Exact methods and Markov chain Monte Carlo methods of conditional inference for contingency tables

（正確法およびマルコフ連鎖・モンテカルロ法による分割表の条件付推測問題の解法）

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Chapter 1

Introduction

1.1 Background

This thesis concerns conditional inference for contingency tables. In the conditional inference, we use distributions of the sufficient statistic for the parameter that we concern, conditioning on the sufficient statistic for the nuisance parameter in the model. For example, suppose we want to test a null hypothesis H_0 that corresponds to a log-linear model symbolized by $\mathcal{M}_0$, under the assumption that a more general model $\mathcal{M}_1$ holds, corresponding to an alternative hypothesis H_1. Denote minimal sufficient statistics for these models by T_0 and T_1, respectively. Then we use the conditional distribution of T_1 given T_0. From the theory of sufficiency, the conditional distribution does not depend on the nuisance parameter, and a similar test can be constructed. For detail, see Anderson (1974), Lehmann (1986), Agresti (1990, 1992), for example.

The above general story can be applied to analyses of *contingency tables*. To illustrate the problem, we first consider a typical analysis of two-way contingency tables. Let $\mathbb{Z}_{\geq 0} = \{0, 1, 2, \ldots\}$ and suppose cell frequencies $\{x_{ij},\ i \in [I], j \in [J]\}, x_{ij} \in \mathbb{Z}_{\geq 0}$ have a multinomial distribution generated by n independent trials with IJ cell probabilities $\{p_{ij},\ i \in [I], j \in [J]\}$, where we define $[m] = \{1, \ldots, m\}$ for $m \in \mathbb{Z}_{>0} = \{1, 2, \ldots\}$. The nonnegative integer array $\boldsymbol{x} = \{x_{ij}\}, x_{ij} \in \mathbb{Z}_{\geq 0}$ is called as a contingency table of size $I \times J$. In this case, the saturated log-linear model has the form

$$\log p_{ij} = \mu + \alpha_i + \beta_j + \gamma_{ij}.$$

For the identifiability of the parameters, we assume

$$\alpha_I = \beta_J = \gamma_{Ij} = \gamma_{iJ} = 0$$

and then obtain the reverse transformation (see Plackett, 1981, for example)

$$\mu = \log p_{IJ},\ \alpha_i = \log \frac{p_{iJ}}{p_{IJ}},\ \beta_j = \log \frac{p_{Ij}}{p_{IJ}},\ \gamma_{ij} = \log \frac{p_{ij} p_{IJ}}{p_{iJ} p_{Ij}},\ i \in [I-1], j \in [J-1].$$

It should be noted that, if we start with the other sampling model, again the same conditional distribution is derived (Plackett, 1981). Another typical situation is, for example, $\boldsymbol{x} = \{x_{ij}\}$ are independent Poisson random variables with parameters $\{np_{ij}\}$.

In the analysis of two-way contingency tables, a hypothesis of statistical independence between the row and column is most familiar and is often considered. Since the association between the row and column is represented as the cross-product ratios $\{\gamma_{ij}\}$, the other parameters, $\mu, \{\alpha_i\}, \{\beta_j\}$, are nuisance parameters in this case (see Altham, 1970). An direct calculation shows that the sufficient statistics are $n = x_{\cdot\cdot}$ for μ, $x_{i\cdot}$ for α_i, $x_{\cdot j}$ for β_j and x_{ij} for γ_{ij}. Then to conduct the inference about $\{\gamma_{ij}\}$, we consider the conditional distribution of $\{x_{ij}, i \in [I-1], j \in [J-1]\}$ given $x_{\cdot\cdot}, \{x_{i\cdot}, i \in [I-1]\}, \{x_{\cdot j}, j \in [J-1]\}$. This conditional distribution is written as

$$p(\boldsymbol{x}) = \frac{\exp\left(\sum_{i\in[I-1]}\sum_{j\in[J-1]} x_{ij}\gamma_{ij}\right)}{\prod_{i\in[I]}\prod_{j\in[J]} x_{ij}!} \Bigg/ \sum_{\boldsymbol{y}\in\mathcal{F}} \left\{ \frac{\exp\left(\sum_{i\in[I-1]}\sum_{j\in[J-1]} y_{ij}\gamma_{ij}\right)}{\prod_{i\in[I]}\prod_{j\in[J]} y_{ij}!} \right\}, \tag{1.1}$$

where

$$\mathcal{F} = \{\boldsymbol{y} = \{y_{ij}\} \mid y_{ij} \in \mathbb{Z}_{\geq 0},\ y_{i\cdot} = x_{i\cdot}, y_{\cdot j} = x_{\cdot j},\ i \in [I], j \in [J]\}$$

is the *reference set* of all possible contingency tables having the same marginal totals to $\boldsymbol{x}$.

To test the statistical independence of the row and column, we use this conditional distribution under the null hypothesis

$$\mathrm{H}_0 : \gamma_{ij} = 0 \text{ for } i \in [I-1], j \in [J-1].$$

It should be noted that, under the null hypothesis, (1.1) can be written as

$$p(\boldsymbol{x}; \gamma_{ij} = 0) = h(\boldsymbol{x}) = \prod_{j\in[J]} \binom{x_{\cdot j}}{x_{1j}, \cdots, x_{Ij}} \Bigg/ \binom{x_{\cdot\cdot}}{x_{1\cdot}, \cdots, x_{I\cdot}}, \tag{1.2}$$

which is the hypergeometric distribution. To complete a test, we need to specify a test statistic and the way to compute the p value. One of the most widely used statistics is the Pearson chi-squared statistic for testing the goodness-of-fit of the independence model,

$$\chi^2(\boldsymbol{x}) = \sum_{i\in[I]}\sum_{j\in[J]} \frac{(x_{ij} - x_{i\cdot}x_{\cdot j}/x_{\cdot\cdot})^2}{x_{i\cdot}x_{\cdot j}/x_{\cdot\cdot}}.$$

It is also known that the asymptotic distribution of this statistic under the null hypothesis is the chi square distribution with the degree of freedom $(I-1)(J-1)$. Then comparing the tail probability of the observed value of the statistic for $\chi^2_{(I-1)(J-1)}$ to the prespecified value of α, we can derive a statistical decision, i.e., whether the null hypothesis is rejected or accepted.

Traditionally, as we have seen in the above example, statistical conditional inference for contingency tables has relied heavily on large-sample approximations for sampling distribution of the test statistics. However, many works have shown that large-sample approximations can be very poor when the contingency table contains both small and large expected frequencies even when the sample size is large. See Haberman (1988) and Agresti (1992), for example. In this thesis, we consider several methods, in which we calculate sampling distributions of test statistics by not using large-sample theories. As for the above example, we want to calculate the *exact* p value of $\chi^2(\boldsymbol{x})$, i.e., the probability that $\chi^2(\boldsymbol{x})$ is equal to or greater than the observed value $\chi^2(\boldsymbol{x}^o)$ for some observed data $\boldsymbol{x}^o$ under the null hypothesis. Note that the p value is calculated using the distribution of the test statistic that is induced by the exact conditional distribution of cell frequencies $\boldsymbol{x}$. For example, the exact p value of the Pearson chi-squared statistic $\chi^2(\boldsymbol{x})$ is calculated as

$$p = \sum_{\boldsymbol{x} \in \mathcal{T}} h(\boldsymbol{x}),$$

where

$$\mathcal{T} = \{\boldsymbol{x} \mid \boldsymbol{x} \in \mathcal{F},\ \chi^2(\boldsymbol{x}) \geq \chi^2(\boldsymbol{x}^o)\}$$

is the *contribution region* of this case, i.e., the set of tables which contribute to the p value, and $h(\boldsymbol{x})$ is the conditional distribution of $\boldsymbol{x}$ under the null hypothesis given by (1.2).

Though we mainly consider computation of p values in this thesis, we give a generalization of the above argument as follows. Suppose $\boldsymbol{x} \in \mathbb{Z}^d_{\geq 0}$ is a contingency table, i.e., an array of nonnegative cell frequencies, where d denotes the number of cells. In the case of $I_1 \times I_2 \times \cdots \times I_k$ k-way contingency tables, $d = I_1 \times I_2 \times \cdots \times I_k$. Let $Q(\boldsymbol{x})$ is some real valued function, which is determined by the contribution region of the problem, and $T(\boldsymbol{x})$ is a vector-valued function. Suppose $p(\boldsymbol{x})$ is the null distribution of $\boldsymbol{x}$ conditioning the values $T(\boldsymbol{x})$ on $T(\boldsymbol{x}^o)$ for some observed data $\boldsymbol{x}^o$. Then substantial wide class of the problems for the analysis of contingency tables are formalized as the inference of the conditional expectation,

$$E[Q(\boldsymbol{x}) \mid T(\boldsymbol{x}) = T(\boldsymbol{x}^o)] = \sum_{\boldsymbol{x} \in \mathcal{F}} Q(\boldsymbol{x})p(\boldsymbol{x}), \tag{1.3}$$

where

$$\mathcal{F} = \{\boldsymbol{x} \mid \boldsymbol{x} \in \mathbb{Z}^d_{\geq 0},\ T(\boldsymbol{x}) = T(\boldsymbol{x}^o)\}. \tag{1.4}$$

The above example of the Pearson chi-squared test corresponds to the special case that $d = IJ$,

$$Q(\boldsymbol{x}) = \begin{cases} 1, & \text{if } \chi^2(\boldsymbol{x}) \geq \chi^2(\boldsymbol{x}^o), \\ 0, & \text{otherwise,} \end{cases}$$

$$T(\boldsymbol{x}) = (x_{\cdot\cdot}, x_{1\cdot}, \ldots, x_{I-1\cdot}, x_{\cdot 1}, \ldots, x_{\cdot J-1})$$

and $p(\boldsymbol{x})$ is the hypergeometric distribution (1.2).

Now we have a generalized description of the problem, i.e., conditional inference for the contingency tables as (1.3) and (1.4), which we consider in this thesis. What we should note here is that actual computations of (1.3) require working with all the elements in the reference set (1.4), i.e., the set of contingency tables having the given values of the sufficient statistic for the nuisance parameter. However, the huge cardinality of the reference set often prevents performing the exact conditional inference. Even for the case of $I \times J$ two-way contingency tables, it is known that, for given I and J and marginal proportions, the number of tables in the reference set of $I \times J$ contingency tables having those fixed marginal proportions increases exponentially in the sample size n. Moreover, for given n, the number of tables also increases rapidly as I and J increase or as the row and column proportions become more homogeneous. For this two-way setting, Good (1977) and Gail and Mantel (1977) gave approximate methods of counting number of tables with fixed marginals. Their works clearly show the complexity of this problem. For this reason, algorithms that provide total enumeration of the reference set (e.g., March, 1972 or Baker, 1977) are very time-consuming, and adequate only for small problems. Such a problem of the huge cardinality of the reference sets also arises for problems of higher dimensional contingency tables in far more serious ways.

Then, how can we compute the conditional expectation (1.3) ? The approach can be classified into the following two areas:

- invent some ingenious enumeration schemes that do not require the total enumeration of the reference set and enable the exact computation in feasible computing times,
- generate random samples $\boldsymbol{x}_1, \ldots, \boldsymbol{x}_M$ from $p(\boldsymbol{x})$ and estimate (1.3) as, say,

$$\hat{p} = \frac{1}{M} \sum_{m=1}^{M} Q(\boldsymbol{x}_m).$$

In this thesis we call the above two methods as the *exact method* and the *Monte Carlo method*, respectively. In the analysis of two-way contingency tables, there are several algorithms to compute the exact p values of the generalized Fisher's exact test (Freeman-Halton test), including Pagano and Halvorsen (1981). However, the most popular and adaptable algorithm is the *network algorithm* proposed by Mehta and Patel (1983), which we consider in this thesis. Note that the possibility of constructing efficient exact algorithms relies heavily on the characteristic of the function $Q(\boldsymbol{x})$, i.e., test statistics. For example, when the test statistic has a good property such as a *Markov property*, some efficient algorithms to compute the exact p values have been proposed. See Hirotsu *et al.* (2001), for example, which proposed an efficient algorithm to compute the exact p values for the multiple comparison type test statistics for the analysis of the three-factor interaction in the $2 \times J \times K$ contingency tables. Unfortunately, however, construction of the exact methods for higher-dimensional tables are difficult in general, and at an infant stage nowadays. For such data sets, i.e., for sparse and high-dimensional data sets where total enumeration becomes infeasible and the large-sample approximation is not adequate, approximation of the p values by Monte Carlo methods may be the only feasible approach. Note that, theoretically, we can estimate p values in arbitrary accuracy by adjusting sample sizes. In this thesis we also consider the Monte Carlo method, with special interest in the *Markov chain Monte Carlo method*.

1.2 Our contributions

1.2.1 Exact methods

In the *exact methods* part of this thesis (Chapter 2), we consider two topics of computing exact p values. The first topic (Section 2.1) is the Freeman-Halton test of the independence between the row and column in two-way contingency tables, and the second topic (Section 2.2) is the exact test of the Hardy-Weinberg proportion for multiple alleles, which appears in the analysis of allele frequency data in population genetics. For both problems, we consider the network algorithm that is originally proposed by Mehta and Patel (1983). As we have stated, the network algorithm is the most popular and adaptable algorithm for the Freeman-Halton test. In this thesis we give an improvement of this algorithm first, and give an extension of this algorithm to the analysis of the allele frequency data. These results are published separately as Aoki (2002) and Aoki (2003).

The essential feature of the network algorithm is the evaluation of some maximization and minimization problems. In the improvement upon the work of Mehta and Patel (1983), we give another upper bound for this maximization problem. The idea of this improvement is based on the differential geometry, and it will be shown that the proposed bound performs well regardless of the types of problems, i.e., the pattern of marginal totals of observed data. As for the extension of the network algorithm to the test of Hardy-Weinberg proportion, the same idea can be applied and an upper bound for the corresponding maximization problem is presented. In addition, some interesting new theorems are proved and the closed form expression of the optimal solution for the minimization problem is given. Some numerical examples show that the efficacy of the computation is greatly improved by our algorithm compared to the total enumeration algorithm.

1.2.2 Markov chain Monte Carlo methods

In Chapter 3 of this thesis, we consider the *Markov chain Monte Carlo methods*. As we have stated, for sparse data sets where enumeration becomes infeasible and the large-sample approximation is not adequate, approximation of the p values by Monte Carlo methods may be the only feasible approach. For some models, random samples can be easily generated from the conditional distribution. A primary example is decomposable log-linear models (e.g., Section 4.4 of Lauritzen, 1996) in multi-way contingency tables. In decomposable models, random samples can be easily generated by exploiting the nesting structure of conditional independence. On the other hand, for testing more general hierarchical log-linear models in multi-way contingency tables, direct generation of random samples is difficult. In this case Markov chain Monte Carlo techniques can be used.

As an example, consider testing the null hypothesis of no three-factor interactions in the log-linear model of three-way contingency tables. This is the simplest case of non-decomposable hierarchical log-linear model for multi-way contingency tables. According to the general theory of the similar tests described in Section 1.1, we want to sample from the hypergeometric distribution over three-way contingency tables with all two-dimensional marginal frequencies fixed. This problem is surprisingly difficult. Not only the direct generation of random samples but also the construction of an appropriate connected Markov chain is difficult as shown in Diaconis and Sturmfels (1998). This interesting example motivated us to investigate this topic. In Section 3.1 we illustrate the difficulty of this problem in detail and review some related works. In Section 3.2 and Section 3.3, we consider this interesting problem for some small contingency tables, i.e., $3 \times 4 \times K, 4 \times 4 \times 4$, and so on. These sections correspond to our two papers, Aoki and Takemura (2003a) and Aoki and Takemura (2003c), respectively.

For the case of two-way contingency tables, on the other hand, it is rather simple to describe a connected Markov chain over two-way contingency tables with fixed one-dimensional marginals, if there are no additional restrictions on individual cells. However, if there are additional restrictions on the cell frequencies such as structural zeros in two-way contingency tables, description of a connected Markov chain becomes more complicated. We consider such situations in Section 3.4, which corresponds to our paper, Aoki and Takemura (2002). See also

Chapter 5 of Bishop et al. (1975) for comprehensive treatment of structural zeros in contingency tables.

Section 3.5 and Section 3.6 give some basic and theoretical results for the problem of constructing a connected Markov chain. As we will see in Section 3.1, it is summarized that our purpose is to compute a *Markov basis*. These two sections relate a *minimality* and its *uniqueness* of the Markov basis.

In Section 3.5, we derive some basic characterizations of minimal Markov basis for a connected Markov chain for sampling from conditional distributions, which we published as Takemura and Aoki (2004). Our arguments are totally elementary. We also give a necessary and sufficient condition for the uniqueness of minimal Markov basis. Our approach is basically constructive and it clarifies a partially ordered structure of minimal Markov basis. At present, our result is not powerful enough to completely characterize a minimal Markov basis for a given problem, but with further refinement it might be possible to implement an alternative algorithm for constructing a Markov basis for a connected Markov chain over a given sample space.

Moreover, in Section 3.6, we consider a *symmetry* of the Markov basis. We treat the permutation of indices of each axis of contingency tables as an action of a direct product of symmetric groups to the basis elements and define an invariant Markov basis. Logically important point is that if a unique minimal Markov basis exists then it is also the unique invariant Markov basis. On the other hand, if a minimal Markov basis is not unique, an invariant minimal Markov basis is important, since a minimal Markov basis is usually not symmetric. We combine the results of Section 3.5 with the theory of transformation groups to study minimality of invariant Markov bases and give some characterizations of invariant Markov basis and its minimality. We also give a necessary and sufficient condition for uniqueness of invariant minimal Markov basis. The main part of this section is that of Aoki and Takemura (2003b).

Chapter 2

Exact methods

This chapter provides two topics of the exact methods of computing p values. Both topics are concerned with the network algorithm, which is originally proposed by Mehta and Patel (1983) in the framework of computing p values for Freeman-Halton exact tests. First we give an improvement of the original algorithm of Mehta and Patel (1983) in Section 2.1, and then give an extension of this algorithm to the exact test of the Hardy-Weinberg proportion for multiple alleles in Section 2.2, which appears in the analysis of allele frequency data in population genetics.

2.1 Network algorithm for Fisher's exact test in two-way contingency tables

This section provides an improvement of the network algorithm for calculating the exact p value of Freeman-Halton exact tests in two-way contingency tables. We give a new exact upper bound and an approximate upper bound for the maximization problems encountered in the network algorithm. The approximate bound has some very desirable computational properties and the meaning is elucidated from a viewpoint of differential geometry. Our proposed procedure performs well regardless of the pattern of marginal totals of data.

2.1.1 Historical background

In testing the independence of the row and column effects in two-way contingency tables, one would, in general, prefer to report the exact p value of the generalized Fisher's exact test (Freeman-Halton test), especially when the entries in each cell are small. It is more common, however, to report the tail probability of the Pearson's χ^2 statistic because of computational feasibility. In fact, calculating the exact p value requires working with the set of contingency tables having the given values of the sufficient statistics and algorithms based on total enumeration of the reference set (e.g., March, 1972; Baker, 1977) are often very time-consuming. Gail and Mantel (1977) gave an approximate method of counting the number of tables with fixed marginals. Their work clearly shows the complexity of this problem.

There are several algorithms, including Pagano and Halvorsen (1981), that do not require total enumeration of the reference set. However, the most popular and adaptable algorithm is the network algorithm proposed by Mehta and Patel (1983). This algorithm has been applied to many problems other than the Freeman-Halton test. For example, see Mehta, Patel and Tsiatis (1984) for exact tests for $2 \times J$ tables; Mehta, Patel and Gray (1985) for inference for the common odds ratio in $2 \times 2 \times K$ tables; Hirji, Mehta and Patel (1987) for exact logistic regression; Agresti, Mehta and Patel (1990) for exact inference in $I \times J$ tables with ordered categories; Mehta, Patel and Senchaudhuri (1991) for inference for $2 \times J \times K$ tables; and Hilton, Mehta and Patel (1991) for Smirnov tests for categorical or continuous data.

This section improves upon the work of Mehta and Patel (1983), which applies the network algorithm to the Freeman-Halton exact test. Another upper bound is given for some maximization problems encountered in the network algorithm. The evaluation of this maximization problem plays an important role in the network algorithm. We also give a closed form for an approximate upper bound that makes it possible to compute sufficiently accurate p values. It will be shown that this bound performs well regardless of the pattern of marginal totals of data.

The construction of this section is as follows. In Section 2.1.2, a brief outline of the network algorithm is provided. We refer the reader to the original article by Mehta and Patel (1983) for technical details of the algorithm. In Section 2.1.3, the new approach is described. In Section 2.1.4, we demonstrate desirable properties of our bound through some computation-based examples.

2.1.2 The network algorithm

Let $\boldsymbol{x} \in \mathbb{Z}_{\geq 0}^{IJ}$ be an $I \times J$ contingency table and let $x_{ij}, i \in [I], j \in [J]$ be the entry in row i and column j. Let $R_i = \sum_{j=1}^{J} x_{ij}$ and $C_j = \sum_{i=1}^{I} x_{ij}$ be the marginal totals and let $\mathcal{F}$ denote the reference set of all possible $I \times J$ contingency tables with the same marginal totals as $\boldsymbol{x}$. Thus

$$\mathcal{F} = \left\{ \boldsymbol{y} = \{y_{ij}\} \;\middle|\; \boldsymbol{y} \in \mathbb{Z}_{\geq 0}^{IJ}, \sum_{j=1}^{J} y_{ij} = R_i, \sum_{i=1}^{I} y_{ij} = C_j \right\}.$$

We define $N = \sum_{i=1}^{I} R_i = \sum_{j=1}^{J} C_j$ and $D = N!/\{(\prod_{i=1}^{I} R_i!)(\prod_{j=1}^{J} C_j!)\}$ for later use. Under the null hypothesis of row and column independence, the conditional probability of observing any $\boldsymbol{y} \in \mathcal{F}$ is expressed as

$$P(\boldsymbol{y}) = \frac{\left(\prod_{i=1}^{I} R_i!\right)\left(\prod_{j=1}^{J} C_j!\right)}{N! \prod_{i=1}^{I} \prod_{j=1}^{J} y_{ij}!} = \frac{1}{D} \left(\prod_{i=1}^{I} \prod_{j=1}^{J} y_{ij}! \right)^{-1}.$$

Freeman and Halton (1951) defined the p value for the conditional test of independence to be the sum of the probabilities of all the tables in $\mathcal{F}$ that are no more likely than $\boldsymbol{x}$, that is,

$$p = \sum_{\boldsymbol{y} \in \mathcal{T}} P(\boldsymbol{y}),$$

where $\mathcal{T} = \{\boldsymbol{y} \mid \boldsymbol{y} \in \mathcal{F},\ P(\boldsymbol{y}) \leq P(\boldsymbol{x})\}$ is the contribution region of this case. This test is also known as the generalized Fisher's exact test in two-way contingency tables.

The network representation of the reference set for $\mathcal{F}$ consists of *nodes* and *arcs* constructed in $J+1$ stages. For $j = J, J-1, ..., 0$, the nodes at stage j have the form $(j, \boldsymbol{R}_j)$, where

$\boldsymbol{R}_j = (R_{1,j}, ..., R_{I,j})$. There are as many nodes at stage j as there are possible partial sums for the first j columns of the tables. Arcs emanate from each node at stage j and every arc is connected to only one node at stage $j-1$. The network is constructed recursively by specifying all successive nodes $(j-1, \boldsymbol{R}_{j-1})$ that are connected by arcs to each node $(j, \boldsymbol{R}_j)$. A path $(J, R_1, ..., R_I) = (J, \boldsymbol{R}_J) \to (c-1, \boldsymbol{R}_{c-1}) \to \cdots \to (0, \boldsymbol{R}_0) = (0, 0, ..., 0)$ represents a distinct table in $\mathcal{F}$, with $y_{ij} = R_{i,j} - R_{i,j-1}, i \in [I], j \in [J]$. Figure 2.1 shows the network representation for all the 3×3 contingency tables with $(R_1, R_2, R_3) = (2, 1, 6), (C_1, C_2, C_3) = (3, 3, 3)$. The dotted path gives the contingency table of counts $\boldsymbol{x} = (x_{11}, x_{12}, x_{13}, x_{21}, x_{22}, x_{23}, x_{31}, x_{32}, x_{33}) = (1, 0, 1, 0, 1, 0, 2, 2, 2)$.

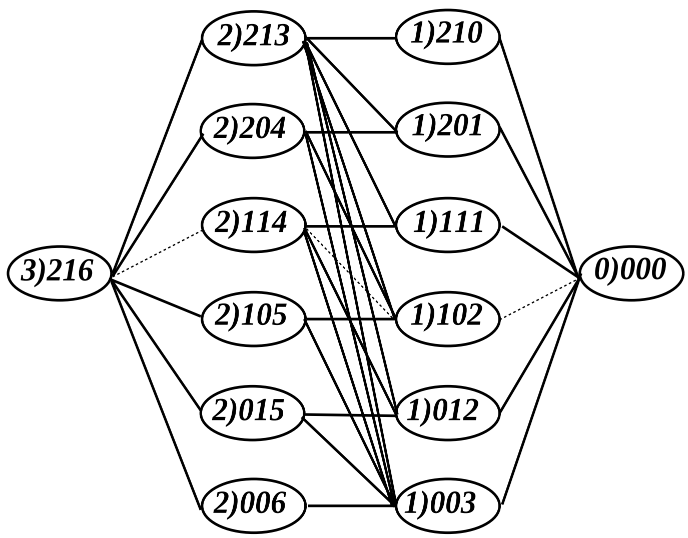

Figure 2.1: Network representation for all the 3×3 contingency tables with $(R_1, R_2, R_3) = (2, 1, 6), (C_1, C_2, C_3) = (3, 3, 3)$.

We define the length of an arc from node $(j, \boldsymbol{R}_j)$ to node $(j-1, \boldsymbol{R}_{j-1})$ by $\{(R_{1,j} - R_{1,j-1})! \times \cdots \times (R_{I,j} - R_{I,j-1})!\}^{-1}$ and the length of the path or sub-path by the product of the corresponding arc lengths. Then we can readily verify that the length of the complete path from $(J, \boldsymbol{R}_J)$ to $(0, \boldsymbol{R}_0)$ is equal to $D \cdot P(\boldsymbol{y})$. Now our goal is to identify and sum all paths whose lengths do not exceed $D \cdot P(\boldsymbol{x})$.

For calculating the p value efficiently, we compute at each node $(j, \boldsymbol{R}_j)$ the shortest and longest lengths of the sub-path from node $(j, \boldsymbol{R}_j)$ to $(0, \boldsymbol{R}_0)$. We call these items as LP or SP (longest / shortest sub-path) according to Mehta and Patel (1983). Using these values, we can determine tables that necessarily do or do not contribute to the p value, without processing the remaining parts of paths in the network passing through that node.

If we can evaluate LP and SP exactly, we can *trim* paths perfectly. It is worth pointing out, however, that if we can only evaluate an upper bound for LP and a lower bound for SP, we can trim paths incompletely. Hence both the quality of the bounds and the time for computing the bounds influence the efficiency of the algorithm. Mehta and Patel (1983) evaluated the upper bound for LP by using the closed form of LP when all the C_j's are equal. This upper bound works well when the C_j's are equal, or nearly equal. On the other hand, when the pattern of C_j's is imbalanced, the quality of this upper bound is poor, i.e., this upper bound is much larger than LP. In this section, we propose another upper bound. We demonstrate that our new method performs well regardless of the pattern of C_j's and makes it possible to compute the exact p values more efficiently.

2.1.3 Numerical computation of the upper bound for longest paths from any node to the terminal node

In Section 2.1.3, we present a new upper bound for LP. First we define the continuous relaxation problem that gives the upper bound for the optimal solution of the original maximization problem. Next we show how to evaluate the optimal solution of the relaxation problem. And at last, we provide how to determine the initial vector. The choice of the initial vector is very important for our improved upper bound.

Relaxation problem

The problem that we consider can be written in the following form:

$$\text{P:}\quad \text{minimize} \sum_{i=1}^{I}\sum_{j=1}^{J} \log y_{ij}!$$

subject to

$$\sum_{j=1}^{J} y_{ij} = R_i, \quad i \in [I], \quad \sum_{i=1}^{I} y_{ij} = C_j, \quad j \in [J], \tag{2.1}$$

$$y_{ij} \in \mathbb{Z}_{\geq 0}, \quad i \in [I],\ j \in [J].$$

This integer programming problem is equivalent to the original problem for LP discussed in Mehta and Patel (1983), and we fixed the number of columns at J for simplicity. Corresponding to an upper bound for LP, we consider the following relaxation problem:

$$\text{P}':\ \text{minimize} \sum_{i=1}^{I}\sum_{j=1}^{J} g(y_{ij}) \ \text{ subject to (2.1) and } y_{ij} \geq 0 \ \text{ for all } i, j,$$

where the function $g(y) : [0, \infty) \mapsto \mathbb{R}$ is a convex function of class C^1 which satisfies

$$g(n) = \log n! \ \text{ for all } n \in \mathbb{Z}_{\geq 0}. \tag{2.2}$$

One simple method of specifying $g(y)$ is to fit a piecewise quadratic function. We show that a closed form of the piecewise quadratic function satisfying (2.2) can be uniquely obtained using the following lemma. For future use, we define

$$n!! = \begin{cases} n(n-2)(n-4) \times \cdots \times 4 \times 2, & \text{if } n \text{ is even}, \\ n(n-2)(n-4) \times \cdots \times 3 \times 1, & \text{if } n \text{ is odd}, \end{cases}$$

$$0!! \equiv (-1)!! \equiv 1.$$

Lemma 2.1.1 *Let $I_{[n,n+1)}(y)$ be the indicator function given by*

$$I_{[n,n+1)}(y) = \begin{cases} 1, & \text{if } n \le y < n+1, \\ 0, & \text{otherwise} \end{cases}$$

and let $g_n(y)$ be quadratic in y. Then the piecewise quadratic function

$$g(y) = \sum_{n=0}^{\infty} I_{[n,n+1)}(y) g_n(y)$$

is a convex function of class C^1 satisfying the condition (2.2) if and only if

$$g_n(y) = \log n! + v_n(y-n) + \frac{1}{2}\Delta v_n (y-n)^2, \quad n = 0, 1, 2, ...,$$

where

$$v_n = (-1)^n \log \frac{2}{\pi} + 2 \log \frac{n!!}{(n-1)!!}, \quad \Delta v_n = v_{n+1} - v_n.$$

Proof. Because $g(y)$ satisfies condition (2.2), $g_n(y)$ must be written as

$$g_n(y) = \log n! + v_n(y-n) + A_n(y-n)^2$$

where $v_n \equiv g_n'(y)|_{y=n}$. From the continuity of $g_n(y)$ and $g_n'(y)$ at $y = n+1$, we have

$$g_n(n+1) = \log n! + v_n + A_n = \log(n+1)!,$$

$$g_n'(y)|_{y=n+1} = v_n + 2A_n = v_{n+1}$$

and hence we obtain

$$A_n = \frac{1}{2}(v_{n+1} - v_n) = \frac{1}{2}\Delta v_n,$$

$$v_{n+1} + v_n = 2\log(n+1). \tag{2.3}$$

The recurrence formula (2.3) can be easily solved as $v_n = (-1)^n v_0 + 2\log\{n!!/(n-1)!!\}$. Now we will show that v_0 is determined uniquely from the convexity of $g(y)$. If $n = 2m$, we have

$$\Delta v_{2m} - \Delta v_{2m-2} = 2 \log \left(1 - \frac{1}{4m^2}\right) < 0$$

and

$$\lim_{m\to\infty} \Delta v_{2m} = -2v_0 + 2\log\frac{2}{\pi} \quad \text{(Wallis' formula)}.$$

Hence $\Delta v_0 > \Delta v_2 > \Delta v_4 > \cdots \ge 0$ holds if and only if $v_0 \le \log \frac{2}{\pi}$. Similarly, if $n = 2m-1$, we have

$$\Delta v_{2m-1} - \Delta v_{2m-3} = 2 \log \left\{1 - \frac{1}{(2m-1)^2}\right\} < 0$$

and

$$\lim_{m\to\infty} \Delta v_{2m-1} = 2v_0 - 2\log\frac{2}{\pi} \quad \text{(Wallis' formula)}.$$

Hence $\Delta v_1 > \Delta v_3 > \Delta v_5 > \cdots \geq 0$ holds if and only if $v_0 \geq \log \dfrac{2}{\pi}$. Consequently, v_0 can be determined uniquely as $v_0 = \log \dfrac{2}{\pi}$. Q.E.D.

Because the objective function of the problem P' is convex, the optimal solution of this problem can be obtained by a technique of a convex programming. Our approach is to solve P' numerically by a gradient method. For convenience, we regard $\boldsymbol{y}$ as the column vector $\boldsymbol{y} = (y_{11}, ..., y_{1J}, ..., y_{I1}, ..., y_{IJ})'$ and rewrite P' in the vector notation as

$$\mathrm{P}'': \text{ minimize } f(\boldsymbol{y}) \text{ subject to } A\boldsymbol{y} = \boldsymbol{b} \text{ and } \boldsymbol{y} \geq \boldsymbol{0},$$

where the function $f : \mathbb{R}^{rc} \mapsto \mathbb{R}$ is defined as $f = \sum_{i=1}^{I} \sum_{j=1}^{J} g(y_{ij})$ and A is an $(I+J-1) \times IJ$ matrix such that $A\boldsymbol{y}$ forms a set of linearly independent marginals. For example, we can select A and $\boldsymbol{b}$ as

$$A = \begin{bmatrix} I_{I-1} \otimes \boldsymbol{j}_J' \mid O_{(I-1)\times J} \\ \boldsymbol{j}_I' \otimes I_J \end{bmatrix}, \quad \boldsymbol{b} = (R_1, ..., R_{I-1}, C_1, ..., C_J)',$$

where I_n is an $n \times n$ identity matrix, $\boldsymbol{j}_n$ is an $n \times 1$ column vector with all the elements equal to one and $O_{(I-1)\times J}$ is an $(I-1) \times J$ zero matrix. We also define *the feasible region* S as $S = \{\boldsymbol{y} \mid A\boldsymbol{y} = \boldsymbol{b},\ \boldsymbol{y} \geq \boldsymbol{0}\} \subset \boldsymbol{R}^{IJ}$. Our algorithm is to construct the sequence $\boldsymbol{y}^0, \boldsymbol{y}^1, ... \in S$ which satisfies $f(\boldsymbol{y}^{k+1}) < f(\boldsymbol{y}^k),\quad k = 0, 1, 2, \cdots$, by the formula

$$\boldsymbol{y}^{k+1} = \boldsymbol{y}^k + \alpha^k \boldsymbol{d}^k, \tag{2.4}$$

beginning with some initial vector $\boldsymbol{y}^0 \in S$. We show how to determine $\boldsymbol{d}^k$, α^k and $\boldsymbol{y}^0$ in the followings.

The direction vector and the step size

For $\boldsymbol{y} \in S$, we want to determine the direction vector $\boldsymbol{d}^k \in \mathbb{R}^{IJ}$ which satisfies

$$\exists \overline{\alpha}, \text{ s. t. } \boldsymbol{y}^k + \alpha \boldsymbol{d}^k \in S \text{ and } f(\boldsymbol{y}^k + \alpha \boldsymbol{d}^k) < f(\boldsymbol{y}^k) \text{ for } \forall \alpha \in [0, \overline{\alpha}]. \tag{2.5}$$

Such a vector $\boldsymbol{d}^k$ can be determined as the orthogonal projection of

$$-\nabla f(\boldsymbol{y}^k) = -\left(\frac{\partial f(\boldsymbol{y}^k)}{\partial {y_{11}}^k}, \cdots, \frac{\partial f(\boldsymbol{y}^k)}{\partial {y_{IJ}}^k}\right)' = -\left(\frac{\partial g({y_{11}}^k)}{\partial {y_{11}}^k}, \cdots, \frac{\partial g({y_{IJ}}^k)}{\partial {y_{IJ}}^k}\right)'$$

to the subspace which is defined by the *active constraints* at $\boldsymbol{y}^k$ (gradient projection method, Rosen, 1960).

First we consider the case that all the elements of $\boldsymbol{y}^k$ are positive.

Lemma 2.1.2 *If $\boldsymbol{y}^k > \boldsymbol{0}$, then*

$$\boldsymbol{d}^k = -\{I - A'(AA')^{-1}A\}\nabla f(\boldsymbol{y}^k) \tag{2.6}$$

is a direction vector which satisfies condition (2.5).

Proof. For any $\boldsymbol{y}^k(> \mathbf{0}) \in S$, we can see that $\exists \overline{\alpha} > 0$, s. t. $\boldsymbol{y}^k + \alpha \boldsymbol{d}^k \in S$ for $\forall \alpha \in [0, \overline{\alpha}]$ because $P = I - A^{'}(AA^{'})^{-1}A$ is an orthogonal projector from $\mathbb{R}^{IJ}$ to the $IJ - (I + J - 1)$ dimensional subspace $M = \{\boldsymbol{y} \mid A\boldsymbol{y} = \mathbf{0},\ \boldsymbol{y} \in \mathbb{R}^{IJ}\}$. Now we show that (2.6) satisfies the latter part of (2.5). Using the properties $P^2 = P$, $P' = P$, we can derive

$$\nabla^{'} f(\boldsymbol{y}^k)\boldsymbol{d}^k = -\nabla^{'} f(\boldsymbol{y}^k)P\nabla f(\boldsymbol{y}^k) = -\|P\nabla f(\boldsymbol{y}^k)\|^2 = -\|\boldsymbol{d}^k\|^2 < 0. \tag{2.7}$$

On the other hand, the mean value theorem produces

$$\forall \alpha,\ \exists \theta \in [0, 1],\ \text{s. t.}\ \ f(\boldsymbol{y}^k + \alpha \boldsymbol{d}^k) - f(\boldsymbol{y}^k) = \alpha \nabla^{'} f(\boldsymbol{y}^k + \theta\alpha \boldsymbol{d}^k)\boldsymbol{d}^k. \tag{2.8}$$

From the continuity of $\nabla^{'} f(\boldsymbol{y}^k)$ and (2.7), the left hand side of (2.8) is negative for all $\alpha \in (0, \overline{\alpha}]$ if we choose $\overline{\alpha}$ that is sufficiently small. Q.E.D.

Following this lemma, we can write the direction vector as ${d_{ij}}^k = {f_{ij}}^k - I^{-1}\sum_{i=1}^{I} {f_{ij}}^k - J^{-1}\sum_{j=1}^{J} {f_{ij}}^k + (IJ)^{-1}\sum_{i=1}^{I}\sum_{j=1}^{J} {f_{ij}}^k$ where $\boldsymbol{d}^k = ({d_{11}}^k, ..., {d_{IJ}}^k)'$ and $\nabla f(\boldsymbol{y}^k) = ({f_{11}}^k, ..., {f_{IJ}}^k)'$.

Next consider the case that only one element of $\boldsymbol{y}^k$ is zero. Let us assume that ${y_{11}}^k = 0$, ${y_{ij}}^k > 0$, $(i, j) \neq (1, 1)$, and define

$$\widetilde{A}^{'} = \left[A^{'}|\boldsymbol{e}_{11}\right],\quad \boldsymbol{e}_{11} = (1, 0, ..., 0)^{'} \in \mathbb{R}^{IJ}. \tag{2.9}$$

Then similarly to Lemma 2.1.2, it can be shown that the direction vector $\boldsymbol{d}^k$ can be obtained as the orthogonal projection of $-\nabla f(\boldsymbol{y}^k)$ to the $IJ - (I+J)$ dimensional subspace $\widetilde{M} = \{\boldsymbol{y} \mid \widetilde{A}\boldsymbol{y} = \mathbf{0},\ \boldsymbol{y} \in \mathbb{R}^{IJ}\}$, that is, $\boldsymbol{d}^k = -\widetilde{P}\nabla f(\boldsymbol{y}^k) = -\{I - \widetilde{A}^{'}(\widetilde{A}\widetilde{A}^{'})^{-1}\widetilde{A}\}\nabla f(\boldsymbol{y}^k)$. The next lemma is useful to calculate the orthogonal projector $\widetilde{P}$.

Lemma 2.1.3 *$\widetilde{P}$ is obtained from P and $\boldsymbol{e}_{11}$ as $\widetilde{P} = P - P\boldsymbol{e}_{11}\boldsymbol{e}_{11}^{'}P/(\boldsymbol{e}_{11}^{'}P\boldsymbol{e}_{11})$.*

Proof. Substituting (2.9) into $\widetilde{P} = I - \widetilde{A}^{'}(\widetilde{A}\widetilde{A}^{'})^{-1}\widetilde{A}$ and simplifying it, using $P = I - A^{'}(AA^{'})^{-1}A$ yields the lemma. Q.E.D.

If there is more than one zero element in $\boldsymbol{y}^k$, we can obtain the orthogonal projector in a similar way by using Lemma 2.1.3 repeatedly.

Finally we discuss how to determine the step size α^k according to $\boldsymbol{y}^k$ and $\boldsymbol{d}^k$. The optimal value of α^k can be defined as $\alpha^* = \arg\min_\alpha f(\boldsymbol{y}^k + \alpha \boldsymbol{d}^k)$.

We first assume that we know the interval $[\underline{\alpha}, \overline{\alpha}]$ which includes α^*, that is, $\alpha^* \in [\underline{\alpha}, \overline{\alpha}]$. Since $f(\boldsymbol{y}^k + \alpha \boldsymbol{d}^k)$ is a unimodal function of α in the interval $[\underline{\alpha}, \overline{\alpha}]$, for all interior points $\alpha_1, \alpha_2 \in [\underline{\alpha}, \overline{\alpha}]$, $\alpha_1 < \alpha_2$ we can see that

$$\begin{array}{lll}
\text{if} & f(\boldsymbol{y}^k + \alpha_1 \boldsymbol{d}^k) > f(\boldsymbol{y}^k + \alpha_2 \boldsymbol{d}^k) & \text{then } \alpha^* \in [\alpha_1, \overline{\alpha}], \\
\text{if} & f(\boldsymbol{y}^k + \alpha_1 \boldsymbol{d}^k) = f(\boldsymbol{y}^k + \alpha_2 \boldsymbol{d}^k) & \text{then } \alpha^* \in [\alpha_1, \alpha_2], \\
\text{if} & f(\boldsymbol{y}^k + \alpha_1 \boldsymbol{d}^k) < f(\boldsymbol{y}^k + \alpha_2 \boldsymbol{d}^k) & \text{then } \alpha^* \in [\underline{\alpha}, \alpha_2].
\end{array}$$

Using this relation repeatedly, we can shorten the interval which includes α^* and obtain α^* with any accuracy.

Obviously, the initial value of $\underline{\alpha}$ should be zero. A simple initial value of $\overline{\alpha}$ is $\overline{\alpha} = \min\left\{-{y_{ij}}^k/{d_{ij}}^k \;\middle|\; {d_{ij}}^k < 0\right\}$. We can also obtain better initial value of $\overline{\alpha}$ by a bracketing procedure.

It is known that if we select the interior points α_1, α_2 according to a golden section ratio (Bazaraa et al. 1993, pp. 270-271), we can shorten the interval which includes α^* most efficiently.

The initial vector

Here we discuss our choice of the initial vector $\boldsymbol{y}^0$. A very good initial vector is given by

$$ {y_{ij}}^0 = \frac{R_i C_j}{N}, \; i \in [I], \; j \in [J]. \tag{2.10} $$

The meaning of (2.10) can be understood as follows. The objective function of the original integer programming problem P can be approximated to

$$ \begin{aligned} \sum_{i=1}^{I}\sum_{j=1}^{J} \log y_{ij}! &\simeq \sum_{i=1}^{I}\sum_{j=1}^{J} \log\left(\sqrt{2\pi}{y_{ij}}^{y_{ij}+\frac{1}{2}}\mathrm{e}^{-y_{ij}}\right) \\ &= \text{Const.} + \sum_{i=1}^{I}\sum_{j=1}^{J}\left(y_{ij}+\frac{1}{2}\right)\log y_{ij} \end{aligned} \tag{2.11} $$

by replacing the factorial with Stirling's formula. We can see that except for the constant term the right hand side of (2.11) is a negative entropy if we ignore the factor $\frac{1}{2}$. It follows that the problem P is approximately equivalent to the maximizing entropy problem.

We can interpret this problem from a viewpoint of differential geometry. Let P_1 be the reference empirical distribution given by $p_{ij} = y_{ij}/N, \; i \in [I], \; j \in [J]$ and P_U be the uniform distribution given by $p_{ij} = 1/IJ, \; i \in [I], \; j \in [J]$. We also define the Kullback-Leibler divergence from P_1 to P_U as $D(P_1, P_U)$. It is well known that the maximum entropy is obtained when the occurrence probability from the uniform distribution is maximum, in other words, $D(P_1, P_U)$ is minimum. The important property of the divergence $D(P_1, P_U)$ is the following Pythagorean decomposition

$$ D(P_1, P_U) = D(P_1, P_M) + D(P_M, P_U) \tag{2.12} $$

where P_M is the maximum likelihood estimate under the model of no interaction between the row and column given by $p_{ij} = R_i C_j/N^2, \; i \in [I], \; j \in [J]$. This can be easily checked by direct calculation. The Pythagorean decomposition can be derived from a dually flat structure of the parameter space. A meaning of this decomposition is elucidated from the differential geometrical point of view. For details, see Amari (1985, 1989), for example. Since the second term of the right hand side of (2.12) is constant, we only have to consider the minimizing $D(P_1, P_M)$. This naturally implies (2.10).

Of course, we can rewrite $D(P_1, P_M)$ directly as

$$ D(P_1, P_M) = \sum_{i=1}^{I}\sum_{j=1}^{J}\frac{y_{ij}}{N}\left(\log\frac{y_{ij}}{N} - \log\frac{R_i C_j}{N^2}\right) = \frac{1}{N}\sum_{i=1}^{I}\sum_{j=1}^{J} y_{ij}\log y_{ij} + \text{Const.} $$

and again we can see that minimizing the divergence $D(P_1, P_U)$ corresponds to maximizing entropy. See also Lemma 2.2 of Darroch and Speed (1983).

2.1.4 Some computational results

We present exact p values by the network algorithm for some problems. In this study, contingency tables of three or four rows were considered. All the algorithms were programmed by C on a PC running on Linux (Pentium III, 930 MHz). We compared our algorithm only with the algorithm by Mehta and Patel (1983), since their algorithm already yields considerable improvements over previously published algorithm, e.g., Pagano and Halvorsen's algorithm (1981).

We must check the quality of the upper bound for LP carefully, because our upper bound, the optimal solution of the relaxation problem, relies on numerical optimization. We compared four upper bounds for LP:

- UB_{MP}: the upper bound proposed by Mehta and Patel (1983),
- UB_0: the approximate upper bound attained at (2.10),
- UB_1: the modification of UB_0 by using (2.4) once,
- UB_k: the modification of UB_0 by using (2.4) recursively according to some stopping rule.

We have determined the stopping rule of UP_k as

$$\|\boldsymbol{d}^k\| < \varepsilon \;\Rightarrow\; \text{stop},$$

where ε is specified in advance.

As for the SP, we estimated its lower bound in the same way as Mehta and Patel (1983), that is, we estimated the lower bound as a basic feasible solution to a set of constraints when the C_j's are equal. This bound also arises in the transportation problem of linear programming. For detail, see Hadley (1962).

We first considered some examples discussed in Mehta and Patel (1983). Table 2.1 shows the p values and CPU times.

As for UB_k, we calculated the p values for $\varepsilon = 0.01, 0.001$, and 0.0001, though only the cases of $\varepsilon = 0.0001$ were displayed in Table 2.1. Actually, we observed that the p values were not affected by ε, whereas the CPU times were affected. For example, the CPU times for computing the p values of problem 4 of Mehta and Patel (1983) for several values of ε were 8:14.65 for $\varepsilon = 0.01$, 8:50.14 for $\varepsilon = 0.001$, and 8:50.60 for $\varepsilon = 0.0001$, although all the obtained p values were the same ($p = 0.0353520690$). In our study, we did not examine the relation between the threshold value ε and the CPU times in detail because even the initial vector $\boldsymbol{y}_0$ is satisfactory and a tight stopping rule was not needed to calculate the exact p values.

Table 2.1 shows two things. First, the proposed algorithm gives exact (strictly speaking, sufficiently accurate) p values, even when we use UB_0. This implies that the approximate upper bound attained at (2.10) is quite good in practice. Second, in these examples, the proposed algorithms do not improve the computational efficacy compared to the method by Mehta and Patel (1983). This is due to the *well balanced* values of the column sums, since the upper bound

Table 2.1: Computing results with the network algorithm for balanced column sum cases.

table	upper bound	p values	CPU time[a]
(problem 2 of Mehta and Patel)			
20126	UB_{MP}	0.0911177720	0:01.48
13111	UB_0	0.0911177720	0:01.66
10310	UB_1	0.0911177720	0:01.70
12120	$UB_k{}^b$	0.0911177720	0:02.13
(problem 3 of Mehta and Patel)			
201265	UB_{MP}	0.0453742835	0:44.19
131112	UB_0	0.0453742835	0:48.15
103100	UB_1	0.0453742835	0:48.96
121200	$UB_k{}^b$	0.0453742835	0:51.48
(problem 4 of Mehta and Patel)			
111000124	UB_{MP}	0.0353520690	7:37.04
444555650	UB_0	0.0353520690	8:10.76
111000124	UB_1	0.0353520690	8:17.88
	$UB_k{}^b$	0.0353520690	8:50.60

[a]CPU time is represented by min:sec.millisec.
[b]Using the stopping rule with $\varepsilon = 0.0001$.

by Mehta and Patel (1983) is evaluated by the optimal value when the column sums are equal. But the inferiority of the proposed method, especially when using UB_0, is quite small.

Next we consider the cases of imbalanced column sums. The values of column sums that we treated here are $(C_1, C_2, C_3, C_4, C_5, C_6) = (5, 5, 10, 10, 20, 20)$ for 3×6 contingency tables and $(C_1, C_2, C_3, C_4, C_5) = (5, 5, 10, 10, 20)$ for 4×5 contingency tables. For both patterns of the marginals, we considered the examples of large (larger than 0.8), middle (around 0.5) and small (less than 0.05) p values, even though examples of only small p values had been considered in Mehta and Patel (1983). This is because the analyses of examples of large p values are considered to be more suitable for the purpose of comparing the quality of the upper bounds. The p values and CPU times for the imbalanced case are shown in Table 2.2. Table 2.2 also shows the number of trimmings by the upper bounds.

Table 2.2 again shows that our algorithms gave exact p values, even when we use UB_0 for the upper bound. The CPU times show that UB_0 performed uniformly better and UB_1 performed better for most cases than UP_{MP}. As for UB_k, it was not as good as UP_{MP} for a 4×5 case. It does not, however, explain the relation between the size of table and the efficacy of the methods since the CPU time for the case of UB_k is affected by ε. The number of trimmings clearly shows the good quality of our upper bounds. It is observed that our upper bounds enabled a more efficient trimming in the early stage, especially in stage $J - 1$, of the algorithm and hence the total number of paths to be considered in the algorithm decreases. The number of trimmings also shows that UB_0 and UB_1 did not reach the optimal solution of the relaxation problem. It should be noticed, however, that this fact does not indicate over-trimming. Over-trimming may occur only if these values are smaller than the optimal solution of the original problem. The accuracy of p values in Table 2.2 shows that the values of UB_0 or UB_1 were at least larger

Table 2.2: Computing results with the network algorithm for unbalanced column sum cases.

				# of trimming by the upper bound			
table	upper bound	p values	CPU time[a]	stag e 5	stage 4	stage 3	stage 2
012278	UB_{MP}	0.8200735203	0:02.89	21	24946	362928	2954230
424578	UB_0	0.8200735203	0:00.61	185	7578	51358	274554
124364	UB_1	0.8200735203	0:00.65	185	7574	51540	275996
	${UB_k}^b$	0.8200735203	0:00.86	185	7574	51524	276456
003269	UB_{MP}	0.4783413730	0:05.83	14	22483	430003	4950199
335388	UB_0	0.4783413730	0:02.65	157	11164	107840	889258
222563	UB_1	0.4783413730	0:02.70	157	11160	108018	890380
	${UB_k}^b$	0.4783413730	0:02.92	157	11156	108132	891356
201359	UB_{MP}	0.0129408780	0:33.04	6	12662	441645	10965868
341688	UB_0	0.0129408780	0:29.17	79	15405	285220	4161458
018173	UB_1	0.0129408780	0:29.29	79	15383	284724	4176262
	${UB_k}^b$	0.0129408780	0:29.34	79	15285	283074	4210124
00235	UB_{MP}	0.8892778315	0:03.35		536	102958	3058464
32226	UB_0	0.8892778315	0:01.12		1090	34083	406826
12444	UB_1	0.8892778315	0:01.27		1090	34071	407902
11215	${UB_k}^b$	0.8892778315	0:10.48		1090	34031	412310
11215	UB_{MP}	0.4972713811	0:08.31		363	97113	5057688
02355	UB_0	0.4972713811	0:05.90		916	56346	1386424
32433	UB_1	0.4972713811	0:06.15		916	55918	1406148
10117	${UB_k}^b$	0.4972713811	0:15.78		916	55764	1418840
10027	UB_{MP}	0.0354175392	0:35.08		116	59345	6904807
03543	UB_0	0.0354175392	0:34.69		484	71236	3406770
41433	UB_1	0.0354175392	0:35.47		480	70208	3470314
01117	${UB_k}^b$	0.0354175392	0:43.86		464	70805	3487145

[a]CPU time is represented by min:sec.millisec.
[b]Using the stopping rule with $\varepsilon = 0.0001$.

than the optimal solution of the original problem in most cases, or if not, that its influence was negligible.

2.1.5 Discussion

The essential feature of the network algorithm is the evaluation of an upper bound for LP and a lower bound for SP. Mehta and Patel (1983) evaluate an upper bound for LP by using the closed form of LP when all the column sums are equal. In this study, we have given an improved method of evaluating an upper bound for LP.

There are other methods of evaluating an upper bound. We can calculate LP directly by a dynamic programming procedure, for example. Computational efficiency, however, depends on both (i) time needed for calculating (an upper bound for) LP and (ii) efficiency of trimming. If we calculate LP exactly, we can trim paths most efficiently but we may need a comparatively long time to evaluate it. On the other hand, we can evaluate an upper bound in a simple way, which leads to incomplete trimming. Both approaches by Mehta and Patel (1983) and by us are the latter one.

An important point of our method is that we obtain the closed form of the approximately optimal solution of the relaxation problem. As we have seen in Section 2.1.4, this approximate bound gave sufficiently accurate p values and the number of trimmings in Table 2.2 shows that this bound enabled much more efficient trimmings than the bound by Mehta and Patel (1983). From these results, we recommend using the new method to calculate the p values when the column sums are imbalanced. Our new method is recommended in particular when some extremely large values are included in the column sums, because the Mehta and Patel's upper bound is inevitably affected by $\max C_j$. Considering the fact that for the inferiority of our method in Table 2.1 when the column sums are balanced is quite small, our method can be used for most cases in the practical applications.

Finally, it is worth pointing out that this idea of evaluating an approximate optimal solution as the value at maximum likelihood estimator can be applied to a variety of optimizing problems. The most straightforward extension may be a case of higher dimensional tables. For example, consider the three-way contingency table. The maximizing problem:

$$\text{maximize} \quad \prod_i \prod_j \prod_k (y_{ijk}!)^{-1} \quad \text{subject to } y_{ij\cdot}, y_{i\cdot k}, y_{\cdot jk} \text{ are fixed}$$

can be again interpreted as a maximizing probability problem under the hypothesis of no three-way interaction. The relaxation approach of this section can be applied to this maximization problem.

2.2 Network algorithm for the exact test of Hardy-Weinberg proportion for multiple alleles

2.2.1 Historical background

Since its discovery in the early 1900s, the Hardy-Weinberg law plays an important role in the field of population genetics and often serves as a basis for genetic inference (see, for example, Crow, 1988). This law states that in a large random-mating population with no selection, mutation or migration, the allele frequencies and the genotype frequencies are constant from generation to generation and that there is a simple relationship between the allele frequencies and the genotype frequencies. For an r-allele autosomal locus with alleles $A_1, A_2, ..., A_r$, the probability that a random individual from random breeding population will be A_iA_j is $p_i^2(i = j)$ or $2p_ip_j(i \neq j)$, where p_i is the proportion of type A_i, which are known as the Hardy-Weinberg equilibrium probabilities. Because of its importance, much attention has been paid to tests of the hypothesis that a population being sampled is in Hardy-Weinberg equilibrium against the alternative hypothesis that disturbing forces any deviation from this Hardy-Weinberg ratio.

For testing Hardy-Weinberg proportion, various large-sample goodness-of-fit tests, such as Pearson's statistic, likelihood ratio statistic or Freeman-Tukey statistic, are often used. It has been recognized, however, that the adequacy of applying these goodness-of-fit tests of Hardy-Weinberg proportion is often questionable when the sample size or some genotypic frequencies are small (see, for example, Emigh, 1980). Although a variety of corrections for small sample sizes are proposed (Emigh and Kempthorne, 1975; Elston and Forthofer, 1977; Smith, 1986), it is found that they usually do not greatly improve the results obtained from the traditional goodness-of-fit tests (Emigh, 1980; Hernández and Weir, 1989). Moreover, with the advent of variable number of tandem repeats (VNTRs) or micro-satellite marker, genetic loci with 10 or more alleles are not uncommon nowadays. In Section 2.2.5, we will treat 6 alleles or 8 alleles examples (genotype frequency data from Cazeneuve et al., 1999) involving some small and zero genotype counts. We show that large-sample inference does not work well for these examples, yielding incorrect p values. For these reasons, use of exact tests, which do not rely on asymptotic theory, is desirable.

Levene (1949) obtained the conditional distribution of a sample drawn from a population in Hardy-Weinberg equilibrium for an arbitrary number of alleles and Emith (1980) used Levene's distribution for the case of two alleles in his comparison of many statistical tests of Hardy-Weinberg hypothesis. Louis and Dempster (1987) proposed an algorithm for generating all possible samples for the exact distribution. Their algorithm works well when the number of alleles is small (say, four or five). However, it is not of practical use for loci with more than a few alleles since the number of possible samples with the same gene frequencies and sample sizes grows exponentially with the number of alleles (Hernández and Weir, 1989). An alternative approach that avoids complete enumeration is the simulated method such as a conventional Monte Carlo method or a Markov chain method (Guo and Thompson, 1992). Although Monte Carlo methods yield an unbiased estimate of the exact p value to arbitrary accuracy, there is currently no widely-used method that allows efficient computation of the exact p value, itself.

Our work builds on Louis and Dempster (1987) to provide an efficient method for exact inference. In this section, we propose a new technique that considerably extends the bounds of computational feasibility of the exact test. Our algorithm is constructed analogously to a network algorithm proposed by Mehta and Patel (1983) for Freeman-Halton exact test (Freeman and Halton, 1951) in two-way contingency tables. As in their application of the network algorithm, the computation of the smallest and largest values for the statistic plays an important role in our algorithm and some interesting new theorems are proved for computing these values.

The construction of this section is as follows. In Section 2.2.2, an exact test of Hardy-Weinberg proportion for multiple alleles is formulated. In Section 2.2.3, the network algorithm for computing the exact p values is given. In Section 2.2.4, several new theorems for some optimizing problems are proved. Some numerical examples are given in Section 2.2.5 to illustrate the practicality of our algorithm.

2.2.2 Exact test for multiple alleles

We assume that there are r distinct alleles, $A_1, A_2, ..., A_r$, of a given gene. If a sample of size N is drawn from a population of interest, the data can be expressed as the upper triangular array

$$
\begin{array}{c|c|c|c|c|}
\cline{2-5}
A_1 & x_{11}^o & x_{12}^o & \cdots & x_{1r}^o \\
\cline{2-5}
A_2 & \multicolumn{1}{c}{} & x_{22}^o & \cdots & x_{2r}^o \\
\cline{3-5}
\vdots & \multicolumn{1}{c}{} & \multicolumn{1}{c|}{} & \cdots & \cdots \\
\cline{4-5}
A_r & \multicolumn{1}{c}{} & \multicolumn{1}{c}{} & \multicolumn{1}{c|}{} & x_{rr}^o \\
\cline{5-5}
\multicolumn{1}{c}{} & \multicolumn{1}{c}{A_1} & \multicolumn{1}{c}{A_2} & \multicolumn{1}{c}{\cdots} & \multicolumn{1}{c}{A_r}
\end{array}
$$

where x_{ij}^o $(1 \le i \le j \le r)$ is the observed count of genotype A_iA_j in the sample. Throughout this section we will use a vector notation $\boldsymbol{x} = (x_{ij})$ to designate this type of table. For notational convenience, we write $x_{ij} = x_{ji}$ for $i > j$. We also define $\boldsymbol{y} = (y_1, y_2, ..., y_r)$ with $y_i = x_{ii}^o + \sum_{j=1}^r x_{ij}^o$, $i \in [r]$. y_i is the number of A_i genes in the sample. Clearly we have $\sum_{i \le j} x_{ij}^o = N$ and $\sum_{i=1}^r y_i = 2N$. Let $\mathcal{F}$ denote the reference set of all possible counts of genotype with the same gene counts as $\boldsymbol{x}^o$:

$$\mathcal{F} = \left\{ \boldsymbol{x} \mid \boldsymbol{x} = (x_{11}, x_{12}, x_{22}, ..., x_{rr}),\ x_{ii} + \sum_{j=1}^{r} x_{ij} = y_i \text{ for } i \in [r] \right\}.$$

We denote the number of elements in $\mathcal{F}$ by $\#\mathcal{F}$. Write $D = (2N)!/(N! \prod_{i=1}^r y_i!)$ for later use. Then, under Hardy-Weinberg proportions and conditional on $\boldsymbol{y}$, the probability of observing any $\boldsymbol{x} \in \mathcal{F}$ is expressed as (Levene, 1949)

$$P(\boldsymbol{x}) = \frac{N! \prod_{i=1}^r y_i!}{(2N)! \prod_{i \le j} x_{ij}!} 2^z = \frac{1}{D} \frac{2^z}{\prod_{i \le j} x_{ij}!}, \tag{2.13}$$

where $z = \sum_{i<j} x_{ij} = N - \sum_{i=1}^r x_{ii}$ is the number of heterozygotes in the sample.

The p value for the conditional test of Hardy-Weinberg proportions is defined as the sum of probabilities of all the counts of genotype in $\mathcal{F}$ that are no more likely than $\boldsymbol{x}^o$ (see, for example, Chapco, 1976), that is,

$$p = \sum_{\boldsymbol{x} \in \mathcal{T}} P(\boldsymbol{x}), \tag{2.14}$$

where $\mathcal{T} = \{\boldsymbol{x} \mid \boldsymbol{x} \in \mathcal{F},\ P(\boldsymbol{x}) \le P(\boldsymbol{x}^o)\}$ is the contribution region of this case. Acceptance or rejection is based on a comparison of this value with some preset α level as in any statistical test. This test corresponds to the two-sided version of Fisher's exact test for 2×2 contingency table, or Freeman-Halton exact test for two-way contingency table.

2.2.3 The network representation and the algorithm

For calculating the p value defined by (2.14), one simple approach is to generate all the samples in $\mathcal{F}$. Louis and Dempster (1987) described how to generate all the samples in $\mathcal{F}$ and computed the exact p values for some examples with three or four alleles. Their algorithm is, however, very time-consuming if $\#\mathcal{F}$ is large. In our study, we propose a new algorithm that does not require total enumeration of the reference set. This algorithm is a natural extension of the network algorithm for computing Freeman-Halton exact p values for two-way contingency table (Mehta and Patel, 1983). Similarly as in Section 2.1, first we provide a network representation of the reference set $\mathcal{F}$.

The network representation consists of *nodes* and *arcs* constructed in $r+1$ stages in this situation. For $k = r, r-1, ..., 1, 0$, the nodes at stage k have the form $(k, Y_{1,k}, Y_{2,k}, ..., Y_{k,k}) \equiv (k, \boldsymbol{Y}_k)$. There are as many nodes at stage k as there are possible partial sums of genes for the first k alleles. Arcs emanate from each node at stage k and every arc is connected to only one node at stage $k-1$. The network is constructed recursively by specifying all successor nodes $(k-1, \boldsymbol{Y}_{k-1})$ that are connected by arcs to each node $(k, \boldsymbol{Y}_k)$. The range of $Y_{i,k},\ i = 1, ..., k$, for these successor nodes is obtained from using the algorithm of Louis and Dempster (1987). There is only one node at stage r, the initial node, which is labeled $(r, \boldsymbol{Y}_r) \equiv (r, Y_{1,r}, ..., Y_{r,r}) = (r, y_1, ..., y_r) = (r, \boldsymbol{y})$. There is also only one node at stage 0, the terminal node, which is labeled (0). A path through the network is a sequence of arcs

$$(r, \boldsymbol{Y}_r) \to (r-1, \boldsymbol{Y}_{r-1}) \to \cdots \to (2, \boldsymbol{Y}_2) \to (1, \boldsymbol{Y}_1) \to (0).$$

One can verify that each path represents a distinct element in $\mathcal{F}$, with the relations

$$x_{11} = \frac{1}{2} Y_{1,1}, \tag{2.15}$$

$$x_{ik} = Y_{i,k} - Y_{i,k-1}, \quad i = 1, ..., k-1, \quad k = 2, ..., r, \tag{2.16}$$

and

$$x_{kk} = \frac{1}{2}\left(Y_{k,k} - \sum_{i=1}^{k-1} x_{ik}\right), \quad k = 2, ..., r. \tag{2.17}$$

Figure 2.2 shows the network representation for three alleles case with gene counts $(y_1, y_2, y_3) = (6, 5, 3)$. The dotted path gives the array of counts $\boldsymbol{x} = (x_{11}, x_{12}, x_{13}, x_{22}, x_{23}, x_{33}) = (2, 1, 1, 2, 0, 1)$.

We define the length of an arc from node $(k, \boldsymbol{Y}_k)$ to $(k-1, \boldsymbol{Y}_{k-1})$ by

$$ARC(k, \boldsymbol{Y}_k, \boldsymbol{Y}_{k-1}) = \frac{2^{\sum_{i=1}^{k-1}(Y_{i,k} - Y_{i,k-1})}}{\left[\frac{1}{2}\{Y_{k,k} - \sum_{i=1}^{k-1}(Y_{i,k} - Y_{i,k-1})\}\right]! \times \prod_{i=1}^{k-1}(Y_{i,k} - Y_{i,k-1})!}.$$

The length of path or sub-path is defined as the product of the corresponding arc lengths. Then it is straightforward to verify that the length of complete path from the initial node to the terminal node is equal to $D \cdot P(\boldsymbol{x})$ by using the relations (2.15), (2.16) and (2.17).

Now our goal is to identify and sum all paths whose length do not exceed $D \cdot P(\boldsymbol{x}^o)$. If we systematically enumerate each path through the network, compute its length and sum the path lengths that does not exceed $D \cdot P(\boldsymbol{x}^o)$, we are in effect considering all the elements in $\mathcal{F}$. This is the algorithm of Louis and Dempster (1987) and is usually computationally infeasible if $\#\mathcal{F}$ is large.

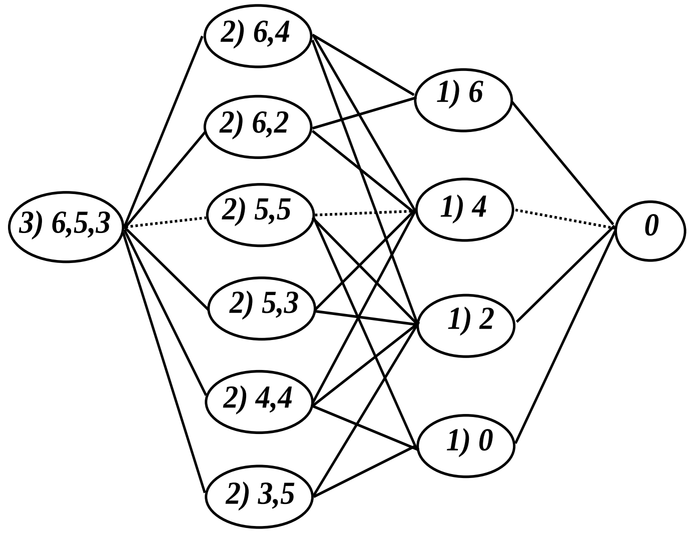

Figure 2.2: Network representation for three alleles case with $(y_1, y_2, y_3) = (6, 5, 3)$.

To avoid such total enumeration, we compute at each node $(k, \boldsymbol{Y}_k)$ the shortest and longest values of the sub-path from the node $(k, \boldsymbol{Y}_k)$ to the terminal node. We call these sub-paths as LP (longest sub-path) or SP (shortest sub-path) similarly as in Section 2.1. On the other hand, the length of the sub-path from the initial node to the current node $(k, \boldsymbol{Y}_k)$ is calculated from the labels $(r, \boldsymbol{Y}_r), ..., (k, \boldsymbol{Y}_k)$ as

$$PAST = \prod_{j=k+1}^{r} ARC(j, \boldsymbol{Y}_j, \boldsymbol{Y}_{j-1}).$$

Now we can determine whether all the paths having a common sub-path $(r, \boldsymbol{Y}_r) \to \cdots \to (k, \boldsymbol{Y}_k)$ do or do not contribute to the p value, without processing the remaining parts of paths as follows.

- Case 1. If
$$PAST \cdot LP(k, \boldsymbol{Y}_k) \le D \cdot P(\boldsymbol{x}^o), \tag{2.18}$$
then the lengths of all paths having common sub-path $(r, \boldsymbol{Y}_r) \to \cdots \to (k, \boldsymbol{Y}_k)$ are not greater than $D \cdot P(\boldsymbol{x}^o)$. Hence the lengths of all these paths contribute the p value.

- Case 2. If
$$PAST \cdot SP(k, \boldsymbol{Y}_k) > D \cdot P(\boldsymbol{x}^o), \tag{2.19}$$
then the lengths of all paths having common sub-path $(r, \boldsymbol{Y}_r) \to \cdots \to (k, \boldsymbol{Y}_k)$ exceed $D \cdot P(\boldsymbol{x}^o)$. Hence none of these paths contributes to the p value.

- Case 3. Otherwise, we consider the next stage (stage $k-1$).

It should be noted that the sum of all the sub-path lengths from the node $(k, \boldsymbol{Y}_k)$ to the terminal node is equal to $(2N_k)!/(N_k! \prod_{i=1}^{k} Y_{i,k})$, where $N_k = \frac{1}{2} \sum_{i=1}^{k} Y_{i,k}$. This relation is derived in the same manner as Levene (1949). Then the contribution to the p value in Case 1 equals

$PAST \cdot (2N_k)!/(N_k! \prod_{i=1}^{k} Y_{i,k})$. Consequently, we need not enumerate the remaining parts of paths for Case 1 or 2. In Case 3, we consider the common sub-path to a node $(k-1, \boldsymbol{Y}_{k-1})$ at stage $k-1$ which is connected to the node $(k, \boldsymbol{Y}_j)$, and proceed to verify (2.18) and (2.19) in the same manner as before.

The only remaining problem is to compute LP and SP at each node. If we can evaluate LP and SP exactly, we can ignore paths whose associated tables completely do or do not contribute to the p value. (We can *trim* paths.) It is worth pointing out, however, that if we can only evaluate an upper bound for LP or a lower bound for SP, we can make incomplete trimming. For Freeman-Halton exact test in two-way contingency table, Mehta and Patel (1983) evaluated an upper bound for LP and a lower bound for SP. For the Hardy-Weinberg case, we obtain the closed form expression of exact SP value in the following. As for LP, although no closed form of exact LP value is available, we present two upper bounds for LP.

2.2.4 Computing the shortest and longest paths from any node to the terminal node

A closed form expression of SP

First we present a closed form expression of $SP(k, \boldsymbol{Y}_k)$. Before we state a theorem we define $I = [k]$, $I_e = \{i \mid Y_{i,k} \text{ is even}\}$ and $I_o = \{i \mid Y_{i,k} \text{ is odd}\}$. We also define the following decomposition of the set I_o as $I_o = I_o^* \cup \widetilde{I}_o$, $I_o^* \cap \widetilde{I}_o = \emptyset$, where I_o^* is the maximal set made from the unions of pair (i,j) such that $Y_{i,k} = Y_{j,k}$ and $\widetilde{I}_o = I_o - I_o^*$ is the remaining set satisfying $Y_{i,k} \neq Y_{j,k}$ for all $i, j \in \widetilde{I}_o$, $i \neq j$. If $\boldsymbol{Y}_k = (13, 12, 11, 11, 11, 10, 9, 8, 5, 5, 3, 3, 3)$, for example, we have $I_e = \{2, 6, 8\}$, $I_o^* = \{3, 4, 9, 10, 11, 12\}$ and $\tilde{I}_o = \{1, 5, 7, 13\}$. (Although the elements of $\tilde{I}_o$ and I_o^* are not unique, corresponding values of $Y_{i,k}$ are uniquely determined.) It should be noted that, by definition, $Y_{1,k} + \cdots + Y_{k,k}$, $\#I_o$, $\#\widetilde{I}_o$ and $\#I_o^*$ are all even numbers. Using these sets, our problem can be written in the following form:

$$\mathrm{P}_1 : \text{minimize } \frac{2^z}{\prod_{1 \le i \le j \le k} x_{ij}!}, \quad z = \sum_{1 \le i < j \le k} x_{ij}, \tag{2.20}$$

subject to

$$x_{ii} + \sum_{j=1}^{k} x_{ij} = 2m_i, \quad \text{for } i \in I_e, \tag{2.21}$$

$$x_{ii} + \sum_{j=1}^{k} x_{ij} = 2m_i + 1, \quad \text{for } i \in I_o, \tag{2.22}$$

$$x_{ji} = x_{ij}, \tag{2.23}$$

$$x_{ij} \in \mathbb{Z}_{\ge 0} \text{ for } i, j \in [k]. \tag{2.24}$$

A solution of P_1 is given in the following theorem.

Theorem 2.2.1 *The optimal objective function value of P_1 is given by*

$$2^{z^*}\left(\prod_{i\in I_e}\frac{1}{m_i!}\right)\left(\prod_{i\in \widetilde{I}_o}\frac{1}{m_i!}\right)\left\{\prod_{i\in I_o^*}\frac{1}{(2m_i+1)!}\right\}^{1/2}, \ \textit{where} \ \ z^*=\frac{1}{2}\left\{\sum_{i\in I_o^*}(2m_i+1)+\#\widetilde{I}_o\right\}. \tag{2.25}$$

Hereafter, we define $\boldsymbol{x}^* = (x^*_{11}, x^*_{12}, x^*_{22}, ..., x^*_{kk})$ as one of the solutions of P_1 that minimizes (2.20) subject to (2.21), (2.22), (2.23) and (2.24). To prove the above theorem, we prepare the following lemma.

Lemma 2.2.1 *The optimal solution $\boldsymbol{x}^*$ satisfies the following conditions.*
(a) x^*_{ij}, $i \neq j$, cannot be a positive even number.
(b) $\{x^*_{i1}, ..., x^*_{ii-1}, x^*_{ii+1}, ..., x^*_{ik}\}$ includes at most one odd number for all i.

Proof of Lemma 2.2.1.
(a) Suppose that $x^*_{ij} = 2n, n \geq 1$, for some i, j $(i \neq j)$. Consider another solution $\boldsymbol{x}' = (x'_{11}, ..., x'_{kk})$, where

$$\begin{cases} x'_{ii} = x^*_{ii} + n, \ x'_{jj} = x^*_{jj} + n, \ x'_{ij} = 0, \\ x'_{ij} = x^*_{ij} \ \text{ for all the other } i, j. \end{cases}$$

Clearly, $\boldsymbol{x}'$ satisfies (2.21),(2.22),(2.23) and (2.24). Let OF^* be the value of the objective function under $\boldsymbol{x}^*$ and OF' be the value of the objective function under $\boldsymbol{x}'$. Then we have

$$\frac{OF^*}{OF'} = \frac{2^{2n}(n!)^2}{(2n)!}\begin{pmatrix} x^*_{ii}+n \\ x^*_{ii}\end{pmatrix}\begin{pmatrix} x^*_{jj}+n \\ x^*_{jj}\end{pmatrix} \geq \frac{2^{2n}(n!)^2}{(2n)!} \equiv f_1(n),$$

$$\frac{f_1(n+1)}{f_1(n)} = \frac{2(n+1)}{2n+1} > 1$$

and $f_1(n) > f_1(n-1) > \cdots > f_1(1) = 2 > 1$. Hence $OF^* > OF'$ holds. This contradicts that OF^* is the optimal objective function value.

(b) Suppose that $x^*_{ij_1} = 2n_1+1, x^*_{ij_2} = 2n_2+1, \ n_1, n_2 \geq 0, j_1 \neq i, j_2 \neq i$ for some j_1, j_2 $(j_1 \neq j_2)$. Consider another solution $\boldsymbol{x}'$, where

$$\begin{cases} x'_{ii} = x^*_{ii} + n_1 + n_2 + 1, \ x'_{j_1j_1} = x^*_{j_1j_1} + n_1, \ x'_{j_2j_2} = x^*_{j_2j_2} + n_2, \\ x'_{ij_1} = x'_{ij_2} = 0, \ x'_{j_1j_2} = x^*_{j_1j_2} + 1, \\ x'_{ij} = x^*_{ij} \ \text{ for all the other } i, j. \end{cases}$$

Clearly, $\boldsymbol{x}'$ satisfies (2.21),(2.22),(2.23) and (2.24). Let OF' be the value of the objective function under $\boldsymbol{x}'$. Then we have

$$\begin{aligned} \frac{OF^*}{OF'} &= \frac{2^{2n_1+2n_2+1}n_1!n_2!(n_1+n_2+1)!}{(2n_1+1)!(2n_2+1)!}\begin{pmatrix} x^*_{ii}+n_1+n_2+1 \\ x^*_{ii}\end{pmatrix}\begin{pmatrix} x^*_{j_1j_1}+n_1 \\ x^*_{j_1j_1}\end{pmatrix} \\ &\qquad\qquad \times \begin{pmatrix} x^*_{j_2j_2}+n_2 \\ x^*_{j_2j_2}\end{pmatrix}(x^*_{j_1j_2}+1) \\ &\geq \frac{2^{2n_1+2n_2+1}n_1!n_2!(n_1+n_2+1)!}{(2n_1+1)!(2n_2+1)!} \equiv f_2(n_1, n_2) \end{aligned}$$

and

$$\frac{f_2(n_1+1,n_2)}{f_2(n_1,n_2)} = \frac{2(n_1+n_2+2)}{2n_1+3} \geq \frac{2(n_1+2)}{2n_1+3} > 1.$$

Similarly we have $\dfrac{f_2(n_1,n_2+1)}{f_2(n_1,n_2)} > 1$. Hence $f_2(n_1,n_2) > f_2(0,0) = 2 > 1$ and $OF^* > OF'$ holds. This contradicts that OF^* is the optimal objective function value. Q.E.D.

Now we prove Theorem 2.2.1 using the above lemma.

Proof of Theorem 2.2.1.
As a direct result of the Lemma 2.2.1, we have $x^*_{ii} = m_i,\ x^*_{ij} = 0,\ j \neq i,$ for all $i \in I_e$ since the number of odd values in $\{x^*_{i1}, ..., x^*_{ii-1}, x^*_{ii+1}, ..., x^*_{ik}\}$ is even for all $i \in I_e$. On the other hand, we see that the elements of I_o are separated into *pairs* as $(i_1,j_1),(i_2,j_2),...,(i_p,j_p)$ such that

$$x^*_{ij} \quad \begin{array}{ll} > 0, & \text{if } (i,j) \text{ is a pair,} \\ = 0, & \text{otherwise,} \end{array}$$

and $p = \#I_o/2$ is the number of the pairs. Then the optimal objective function value of P_1 can be written as

$$2^{z^*}\left(\prod_{i\in I_e}\frac{1}{m_i!}\right)\left(\prod_{n=1}^{p}\frac{1}{x^*_{i_ni_n}!x^*_{j_nj_n}!x^*_{i_nj_n}!}\right), \quad z^* = \sum_{n=1}^{p} x^*_{i_nj_n}. \tag{2.26}$$

Hereafter we call (i,j) an *identical pair* if $m_i = m_j$ and a *different pair* if $m_i \neq m_j$. It is worth pointing out that $i,j \in I^*_o$ for all identical pairs (i,j).

First we consider the identical pair (i,j). Let $m_i = m_j \equiv m$ and

$$x^*_{ij} = 2(m-n)+1, \quad x^*_{ii} = x^*_{jj} = n \tag{2.27}$$

for these i,j. Now we show that n has to be zero, that is, $\min\limits_{0\leq n\leq m} OF(n) = OF(0)$, where $OF(n)$ is the objective function value when x^*_{ij}, x^*_{ii} and x^*_{jj} of $\boldsymbol{x}^*$ are given by (2.27) for $n = 0,...,m$. We have

$$\frac{OF(n+1)}{OF(n)} = \frac{(2m-2n+1)(m-n)}{2(n+1)^2}.$$

If we compare this ratio to 1 for $n = 0,1,...,m$, then we have

$$\frac{OF(n+1)}{OF(n)} < 1 \text{ for } n > \frac{2m^2+m-2}{4m+5}$$

and

$$\frac{OF(n+1)}{OF(n)} > 1 \text{ for } n < \frac{2m^2+m-2}{4m+5}$$

and hence $\min\limits_{0\leq n\leq m} OF(n) = \min\{OF(0), OF(m)\}$. Besides we have

$$\frac{OF(m)}{OF(0)} = \frac{(2m+1)!}{2^{2m}(m!)^2} \equiv f_3(m)$$

and

$$\frac{f_3(m+1)}{f_3(m)} = \frac{2m+3}{2(m+1)} > 1.$$

Hence

$$f_3(m) > f_3(m-1) > \cdots > f_3(0) = 1 \tag{2.28}$$

and $OF(m) > OF(0)$. We have now shown that

$$\begin{cases} x^*_{ij} = 2m_i + 1, \\ x_{is} = 0, \text{ for } s \neq j, \\ x_{js} = 0, \text{ for } s \neq i, \end{cases} \tag{2.29}$$

for the identical pair (i, j).

Next we consider the different pair (i, j). We can assume $m_i > m_j$ without loss of generality. Similarly to the case of the identical pair, we denote

$$x^*_{ii} = m_i - n, \quad x^*_{jj} = m_j - n, \quad x^*_{ij} = 2n + 1$$

and consider the sequence $OF(n), n = 0, 1, ..., m_j$. The ratio is written as

$$\frac{OF(n)}{OF(0)} = \prod_{k=0}^{n-1} \left\{ \frac{2(m_i - k)}{2(n-k)+1} \times \frac{m_j - k}{n-k} \right\} \geq \prod_{k=0}^{n-1} \frac{2(m_i - k)}{2(n-k)+1}.$$

From $m_i > m_j$, we have $m_i - n > m_j - n \geq 0$ and then $m_i \geq n + 1$ holds. Hence we have

$$\frac{OF(n)}{OF(0)} \geq \prod_{k=0}^{n-1} \frac{2(n+1-k)}{2(n-k)+1} > 1$$

and $OF(n) > OF(0)$. We have shown that

$$\begin{cases} x^*_{ii} = m_i, \; x^*_{jj} = m_j, \; x^*_{ij} = 1, \\ x_{is} = x_{js} = 0 \text{ for } s \neq i, j \end{cases} \tag{2.30}$$

for the different pair (i, j).

Now we show that the pairs have to be constructed in such a way that the number of identical pairs is maximized. Clearly it is sufficient to consider the case of four alleles, $\boldsymbol{Y}_k = (Y_{1,k}, Y_{2,k}, Y_{3,k}, Y_{4,k}) = (2m_1 + 1, 2m_1 + 1, 2m_3 + 1, 2m_4 + 1)$ where $m_1 \neq m_3$ and $m_1 \neq m_4$.

(i) If we make pairs as $(1, 3)$ and $(2, 4)$, then the optimal $\boldsymbol{x}^*$ is obtained from (2.30) as

$$\begin{cases} x^*_{11} = x^*_{22} = m_1, \; x^*_{33} = m_3, \; x^*_{44} = m_4, \; x^*_{13} = x^*_{24} = 1, \\ \text{otherwise } x^*_{ij} = 0. \end{cases}$$

(ii) Similarly, if we make pairs as $(1, 2)$ and $(3, 4)$, $\boldsymbol{x}^*$ is written as follows:

- If $m_3 = m_4$, then

$$\begin{cases} x^*_{12} = 2m_1 + 1, \; x^*_{34} = 2m_3 + 1, \\ \text{otherwise } x^*_{ij} = 0. \end{cases}$$

- If $m_3 \neq m_4$, then

$$\begin{cases} x_{12}^* = 2m_1 + 1, \; x_{33}^* = m_3, \; x_{44}^* = m_4, \; x_{34}^* = 1, \\ \text{otherwise } x_{ij}^* = 0. \end{cases}$$

Let OF_i and OF_{ii} denote the objective function values corresponding to *(i)* and *(ii)*, respectively.

- If $m_3 = m_4$, then

$$\frac{OF_i}{OF_{ii}} = \frac{(2m_1+1)!}{2^{2m_1}(m_1!)^2} \cdot \frac{(2m_3+1)!}{2^{2m_3}(m_3!)^2} = f_3(m_1)f_3(m_3).$$

  From (2.28), we have $OF_i > OF_{ii}$ in this case.

- If $m_3 \neq m_4$, then

$$\frac{OF_i}{OF_{ii}} = \frac{(2m_1+1)!}{2^{2m_1}(m_1!)^2} = f_3(m_1).$$

  Again from (2.28), we have $OF_i > OF_{ii}$.

From these considerations, it is shown that the case of *(i)* is not optimal. In other words, all the different pairs have to be included in $\widetilde{I}_o$ and all the identical pairs have to be included in I_o^*. Substitution of (2.29) and (2.30) into (2.26) corresponding to $\widetilde{I}_o$ and I_o^* and some simplification yields (2.25). Q.E.D.

Some upper bounds for LP

Next we consider $LP(k, \boldsymbol{Y}_k)$. The problem we consider is

$$\mathrm{P}_2 : \text{maximize } \frac{2^z}{\prod_{1 \le i \le j \le k} x_{ij}!}, \quad z = \sum_{1 \le i < j \le k} x_{ij},$$

subject to

$$x_{ii} + \sum_{j=1}^{k} x_{ij} = Y_{i,k}, \quad \text{for } i = 1, ..., k \tag{2.31}$$

and (2.23),(2.24). Unfortunately the closed form expression of $LP(k, \boldsymbol{Y}_k)$ in not available except for small k. In this study, two upper bounds for $LP(k, \boldsymbol{Y}_k)$ and closed form of $LP(2, \boldsymbol{Y}_2)$ are provided.

Theorem 2.2.2 *An upper bound for the optimal objective function value of* P_2 *is given by*

$$\max_{0 \le z \le N_k} \frac{2^z}{(d_1+1)^{N_k - z - kd_1}(d_1!)^k (d_2+1)^{z - k(k-1)d_2/2}(d_2!)^{k(k-1)/2}}, \tag{2.32}$$

where $d_1 = [(N_k - z)/k]\,, \; d_2 = [2z/\{k(k-1)\}]\,, \; N_k = \frac{1}{2}\sum_{i=1}^{k} Y_{i,k}$, *and* $[x]$ *denotes the largest integer less than or equal to* x.

Proof. Fixing z and ignoring the constraints (2.31), we can easily show that the object function value

$$\frac{2^z}{\prod_{i\le j} x_{ij}!} = \frac{2^z}{\left(\prod_{i=1}^k x_{ii}!\right)\left(\prod_{i<j} x_{ij}!\right)} \tag{2.33}$$

is maximized when $|x_{ii} - x_{jj}| \le 1$ for all i, j and $|x_{ij} - x_{i'j'}| \le 1$ for all $i < j,\ i' < j'$. Therefore under the constraints $\sum_{i=1}^k x_{ii} = N_k - z$ and $\sum_{i<j} x_{ij} = z$, $N_k - z - kd_1$ elements in $\{x_{11}, ..., x_{kk}\}$ are equal to $d_1 + 1$ and the rest are equal to d_1, and $z - k(k-1)d_2/2$ elements in $\{x_{12}, ..., x_{k-1k}\}$ are equal to $d_2 + 1$ and the rest are equal to d_2. Substituting these values into (2.33) and maximizing with respect to z yields (2.32). Since (2.32) is the maximum objective function value for the relaxation problem of P_2 where the constraints (2.31) are ignored, it is indeed an upper bound for the optimal objective function value of P_2. Q.E.D.

We can see that the upper bound given in Theorem 2.2.2 is equal to the exact $LP(k, \boldsymbol{Y}_k)$ value when the components of $\boldsymbol{Y}_k$ is equal or nearly equal to each other. For this reason, this upper bound is a natural analogue of an upper bound for LP given by Mehta and Patel (1983) for Freeman-Halton case.

Next we provide another (approximate) upper bound which has good property regardless of the pattern of $\boldsymbol{Y}_k$ in the following Theorem.

Theorem 2.2.3 *An approximate upper bound for the optimal objective function value of P_2 is given by*

$$\frac{2^{z^*}}{\prod_{i\le j} g(x_{ij}^*)}, \quad z^* = \sum_{i<j} x_{ij}^*,$$

where

$$x_{ii}^* = \frac{Y_{i,k}^2}{4N_k}, \quad x_{ij}^* = \frac{Y_{i,k}Y_{j,k}}{2N_k}, \quad i \ne j, \tag{2.34}$$

and $g(x)$ is an arbitrary continuous function satisfying $g(n) = n!$ if n is an integer.

Proof. Replacing $x!$ with the function $g(x)$ defined above and ignoring the constraint that x_{ij} is integer, the continuous relaxation problem of P_2 is obtained as

$$\mathrm{P}_2' : \text{maximize } \frac{2^z}{\prod_{i\le j} g(x_{ij})}, \quad z = \sum_{i<j} x_{ij},$$

subject to (2.31),(2.23) and $x_{ij} \ge 0$. Clearly the optimal objective function value of P_2' is an upper bound for the original integer optimizing problem P_2.

On the other hand, the optimal solution of P_2' is approximated by (2.34) for the following reason. Let $\boldsymbol{p}_1$ be the reference empirical distribution given by

$$p_{ij} = x_{ij}/N_k, \quad i = 1, ..., k,\ j = i, ..., k,$$

where x_{ij} satisfies (2.31) and $\boldsymbol{p}_0$ be the Hardy-Weinberg distribution given by

$$p_{ii} = p_i^2, \quad i = 1, ..., k,$$
$$p_{ij} = 2p_i p_j, \quad i = 1, ..., k-1, \ j = i+1, ..., k.$$

We denote the Kullback-Leibler divergence from $\boldsymbol{p}_1$ to $\boldsymbol{p}_0$ as $D(\boldsymbol{p}_1, \boldsymbol{p}_0)$. Since the optimal solution of P_2 corresponds to $\boldsymbol{p}_1$ whose occurrence probability is maximum when the true distribution is $\boldsymbol{p}_0$, P_2 is approximately equivalent to minimizing $D(\boldsymbol{p}_1, \boldsymbol{p}_0)$. Here the decomposition

$$D(\boldsymbol{p}_1, \boldsymbol{p}_0) = D(\boldsymbol{p}_1, \boldsymbol{p}_M) + D(\boldsymbol{p}_M, \boldsymbol{p}_0) \tag{2.35}$$

holds where $\boldsymbol{p}_M$ is the conditional maximum likelihood estimate under the Hardy-Weinberg model given by $p_{ij} = x_{ij}/N_k$ where x_{ij} is given by (2.34). This prove the theorem. Q.E.D.

The decomposition (2.35) is an important property of the divergence $D(\boldsymbol{p}_1, \boldsymbol{p}_0)$ and can be derived directly for the present case. The meaning of this decomposition is elucidated from the differential geometrical point of view. For detail, see Amari (1985, 1989) for example.

The standard example of $g(x)$ is Gamma function, $g(x) = \Gamma(x+1)$. However, similarly as in Section 2.1, even simpler function such as piecewise linear or piecewise quadratic function can also be used.

As the last result of this section, we provide the closed form expression of $LP(2, \boldsymbol{Y}_2)$. The problem that we consider is written as

$$\mathrm{P}_3 : \text{maximize } \frac{2^{x_{12}}}{x_{11}!x_{12}!x_{22}!} \ ,$$

subject to

$$2x_{11} + x_{12} = Y_{1,2}, \quad 2x_{22} + x_{12} = Y_{2,2},$$
$$x_{11}, x_{12}, x_{22} \in \mathbb{Z}_{\geq 0}.$$

Theorem 2.2.4 *The optimal solution $\boldsymbol{x}^* = (x_{11}^*, x_{12}^*, x_{22}^*)$ of P_3 is given as follows.*

1. *If $Y_{1,2}, Y_{2,2}$ are both even numbers, let $a(\boldsymbol{Y}_2) = (Y_{1,2}Y_{2,2} - 2)/\{2(Y_{1,2} + Y_{2,2} + 3)\}$. The optimal solution is*

$$x_{11}^* = \frac{Y_{1,2}}{2} - n, \quad x_{22}^* = \frac{Y_{2,2}}{2} - n, \quad x_{12}^* = n,$$

where

$$\begin{cases} n = a(\boldsymbol{Y}_2) \ \text{or} \ a(\boldsymbol{Y}_2) + 1, & \text{if} \ \ a(\boldsymbol{Y}_2) \ \ \text{is integer}, \\ n = \lfloor a(\boldsymbol{Y}_2) + 1 \rfloor, & \text{otherwise}. \end{cases}$$

2. *If $Y_{1,2}, Y_{2,2}$ are both odd numbers, let $a(\boldsymbol{Y}_2) = \{(Y_{1,2}-1)(Y_{2,2}-1)-6\}/\{2(Y_{1,2}+Y_{2,2}+3)\}$. The optimal solution is*

$$x_{11}^* = \frac{Y_{1,2} - 1}{2} - n, \quad x_{22}^* = \frac{Y_{2,2} - 1}{2} - n, \quad x_{12}^* = 2n + 1,$$

where

$$\begin{cases} n = a(\boldsymbol{Y}_2) \ \text{or} \ a(\boldsymbol{Y}_2) + 1, & \text{if} \ \ a(\boldsymbol{Y}_2) \ \ \text{is integer}, \\ n = \lfloor a(\boldsymbol{Y}_2) + 1 \rfloor, & \text{otherwise}. \end{cases}$$

The proof of this theorem is straightforward and omitted.

Table 2.3: Genotype frequency data from Guo and Thompson (1992).

Genotype	No
A_1A_1	3
A_1A_2	4
A_1A_3	2
A_1A_4	3
A_2A_2	2
A_2A_3	2
A_2A_4	3
A_2A_5	1
A_3A_3	2
A_3A_4	2
A_3A_7	1
A_4A_4	1
A_4A_8	2
A_5A_8	1
A_6A_6	1
Total	30

2.2.5 Some numerical examples

We computed exact p values for problems of various sizes by the network algorithm. All the algorithms were programmed using C language on a PC running on Linux (Pentium III, 930MHz).

First we analyze the data of $r = 8, N = 30, \boldsymbol{y} = (15, 14, 11, 12, 2, 2, 1, 3)$, displayed in Table 2.3. This data is taken from Figure 1 of Guo and Thompson (1992). Since the size of this data is moderately large, they could not calculate the exact p value and instead evaluated the simulated value by Monte Carlo method. We computed the exact p value for this data by using a complete enumeration algorithm proposed by Louis and Dempster (1987), Markov chain Monte Carlo method by Guo and Thompson (1992) and the network algorithm. As for computing upper bounds for LP in the network algorithm, two upper bounds proposed in the previous section (Theorem 2.2.2 and Theorem 2.2.3) were considered. For the Markov chain Monte Carlo method, the dememorization period is $1,000$ steps. We use a batching method to obtain an estimate of variance (Hastings, 1970; Ripley, 1987), that is, we divide the observations into B batches of C consecutive observations each, and use

$$S^2 = \frac{1}{B(B-1)} \sum_{i=1}^{B} (\hat{p}_i - \hat{p})^2$$

as an estimate of variance, where $\hat{p}$ is an estimated p value computed from all the observations and $\hat{p}_i$ is an estimated p value computed from observations in the ith batch. Table 2.4 shows the p values and CPU times. The results of various goodness-of-fit tests are also listed: F^2 is the Freeman-Tukey statistic; G^2, the likelihood ratio statistic; χ^2, Pearson's statistic; $\chi^2_{.5}$, Pearson's statistic with continuity correction of .5; $\chi^2_{.25}$, Pearson's statistic with continuity correction of

Table 2.4: A results of goodness-of-fit and exact tests for the allele frequency data in Table 2.3 ($r = 8, \#\mathcal{F} = 250552020 \sim 2.5 \times 10^8$).

Statistic/Method	Value	p value	S.E.	CPU time[a]
F^2	14.7601	0.9809	—	—
G^2	25.9748	0.5744	—	—
χ^2	51.9302	0.003908	—	—
$\chi^2_{.5}$	71.5300	1.1344 $\times 10^{-5}$	—	—
$\chi^2_{.25}$	39.4041	0.07464	—	—
MCMC ($B = 100, C = 10,000$)	—	0.2253	0.00470	0:03.31
MCMC ($B = 100, C = 100,000$)	—	0.2144	0.00149	0:25.02
MCMC ($B = 100, C = 1,000,000$)	—	0.2157	0.000425	4:13
Complete enumeration	—	0.2159398218	—	44:43
Network (LP by Thm. 2.2.2)	—	0.2159398218	—	10:25
Network (LP by Thm. 2.2.3)	—	0.2159433639	—	8:21

[a]CPU time is represented by min : sec.

.25 as suggested by Emigh(1980). Table 2.4 shows, as is reported by Guo and Thompson (1992), that the different goodness-of-fit statistics employed could lead to completely different conclusions. This implies the need for the exact test. For the exact tests, it takes about 45 minutes to perform the complete enumeration algorithm. By the Markov chain Monte Carlo methods, the exact p values are computed to the accuracy of the two digits in 4 minutes. This implies that the Markov chain Monte Carlo method is a valuable tool if a rough estimate of p value is needed. On the other hand, the network algorithm enables more efficient calculations than the complete enumeration algorithm. To calculate the exact p value, it takes about 10 minutes when using the upper bound proposed in Theorem 2.2.2 and about 8 minutes when using the approximate upper bound proposed in Theorem 2.2.3. These CPU times show that the path was trimmed in Case 1 (in Section 2.2.3) more efficiently when using the approximate upper bound. Strictly speaking, it is not guaranteed that the obtained p value is precise when the approximate upper bound is used. This is because the optimal solution of the relaxation problem P_2' is attained at (2.34) only approximately. Then an over trimming may occur when the optimal solution of the relaxation problem is underestimated than the true optimal solution of the original integer maximization problem. Indeed, the p value by Network (LP by Thm. 2.2.3) in Table 2.4 is slightly larger than the values by Network (LP by Thm. 2.2.2) and the complete enumeration. However, Table 2.4 shows that the p value is computed to the accuracy of the five digits when using the approximate upper bound and it can be considered that the accuracy of the approximation is sufficiently good in practice.

Next we analyze the genotype frequency data at the MEFV locus in Armenian patients from Cazeneuve et al. (1999) displayed in Table 2.5. Note that there is an "unidentified allele" in Table 2.5. In this study, we treat it in two ways. First, we ignore the unidentified allele (and also the complex allele) and calculate p values for the 6 alleles (M694V, V726A, M680I, F479L, E148Q, R761H) data of $N = 76, \boldsymbol{y} = (73, 40, 32, 4, 2, 1)$. Table 2.6 shows the results. Second, we treat the unidentified allele (and also the complex allele) as one allele and calculate p values for the 8 alleles data of $N = 85, \boldsymbol{y} = (75, 42, 33, 12, 4, 2, 1, 1)$. Table 2.7 shows the results.

Table 2.5: Genotype frequency data at the MEFV locus in Armenian patients from Cazeneuve et al. (1999).

Genotype	No	(%)
M694V/M694V	18	(21.2)
M694V/V726A	22	(25.9)
M694V/M680I	13	(15.3)
M726A/M680I	9	(10.6)
M680I/M680I	4	(4.7)
V726A/V726A	3	(3.5)
V726A/F479L	3	(3.5)
M694V/E148Q	2	(2.4)
M680I/R761H	1	(1.2)
M680I/F479L	1	(1.2)
M680I/unidentified allele	1	(1.2)
M694V/unidentified allele	2	(2.4)
complex allele[a]/unidentified allele	1	(1.2)
unidentified allele/unidentified allele	3	(3.5)
Total	85	(100)

[a]E148Q, P369S and R408Q mutations in *cis*.

Table 2.6: A results of goodness-of-fit and exact tests for the MEFV data (6 alleles) in Table 2.5 ($\#\mathcal{F} = 3048176 \sim 3.0 \times 10^6$).

Statistic/Method	Value	p value	S.E.	CPU time[a]
F^2	11.6791	0.7783	—	—
G^2	14.4440	0.5895	—	—
χ^2	13.4047	0.6645	—	—
$\chi^2_{.5}$	132.3692	$< 1.0 \times 10^{-38}$	—	—
$\chi^2_{.25}$	38.4253	0.00024558	—	—
MCMC ($B = 100, C = 10,000$)	—	0.2488	0.00507	0:03.04
MCMC ($B = 100, C = 100,000$)	—	0.2555	0.00172	0:30.10
MCMC ($B = 100, C = 1,000,000$)	—	0.2547	0.000435	5:04
Complete enumeration	—	0.2537322421	—	0:27.68
Network (LP by Thm. 2.2.2)	—	0.2537322421	—	0:02.01
Network (LP by Thm. 2.2.3)	—	0.2537322421	—	0:01.45

[a]CPU time is represented by min : sec.

Table 2.7: A results of goodness-of-fit and exact tests for the MEFV data (8 alleles) in Table 2.5 ($\#\mathcal{F} = 9365418588 \sim 9.4 \times 10^9$).

Statistic/Method	Value	p value	S.E.	CPU time[a]
F^2	22.0452	0.8226	—	—
G^2	31.5254	0.3532	—	—
χ^2	47.0085	0.01251	—	—
$\chi^2_{.5}$	323.1206	$< 1.0 \times 10^{-38}$	—	—
$\chi^2_{.25}$	103.3698	8.4231×10^{-15}	—	—
MCMC ($B = 100, C = 10,000$)	—	0.009833	0.00109	0:02.51
MCMC ($B = 100, C = 100,000$)	—	0.01070	0.000399	0:24.77
MCMC ($B = 100, C = 1,000,000$)	—	0.01080	0.000117	4:14
Complete enumeration	—	0.0109317715	—	1488:17
Network (LP by Thm. 2.2.2)	—	0.0109317226	—	191:39
Network (LP by Thm. 2.2.3)	—	0.0109317318	—	155:10

[a]CPU time is represented by min : sec.

Table 2.6 and Table 2.7 again show that the different goodness-of-fit statistics could lead to different conclusions as we have seen in Table 2.4. Especially, the p values calculated from χ^2 with continuity corrections are erroneously small. Table 2.6 shows that the network algorithms perform quite well for this data: it takes only 1 or 2 seconds to calculate the exact p values by the network algorithm and the accuracy of the p value when using the approximate upper bound is quite good (at least ten digits). It can be concluded that there is no reason for using the Markov chain Monte Carlo method for this data. On the other hand, Table 2.7 shows that it takes a moderately long time to calculate the p values by the network algorithms, though the network algorithms perform much better than the complete enumeration algorithm.

Finally, we compare the network algorithm with the complete enumeration algorithm in detail. For considering the computational feasibility, we analyze data sets of various sizes. Table 2.8 shows the p values and CPU times for the examples of $r = 5$, where the pattern of $\boldsymbol{y}$ is uniform. Table 2.9 shows the p values and CPU times for the various pattern of $\boldsymbol{y}$ for examples of $N = 50$. In each example, the p value close to 0.05 is calculated. The number of all the tables ($\#\mathcal{F}$) and the ratio of CPU time (complete enumeration to network) are also provided when the complete enumeration is feasible.

Table 2.8 and Table 2.9 show that the network algorithm performs uniformly better for all these examples. CPU ratio shows that the efficiency of the network algorithm is more emphasized when the size of the problem is large. We see that the p values of examples of moderate size ($\#\mathcal{F} \sim 10^9$) can be calculated within about 30 minutes by the network algorithm, while it took several hours by the complete enumeration. Comparing the upper bound for LP, we see that the approximate upper bound proposed in Theorem 2.2.3 performs better and the accuracy of the approximation is satisfactory.

It should be noted that the CPU time is greatly effected by p value when using the network algorithm, while it takes same time regardless of p value by the complete enumeration or the Monte Carlo method. In this study p values about 0.05 are mainly considered, however, larger p values can be more easily calculated by the network algorithm. Table 2.10 shows CPU times

Table 2.8: A comparison of the network and the Louis and Dempster algorithms for the allele frequency data of $r = 5$ (uniform case).

$\boldsymbol{y}$	Algorithm	p value	CPU time[a] (ratio[b])	$\#\mathcal{F}$
$(20, 20, 20, 20, 20)$	Complete enumeration	0.0448476262	46:27	3.0×10^8
	Network (LP by Thm. 2.2.2)	0.0448476262	4:55 (9.45)	
	Network (LP by Thm. 2.2.3)	0.0448505876	4:03 (11.47)	
$(22, 22, 22, 22, 22)$	Complete enumeration	0.0443505782	106:56	7.0×10^8
	Network (LP by Thm. 2.2.2)	0.0443505782	9:06 (11.75)	
	Network (LP by Thm. 2.2.3)	0.0443514885	7:27 (14.35)	
$(24, 24, 24, 24, 24)$	Complete enumeration	0.0476068427	230:13	1.5×10^9
	Network (LP by Thm. 2.2.2)	0.0476068428	15:09 (15.20)	
	Network (LP by Thm. 2.2.3)	0.0476073528	12:21 (18.64)	
$(26, 26, 26, 26, 26)$	Complete enumeration		infeasible[c]	
	Network (LP by Thm. 2.2.2)	0.0490752414	27:42	
	Network (LP by Thm. 2.2.3)	0.0490747618	24:20	
$(28, 28, 28, 28, 28)$	Complete enumeration		infeasible[c]	
	Network (LP by Thm. 2.2.2)	0.0502934492	37:29	
	Network (LP by Thm. 2.2.3)	0.0502939082	30:38	
$(30, 30, 30, 30, 30)$	Complete enumeration		infeasible[c]	
	Network (LP by Thm. 2.2.2)	0.0516508563	55:49	
	Network (LP by Thm. 2.2.3)	0.0516511735	45:29	

[a]CPU time is represented by min : sec.
[b]CPU time (complete enumeration) / CPU time (network)
[c]Fail to compute p value within 360 CPU minutes.

Table 2.9: A comparison of the network and the Louis and Dempster algorithms for the allele frequency data of $N = 50, r = 4 \sim 8$.

$\boldsymbol{y}$	Algorithm	p value	CPU time[a](ratio[b])	$\#\mathcal{F}$
(25, 25, 25, 25)	Complete enumeration	0.0526117171	0:02.05	2.3×10^5
	Network (LP by Thm. 2.2.2)	0.0526117171	0:00.46 (4.46)	
	Network (LP by Thm. 2.2.3)	0.0526117171	0:00.40 (5.13)	
(40, 30, 20, 5, 5)	Complete enumeration	0.0566520911	0:18.28	2.0×10^6
	Network (LP by Thm. 2.2.2)	0.0566520911	0:04.25 (4.30)	
	Network (LP by Thm. 2.2.3)	0.0566520911	0:03.64 (5.02)	
(30, 30, 30, 5, 5)	Complete enumeration	0.0479355528	0:26.98	3.0×10^6
	Network (LP by Thm. 2.2.2)	0.0479355528	0:06.13 (4.40)	
	Network (LP by Thm. 2.2.3)	0.0479355528	0:05.48 (4.92)	
(40, 30, 10, 10, 10)	Complete enumeration	0.0682463011	1:41.53	1.1×10^7
	Network (LP by Thm. 2.2.2)	0.0682463011	0:17.50 (5.80)	
	Network (LP by Thm. 2.2.3)	0.0683323439	0:13.66 (7.43)	
(20, 20, 20, 20, 20)	Complete enumeration	0.0448476262	46:27	3.0×10^8
	Network (LP by Thm. 2.2.2)	0.0448476262	4:55 (9.45)	
	Network (LP by Thm. 2.2.3)	0.0448505876	4:03 (11.47)	
(30, 30, 30, 4, 3, 3)	Complete enumeration	0.0449065433	2:16	1.5×10^7
	Network (LP by Thm. 2.2.2)	0.0449065433	0:31 (4.39)	
	Network (LP by Thm. 2.2.3)	0.0449065433	0:28 (4.86)	
(40, 30, 10, 10, 5, 5)	Complete enumeration	0.0606964775	27:47	1.8×10^8
	Network (LP by Thm. 2.2.2)	0.0606964775	4:29 (6.20)	
	Network (LP by Thm. 2.2.3)	0.0607761595	3:28 (8.01)	
(40, 20, 20, 8, 7, 5)	Complete enumeration	0.0435034239	85:03	5.6×10^8
	Network (LP by Thm. 2.2.2)	0.0435027787	16:06 (5.28)	
	Network (LP by Thm. 2.2.3)	0.0435052514	12:12 (6.97)	
(30, 30, 20, 8, 7, 5)	Complete enumeration	0.0521534407	133:05	8.8×10^8
	Network (LP by Thm. 2.2.2)	0.0521534422	22:40 (5.87)	
	Network (LP by Thm. 2.2.3)	0.0521535686	19:16 (6.91)	
(30, 20, 20, 20, 5, 5)	Complete enumeration	0.0426073065	264:41	1.7×10^9
	Network (LP by Thm. 2.2.2)	0.0426073065	43:40 (6.06)	
	Network (LP by Thm. 2.2.3)	0.0426079323	35:39 (7.42)	

Table 2.9: Continued.

$\boldsymbol{y}$	Algorithm	p value	CPU time[a]	(ratio[b])	$\#\mathcal{F}$
$(40, 30, 20, 3, 3, 2, 2)$	Complete enumeration	0.0657281092	4:56		3.3×10^7
	Network (LP by Thm. 2.2.2)	0.0657281092	0:59	(5.02)	
	Network (LP by Thm. 2.2.3)	0.0657315171	0:49	(6.04)	
$(30, 30, 30, 3, 3, 2, 2)$	Complete enumeration	0.0640574757	7:17		4.8×10^7
	Network (LP by Thm. 2.2.2)	0.0640574757	1:22	(5.33)	
	Network (LP by Thm. 2.2.3)	0.0640574757	1:13	(5.99)	
$(40, 30, 10, 10, 5, 3, 2)$	Complete enumeration	0.0480403049	121:27		8.0×10^8
	Network (LP by Thm. 2.2.2)	0.0480403049	21:21	(5.69)	
	Network (LP by Thm. 2.2.3)	0.0480998952	16:48	(7.23)	
$(40, 25, 15, 10, 5, 3, 2)$	Complete enumeration	0.0493349444	228:40		1.5×10^9
	Network (LP by Thm. 2.2.2)	0.0493349444	40:43	(5.62)	
	Network (LP by Thm. 2.2.3)	0.0493396952	31:50	(7.18)	
$(40, 30, 20, 2, 2, 2, 2, 2)$	Complete enumeration	0.0658297002	13:57		9.2×10^7
	Network (LP by Thm. 2.2.2)	0.0658297002	2:38	(5.30)	
	Network (LP by Thm. 2.2.3)	0.0658300956	2:12	(6.34)	
$(40, 25, 25, 2, 2, 2, 2, 2)$	Complete enumeration	0.0531653738	15:37		1.0×10^8
	Network (LP by Thm. 2.2.2)	0.0531653738	3:09	(4.96)	
	Network (LP by Thm. 2.2.3)	0.0531653738	2:40	(5.86)	
$(40, 30, 18, 4, 2, 2, 2, 2)$	Complete enumeration	0.0492180369	45:16		3.0×10^8
	Network (LP by Thm. 2.2.2)	0.0492180369	8:59	(5.04)	
	Network (LP by Thm. 2.2.3)	0.0492180505	7:30	(6.04)	
$(40, 30, 15, 7, 2, 2, 2, 2)$	Complete enumeration	0.0422794862	114:12		7.6×10^8
	Network (LP by Thm. 2.2.2)	0.0422794862	22:58	(4.97)	
	Network (LP by Thm. 2.2.3)	0.0422816826	18:57	(6.03)	
$(40, 30, 15, 5, 4, 2, 2, 2)$	Complete enumeration	0.0641293814	217:22		1.4×10^9
	Network (LP by Thm. 2.2.2)	0.0641293814	33:32	(6.48)	
	Network (LP by Thm. 2.2.3)	0.0641321353	26:34	(8.18)	

Table 2.10: A comparison of the network and the Louis and Dempster algorithms for the allele frequency data of $\boldsymbol{y} = (30, 30, 20, 8, 7, 5)$ for various p values.

		CPU time[a]	
p	Complete enumeration	Network (LP by Thm. 2.2.2)	Network (LP by Thm. 2.2.3)
0.9968	133:12	0:05.89	0:00.19
0.9101	133:09	0:18.56	0:05.82
0.8242	133:11	0:34.76	0:15.24
0.5933	133:09	1:45	1:07
0.4728	133:09	2:56	2:00
0.3178	133:09	5:23	4:02
0.2161	133:25	8:20	6:34
0.1070	133:31	14:58	12:22
0.0522	133:05	22:40	19:16

[a]CPU time is represented by min : sec.millisec

to calculate various p values for the case of $\boldsymbol{y} = (30, 30, 20, 8, 7, 5)$.

2.2.6 Discussion

The contribution of this section is to extend the bounds of computational feasibility of the exact test of Hardy-Weinberg proportion for multiple alleles by the network algorithm. Numerical examples in Section 2.2.5 show that the efficacy of the computation is greatly improved by our algorithm compared to the algorithm proposed by Louis and Dempster. The CPU time required for calculating p values around 0.05 is within 30 minutes by the network algorithm when the size of the problem (the number of all possible counts of genotype with the same gene counts as observed data) is 10^9, while it takes more than 2 hours by the complete enumeration algorithm. Table 2.10 shows that the degree of the improvement increases for large p values. This is because larger p values can be more easily calculated by the network algorithm, while the value of p does not effect the CPU time in the complete enumeration.

The essential features of the network algorithm are the evaluation of LP, the longest path from any node to the terminal node, and SP, the shortest path from any node to the terminal node. In this study, we proved an interesting optimization theorem that leads to the closed form expression for SP. Although no comparable closed form for LP is available, it is shown that two upper bounds for LP are easily evaluated: one is the optimal solution of the one variable maximizing problem, and the other is the approximate optimal solution of the continuity relaxation problem. It is worth pointing out that the latter idea can be applied to a variety of integer optimizing problems, for example Freeman-Halton tests, which we have seen in Section 2.1.

Our numerical examples show that these two upper bounds have their own merits. The approximate upper bound is slightly superior in the CPU times required, however, the approximation may slightly influence the p value. Both the difference of the efficacy between the two methods and the degree of the overestimate of p values caused by the approximation are quite small. It should be noted that the approximation never leads to the underestimate of p values. Therefore in practical use, the influence of the approximation may not be so important because the conservative decision can be done.

The simulation results suggest that most trimming occurs when tables associated with paths emanating from the node are all less probable than the observed table (trimming based on the LP bound) rather than when they are all more probable (trimming based on the SP table). This is true even when the observed data are "rare" under the Hardy-Weinberg equilibrium in the usual sense (i.e., when p values are around $0.05 \sim 0.01$) and more SP-trimming would be expected. One reason for this is related to the shape of the conditional probability function (2.13), where the factorial part of the denominator drastically increases when the table becomes close to the least probable case. Regardless of how probable is the assignment of alleles $A_r, ..., A_{k+1}$, alleles $A_k, ..., A_1$ can be assigned to construct a table which is improbable by making the factorial part of the denominator as large as possible given the assignment for $A_r, ..., A_{k+1}$. Hence SP-trimmings hardly ever occur unless the observed table itself is the least probable case.

Chapter 3

Markov chain Monte Carlo methods

In this chapter we consider the Markov chain Monte Carlo methods. In Section 3.1, we illustrate an outline of the Markov chain Monte Carlo methods in the analysis of contingency tables. We consider the no three-factor interaction model in three-way contingency tables as an example, and show the difficulty in performing the Markov chain Monte Carlo method for this case. Section 3.1 also reviews related works concerning the Markov chain Monte Carlo methods in the analysis of contingency tables, including the important work by Diaconis and Sturmfels (1998). This problem of the no three-factor interaction model in three-way contingency tables is thoroughly investigated in Section 3.2 and Section 3.3 for some problems of relatively small sizes. Section 3.4 concerns problems for two-way contingency tables containing structural zero cells. Section 3.5 and Section 3.6 give some basic and theoretical results.

3.1 Introduction

In this section, we illustrate the problem that we consider in this chapter. First we consider a simple problem of generating two-way contingency tables with fixed row and column totals, which we have seen in Chapter 1. The problem is written as follows. Let $\boldsymbol{x} = \{x_{ij}\} \in \mathbb{Z}_{\geq 0}^{IJ}$ be an $I \times J$ contingency table and

$$\mathcal{F}(\{x_{i\cdot}\}, \{x_{\cdot j}\}) = \{\boldsymbol{y} = \{y_{ij}\} \mid y_{i\cdot} = x_{i\cdot}, y_{\cdot j} = x_{\cdot j},\ y_{ij} \in \mathbb{Z}_{\geq 0}\ i \in [I], j \in [J]\}$$

denote the reference set of all $I \times J$ contingency tables with the same marginal totals as $\boldsymbol{x}$. Under the hypothesis of statistical independence (i.e. $p_{ij} = p_{i\cdot}p_{\cdot j}$), the sufficient statistics are the row and column sums, $x_{i\cdot}, x_{\cdot j},\ i \in [I],\ j \in [J]$. The hypergeometric distribution $h(\boldsymbol{x})$ on $\mathcal{F}(\{x_{i\cdot}\}, \{x_{\cdot j}\})$, which is written as (1.2), is the conditional distribution of $\boldsymbol{x}$, given the sufficient statistics. To test the hypothesis of independence, our approach in this chapter is to generate samples from $h(\boldsymbol{x})$ and calculate the null distribution of various test statistics. An important point is that, if an arbitrary connected Markov chain on $\mathcal{F}(\{x_{i\cdot}\}, \{x_{\cdot j}\})$ is constructed, the chain can be modified to give a connected and aperiodic Markov chain with stationary distribution $h(\boldsymbol{x})$ by the usual Metropolis procedure (Hastings, 1970, for example). Then how can we construct a connected Markov chain on $\mathcal{F}(\{x_{i\cdot}\}, \{x_{\cdot j}\})$?

In this case of two-way contingency tables, a connected Markov chain on $\mathcal{F}(\{x_{i\cdot}\}, \{x_{\cdot j}\})$ is easily constructed as follows. Let $\boldsymbol{x}$ be the current state in $\mathcal{F}(\{x_{i\cdot}\}, \{x_{\cdot j}\})$. The next state is selected by choosing a pair of rows and a pair of columns at random, and modifying $\boldsymbol{x}$ at the four entries where the selected rows and columns intersect as

$$\begin{matrix} + & - \\ - & + \end{matrix} \quad \text{or} \quad \begin{matrix} - & + \\ + & - \end{matrix} \quad \text{with probability } \frac{1}{2} \text{ each.} \tag{3.1}$$

The modification adds or subtracts 1 from each of the four entries, keeping the row and column sums. If the modification forces negative entries, discard it and continue by choosing a new pairs of rows and columns. Hereafter we call such modifications (two-dimensional) *rectangles* or *rectangular moves*. A precise definition of rectangles is given in Section 3.2 (Definition 3.2.5).

Extending the above approach, now consider the three-way case. Let $\boldsymbol{x} = \{x_{ijk}\} \in \mathbb{Z}_{\geq 0}^{IJK}$ be an $I \times J \times K$ contingency table. The reference set is now defined as

$$\mathcal{F}(\{x_{ij\cdot}\}, \{x_{i\cdot k}\}, \{x_{\cdot jk}\}) = \{\boldsymbol{y} \mid y_{ij\cdot} = x_{ij\cdot},\ y_{i\cdot k} = x_{i\cdot k},\ y_{\cdot jk} = x_{\cdot jk},\ y_{ijk} \in \mathbb{Z}_{\geq 0},\ i \in [I], j \in [J], k \in [K]\},$$

and our aim is to construct a connected Markov chain over $\mathcal{F}(\{x_{ij\cdot}\}, \{x_{i\cdot k}\}, \{x_{\cdot jk}\})$. The simple analogue of rectangles in (3.1) is the eight-entries modifications:

$$\begin{array}{ccc} i = i_1 & & \\ j \backslash k & k_1 & k_2 \\ j_1 & +1 & -1 \\ j_2 & -1 & +1 \end{array} \qquad \begin{array}{ccc} i = i_2 & & \\ j \backslash k & k_1 & k_2 \\ j_1 & -1 & +1 \\ j_2 & +1 & -1 \end{array} \,. \tag{3.2}$$

However, a chain constructed from this type of modifications is known to be *not* connected. A simple counter-example is given by the following $3 \times 3 \times 3$ contingency table.

$$\begin{array}{|ccc|} \hline m & 0 & 0 \\ 0 & m & 0 \\ 0 & 0 & m \\ \hline \end{array} \qquad \begin{array}{|ccc|} \hline 0 & m & 0 \\ 0 & 0 & m \\ m & 0 & 0 \\ \hline \end{array} \qquad \begin{array}{|ccc|} \hline 0 & 0 & m \\ m & 0 & 0 \\ 0 & m & 0 \\ \hline \end{array}$$

For this table, the two-dimensional marginals have the same value, i.e., $x_{ij\cdot} = x_{i\cdot k} = x_{\cdot jk} = m$ for $1 \leq i, j, k \leq 3$. It is clear that this state is not connected to any other states in $\mathcal{F}(\{x_{ij\cdot}\}, \{x_{i\cdot k}\}, \{x_{\cdot jk}\})$ by the eight-entries modification described in (3.2) for any m, i.e., we cannot modify any set of eight entries of the position described as (3.2) without causing negative entries. This simple $3 \times 3 \times 3$ example clearly describes the difficulty of this problem.

The Markov chain Monte Carlo approach is extensively used in various two-way settings, for example, Smith, Forster and McDonald (1996) for tests of independence, quasi-independence and quasi-symmetry for square two-way contingency tables; Guo and Thompson (1992) for exact tests of Hardy-Weinberg proportions (triangular two-way contingency tables). There are also many works that discuss the convergence of the chain, for example, Diaconis and Saloff-Coste (1995) for two-way contingency tables; Hernek (1998), Dyer and Greenhill (2000) for $2 \times J$ contingency tables. On the other hand, there are only a few works dealing with high dimensional tables. For example see Besag and Clifford (1989) for the Ising model and Forster, McDonald and Smith (1996) for general 2^d tables.

Diaconis and Sturmfels (1998) presented a general algorithm for computing a *Markov basis* (we give precise definition afterward) in the setting of a general discrete exponential family of distribution. Their approach relies on the existence of a Gröbner basis of a well specified polynomial ideal. For the above setting of three-way contingency tables, the argument is summarized as follows. Let $\mathbb{K}$ be a field and consider the map of polynomial rings

$$\phi : \mathbb{K}[x_{ijk}, i \in [I], j \in [J], k \in [K]] \to \mathbb{K}[a_{ij}, b_{ik}, c_{jk}, i \in [I], j \in [J], k \in [K]],$$

$$x_{ijk} \mapsto a_{ij}b_{ik}c_{jk}, \ \ i \in [I], j \in [J], k \in [K].$$

Then the Markov basis for this problem corresponds to generators for the kernel of ϕ. See also Dinwoodie (1998) for a clear exposition of the Gröbner basis technique.

Their approach is extremely appealing because, in principle, it can be used for the problems of any dimension. Despite its generality, however, the power of their procedure is limited for the following two reasons; the computational feasibility and outputs of redundant basis elements. The first one stems from the computational complexity of computing Gröbner bases. Although intensive research is being conducted for improving the efficiency of Gröbner bases computation (e.g. Sturmfels, 1995; Boffi and Rossi, 2001), it is still difficult to obtain a Gröbner basis by standard packages even for problems of moderate sizes. We also note that the computational complexity of the Buchberger algorithm increases double exponentially with the number of variables as well as the number of categories per variable (see Dobra, 2003). The second one, which we especially consider in this thesis, stems from the lack of minimality and symmetry of a reduced Gröbner basis. Gröbner basis is in general not symmetric because it depends on the particular term order. For example, Diaconis and Sturmfels reported in their paper that the reduced Gröbner basis for the $3 \times 3 \times 3$ case contains moves of

$$\text{28 relations of the form} \quad \begin{array}{|ccc|}\hline 0 & 0 & 0 \\ 0 & -1 & +1 \\ 0 & +1 & -1 \\ \hline\end{array} \qquad \begin{array}{|ccc|}\hline +1 & 0 & -1 \\ -1 & +1 & 0 \\ 0 & -1 & +1 \\ \hline\end{array} \qquad \begin{array}{|ccc|}\hline -1 & 0 & +1 \\ +1 & 0 & -1 \\ 0 & 0 & 0 \\ \hline\end{array} \tag{3.3}$$

and

$$\text{1 relation of the form} \quad \begin{array}{|ccc|}\hline -2 & +1 & +1 \\ +1 & 0 & -1 \\ +1 & -1 & 0 \\ \hline\end{array} \qquad \begin{array}{|ccc|}\hline +1 & 0 & -1 \\ 0 & 0 & 0 \\ -1 & 0 & +1 \\ \hline\end{array} \qquad \begin{array}{|ccc|}\hline +1 & -1 & 0 \\ -1 & 0 & +1 \\ 0 & +1 & -1 \\ \hline\end{array}\ . \tag{3.4}$$

However, as remarked by Diaconis and Sturmfels, the moves of the above types are not essential in view of the connectedness of the chain. We also consider this point in Section 3.2. As another example, Sakata and Sawae (2000) reports that for $4 \times 4 \times 4$ tables with fixed two-dimensional marginals, their lattice based algorithm was not able to produce the Gröbner basis after two months of computation and the incomplete basis at that time already contained more than 340,000 basis elements. Furthermore the resulting Gröbner basis may not be easily interpretable due to the redundant elements and the dependence on the chosen term order. On the other hand, we show in Section 3.3 that there are exactly 14 types of moves, which constitute the unique minimal basis for $4 \times 4 \times 4$ tables. All these points are related to the notion of minimality of Markov basis as defined below.

Now we give a a definition of *Markov basis* and its *minimality* according to Diaconis and Sturmfels (1998) in this three-way setting. Let $\mathcal{F}_0$ be a set of $I \times J \times K$ integer arrays with zero two-way marginal totals

$$\mathcal{F}_0 = \{\boldsymbol{z} = \{z_{ijk}\} \mid z_{ij\cdot} = z_{i\cdot k} = z_{\cdot jk} = 0, \ z_{ijk} \in \mathbb{Z}, \ i \in [I], j \in [J], k \in [K]\},$$

where $\mathbb{Z} = \{\ldots, -2, -1, 0, 1, 2, \ldots\}$. Elements of $\mathcal{F}_0$ are called *moves* in this thesis.

Definition 3.1.1 *A Markov basis is a set $\mathcal{B} = \{\boldsymbol{z}_1, \dots, \boldsymbol{z}_L\}$ of $I \times J \times K$ integer arrays $\boldsymbol{z}_\ell \in \mathcal{F}_0$, $\ell \in [L]$, such that, for any $\{x_{ij\cdot}\}, \{x_{i\cdot k}\}, \{x_{\cdot jk}\}$ and $\boldsymbol{x}, \boldsymbol{x}' \in \mathcal{F}(\{x_{ij\cdot}\}, \{x_{i\cdot k}\}, \{x_{\cdot jk}\})$, there exist $A > 0$, $(\varepsilon_1, \boldsymbol{z}_{t_1}), \dots, (\varepsilon_A, \boldsymbol{z}_{t_A})$ with $\varepsilon_s = \pm 1$, such that*

$$\boldsymbol{x}' = \boldsymbol{x} + \sum_{s=1}^{A} \varepsilon_s \boldsymbol{z}_{t_s} \quad \textit{and} \quad \boldsymbol{x} + \sum_{s=1}^{a} \varepsilon_s \boldsymbol{z}_{t_s} \in \mathcal{F}(\{x_{ij\cdot}\}, \{x_{i\cdot k}\}, \{x_{\cdot jk}\}) \ \textit{for}\ 1 \le a \le A.$$

A Markov basis $\mathcal{B}$ is minimal if no proper subset of $\mathcal{B}$ is a Markov basis. A minimal Markov basis is unique if there exists only one minimal Markov basis.

If a Markov basis is obtained, a connected Markov chain over $\mathcal{F}(\{x_{ij\cdot}\}, \{x_{i\cdot k}\}, \{x_{\cdot jk}\})$ is easily constructed. As Diaconis and Sturmfels (1998) mentioned, it may be preferable to run the chain by selecting a Markov basis element, say $\boldsymbol{z}$, calculating the collection of points, $\{c_i\}$, so that $\boldsymbol{x}+c_i\boldsymbol{z}$ contains no negative entries, and selecting amongst these points with probability

$$p_i = f(\boldsymbol{x} + c_i \boldsymbol{z}) \ / \sum_j f(\boldsymbol{x} + c_j \boldsymbol{z}),$$

where f is the null probability function of $\boldsymbol{x}$.

The above definition of a Markov basis is written in the three-way setting. We postponed a more general definition of a Markov basis to Section 3.5, since we consider this three-way problem for a while. It should be noted that, this no three-way interaction model is the simplest model of the non-decomposable hierarchical log-linear models for multi-way contingency tables, and hence is important in applications. For a general three-way setting, i.e., for general an $I \times J \times K$ case, a closed-form expression of the Markov basis is very complicated, except for the case that $\min(I, J, K) = 2$ (see Diaconis and Sturmfels, 1998, Section 4). In Section 3.2 and Section 3.3, we give the unique minimal Markov basis for problems of relatively small sizes.

3.2 Construction of a connected Markov chain over $3 \times 3 \times K$ contingency tables with fixed two-dimensional marginals

3.2.1 Representation of the unique minimal Markov basis for $3\times3\times K$ tables

First we derive a closed-form expression of the unique minimal Markov basis for $3 \times 3 \times K$ tables in Section 3.2.1. Theorem 3.2.1 gives the unique minimal basis for the $3 \times 3 \times 3$ case. Theorem 3.2.2 is for the $3 \times 3 \times 4$ case, Theorem 3.2.3 is for the $3 \times 3 \times 5$ case, and finally our main result in Theorem 3.2.4 gives the unique minimal basis for the $3 \times 3 \times K$ case. Proofs of these theorems are postponed to Section 3.2.2.

The *degree* of $\boldsymbol{z} \in \mathcal{F}_0$ is defined according to Diaconis and Sturmfels (1998). Write $\boldsymbol{z} = \boldsymbol{z}^+ - \boldsymbol{z}^-$ where $\boldsymbol{z}^+$ and $\boldsymbol{z}^-$ are the positive and the negative part of $\boldsymbol{z}$ having the elements $z^+_{ijk} = \max(z_{ijk}, 0)$, $z^-_{ijk} = \max(-z_{ijk}, 0)$ and define $\deg \boldsymbol{z} = \sum_{i,j,k} z^+_{ijk} = \sum_{i,j,k} z^-_{ijk}$.

For an $I \times J \times K$ contingency table $\boldsymbol{y} = \{y_{ijk}\}$, *i-slice* (or $i = i_0$ slice) of $\boldsymbol{y}$ is the two-dimensional slice $\boldsymbol{y}_{i=i_0} = \{y_{i_0jk}\}_{j\in[J],\ k\in[K]}$, where $i = i_0$ is fixed. We similarly define j-slice and k-slice. To display $3 \times 3 \times K$ contingency tables, we write three i-slices of size $3 \times K$ as follows:

$$
\begin{array}{llll}
i=1 & & & \\
j\backslash k & 1 & \cdots & K \\
1 & & & \\
2 & & & \\
3 & & &
\end{array}
\qquad
\begin{array}{llll}
i=2 & & & \\
j\backslash k & 1 & \cdots & K \\
1 & & & \\
2 & & & \\
3 & & &
\end{array}
\qquad
\begin{array}{llll}
i=3 & & & \\
j\backslash k & 1 & \cdots & K \\
1 & & & \\
2 & & & \\
3 & & &
\end{array}
$$

In the following, it is always assumed that the indices are integers such that

$$
\begin{array}{ll}
1 \le i_1, i_2, i_3 \le 3, \ i_1, i_2, i_3 & \text{all distinct;} \\
1 \le j_1, j_2, j_3 \le 3, \ j_1, j_2, j_3 & \text{all distinct;} \\
1 \le k_1, k_2, ..., k_K \le K, \ k_1, k_2, ..., k_K & \text{all distinct.}
\end{array}
$$

Moves of degree 4 (basic moves)

First we define the most elementary eight-entries move that is already discussed in (3.2).

Definition 3.2.1 *A move of degree 4 is a* $3 \times 3 \times K$ *integer array* $\boldsymbol{m}_4(i_1i_2, j_1j_2, k_1k_2) \in \mathcal{F}_0$, *where* $\boldsymbol{m}_4(i_1i_2, j_1j_2, k_1k_2)$ *has the elements*

$$
m_{i_1j_1k_1} = m_{i_1j_2k_2} = m_{i_2j_1k_2} = m_{i_2j_2k_1} = 1,
$$

$$
m_{i_1j_1k_2} = m_{i_1j_2k_1} = m_{i_2j_1k_1} = m_{i_2j_2k_2} = -1,
$$

and all the other elements are zero.

We call this move a *basic move*. Figure 3.1 gives a three-dimensional view of the basic move.

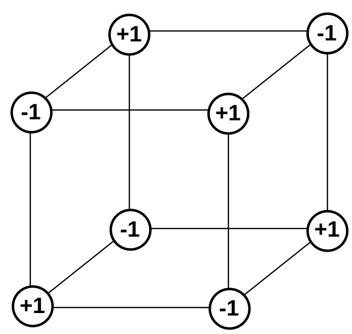

Figure 3.1: Basic move

From the definition, the relation

$$
\boldsymbol{m}_4(i_1i_2, j_1j_2, k_1k_2) = \boldsymbol{m}_4(i_1i_2, j_2j_1, k_2k_1) = \boldsymbol{m}_4(i_2i_1, j_1j_2, k_2k_1) = -\boldsymbol{m}_4(i_2i_1, j_1j_2, k_1k_2)
$$

is derived.

The moves of degree 4 are the most elemental moves in the sense that all the other moves of higher degree in $\mathcal{F}_0$ are written as linear combinations of degree 4 moves with integral coefficients.

Moves of degree 6

As we have seen in Section 3.1, a connected Markov chain cannot be constructed by the set of basic moves alone in the case of $\min(I,J,K) \geq 3$. Here we consider patterns of moves that are composed of two basic moves.

As preparations, we provide a complete list of the patterns that are obtained by the sum of two overlapping basic moves. For two basic moves, $\boldsymbol{m}_4(i_1i_2, j_1j_2, k_1k_2)$ and $\boldsymbol{m}_4(i'_1i'_2, j'_1j'_2, k'_1k'_2)$, define

$$\Delta_I = \delta_{i_1i'_1} + \delta_{i_1i'_2} + \delta_{i_2i'_1} + \delta_{i_2i'_2},$$

$$\Delta_J = \delta_{j_1j'_1} + \delta_{j_1j'_2} + \delta_{j_2j'_1} + \delta_{j_2j'_2},$$

$$\Delta_K = \delta_{k_1k'_1} + \delta_{k_1k'_2} + \delta_{k_2k'_1} + \delta_{k_2k'_2}$$

and

$$\Delta = \Delta_I + \Delta_J + \Delta_K,$$

where $\delta_{ij} = 1$ if $i = j$; and $= 0$ otherwise. Since two moves are overlapping, $\Delta_I, \Delta_J, \Delta_K \geq 1$. Furthermore $\Delta_I \leq 2$, because $i_1 \neq i_2$ and $i'_1 \neq i'_2$. Similarly, $\Delta_J, \Delta_K \leq 2$, therefore, $\Delta \in \{3,4,5,6\}$. Corresponding to the values of Δ, all the patterns are classified as follows.

- $\Delta = 3$: $\boldsymbol{m}_4(i_1i_2, j_1j_2, k_1k_2)$ and $\boldsymbol{m}_4(i'_1i'_2, j'_1j'_2, k'_1k'_2)$ overlap at one nonzero entry. We call this case a *combination of type 1* or a *type*-1 *combination*. If the signs of this overlapped cell are opposite, a move of degree 7 is obtained. Figure 3.2 gives a three-dimensional view of this type of move. Note that (3.3) in Section 3.1 is this type of move.

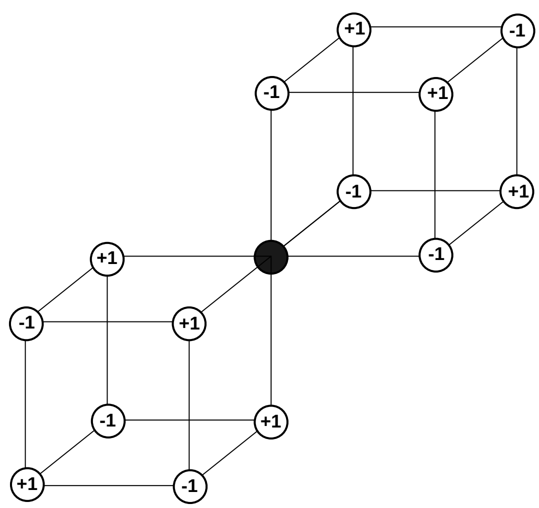

Figure 3.2: $3 \times 3 \times 3$ move of degree 7

- $\Delta = 4$: $\boldsymbol{m}_4(i_1i_2, j_1j_2, k_1k_2)$ and $\boldsymbol{m}_4(i'_1i'_2, j'_1j'_2, k'_1k'_2)$ overlap at two nonzero entries. We call this case a *combination of type 2* or a *type*-2 *combination*. If the pairs of signs of these two cells are opposite, a move of degree 6 is obtained. Figure 3.3 gives a three-dimensional view of this type of move.

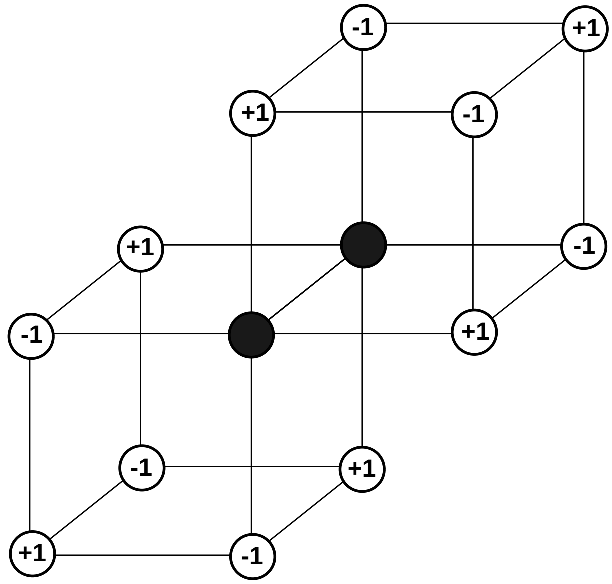

Figure 3.3: $2 \times 3 \times 3$ move of degree 6

- $\Delta = 5$: $\boldsymbol{m}_4(i_1 i_2, j_1 j_2, k_1 k_2)$ and $\boldsymbol{m}_4(i_1' i_2', j_1' j_2', k_1' k_2')$ overlap at four nonzero entries along a two-dimensional rectangle. If all the pairs of signs are canceled, a basic move is again obtained as

$$\left.\begin{array}{rcl} \boldsymbol{m}_4(i_1 i_2, j_1 j_2, k_1 k_2) & = & \boldsymbol{m}_4(i_1 i_2, j_1 j_2, k_1 k_3) + \boldsymbol{m}_4(i_1 i_2, j_1 j_2, k_3 k_2) \\ & = & \boldsymbol{m}_4(i_1 i_2, j_1 j_3, k_1 k_2) + \boldsymbol{m}_4(i_1 i_2, j_3 j_2, k_1 k_2) \\ & = & \boldsymbol{m}_4(i_1 i_3, j_1 j_2, k_1 k_2) + \boldsymbol{m}_4(i_3 i_2, j_1 j_2, k_1 k_2). \end{array}\right\} \qquad (3.5)$$

- $\Delta = 6$: $\boldsymbol{m}_4(i_1 i_2, j_1 j_2, k_1 k_2)$ and $\boldsymbol{m}_4(i_1' i_2', j_1' j_2', k_1' k_2')$ overlap completely.

The relation (3.5) suggests the difficulty of the concept of decomposing a larger move into several basic moves. If we call a move of degree 6 or 7 as a ‘two-step move’, it means that *at least two* basic moves are needed to construct these moves. Among the above list, a combination of type 2 is the most important case from the viewpoint of a connected Markov chain. It is discussed in the next definition and in Theorem 3.2.1 below.

Definition 3.2.2 *A move of degree 6 is a* $3 \times 3 \times K$ *integer array* $\boldsymbol{m}_6^I(i_1 i_2, j_1 j_2 j_3, k_1 k_2 k_3) \in \mathcal{F}_0$ *with elements*

$$\begin{array}{l} m_{i_1 j_1 k_1} = m_{i_1 j_2 k_2} = m_{i_1 j_3 k_3} = m_{i_2 j_1 k_2} = m_{i_2 j_2 k_3} = m_{i_2 j_3 k_1} = 1, \\ m_{i_1 j_1 k_2} = m_{i_1 j_2 k_3} = m_{i_1 j_3 k_1} = m_{i_2 j_1 k_1} = m_{i_2 j_2 k_2} = m_{i_2 j_3 k_3} = -1, \end{array}$$

and all the other elements are zero. $\boldsymbol{m}_6^J(i_1 i_2 i_3, j_1 j_2, k_1 k_2 k_3)$ *and* $\boldsymbol{m}_6^K(i_1 i_2 i_3, j_1 j_2 j_3, k_1 k_2)$ *are defined similarly.*

Examples for the $3 \times 3 \times 4$ case are displayed as follows.

$$\boldsymbol{m}_6^I(12, 123, 123): \quad \begin{array}{|cccc|} \hline +1 & -1 & 0 & 0 \\ 0 & +1 & -1 & 0 \\ -1 & 0 & +1 & 0 \\ \hline \end{array} \quad \begin{array}{|cccc|} \hline -1 & +1 & 0 & 0 \\ 0 & -1 & +1 & 0 \\ +1 & 0 & -1 & 0 \\ \hline \end{array} \quad \begin{array}{|cccc|} \hline 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ \hline \end{array}$$

$$
\boldsymbol{m}_6^J(123,12,123):\quad
\begin{array}{|cccc|}\hline +1 & -1 & 0 & 0 \\ -1 & +1 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ \hline\end{array}
\quad
\begin{array}{|cccc|}\hline 0 & +1 & -1 & 0 \\ 0 & -1 & +1 & 0 \\ 0 & 0 & 0 & 0 \\ \hline\end{array}
\quad
\begin{array}{|cccc|}\hline -1 & 0 & +1 & 0 \\ +1 & 0 & -1 & 0 \\ 0 & 0 & 0 & 0 \\ \hline\end{array}
$$

$$
\boldsymbol{m}_6^K(123,123,12):\quad
\begin{array}{|cccc|}\hline +1 & -1 & 0 & 0 \\ -1 & +1 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ \hline\end{array}
\quad
\begin{array}{|cccc|}\hline 0 & 0 & 0 & 0 \\ +1 & -1 & 0 & 0 \\ -1 & +1 & 0 & 0 \\ \hline\end{array}
\quad
\begin{array}{|cccc|}\hline -1 & +1 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ +1 & -1 & 0 & 0 \\ \hline\end{array}
$$

Similarly as in the basic move, the relations

$$
\boldsymbol{m}_6^I(i_1i_2, j_1j_2j_3, k_1k_2k_3) = \boldsymbol{m}_6^I(i_1i_2, j_2j_3j_1, k_2k_3k_1) = \boldsymbol{m}_6^I(i_2i_1, j_1j_3j_2, k_2k_1k_3),
$$

$$
\boldsymbol{m}_6^I(i_1i_2, j_1j_2j_3, k_1k_2k_3) = -\boldsymbol{m}_6^I(i_2i_1, j_1j_2j_3, k_1k_2k_3),
$$

and similar relations for $\boldsymbol{m}_6^J(i_1i_2i_3, j_1j_2, k_1k_2k_3)$ and $\boldsymbol{m}_6^K(i_1i_2i_3, j_1j_2j_3, k_1k_2)$ are derived from the definition.

The expression of the move of degree 6 as a type-2 combination of two basic moves is not unique. Figure 3.4 illustrates the same move of degree 6 shown in Figure 3.3, but the overlapping cells of the two basic moves are different.

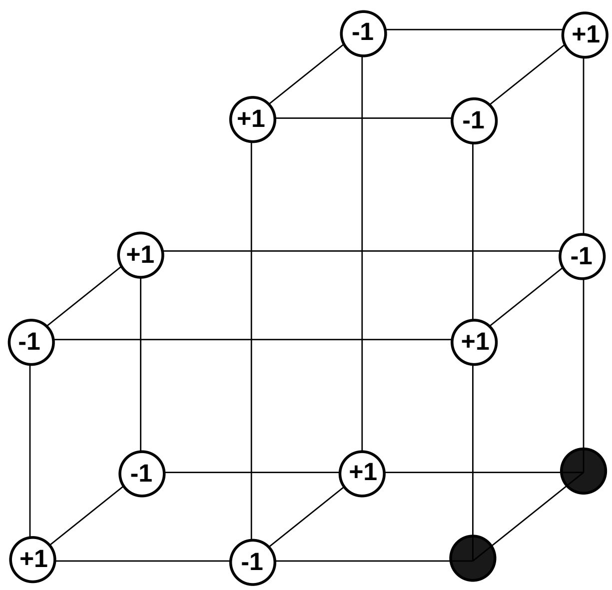

Figure 3.4: $2 \times 3 \times 3$ move of degree 6 (as another combination of type 2)

We now give the unique minimal basis for a connected Markov chain over $3 \times 3 \times 3$ tables.

Theorem 3.2.1 *A set of basic moves* $\boldsymbol{m}_4(i_1i_2, j_1j_2, k_1k_2)$ *and moves of degree* 6, $\boldsymbol{m}_6^I(i_1i_2, j_1j_2j_3, k_1k_2k_3), \boldsymbol{m}_6^J(i_1i_2i_3, j_1j_2, k_1k_2k_3), \boldsymbol{m}_6^K(i_1i_2i_3, j_1j_2j_3, k_1k_2)$ *constitute the unique minimal Markov basis for* $3 \times 3 \times 3$ *tables.*

This theorem shows that a move of degree 7 is not needed to construct a connected Markov chain. To demonstrate this point, consider the following two $3 \times 3 \times 3$ contingency tables.

$$
\boldsymbol{x}:\quad
\begin{array}{|ccc|}\hline 0 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \\ \hline\end{array}
\qquad
\begin{array}{|ccc|}\hline 0 & 0 & 1 \\ 1 & 0 & 0 \\ 0 & 1 & 0 \\ \hline\end{array}
\qquad
\begin{array}{|ccc|}\hline 1 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & 0 & 0 \\ \hline\end{array}
$$

$$\boldsymbol{y}: \quad \begin{array}{|ccc|}\hline 0 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & 1 & 0 \\ \hline \end{array} \qquad \begin{array}{|ccc|}\hline 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \\ \hline \end{array} \qquad \begin{array}{|ccc|}\hline 0 & 0 & 1 \\ 1 & 0 & 0 \\ 0 & 0 & 0 \\ \hline \end{array}$$

These two contingency tables are the negative part and the positive part of the move of degree 7 in (3.3) and mutually accessible by the move of degree 7. However, instead of adding (3.3) to $\boldsymbol{x}$, $\boldsymbol{m}_4(23, 12, 13)$ can be added to $\boldsymbol{x}$, and then, $\boldsymbol{m}_4(12, 23, 32)$ can be added to $\boldsymbol{x} + \boldsymbol{m}_4(23, 12, 13)$, to obtain $\boldsymbol{y}$. Note that move (3.3) is a type-1 combination of $\boldsymbol{m}_4(23, 12, 13)$ and $\boldsymbol{m}_4(12, 23, 32)$, and $\boldsymbol{x} + \boldsymbol{m}_4(23, 12, 13)$ does not contain a negative entry, while $\boldsymbol{x} + \boldsymbol{m}_4(12, 23, 32)$ contains a negative entry at the cell $(2, 2, 3)$. Note also that $\boldsymbol{m}_4(23, 12, 13)$ and $\boldsymbol{m}_4(12, 23, 32)$ overlap at this cell. Because the two basic moves are canceling at this cell, it is obvious that at least one of these basic moves (that has $+1$ at this cell) can be added without causing negative cells.

On the other hand, because the type-2 combination has two overlapped cells, it cannot be avoided that one of these two cells must become negative in adding basic moves one by one. For this reason, the type-2 combination is essential.

Concerning the move of degree 9 displayed as (3.4) of Section 3.1, it can be written as type-1 combination of a basic move and a move of degree 6, $\boldsymbol{m}_4(12, 13, 31) + \boldsymbol{m}_6^I(31, 132, 123)$, and hence is not needed for the same reason as that in the case of the degree 7 move.

Moves of degree 8

The next essential move is a *three-step move*. For the case of a general $I \times J \times K$ contingency table, there are several types of such a move. One is a $2 \times 4 \times 4$ move of degree 8 already discussed in Diaconis and Sturmfels (1998, equation (4.6)). Another one is a $3 \times 4 \times 4$ move of degree 9, which is discussed in Section 3.2.4. For the $3 \times 3 \times K$ case, the following type of move is needed.

Definition 3.2.3 *A move of degree 8 is a $3 \times 3 \times K$ integer array $\boldsymbol{m}_8(i_1i_2i_3, j_1j_2j_3, k_1k_2k_3k_4) \in \mathcal{F}_0$ with the elements*

$$\begin{aligned} m_{i_1j_1k_1} = m_{i_1j_2k_2} = m_{i_2j_1k_3} = m_{i_2j_2k_1} = m_{i_2j_3k_4} = m_{i_3j_1k_2} = m_{i_3j_2k_4} = m_{i_3j_3k_3} = 1, \\ m_{i_1j_1k_2} = m_{i_1j_2k_1} = m_{i_2j_1k_1} = m_{i_2j_2k_4} = m_{i_2j_3k_3} = m_{i_3j_1k_3} = m_{i_3j_2k_2} = m_{i_3j_3k_4} = -1, \end{aligned}$$

and all the other elements are zero.

For example, $\boldsymbol{m}_8(123, 123, 1234)$ is displayed as follows.

$$\begin{array}{|cccc|}\hline +1 & -1 & 0 & 0 \\ -1 & +1 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ \hline \end{array} \qquad \begin{array}{|cccc|}\hline -1 & 0 & +1 & 0 \\ +1 & 0 & 0 & -1 \\ 0 & 0 & -1 & +1 \\ \hline \end{array} \qquad \begin{array}{|cccc|}\hline 0 & +1 & -1 & 0 \\ 0 & -1 & 0 & +1 \\ 0 & 0 & +1 & -1 \\ \hline \end{array}$$

Figure 3.5 gives a three-dimensional view of this type of move.

From the definition, the relation

$$\boldsymbol{m}_8(i_1i_2i_3, j_1j_2j_3, k_1k_2k_3k_4) = \boldsymbol{m}_8(i_1i_3i_2, j_2j_1j_3, k_2k_1k_4k_3) = -\boldsymbol{m}_8(i_1i_3i_2, j_1j_2j_3, k_2k_1k_3k_4)$$

is derived.

Now we state a theorem for the $3 \times 3 \times 4$ case.

Theorem 3.2.2 *A set of basic moves $\boldsymbol{m}_4(i_1i_2, j_1j_2, k_1k_2)$, moves of degree 6, $\boldsymbol{m}_6^I(i_1i_2, j_1j_2j_3, k_1k_2k_3)$, $\boldsymbol{m}_6^J(i_1i_2i_3, j_1j_2, k_1k_2k_3)$, $\boldsymbol{m}_6^K(i_1i_2i_3, j_1j_2j_3, k_1k_2)$, and moves of degree 8, $\boldsymbol{m}_8(i_1i_2i_3, j_1j_2j_3, k_1k_2k_3k_4)$) constitute the unique minimal Markov basis for $3 \times 3 \times 4$ tables.*

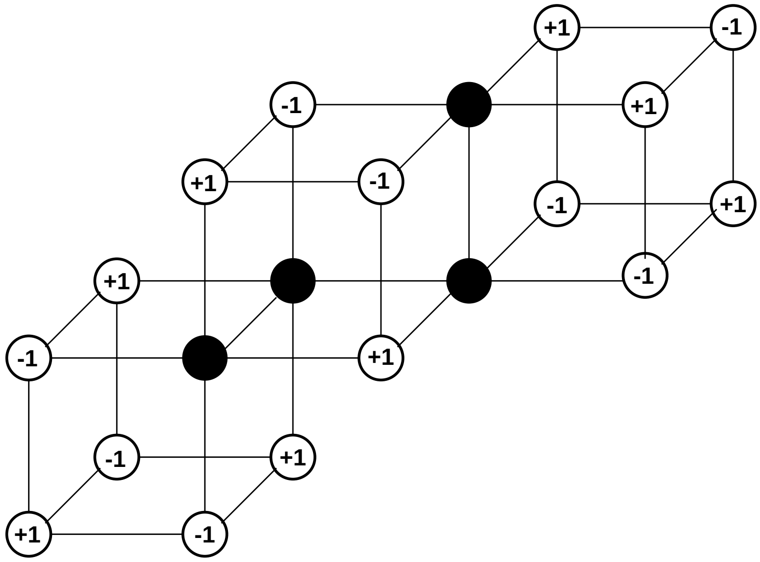

Figure 3.5: $3 \times 3 \times 4$ move of degree 8

Moves of degree 10

Continuing the above discussion, next we consider a *four-step move.* For the case of a $3 \times 3 \times K$ contingency table, only a move of the following type needs to be considered.

Definition 3.2.4 *A move of degree 10 is a* $3 \times 3 \times K$ *integer array* $\boldsymbol{m}_{10}(i_1 i_2 i_3, j_1 j_2 j_3, k_1 k_2 k_3 k_4 k_5) \in \mathcal{F}_0$ *with the elements*

$$\begin{aligned} m_{i_1 j_1 k_1} &= m_{i_1 j_2 k_2} = m_{i_1 j_2 k_5} = m_{i_1 j_3 k_4} = m_{i_2 j_1 k_3} \\ &= m_{i_2 j_2 k_1} = m_{i_2 j_3 k_5} = m_{i_3 j_1 k_2} = m_{i_3 j_2 k_4} = m_{i_3 j_3 k_3} = 1, \\ m_{i_1 j_1 k_2} &= m_{i_1 j_2 k_1} = m_{i_1 j_2 k_4} = m_{i_1 j_3 k_5} = m_{i_2 j_1 k_1} \\ &= m_{i_2 j_2 k_5} = m_{i_2 j_3 k_3} = m_{i_3 j_1 k_3} = m_{i_3 j_2 k_2} = m_{i_3 j_3 k_4} = -1, \end{aligned}$$

and all the other elements are zero.

For example, $\boldsymbol{m}_{10}(123, 123, 12345)$ is displayed as follows.

$$\boxed{\begin{array}{ccccc} +1 & -1 & 0 & 0 & 0 \\ -1 & +1 & 0 & -1 & +1 \\ 0 & 0 & 0 & +1 & -1 \end{array}} \quad \boxed{\begin{array}{ccccc} -1 & 0 & +1 & 0 & 0 \\ +1 & 0 & 0 & 0 & -1 \\ 0 & 0 & -1 & 0 & +1 \end{array}} \quad \boxed{\begin{array}{ccccc} 0 & +1 & -1 & 0 & 0 \\ 0 & -1 & 0 & +1 & 0 \\ 0 & 0 & +1 & -1 & 0 \end{array}}$$

Figure 3.6 gives a three-dimensional view of this type of move.

From the definition, the relation

$$\begin{aligned} \boldsymbol{m}_{10}(i_1 i_2 i_3, j_1 j_2 j_3, k_1 k_2 k_3 k_4 k_5) &= \boldsymbol{m}_{10}(i_1 i_3 i_2, j_3 j_2 j_1, k_4 k_5 k_3 k_1 k_2) \\ &= -\boldsymbol{m}_{10}(i_1 i_2 i_3, j_3 j_2 j_1, k_5 k_4 k_3 k_2 k_1) \end{aligned}$$

is derived.

As for a connected Markov chain, the next theorem holds for the $3 \times 3 \times 5$ case.

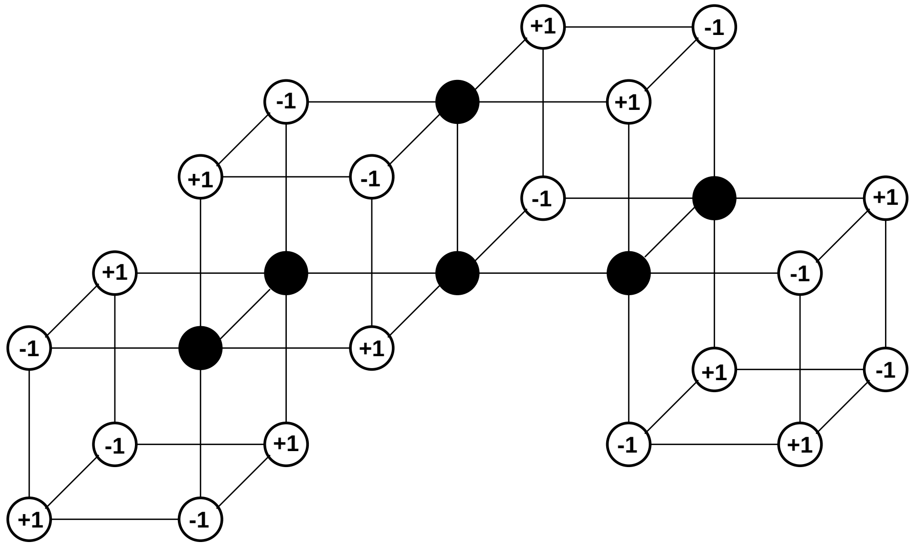

Figure 3.6: $3 \times 3 \times 5$ move of degree 10

Theorem 3.2.3 *A set of basic moves* $\boldsymbol{m}_4(i_1i_2, j_1j_2, k_1k_2)$*, moves of degree* 6*,* $\boldsymbol{m}_6^I(i_1i_2, j_1j_2j_3, k_1k_2k_3)$*,* $\boldsymbol{m}_6^J(i_1i_2i_3, j_1j_2, k_1k_2k_3), \boldsymbol{m}_6^K(i_1i_2i_3, j_1j_2j_3, k_1k_2)$*, degree* 8*,* $\boldsymbol{m}_8(i_1i_2i_3, j_1j_2j_3, k_1k_2k_3k_4))$*, and degree* 10*,* $\boldsymbol{m}_{10}(i_1i_2i_3, j_1j_2j_3, k_1k_2k_3k_4k_5)$ *constitute the unique minimal Markov basis for* $3 \times 3 \times 5$ *tables.*

Finally, it can be shown that for the case $K \geq 6$, no more new moves are needed to construct a connected Markov chain. We now state the main result of this section in the following theorem.

Theorem 3.2.4 *A set of basic moves* $\boldsymbol{m}_4(i_1i_2, j_1j_2, k_1k_2)$*, moves of degree* 6*,* $\boldsymbol{m}_6^I(i_1i_2, j_1j_2j_3, k_1k_2k_3), \boldsymbol{m}_6^J(i_1i_2i_3, j_1j_2, k_1k_2k_3), \boldsymbol{m}_6^K(i_1i_2i_3, j_1j_2j_3, k_1k_2)$*, degree* 8*,* $\boldsymbol{m}_8(i_1i_2i_3, j_1j_2j_3, k_1k_2k_3k_4))$*, and degree* 10*,* $\boldsymbol{m}_{10}(i_1i_2i_3, j_1j_2j_3, k_1k_2k_3k_4k_5)$ *constitute the unique minimal Markov basis for* $3 \times 3 \times K$ $(K \geq 5)$ *tables.*

3.2.2 Proofs of the theorems

The proofs of the theorems in Section 3.2.1 are given here. Our proofs are based on exhaustive investigations of possible patterns and all the proofs are similar and repetitive. However, the whole proofs, without any abbreviations, are shown for the sake of completeness.

Ingredients of our proofs

Let $\boldsymbol{x}$ and $\boldsymbol{y}$ denote three-dimensional contingency tables of the same size with the same two-dimensional marginal totals. Note that all the marginal totals of $\boldsymbol{x} - \boldsymbol{y}$ are zero. We also define $|\boldsymbol{x}| = \sum_{i,j,k} |x_{ijk}|$. The idea of our proofs is based on the following simple observation. Suppose that a set of moves $\mathcal{B} = \{\boldsymbol{z}_1, \ldots, \boldsymbol{z}_L\}$ is given. If $\boldsymbol{x}$ and $\boldsymbol{y}$ are made as close as possible, in other words, make $|\boldsymbol{x}-\boldsymbol{y}|$ as small as possible, by applying moves $\boldsymbol{z}_{i_1}, \boldsymbol{z}_{i_2}, \ldots \in \mathcal{B}$ without causing negative entries on the way, it follows that

$$|\boldsymbol{x}-\boldsymbol{y}| \text{ can be decreased to } 0 \iff \mathcal{B} \text{ is a Markov basis.}$$

This shows that only the patterns of $\boldsymbol{x}-\boldsymbol{y}$ have to be considered, after making $|\boldsymbol{x}-\boldsymbol{y}|$ as small as possible by applying moves from $\mathcal{B}$.

Minimality of the bases given in the theorems in Section 3.2.1 will be clear from our proofs. Our argument for the minimality is as follows. Suppose that $\mathcal{B} = \{\boldsymbol{z}_1, \ldots, \boldsymbol{z}_L\}$ is shown to be a Markov basis. To prove its minimality, it is sufficient to show that $\mathcal{B} \setminus \boldsymbol{z}_i$ is not a Markov basis for each i. Let $\boldsymbol{x} = \boldsymbol{z}_i^+$ be the positive part of $\boldsymbol{z}_i$. In our proofs it will be clear that none of $\boldsymbol{z}_j, j \neq i$, can be added to this $\boldsymbol{x}$ without causing negative entries. Therefore $\boldsymbol{x} = \boldsymbol{z}_i^+$ is not connected to any other states in $\mathcal{F}(\{x_{ij\cdot}\}, \{x_{i\cdot k}\}, \{x_{\cdot jk}\})$ by $\mathcal{B} \setminus \boldsymbol{z}_i$ and the minimality of $\mathcal{B}$ follows. The uniqueness of the minimal basis is again clear from the fact that the move $\boldsymbol{z}_i$ is needed to move from $\boldsymbol{x} = \boldsymbol{z}_i^+$ to $\boldsymbol{y} = \boldsymbol{z}_i^-$ and hence $\boldsymbol{z}_i$ has to belong to each Markov basis. Properties and uniqueness of a minimal basis is investigated in Section 3.5.

Hereafter the following abbreviations are used: ‘without loss of generality’ (wlog); and ‘without causing negative entries’ (wcne).

The following definition for describing patterns of two-dimensional slices of $\boldsymbol{y}-\boldsymbol{x}$ is given below.

Definition 3.2.5 *Let A be a two-dimensional matrix with elements a_{ij}. Then a rectangle is a set of four entries $(a_{i_1j_1}, a_{i_2j_1}, a_{i_2j_2}, a_{i_1j_2})$ with alternating signs. Similarly, a 6-cycle is a set of six entries $(a_{i_1j_1}, a_{i_2j_1}, a_{i_2j_2}, a_{i_3j_2}, a_{i_3j_3}, a_{i_1j_3})$ with alternating signs.*

Using the fact that all the marginal totals of $\boldsymbol{z} = \boldsymbol{x}-\boldsymbol{y}$ are zero, it can be easily shown that any nonzero entry of $\boldsymbol{z}$ has to be a member of either a rectangle or a 6-cycle in all of the i-, j- and k-slices when $\boldsymbol{x}$ and $\boldsymbol{y}$ are $3 \times 3 \times K$ contingency tables.

The following useful lemma concerning patterns of two-dimensional slices of $\boldsymbol{z}$ can now be proved.

Lemma 3.2.1 *Let $\boldsymbol{x}$ and $\boldsymbol{y}$ be $3 \times 3 \times K$ contingency tables and let $\boldsymbol{z} = \boldsymbol{x}-\boldsymbol{y}$. Consider $\boldsymbol{z}$ after minimizing $|\boldsymbol{z}|$ by applying the basic moves and the moves of degree 6 wcne on the way. Then*

(a) each k-slice of $\boldsymbol{z}$ does not contain 6-cycles, and

(b) there is at least one rectangle in either an i-slice or a j-slice unless $\boldsymbol{z} = 0$.

Proof. In the proof of this lemma, we display k-slices of $\boldsymbol{z}$ instead of our usual display of i-slices.

To prove (a), suppose that wlog $k = 1$ slice of $\boldsymbol{z}$ contains the following 6-cycle

$$\begin{array}{c|ccc|} i\backslash j & 1 & 2 & 3 \\ \hline 1 & + & - & * \\ 2 & - & * & + \\ 3 & * & + & - \\ \hline \end{array}\ .$$

Since $z_{11\cdot} = 0$, there exists at least one negative element in $z_{112}, z_{113}, \ldots, z_{11K}$. Let $z_{112} < 0$ wlog. As is shown above, z_{112} has to be an element of either a rectangle or a 6-cycle in the $k = 2$ slice. The two cases are considered respectively as follows.

Case 1: z_{112} is an element of a 6-cycle

It is seen that the negative entries in the 6-cycle in the $k=2$ slice, which includes z_{112}, can be either (i) $(z_{112}, z_{222}, z_{332})$ or (ii) $(z_{112}, z_{232}, z_{322})$. In case (i), $\boldsymbol{m}_4(12, 12, 12)$ can be added to $\boldsymbol{y}$ wcne to make $|\boldsymbol{z}|$ smaller since $y_{121}, y_{211}, y_{112}, y_{222} > 0$. On the other hand, in case (ii), $\boldsymbol{m}_6^K(132, 123, 12)$ can be added to $\boldsymbol{y}$ wcne to make $|\boldsymbol{z}|$ smaller since $y_{121}, y_{211}, y_{331}, y_{112}, y_{232}, y_{322} > 0$. These imply that Case 1 is a contradiction.

Case 2: z_{112} is an element of a rectangle

It is seen that the negative entries in the rectangle, which includes z_{112}, can be either (i) (z_{112}, z_{222}), (ii) (z_{112}, z_{232}), (iii) (z_{112}, z_{322}) or (iv) (z_{112}, z_{332}). In case (i), $\boldsymbol{m}_4(12, 12, 12)$ can be added to $\boldsymbol{y}$ wcne and $|\boldsymbol{z}|$ can be made smaller as in (i) of Case 1. In case (ii), it follows that $z_{132}, z_{212} > 0$ and $\boldsymbol{m}_4(12, 13, 21)$ can be added to $\boldsymbol{x}$ wcne and make $|\boldsymbol{z}|$ smaller since $x_{111}, x_{231}, x_{132}, x_{212} > 0$. Case (iii) is the symmetric case of (ii). In case (iv), the two k-slices, $\{z_{ij1}\}$ and $\{z_{ij2}\}$ are represented as

$$\{z_{ij1}\}: \begin{array}{c|ccc|} i\backslash j & 1 & 2 & 3 \\ \hline 1 & + & - & * \\ 2 & - & * & + \\ 3 & * & + & - \\ \hline \end{array} \qquad \{z_{ij2}\}: \begin{array}{c|ccc|} i\backslash j & 1 & 2 & 3 \\ \hline 1 & - & * & + \\ 2 & * & * & * \\ 3 & + & * & - \\ \hline \end{array}$$

In this case, since $z_{331}, z_{332} < 0$, at least one of $z_{333}, \ldots, z_{33K}$ has to be positive. Let $z_{333} > 0$ wlog. Here, z_{333} is again an element of either a rectangle or a 6-cycle. But as already seen in Case 1, there cannot be another 6-cycle in the $k \neq 1$ slice. Thus z_{333} has to be a member of a rectangle. Moreover, for the same reason as (i)–(iii) of Case 2, the $k=3$ slice has to be a mirror image of the $k=2$ slice:

$$\{z_{ij1}\}: \begin{array}{c|ccc|} i\backslash j & 1 & 2 & 3 \\ \hline 1 & + & - & * \\ 2 & - & * & + \\ 3 & * & + & - \\ \hline \end{array} \qquad \{z_{ij2}\}: \begin{array}{c|ccc|} i\backslash j & 1 & 2 & 3 \\ \hline 1 & - & * & + \\ 2 & * & * & * \\ 3 & + & * & - \\ \hline \end{array} \qquad \{z_{ij3}\}: \begin{array}{c|ccc|} i\backslash j & 1 & 2 & 3 \\ \hline 1 & + & * & - \\ 2 & * & * & * \\ 3 & - & * & + \\ \hline \end{array}$$

However, $\boldsymbol{m}_4(13, 13, 23)$ can be added to $\boldsymbol{x}$ or $\boldsymbol{m}_4(13, 13, 32)$ can be added to $\boldsymbol{y}$ wcne and $|\boldsymbol{z}|$ can be made smaller, which contradicts the assumption. These imply that Case 2 also is a contradiction. These considerations indicate that the 6-cycle cannot be included in any 3×3 slices and the proof of (a) is completed.

Next (b) is proved. Suppose $\boldsymbol{z}$ has nonzero entries and let $z_{111} > 0$ wlog. It is known that z_{111} is a member of a rectangle in the $k=1$-slice from (a). Then let the $k=1$-slice be represented as

$$\begin{array}{c|ccc|} i\backslash j & 1 & 2 & 3 \\ \hline 1 & + & - & * \\ 2 & - & + & * \\ 3 & * & * & * \\ \hline \end{array}$$

wlog. We are assuming that there exists no rectangle in the $3 \times K$ i-slices or j-slices of $\boldsymbol{z}$. Write

$z_{112} < 0$ wlog since $z_{11\cdot} = 0$.

$$\{z_{ij1}\}: \begin{array}{c|ccc|} i\backslash j & 1 & 2 & 3 \\ \hline 1 & + & - & \ast \\ 2 & - & + & \ast \\ 3 & \ast & \ast & \ast \\ \hline \end{array} \qquad \{z_{ij2}\}: \begin{array}{c|ccc|} i\backslash j & 1 & 2 & 3 \\ \hline 1 & - & \ast & \ast \\ 2 & \ast & \ast & \ast \\ 3 & \ast & \ast & \ast \\ \hline \end{array}$$

From the assumption, it follows that $z_{122}, z_{212} \leq 0$ because otherwise either $i = 1$-slice or $j = 1$-slice has a rectangle. We also write $z_{222} \geq 0$ because otherwise we can add $\boldsymbol{m}_4(12, 12, 12)$ to $\boldsymbol{y}$ wcne and make $|\boldsymbol{z}|$ smaller. Hereafter we display non-negative elements by $0+$ and non-positive elements by $0-$.

$$\{z_{ij1}\}: \begin{array}{c|ccc|} i\backslash j & 1 & 2 & 3 \\ \hline 1 & + & - & \ast \\ 2 & - & + & \ast \\ 3 & \ast & \ast & \ast \\ \hline \end{array} \qquad \{z_{ij2}\}: \begin{array}{c|ccc|} i\backslash j & 1 & 2 & 3 \\ \hline 1 & - & 0- & \ast \\ 2 & 0- & 0+ & \ast \\ 3 & \ast & \ast & \ast \\ \hline \end{array}$$

Since z_{112} has to be an element of a rectangle in a $k = 2$ slice, $z_{132} > 0, z_{312} > 0$ and $z_{332} < 0$ are derived.

$$\{z_{ij1}\}: \begin{array}{c|ccc|} i\backslash j & 1 & 2 & 3 \\ \hline 1 & + & - & \ast \\ 2 & - & + & \ast \\ 3 & \ast & \ast & \ast \\ \hline \end{array} \qquad \{z_{ij2}\}: \begin{array}{c|ccc|} i\backslash j & 1 & 2 & 3 \\ \hline 1 & - & 0- & + \\ 2 & 0- & 0+ & \ast \\ 3 & + & \ast & - \\ \hline \end{array}$$

It is seen that if $z_{131} < 0$, there appears a rectangle in the $i = 1$ slice; and if $z_{311} < 0$, there appears a rectangle in the $j = 1$ slice. This contradicts the assumption. Then it follows $z_{131}, z_{311} \geq 0$. Here we write $z_{123} > 0$ wlog, since $z_{12\cdot} = 0$.

$$\{z_{ij1}\}: \begin{array}{c|ccc|} i\backslash j & 1 & 2 & 3 \\ \hline 1 & + & - & 0+ \\ 2 & - & + & \ast \\ 3 & 0+ & \ast & \ast \\ \hline \end{array} \qquad \{z_{ij2}\}: \begin{array}{c|ccc|} i\backslash j & 1 & 2 & 3 \\ \hline 1 & - & 0- & + \\ 2 & 0- & 0+ & \ast \\ 3 & + & \ast & - \\ \hline \end{array} \qquad \{z_{ij3}\}: \begin{array}{c|ccc|} i\backslash j & 1 & 2 & 3 \\ \hline 1 & \ast & + & \ast \\ 2 & \ast & \ast & \ast \\ 3 & \ast & \ast & \ast \\ \hline \end{array}$$

It is seen that if $z_{113} < 0$, there appears a rectangle in the $i = 1$ slice; and if $z_{223} < 0$, there appears a rectangle in the $j = 2$ slice. This contradicts the assumption. Then it follows $z_{113}, z_{223} \geq 0$.

$$\{z_{ij1}\}: \begin{array}{c|ccc|} i\backslash j & 1 & 2 & 3 \\ \hline 1 & + & - & 0+ \\ 2 & - & + & \ast \\ 3 & 0+ & \ast & \ast \\ \hline \end{array} \qquad \{z_{ij2}\}: \begin{array}{c|ccc|} i\backslash j & 1 & 2 & 3 \\ \hline 1 & - & 0- & + \\ 2 & 0- & 0+ & \ast \\ 3 & + & \ast & - \\ \hline \end{array} \qquad \{z_{ij3}\}: \begin{array}{c|ccc|} i\backslash j & 1 & 2 & 3 \\ \hline 1 & 0+ & + & \ast \\ 2 & \ast & 0+ & \ast \\ 3 & \ast & \ast & \ast \\ \hline \end{array}$$

Since z_{123} has to be an element of a rectangle in the $k = 3$ slice, $z_{133}, z_{323} < 0$ and $z_{333} > 0$ are derived.

$$\{z_{ij1}\}: \begin{array}{c|ccc|} i\backslash j & 1 & 2 & 3 \\ \hline 1 & + & - & 0+ \\ 2 & - & + & \ast \\ 3 & 0+ & \ast & \ast \\ \hline \end{array} \qquad \{z_{ij2}\}: \begin{array}{c|ccc|} i\backslash j & 1 & 2 & 3 \\ \hline 1 & - & 0- & + \\ 2 & 0- & 0+ & \ast \\ 3 & + & \ast & - \\ \hline \end{array} \qquad \{z_{ij3}\}: \begin{array}{c|ccc|} i\backslash j & 1 & 2 & 3 \\ \hline 1 & 0+ & + & - \\ 2 & \ast & 0+ & \ast \\ 3 & \ast & - & + \\ \hline \end{array}$$

But there appears a rectangle $(z_{132}, z_{133}, z_{333}, z_{332})$ in the $j = 3$ slice, which contradicts the assumption and the proof of (b) is completed. Q.E.D.

We now carry out proofs of the theorems in Section 3.2.1 using the above lemma.

Proof of Theorem 3.2.1.

It has already been shown that a set of basic moves is not a Markov basis for the $3 \times 3 \times 3$ case in Section 3.1. It is also obvious that a minimal Markov basis includes a set of basic moves and degree 6 moves. Accordingly, to prove Theorem 3.2.1, it is only needed to show that the elements of $\boldsymbol{z} = \boldsymbol{x} - \boldsymbol{y}$ have to be all zero after minimizing $|\boldsymbol{z}|$ by applying the basic moves or the moves of degree 6 wcne on the way.

Suppose $\boldsymbol{z}$ has nonzero entries. Let $z_{111} > 0$ wlog. From Lemma 3.2.1(a), z_{111} has to be an element of rectangles, in each of the $i = 1, j = 1$ and $k = 1$ slices. We can take one of these rectangles in the $i = 1$ slice as $(z_{111}, z_{112}, z_{122}, z_{121})$ wlog.

$$\boxed{\begin{array}{ccc} + & - & * \\ - & + & * \\ * & * & * \end{array}} \qquad \boxed{\begin{array}{ccc} * & * & * \\ * & * & * \\ * & * & * \end{array}} \qquad \boxed{\begin{array}{ccc} * & * & * \\ * & * & * \\ * & * & * \end{array}}$$

Next consider the $j = 1$ slice. We claim that z_{111} and z_{112} are elements of the same rectangle in $j = 1$ slice. To prove this, consider the sign of z_{113}. If $z_{113} \geq 0$, the rectangle containing z_{111} in the $j = 1$ slice contains z_{112}, and if $z_{113} < 0$, the rectangle containing z_{112} in the $j = 1$ slice contains z_{111}. Therefore, z_{111} and z_{112} are elements of the same rectangle in the $j = 1$ slice and the rectangle can be taken as $(z_{111}, z_{112}, z_{212}, z_{211})$ wlog.

$$\boxed{\begin{array}{ccc} + & - & * \\ - & + & * \\ * & * & * \end{array}} \qquad \boxed{\begin{array}{ccc} - & + & * \\ * & * & * \\ * & * & * \end{array}} \qquad \boxed{\begin{array}{ccc} * & * & * \\ * & * & * \\ * & * & * \end{array}}$$

Now consider the rectangle in the $k = 1$ slice containing z_{111}. For a similar reason as above, this rectangle also contains z_{121}. In addition, if $z_{221} > 0$, $\boldsymbol{m}_4(12, 12, 21)$ can be added to $\boldsymbol{x}$ wcne and $|\boldsymbol{z}|$ can be made smaller, which contradicts the assumption. Hence, the rectangle in the $k = 1$ slice including z_{111} has to be $(z_{111}, z_{121}, z_{321}, z_{311})$.

$$\boxed{\begin{array}{ccc} + & - & * \\ - & + & * \\ * & * & * \end{array}} \qquad \boxed{\begin{array}{ccc} - & + & * \\ 0- & * & * \\ * & * & * \end{array}} \qquad \boxed{\begin{array}{ccc} - & * & * \\ + & * & * \\ * & * & * \end{array}}$$

Next consider the rectangle in the $j = 2$ slice including z_{121}. For a similar reason as above, this rectangle also contains z_{122}. Hence, the rectangle in the $j = 2$ slice including z_{121} has to be $(z_{121}, z_{122}, z_{322}, z_{321})$.

$$\boxed{\begin{array}{ccc} + & - & * \\ - & + & * \\ * & * & * \end{array}} \qquad \boxed{\begin{array}{ccc} - & + & * \\ 0- & * & * \\ * & * & * \end{array}} \qquad \boxed{\begin{array}{ccc} - & * & * \\ + & - & * \\ * & * & * \end{array}}$$

However, $\boldsymbol{m}_4(13,12,12)$ can be added to $\boldsymbol{y}$ wcne and $|\boldsymbol{z}|$ can be made smaller, which contradicts the assumption. From these considerations, a set of the basic moves and the moves of degree 6 is shown to be a Markov basis for the $3 \times 3 \times 3$ case. The minimality and the uniqueness is obvious as discussed in the top of Section 3.2.2. This completes the proof of Theorem 3.2.1. Q.E.D.

Proof of Theorem 3.2.2.

From Theorem 3.2.1, it is also shown that a (minimal) Markov basis for the $3 \times 3 \times 4$ case has to include a set of basic moves and moves of degree 6. In addition, if the pattern of $\boldsymbol{x}$ is expressed as

$$\begin{array}{|cccc|}\hline + & 0 & 0 & 0 \\ 0 & + & 0 & 0 \\ 0 & 0 & 0 & 0 \\ \hline\end{array} \quad \begin{array}{|cccc|}\hline 0 & 0 & + & 0 \\ + & 0 & 0 & 0 \\ 0 & 0 & 0 & + \\ \hline\end{array} \quad \begin{array}{|cccc|}\hline 0 & + & 0 & 0 \\ 0 & 0 & 0 & + \\ 0 & 0 & + & 0 \\ \hline\end{array}$$

and the pattern of $\boldsymbol{y}$ is expressed as

$$\begin{array}{|cccc|}\hline 0 & + & 0 & 0 \\ + & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ \hline\end{array} \quad \begin{array}{|cccc|}\hline + & 0 & 0 & 0 \\ 0 & 0 & 0 & + \\ 0 & 0 & + & 0 \\ \hline\end{array} \quad \begin{array}{|cccc|}\hline 0 & 0 & + & 0 \\ 0 & + & 0 & 0 \\ 0 & 0 & 0 & + \\ \hline\end{array},$$

it is observed that any basic moves or moves of degree 6 cannot be added to $\boldsymbol{x}$ or $\boldsymbol{y}$ wcne. This implies that a set of basic moves and moves of degree 6 is not a Markov basis for the $3 \times 3 \times 4$ case. Accordingly, to prove Theorem 3.2.2, it only has to be shown that the pattern of $\boldsymbol{z} = \boldsymbol{x} - \boldsymbol{y}$ has to be of all zero entries after minimizing $|\boldsymbol{z}|$ by adding the basic moves, the moves of degree 6 or degree 8, wcne on the way.

Suppose $\boldsymbol{z}$ has nonzero entries. Let $z_{111} > 0$ wlog. From Lemma 3.2.1(b) we can also assume that there is a rectangle including z_{111} in either an $i = 1$-slice or a $j = 1$-slice. We can take one of these rectangles in the $i = 1$-slice as $(z_{111}, z_{112}, z_{121}, z_{122})$ wlog. Moreover, $z_{211} < 0, z_{221} > 0$ wlog since it is known from Lemma 3.2.1(a) that z_{111} is an element of a rectangle in the $k = 1$ slice.

$$\begin{array}{|cccc|}\hline + & - & * & * \\ - & + & * & * \\ * & * & * & * \\ \hline\end{array} \quad \begin{array}{|cccc|}\hline - & * & * & * \\ + & * & * & * \\ * & * & * & * \\ \hline\end{array} \quad \begin{array}{|cccc|}\hline * & * & * & * \\ * & * & * & * \\ * & * & * & * \\ \hline\end{array}$$

As in the proof of Theorem 3.2.1, by considering the sign of z_{132}, we see that z_{112} and z_{122} are members of the same rectangle in the $k = 2$ slice. Then (z_{212}, z_{222}) and/or (z_{312}, z_{322}) has to be $(+, -)$. But if $z_{212} > 0$, $\boldsymbol{m}_4(12,12,21)$ can be added to $\boldsymbol{x}$ wcne; and if $z_{222} < 0$, $\boldsymbol{m}_4(12,12,12)$ can be added to $\boldsymbol{y}$ wcne; and $|\boldsymbol{z}|$ can be made smaller. These imply that $z_{312} > 0, z_{322} < 0$ and $z_{212} \leq 0, z_{222} \geq 0$. Similarly, if $z_{311} < 0$, $\boldsymbol{m}_4(13,12,12)$ can be added to $\boldsymbol{y}$ wcne; and if $z_{321} > 0$, $\boldsymbol{m}_4(13,12,21)$ can be added to $\boldsymbol{x}$ wcne; and $|\boldsymbol{z}|$ can be made smaller, which forces $z_{311} \geq 0$ and $z_{321} \leq 0$.

$$\begin{array}{|cccc|}\hline + & - & * & * \\ - & + & * & * \\ * & * & * & * \\ \hline\end{array} \quad \begin{array}{|cccc|}\hline - & 0- & * & * \\ + & 0+ & * & * \\ * & * & * & * \\ \hline\end{array} \quad \begin{array}{|cccc|}\hline 0+ & + & * & * \\ 0- & - & * & * \\ * & * & * & * \\ \hline\end{array}$$

Since $z_{21\cdot} = 0$, let $z_{213} > 0$ wlog, which forces $z_{123} \leq 0$, otherwise, $\boldsymbol{m}_4(12,12,31)$ can be added to $\boldsymbol{x}$ wcne and $|\boldsymbol{z}|$ can be made smaller. That $z_{213} > 0$ also forces $z_{323} \leq 0$, otherwise,

$\boldsymbol{m}_6^J(132, 21, 123)$ can be added to $\boldsymbol{x}$ wcne and $|\boldsymbol{z}|$ can be made smaller.

$$\begin{array}{|cccc|}\hline + & - & * & * \\ - & + & 0- & * \\ * & * & * & * \\ \hline\end{array} \quad \begin{array}{|cccc|}\hline - & 0- & + & * \\ + & 0+ & * & * \\ * & * & * & * \\ \hline\end{array} \quad \begin{array}{|cccc|}\hline 0+ & + & * & * \\ 0- & - & 0- & * \\ * & * & * & * \\ \hline\end{array}$$

Since $z_{\cdot 23} = 0$, it follows $z_{223} \geq 0$. This implies $z_{224}, z_{233} < 0$ since $z_{22\cdot} = z_{2\cdot 3} = 0$.

$$\begin{array}{|cccc|}\hline + & - & * & * \\ - & + & 0- & * \\ * & * & * & * \\ \hline\end{array} \quad \begin{array}{|cccc|}\hline - & 0- & + & * \\ + & 0+ & 0+ & - \\ * & * & - & * \\ \hline\end{array} \quad \begin{array}{|cccc|}\hline 0+ & + & * & * \\ 0- & - & 0- & * \\ * & * & * & * \\ \hline\end{array}$$

From symmetry (in interchanging roles of $+$ and $-$), $z_{114}, z_{314} \geq 0$, otherwise, $\boldsymbol{m}_4(12, 12, 14)$ can be added to $\boldsymbol{y}$ wcne or $\boldsymbol{m}_6^J(132, 12, 124)$ can be added to $\boldsymbol{y}$ wcne and $|\boldsymbol{z}|$ can be made smaller. These also implies $z_{214} \leq 0, z_{234} > 0$ since $z_{\cdot 14} = z_{2\cdot 4} = 0$.

$$\begin{array}{|cccc|}\hline + & - & * & 0+ \\ - & + & 0- & * \\ * & * & * & * \\ \hline\end{array} \quad \begin{array}{|cccc|}\hline - & 0- & + & 0- \\ + & 0+ & 0+ & - \\ * & * & - & + \\ \hline\end{array} \quad \begin{array}{|cccc|}\hline 0+ & + & * & 0+ \\ 0- & - & 0- & * \\ * & * & * & * \\ \hline\end{array} \tag{3.6}$$

Since $z_{31\cdot} = z_{32\cdot} = z_{3\cdot 3} = z_{3\cdot 4} = 0$, it follows that $z_{313} < 0, z_{324} > 0, z_{333} > 0, z_{334} < 0$.

$$\begin{array}{|cccc|}\hline + & - & * & 0+ \\ - & + & 0- & * \\ * & * & * & * \\ \hline\end{array} \quad \begin{array}{|cccc|}\hline - & 0- & + & 0- \\ + & 0+ & 0+ & - \\ * & * & - & + \\ \hline\end{array} \quad \begin{array}{|cccc|}\hline 0+ & + & - & 0+ \\ 0- & - & 0- & + \\ * & * & + & - \\ \hline\end{array}$$

But $\boldsymbol{m}_8(132, 123, 2134)$ can be added to $\boldsymbol{x}$ (or $\boldsymbol{m}_8(123, 123, 1234)$ can be added to $\boldsymbol{y}$) wcne and $|\boldsymbol{z}|$ can be made smaller.

From these considerations, a set of the basic moves, the moves of degree 6 and degree 8 is shown to be a Markov basis for the $3 \times 3 \times 4$ case. The minimality and the uniqueness is obvious as in the proof of Theorem 3.2.1. Q.E.D.

Proof of Theorem 3.2.3.

Theorem 3.2.2 implies that a (minimal) Markov basis for the $3 \times 3 \times 5$ case has to include a set of basic moves, moves of degree 6 and degree 8. In addition, if the pattern of $\boldsymbol{x}$ is expressed as

$$\begin{array}{|ccccc|}\hline + & 0 & 0 & 0 & 0 \\ 0 & + & 0 & 0 & + \\ 0 & 0 & 0 & + & 0 \\ \hline\end{array} \quad \begin{array}{|ccccc|}\hline 0 & 0 & + & 0 & 0 \\ + & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & + \\ \hline\end{array} \quad \begin{array}{|ccccc|}\hline 0 & + & 0 & 0 & 0 \\ 0 & 0 & 0 & + & 0 \\ 0 & 0 & + & 0 & 0 \\ \hline\end{array}$$

and the pattern of $\boldsymbol{y}$ is expressed as

$$\begin{array}{|ccccc|}\hline 0 & + & 0 & 0 & 0 \\ + & 0 & 0 & + & 0 \\ 0 & 0 & 0 & 0 & + \\ \hline\end{array} \quad \begin{array}{|ccccc|}\hline + & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & + \\ 0 & 0 & + & 0 & 0 \\ \hline\end{array} \quad \begin{array}{|ccccc|}\hline 0 & 0 & + & 0 & 0 \\ 0 & + & 0 & 0 & 0 \\ 0 & 0 & 0 & + & 0 \\ \hline\end{array},$$

it is observed that we cannot add any basic move, move of degree 6 and degree 8 to $\boldsymbol{x}$ or $\boldsymbol{y}$ wcne. This implies that a set of basic moves, moves of degree 6 and degree 8 is not a Markov basis for the $3 \times 3 \times 5$ case. Accordingly, to prove Theorem 3.2.3, all we have to show is that the pattern of $\boldsymbol{z} = \boldsymbol{x} - \boldsymbol{y}$ must be of all zero entries after minimizing $|\boldsymbol{z}|$ by adding the basic moves, the moves of degree 6, degree 8 or degree 10, wcne on the way.

Suppose $\boldsymbol{z}$ has nonzero entries. For a similar reason leading to (3.6) in the proof of Theorem 3.2.2, the patterns can be restricted to

$$\begin{array}{|ccccc|}\hline + & - & \ast & 0+ & \ast \\ - & + & 0- & \ast & \ast \\ \ast & \ast & \ast & \ast & \ast \\ \hline \end{array} \qquad \begin{array}{|ccccc|}\hline - & 0- & + & 0- & \ast \\ + & 0+ & 0+ & - & \ast \\ \ast & \ast & - & + & \ast \\ \hline \end{array} \qquad \begin{array}{|ccccc|}\hline 0+ & + & \ast & 0+ & \ast \\ 0- & - & 0- & \ast & \ast \\ \ast & \ast & \ast & \ast & \ast \\ \hline \end{array}$$

wlog. Since $z_{31\cdot} = z_{32\cdot} = 0$, at least z_{313} or z_{315} has to be negative and at least z_{324} or z_{325} has to be positive. But we have already seen that $(z_{313}, z_{324}) = (-, +)$ contradicts the assumption. In addition, if $(z_{315}, z_{325}) = (-, +)$, it follows that $z_{115} \leq 0$ and $z_{125} \geq 0$, (otherwise $\boldsymbol{m}_4(13, 12, 25)$ can be added to $\boldsymbol{x}$ wcne and $\boldsymbol{m}_4(13, 12, 52)$ can be added to $\boldsymbol{y}$ wcne and $|\boldsymbol{z}|$ can be made smaller) and $(z_{215}, z_{225}) = (+, -)$ since $z_{\cdot 15} = z_{\cdot 25} = 0$. But $\boldsymbol{m}_6^J(132, 21, 125)$ can be added to $\boldsymbol{x}$ wcne and $\boldsymbol{m}_6^J(132, 12, 125)$ can be added to $\boldsymbol{y}$ wcne and $|\boldsymbol{z}|$ can be made smaller. All of these contradict the assumption. The remaining patterns are $(z_{313}, z_{325}) = (-, +)$ or $(z_{315}, z_{324}) = (-, +)$. Considering the symmetry, we write $(z_{313}, z_{325}) = (-, +)$ wlog. Then the patterns are wlog summarized as

$$\begin{array}{|ccccc|}\hline + & - & \ast & 0+ & \ast \\ - & + & 0- & \ast & \ast \\ \ast & \ast & \ast & \ast & \ast \\ \hline \end{array} \qquad \begin{array}{|ccccc|}\hline - & 0- & + & 0- & \ast \\ + & 0+ & 0+ & - & \ast \\ \ast & \ast & - & + & \ast \\ \hline \end{array} \qquad \begin{array}{|ccccc|}\hline 0+ & + & - & 0+ & 0+ \\ 0- & - & 0- & 0- & + \\ \ast & \ast & \ast & \ast & \ast \\ \hline \end{array} \; .$$

Since $z_{\cdot 24} = z_{1 \cdot 4} = z_{3 \cdot 3} = z_{3 \cdot 5} = 0$, it follows that $z_{124} > 0, z_{134} < 0, z_{333} > 0, z_{335} < 0$.

$$\begin{array}{|ccccc|}\hline + & - & \ast & 0+ & \ast \\ - & + & 0- & + & \ast \\ \ast & \ast & \ast & - & \ast \\ \hline \end{array} \qquad \begin{array}{|ccccc|}\hline - & 0- & + & 0- & \ast \\ + & 0+ & 0+ & - & \ast \\ \ast & \ast & - & + & \ast \\ \hline \end{array} \qquad \begin{array}{|ccccc|}\hline 0+ & + & - & 0+ & 0+ \\ 0- & - & 0- & 0- & + \\ \ast & \ast & + & \ast & - \\ \hline \end{array}$$

If $z_{225} < 0$, $\boldsymbol{m}_8(123, 123, 1235)$ can be added to $\boldsymbol{y}$ wcne and $|\boldsymbol{z}|$ can be made smaller, which contradicts the assumption. Similarly, if $z_{235} > 0$, $\boldsymbol{m}_8(123, 213, 1253)$ can be added to $\boldsymbol{x}$ wcne and $|\boldsymbol{z}|$ can be made smaller, which contradicts the assumption. These imply $z_{225} \geq 0, z_{234} \leq 0$, which also imply $z_{125} < 0, z_{135} > 0$ since $z_{\cdot 25} = z_{\cdot 35} = 0$.

$$\begin{array}{|ccccc|}\hline + & - & \ast & 0+ & \ast \\ - & + & 0- & + & - \\ \ast & \ast & \ast & - & + \\ \hline \end{array} \qquad \begin{array}{|ccccc|}\hline - & 0- & + & 0- & \ast \\ + & 0+ & 0+ & - & 0+ \\ \ast & \ast & - & + & 0- \\ \hline \end{array} \qquad \begin{array}{|ccccc|}\hline 0+ & + & - & 0+ & 0+ \\ 0- & - & 0- & 0- & + \\ \ast & \ast & + & \ast & - \\ \hline \end{array}$$

But $\boldsymbol{m}_{10}(123, 321, 45321)$ can be added to $\boldsymbol{x}$ (or $\boldsymbol{m}_{10}(123, 123, 12354)$ can be added to $\boldsymbol{y}$) wcne and $|\boldsymbol{z}|$ can be made smaller, which contradict the assumption.

From these considerations, a set of the basic moves, the moves of degree 6, degree 8 and degree 10 is shown to be a Markov basis for $3 \times 3 \times 5$ case. The minimality and the uniqueness is obvious as in the proof of Theorem 3.2.1. Q.E.D.

Proof of Theorem 3.2.4.

Again we can begin with the following pattern.

$$\begin{array}{|cccccc|}\hline + & - & \ast & 0+ & \ast & \ast \\ - & + & 0- & \ast & \ast & \ast \\ \ast & \ast & \ast & \ast & \ast & \ast \\ \hline \end{array} \qquad \begin{array}{|cccccc|}\hline - & 0- & + & 0- & \ast & \ast \\ + & 0+ & 0+ & - & \ast & \ast \\ \ast & \ast & - & + & \ast & \ast \\ \hline \end{array} \qquad \begin{array}{|cccccc|}\hline 0+ & + & \ast & 0+ & \ast & \ast \\ 0- & - & 0- & \ast & \ast & \ast \\ \ast & \ast & \ast & \ast & \ast & \ast \\ \hline \end{array}$$

As we have seen in the proof of Theorem 3.2.3, z_{313} has to be nonnegative and z_{324} has to be nonpositive, since $(z_{313}, z_{326}) = (-,+)$ or $(z_{316}, z_{324}) = (-,+)$ also contradict the assumption. The case of $(z_{316}, z_{326}) = (-,+)$ also contradicts the assumption for a similar reason that $(z_{315}, z_{325}) = (-,+)$ does. Hence the remaining pattern is $(z_{315}, z_{326}) = (-,+)$ or $(z_{316}, z_{325}) = (-,+)$. We write $(z_{315}, z_{326}) = (-,+)$ wlog.

$$
\begin{array}{|cccccc|}\hline
+ & - & \ast & 0+ & \ast & \ast \\
- & + & 0- & \ast & \ast & \ast \\
\ast & \ast & \ast & \ast & \ast & \ast \\ \hline
\end{array}
\quad
\begin{array}{|cccccc|}\hline
- & 0- & + & 0- & \ast & \ast \\
+ & 0+ & 0+ & - & \ast & \ast \\
\ast & \ast & - & + & \ast & \ast \\ \hline
\end{array}
\quad
\begin{array}{|cccccc|}\hline
0+ & + & 0+ & 0+ & - & \ast \\
0- & - & 0- & 0- & \ast & + \\
\ast & \ast & \ast & \ast & \ast & \ast \\ \hline
\end{array}
$$

According to the symmetry in interchanging the roles of $\{+,-\}$, the roles of $\{z_{2jk}, z_{3jk}\}$ and the roles of $\{(z_{ij3}, z_{ij4}), (z_{ij5}, z_{ij6})\}$, the patterns can be restricted to

$$
\begin{array}{|cccccc|}\hline
+ & - & \ast & 0+ & \ast & 0- \\
- & + & 0- & \ast & 0+ & \ast \\
\ast & \ast & \ast & \ast & \ast & \ast \\ \hline
\end{array}
\quad
\begin{array}{|cccccc|}\hline
- & 0- & + & 0- & 0- & 0- \\
+ & 0+ & 0+ & - & 0+ & 0+ \\
\ast & \ast & - & + & \ast & \ast \\ \hline
\end{array}
\quad
\begin{array}{|cccccc|}\hline
0+ & + & 0+ & 0+ & - & 0+ \\
0- & - & 0- & 0- & 0- & + \\
\ast & \ast & \ast & \ast & + & - \\ \hline
\end{array}
$$

for a similar reason to the proof of Theorem 3.2.2. Since $z_{\cdot 13} = z_{\cdot 15} = z_{\cdot 24} = z_{\cdot 26} = 0$, it follows that $z_{113} < 0, z_{115} > 0, z_{124} > 0$ and $z_{126} < 0$. $z_{1\cdot 3} = z_{1\cdot 4} = z_{1\cdot 5} = z_{1\cdot 6} = 0$ also forces $z_{133} > 0, z_{134} < 0, z_{135} < 0$ and $z_{136} > 0$.

$$
\begin{array}{|cccccc|}\hline
+ & - & - & 0+ & + & 0- \\
- & + & 0- & + & 0+ & - \\
\ast & \ast & + & - & - & + \\ \hline
\end{array}
\quad
\begin{array}{|cccccc|}\hline
- & 0- & + & 0- & 0- & 0- \\
+ & 0+ & 0+ & - & 0+ & 0+ \\
\ast & \ast & - & + & \ast & \ast \\ \hline
\end{array}
\quad
\begin{array}{|cccccc|}\hline
0+ & + & 0+ & 0+ & - & 0+ \\
0- & - & 0- & 0- & 0- & + \\
\ast & \ast & \ast & \ast & + & - \\ \hline
\end{array}
$$

But this pattern includes moves of degree 6. We can add $\boldsymbol{m}_6^I(21, 132, 134)$ to $\boldsymbol{x}$, $\boldsymbol{m}_6^I(12, 132, 134)$ to $\boldsymbol{y}$, $\boldsymbol{m}_6^I(13, 132, 256)$ to $\boldsymbol{x}$ or $\boldsymbol{m}_6^I(31, 132, 256)$ to $\boldsymbol{y}$ wcne and make $|\boldsymbol{z}|$ smaller, which contradicts the assumption.

From these considerations, it is shown that a set of the basic moves, the moves of degree 6, degree 8 and degree 10 is also a Markov basis for the $3 \times 3 \times K$ $(K \geq 5)$ case. The minimality and the uniqueness is again obvious. Note that although we have displayed $3 \times 3 \times 6$ tables, the above argument does not involve k-slices for $k \geq 7$. Therefore we obtain the same contradiction for the $3 \times 3 \times K$ $(K \geq 7)$ tables. Q.E.D.

3.2.3 Computational examples

The Markov basis obtained above can be used to perform various tests by the Monte Carlo method. Here we show simple examples of testing the hypothesis of no three-factor interaction. We consider the null distribution of the classical goodness-of-fit chi-squared statistic. It is known that, under the hypothesis of no three-factor interaction, the conditional probability of cell counts is a hypergeometric distribution. Our concern is to compute a finite sample null distribution of the goodness-of-fit chi-squared statistic, without using large-sample theory.

The settings of the examples are as follows. The size of the contingency table is $3 \times 3 \times 8$ and the total frequency $x_{\cdots}$ is taken to be 72 and 216. The marginal totals are assumed to be completely uniform, i.e., $x_{i\cdot k} = x_{\cdot jk} = 3$ or 9 and $x_{ij\cdot} = 8$ or 24 for all i, j and k. For this case, as we have seen, a set of $2 \times 2 \times 2$ basic moves, $2 \times 3 \times 3, 3 \times 2 \times 3, 3 \times 3 \times 2$ moves of degree 6, $3 \times 3 \times 4$ moves of degree 8 and $3 \times 3 \times 5$ moves of degree 10, forms a

Markov basis. For constructing a Markov chain which has a hypergeometric distribution as a stationary distribution, we use the Metropolis procedure described in Diaconis and Sturmfels (1998, Lemma 2.2). After 50 000 burn-in steps, the walk was run for 100 000 steps sampling every 50 steps for a total of 2000 values. To compare the obtained sample to the asymptotic distribution, we made a Q-Q plot of the permutation distribution of the chi-squared statistic versus the limiting chi-squared distribution with 28 degrees of freedom. Figures 3.7 and 3.8 show the cases of $x_{\cdots} = 72$ and 216, respectively. It is clear that the approximation is not good, especially for the case of $x_{\cdots} = 72$.

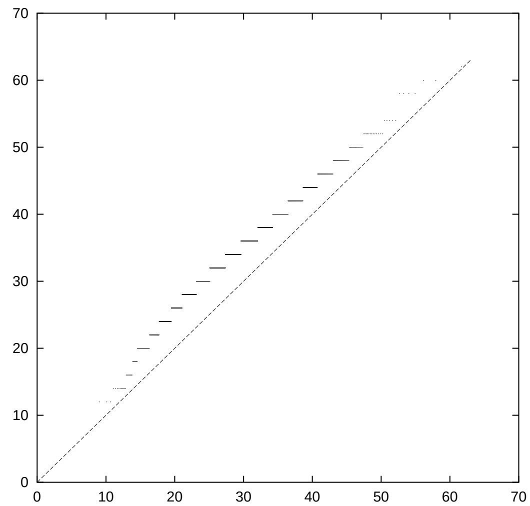

Figure 3.7: Q-Q plot of the permutation distribution of chi-squared statistic versus asymptotic distribution ($x_{\cdots} = 72$).

3.2.4 Discussion

Our main contribution in Section 3.2 is twofold. First, an explicit form of the unique minimal Markov basis for $3 \times 3 \times K$ contingency tables is provided, by considering all the patterns that do not contradict the constraints. These results enable us to construct a connected Markov chain over $3 \times 3 \times K$ contingency tables. Adjusting this chain to have a given stationary distribution by the Metropolis procedure, we can perform various tests by the Monte Carlo method. A typical example of an application is the Monte Carlo simulation of the finite sample distribution of the goodness-of-fit chi-squared statistic under the hypothesis of no three-factor interaction in Section 3.2.3. Our approach is also applicable to the problem of data security, where very sparse contingency tables with fixed marginals are treated. See Irving and Jerrum (1994), for example. Second, a general method to obtain a Markov basis is provided. It is true that our method is laborious one as seen in Section 3.2.2. But Theorem 3.2.4 assures us that no other moves are needed to construct a connected Markov chain regardless of the value of K. This result is attractive since it may not be derived by performing algebraic algorithms, which leads to a general problem suggested by a referee of Aoki and Takemura (2003a).

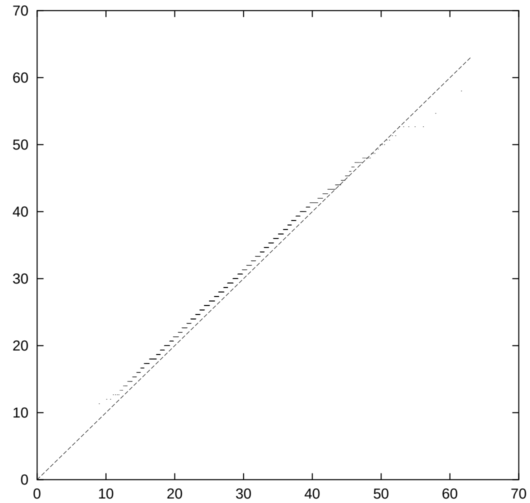

Figure 3.8: Q-Q plot of the permutation distribution of chi-squared statistic versus asymptotic distribution ($x_{\dots} = 216$).

> **Problem** Does there exist a bound $\mu_{I,J}$ depending on I and J, such that for any K the corresponding minimal Markov basis for the three-dimensional $I \times J \times K$ contingency tables with fixed two-dimensional marginals consists of moves whose degree are all less than $\mu_{I,J}$?

From the paper by Diaconis and Sturmfels (1998) it is known that $\mu_{2,J} = 2J$ and we showed that $\mu_{3,3} = 10$. As the next simplest case we consider the case of $3 \times 4 \times K$ tables in Section 3.3.1. Recently Santos and Sturmfels (2002) give an upper bound for $\mu_{I,J}$ using the theory of Graves basis.

Our approach seems to be difficult to generalize to larger tables. For illustration, we here present a Markov basis for the $3 \times 4 \times 4$ case. Similarly as in Section 3.2.2, it can be shown that the unique minimal Markov basis for the $3 \times 4 \times 4$ case is composed of basic moves, moves of degree 6 ($2 \times 3 \times 3, 3 \times 2 \times 3, 3 \times 3 \times 2$), moves of degree 8 ($3 \times 3 \times 4, 3 \times 4 \times 3$), moves of degree 8 ($2 \times 4 \times 4$) like

$$\boxed{\begin{array}{cccc} +1 & -1 & 0 & 0 \\ 0 & +1 & -1 & 0 \\ 0 & 0 & +1 & -1 \\ -1 & 0 & 0 & +1 \end{array}} \quad \boxed{\begin{array}{cccc} -1 & +1 & 0 & 0 \\ 0 & -1 & +1 & 0 \\ 0 & 0 & -1 & +1 \\ +1 & 0 & 0 & -1 \end{array}} \quad \boxed{\begin{array}{cccc} 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{array}},$$

moves of degree 9 ($3 \times 4 \times 4$, Figure 3.9) like

$$\boxed{\begin{array}{cccc} +1 & -1 & 0 & 0 \\ -1 & 0 & +1 & 0 \\ 0 & +1 & -1 & 0 \\ 0 & 0 & 0 & 0 \end{array}} \quad \boxed{\begin{array}{cccc} -1 & +1 & 0 & 0 \\ +1 & 0 & 0 & -1 \\ 0 & 0 & 0 & 0 \\ 0 & -1 & 0 & +1 \end{array}} \quad \boxed{\begin{array}{cccc} 0 & 0 & 0 & 0 \\ 0 & 0 & -1 & +1 \\ 0 & -1 & +1 & 0 \\ 0 & +1 & 0 & -1 \end{array}},$$

and moves of degree 10 ($3 \times 4 \times 4$, Figure 3.10) like

$$\begin{array}{|cccc|}\hline +1 & -1 & 0 & 0 \\ -1 & +1 & 0 & 0 \\ 0 & 0 & +1 & -1 \\ 0 & 0 & -1 & +1 \\ \hline \end{array} \quad \begin{array}{|cccc|}\hline -1 & +1 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ +1 & 0 & -1 & 0 \\ 0 & -1 & +1 & 0 \\ \hline \end{array} \quad \begin{array}{|cccc|}\hline 0 & 0 & 0 & 0 \\ +1 & -1 & 0 & 0 \\ -1 & 0 & 0 & +1 \\ 0 & +1 & 0 & -1 \\ \hline \end{array}\ .$$

Proofs of these results are elementary, but considerably longer and are not reproduced here. Among the newly obtained moves, the $3 \times 4 \times 4$ move of degree 10 is interpreted as a type-2 combination of a basic move and a move of degree 8, which is similar to the $3 \times 3 \times 5$ move of degree 10 shown in Section 3.2.1. However, the $3 \times 4 \times 4$ move of degree 9 is new in the sense that this is a type-2 combination of a basic move and a move of degree 7. Recall that the move of degree 7 itself is not needed to construct a connected Markov chain. In this section, we have only considered combinations of basic moves that happen 'one at a time'. But it might be worthwhile to think of this degree 9 move as a combination of three basic moves that happens 'all at once', and every two of these basic moves are type-1 combinations. The move of degree 9 suggests the difficulty in forming a conjecture on a minimal Markov basis for larger tables.

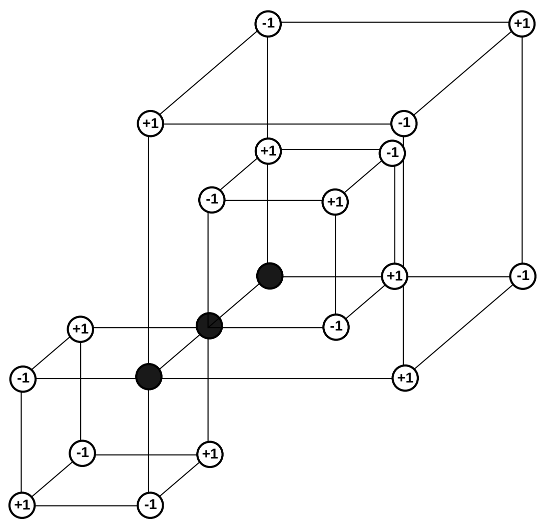

Figure 3.9: $3 \times 4 \times 4$ move of degree 9

3.3 Construction of a connected Markov chain over three-way contingency tables of larger sizes with fixed two-dimensional marginals

We derived an explicit form of unique minimal Markov basis for $3 \times 3 \times K$ tables in Section 3.2.1, by considering all the patterns that do not contradict the constraints as shown in Section 3.2.2. These results enable us to construct a connected Markov chain over $3 \times 3 \times K$ tables, and to perform various tests by the Monte Carlo methods as shown in Section 3.2.3. In Section 3.3, we consider larger tables.

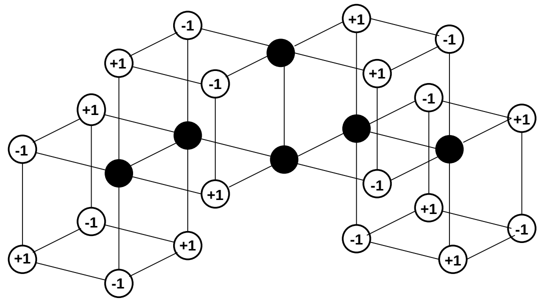

Figure 3.10: $3 \times 4 \times 4$ move of degree 10

As we have seen, our method in Section 3.2.2 is laborious, though it is one of general methods for obtaining a Markov basis. However, as is stated in Section 3.2.4, Theorem 3.2.4 assures us that no other moves are needed for constructing a connected Markov chain, regardless of the value K. This result is attractive since it cannot be derived by performing algebraic algorithms. This is the reason why we dared to perform the similar laborious and exhaustive investigations of possible sign patterns for the next simpler case, $3 \times 4 \times K$ tables. We also considered the more complicated problem, $4 \times 4 \times 4$ tables. We found that, for all these problems, the unique minimal Markov bases exist. Though we give some characterization of a minimal Markov basis and its uniqueness in detail in Section 3.5, we give an important definition here in advance.

Definition 3.3.1 *An indispensable move is a move* $\boldsymbol{z} \in \mathcal{F}_0$ *which is written as* $\boldsymbol{z} = \boldsymbol{x} - \boldsymbol{y}$, *where* $\boldsymbol{x}$ *and* $\boldsymbol{y}$ *constitute a two elements reference set* $\mathcal{F}(\{x_{ij\cdot}\}, \{x_{i\cdot k}\}, \{x_{\cdot jk}\}) = \{\boldsymbol{x}, \boldsymbol{y}\}$.

We use the term *indispensable* for the following reason.

> **Lemma 3.5.3** Every indispensable move belongs to each Markov basis.

This lemma suggests that indispensable moves play an important role in uniqueness of minimal Markov bases. Relations between the indispensable moves and uniqueness of a minimal Markov basis is summarized as follows.

> **Corollary 3.5.2** The unique minimal Markov basis exists if and only if the set of indispensable moves forms a Markov basis. In this case, the set of indispensable moves is the unique minimal Markov basis.

From this corollary, we see that the minimal Markov basis for the $3 \times 3 \times K$ contingency tables is the unique minimal Markov basis since all the basis elements described in Section 3.2.1 are indispensable moves. Similarly, we found that the set of all indispensable moves for $3 \times 4 \times K$ and $4 \times 4 \times 4$ tables constituted the unique minimal Markov basis for these problems.

The organization of Section 3.3 is as follows. In Section 3.3.1, we describe a list of all indispensable moves for the $3 \times 4 \times K$ and $4 \times 4 \times 4$ cases. In Section 3.3.2 we prove a result on combination of two indispensable moves preserving the indispensability and in Section 3.3.3 we prove a result on separation and combination of the two-dimensional slices preserving the indispensability. Some discussion is given in Section 3.3.4. In Appendix we give a (non-exhaustive) list indispensable moves for larger tables.

3.3.1 List of indispensable moves of the unique minimal Markov basis for $3 \times 4 \times K$ and $4 \times 4 \times 4$ tables

In Section 3.3.1, we give a list of all indispensable moves for the $3 \times 4 \times K$ and $4 \times 4 \times 4$ cases. After laborious derivation, we found that these indispensable moves, together with the permutations of indices for each axis and the permutations of axes of these moves, constitute the unique minimal Markov basis for each case. Our approach is similar to that of Section 3.2.2. Note that the permutation of indices for each axis of moves can be considered as an action of a direct product of symmetric groups to the moves. We consider this point in Section 3.6.

Let $\boldsymbol{z} \in \mathcal{F}_0$ be an indispensable move for our problems. Write $\boldsymbol{z} = \boldsymbol{z}^+ - \boldsymbol{z}^-$ where $\boldsymbol{z}^+$ and $\boldsymbol{z}^-$ are the positive and the negative parts of $\boldsymbol{z}$. Similarly as in Section 3.2, to display $I \times J \times K$ moves $\boldsymbol{z}$, we write I i-slices of size $J \times K$ as follows:

$$\begin{array}{c} i=1 \\ \begin{array}{c|ccc|} j\backslash k & 1 & \cdots & K \\ \hline 1 & z_{111} & \cdots & z_{11K} \\ \vdots & \vdots & & \vdots \\ J & z_{1J1} & \cdots & z_{1JK} \\ \hline \end{array} \end{array} \quad \cdots \quad \begin{array}{c} i=I \\ \begin{array}{c|ccc|} j\backslash k & 1 & \cdots & K \\ \hline 1 & z_{I11} & \cdots & z_{I1K} \\ \vdots & \vdots & & \vdots \\ J & z_{IJ1} & \cdots & z_{IJK} \\ \hline \end{array} \end{array} \tag{3.7}$$

We also define the i,j-line (or $i = i_0, j = j_0$-line) of $\boldsymbol{z}$ as the one-dimensional line $\boldsymbol{z}_{i=i_0,j=j_0} = \{z_{i_0 j_0 k}\}_{k\in[K]}$, where $i_0 \in [I]$ and $j_0 \in [J]$ are fixed. We similarly define the i,k-line and the j,k-line of $\boldsymbol{z}$. We label each indispensable move by its *size*, *degree* and *slice degree* defined as follows. The size of $I \times J \times K$ contingency table $\boldsymbol{x}$ is defined as the size of the smallest 3-way subtable containing the support of $\boldsymbol{x}$, defined by

$$\mathrm{supp}(\boldsymbol{x}) = \{(i,j,k) \mid x_{ijk} > 0\} .$$

We call this subtable the *supporting subtable* (or *supporting rectangle*) of $\boldsymbol{x}$ and denote it by

$$R(\boldsymbol{x}) = I_{\boldsymbol{x}} \times J_{\boldsymbol{x}} \times K_{\boldsymbol{x}} \subset [I] \times [J] \times [K],$$

where

$$I_{\boldsymbol{x}} = \{i \in [I] \mid x_{ijk} > 0 \text{ for some } j \in [J], k \in [K]\},$$

and so on. We also define the supporting subtable of a move $\boldsymbol{z}$ as the supporting subtable of its positive and negative parts, i.e., $R(\boldsymbol{z}) = R(\boldsymbol{z}^+) = R(\boldsymbol{z}^-)$. Note that $R(\boldsymbol{z}^+)$ and $R(\boldsymbol{z}^-)$ are equal since $\boldsymbol{z}^+$ and $\boldsymbol{z}^-$ have the same marginal totals. The size of $\boldsymbol{z}$ is defined as the size of $R(\boldsymbol{z})$. We denote the size of $\boldsymbol{z}$ by $s_i \times s_j \times s_k$. We assume that $s_i \le s_j \le s_k$ without loss of generality since other moves can be produced by permutations of axes of these moves. For example, the following $2 \times 3 \times 3$ move is an indispensable move, which we found in Section 3.2.1.

$$\begin{array}{|ccc|}\hline +1 & -1 & 0 \\ -1 & 0 & +1 \\ 0 & +1 & -1 \\ \hline\end{array} \qquad \begin{array}{|ccc|}\hline -1 & +1 & 0 \\ +1 & 0 & -1 \\ 0 & -1 & +1 \\ \hline\end{array} \tag{3.8}$$

By permuting axes of this move, we have other indispensable moves, i.e., $3 \times 2 \times 3$ move

$$\begin{array}{|ccc|}\hline +1 & -1 & 0 \\ -1 & +1 & 0 \\ \hline\end{array} \qquad \begin{array}{|ccc|}\hline -1 & 0 & +1 \\ +1 & 0 & -1 \\ \hline\end{array} \qquad \begin{array}{|ccc|}\hline 0 & +1 & -1 \\ 0 & -1 & +1 \\ \hline\end{array}$$

and $3 \times 3 \times 2$ move

$$\begin{array}{|cc|}\hline +1 & -1 \\ -1 & +1 \\ 0 & 0 \\ \hline \end{array} \qquad \begin{array}{|cc|}\hline -1 & +1 \\ 0 & 0 \\ +1 & -1 \\ \hline \end{array} \qquad \begin{array}{|cc|}\hline 0 & 0 \\ +1 & -1 \\ -1 & +1 \\ \hline \end{array}.$$

In this case, only $2 \times 3 \times 3$ move is included in our list.

We have already defined the degree of move $\boldsymbol{z}$ as the total frequency of $\boldsymbol{z}^+$ or $\boldsymbol{z}^-$, i.e.,

$$\deg(\boldsymbol{z}) = \sum_{i,j,k} z_{ijk}^+ = \sum_{i,j,k} z_{ijk}^- = \frac{1}{2}\sum_{i,j,k} |z_{ijk}|.$$

The slice degree of $\boldsymbol{z}$ (with the size $s_i \times s_j \times s_k$) is the degrees of each slices having the form $\{d_1^i, \dots, d_{s_i}^i\} \times \{d_1^j, \dots, d_{s_j}^j\} \times \{d_1^k, \dots, d_{s_k}^k\}$, where

$$d_{i_0}^i = \deg(\boldsymbol{z}_{i=i_0}) = \sum_{j,k} z_{i_0jk}^+ = \sum_{j,k} z_{i_0jk}^- = \frac{1}{2}\sum_{j,k} |z_{i_0jk}|$$

and so on. For example, the $2 \times 3 \times 3$ move displayed in (3.8) has the degree 6 and the slice degree $\{3,3\} \times \{2,2,2\} \times \{2,2,2\}$. We label this move as

$$2 \times 3 \times 3 \text{ move of degree 6 with slice degree } \{3,3\} \times \{2,2,2\} \times \{2,2,2\}$$

in this thesis. We also assume that

$$d_1^i \le d_2^i \le \dots \le d_{s_i}^i,\ d_1^j \le d_2^j \le \dots \le d_{s_j}^j,\ d_1^k \le d_2^k \le \dots \le d_{s_k}^k$$

without loss of generality since we take account of the permutations of indices for each axis of moves. Therefore our display of the form (3.7) is according to this order of the slice degree. It should be noted that the size, degree and slice degree are examples of invariants for the permutations of indices for each axis of moves and the permutations of axes of moves. Unfortunately, we cannot completely distinguish all indispensable moves by these invariants only. We consider this point in Section 3.3.4.

Closely related notions to indispensability are the notions of fundamental moves and circuits discussed in Ohsugi and Hibi (1999b, 2003). For a move $\boldsymbol{z}$ its support is defined by $\mathrm{supp}(\boldsymbol{z}) = \mathrm{supp}(\boldsymbol{z}^+) \cup \mathrm{supp}(\boldsymbol{z}^-)$. $\boldsymbol{z}$ is called a *circuit* if $\boldsymbol{z}'$ is a move such that $\mathrm{supp}(\boldsymbol{z}') \subset \mathrm{supp}(\boldsymbol{z})$ then $\boldsymbol{z}' = c\boldsymbol{z}$ for some integer c. For a three-way contingency table $\boldsymbol{x}$, let

$$\boldsymbol{t}(\boldsymbol{x}) = \{\{x_{ij\cdot}\}, \{x_{i\cdot k}\}, \{x_{\cdot jk}\}\}$$

denote the marginal frequencies and let $\mathrm{supp}(\boldsymbol{t}(\boldsymbol{x}))$ denote the set of positive marginal cells for $\boldsymbol{x}$. For a move $\boldsymbol{z}$ define $\mathrm{supp}(\boldsymbol{t}(\boldsymbol{z})) = \mathrm{supp}(\boldsymbol{t}(\boldsymbol{z}^+)) = \mathrm{supp}(\boldsymbol{t}(\boldsymbol{z}^-))$. A move $\boldsymbol{z}$ is called *fundamental* if $\boldsymbol{z}'$ is a move such that $\mathrm{supp}(\boldsymbol{t}(\boldsymbol{z}')) \subset \mathrm{supp}(\boldsymbol{t}(\boldsymbol{z}))$ then $\boldsymbol{z}' = c\boldsymbol{z}$ for some integer c. In Ohsugi and Hibi (2003) the following two facts are proved. i) Fundamental moves are indispensable and circuits. ii) There is in general no implications between the notions of indispensability and circuits. Therefore it is of theoretical interest to investigate whether our indispensable moves are fundamental or circuits. We also define a *hidden zero cell* for a move $\boldsymbol{z}$ as

$$\{(i,j,k) \mid z_{ijk} = 0,\ z_{ij\cdot}^+ z_{i\cdot k}^+ z_{\cdot jk}^+ \neq 0\}.$$

Note that a non-fundamental move which has no hidden zero cell is also a non-circuit move by definition.

Now we list all indispensable moves for $3 \times 4 \times K$ and $4 \times 4 \times 4$ tables by their degrees. We found that most of the indispensable moves are at the same time fundamental moves and circuits. Therefore we only give a verbal description if an indispensable move is not fundamental or not a circuit in the list. We also give a more compact information of indispensable moves in the form:

$$((\text{SIZE}), (\text{DEGREE}), (\text{SLICE\_DEGREE}), (\text{PROPERTY}), (\text{HIDDEN\_ZERO}), (\text{CELLS})), \tag{3.9}$$

where PROPERTY means

- f: fundamental, F: not fundamental
- c: circuit, C: not circuit
- s: square free (i.e., consists only of $0, \pm 1$), S: not square free,

HIDDEN_ZERO means the multi-indices of hidden zero cells of $\boldsymbol{z}$ and CELLS means the multi-indices of $\boldsymbol{z}^+$ and $\boldsymbol{z}^-$. In the i-slices display of $\boldsymbol{z}$, we write (0) for a hidden zero cell. All these informations are available from the author's web page:

`http://www.stat.t.u-tokyo.ac.jp/~aoki/list-of-indispensable-moves.html.`

List of indispensable moves for $3 \times 4 \times K$ tables

- $2 \times 2 \times 2$ basic move of degree 4 with slice degree $\{2,2\} \times \{2,2\} \times \{2,2\}$
  $((2,2,2),(4),((2,2),(2,2),(2,2)),(fcs),\emptyset,((111,122,212,221),(112,121,211,222)))$

$$\begin{array}{|cc|}\hline +1 & -1 \\ -1 & +1 \\ \hline\end{array} \qquad \begin{array}{|cc|}\hline -1 & +1 \\ +1 & -1 \\ \hline\end{array}$$

- $2 \times 3 \times 3$ move of degree 6 with slice degree $\{3,3\} \times \{2,2,2\} \times \{2,2,2\}$
  $((2,3,3),(6),((3,3),(2,2,2),(2,2,2)),(fcs),\emptyset,((111,123,132,212,221,233),$
  $(112,121,133,211,223,232)))$

$$\begin{array}{|ccc|}\hline +1 & -1 & 0 \\ -1 & 0 & +1 \\ 0 & +1 & -1 \\ \hline\end{array} \qquad \begin{array}{|ccc|}\hline -1 & +1 & 0 \\ +1 & 0 & -1 \\ 0 & -1 & +1 \\ \hline\end{array}$$

- $2 \times 4 \times 4$ move of degree 8 with slice degree $\{4,4\} \times \{2,2,2,2\} \times \{2,2,2,2\}$
  $((2,4,4),(8),((4,4),(2,2,2,2),(2,2,2,2)),(fcs),\emptyset,((111,122,133,144,212,223,234,241),$
  $(112,123,134,141,211,222,233,244)))$

$$\begin{array}{|cccc|}\hline +1 & -1 & 0 & 0 \\ 0 & +1 & -1 & 0 \\ 0 & 0 & +1 & -1 \\ -1 & 0 & 0 & +1 \\ \hline\end{array} \qquad \begin{array}{|cccc|}\hline -1 & +1 & 0 & 0 \\ 0 & -1 & +1 & 0 \\ 0 & 0 & -1 & +1 \\ +1 & 0 & 0 & -1 \\ \hline\end{array}$$

- $3 \times 3 \times 4$ move of degree 8 with slice degree $\{2,3,3\} \times \{2,3,3\} \times \{2,2,2,2\}$
  $((3,3,4),(8),((2,3,3),(2,3,3),(2,2,2,2)),(fcs),\emptyset,((121,132,214,223,231,313,322,334),$ $(122,131,213,221,234,314,323,332)))$

$$\begin{array}{|cccc|}\hline 0 & 0 & 0 & 0 \\ +1 & -1 & 0 & 0 \\ -1 & +1 & 0 & 0 \\ \hline\end{array} \qquad \begin{array}{|cccc|}\hline 0 & 0 & -1 & +1 \\ -1 & 0 & +1 & 0 \\ +1 & 0 & 0 & -1 \\ \hline\end{array} \qquad \begin{array}{|cccc|}\hline 0 & 0 & +1 & -1 \\ 0 & +1 & -1 & 0 \\ 0 & -1 & 0 & +1 \\ \hline\end{array}$$

- $3 \times 4 \times 4$ move of degree 9 with slice degree $\{3,3,3\} \times \{2,2,2,3\} \times \{2,2,2,3\}$
  $((3,4,4),(9),((3,3,3),(2,2,2,3),(2,2,2,3)),(fcs),\emptyset,((111,124,142,214,233,241,322,$ $334,343),(114,122,141,211,234,243,324,333,342)))$

$$\begin{array}{|cccc|}\hline +1 & 0 & 0 & -1 \\ 0 & -1 & 0 & +1 \\ 0 & 0 & 0 & 0 \\ -1 & +1 & 0 & 0 \\ \hline\end{array} \qquad \begin{array}{|cccc|}\hline -1 & 0 & 0 & +1 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & +1 & -1 \\ +1 & 0 & -1 & 0 \\ \hline\end{array} \qquad \begin{array}{|cccc|}\hline 0 & 0 & 0 & 0 \\ 0 & +1 & 0 & -1 \\ 0 & 0 & -1 & +1 \\ 0 & -1 & +1 & 0 \\ \hline\end{array}$$

- $3 \times 3 \times 5$ move of degree 10 with slice degree $\{3,3,4\} \times \{3,3,4\} \times \{2,2,2,2,2\}$
  $((3,3,5),(10),((3,3,4),(3,3,4),(2,2,2,2,2)),(fcs),\emptyset,((113,125,131,212,223,234,311,$ $324,332,335),(111,123,135,213,224,232,312,325,331,334)))$

$$\begin{array}{|ccccc|}\hline -1 & 0 & +1 & 0 & 0 \\ 0 & 0 & -1 & 0 & +1 \\ +1 & 0 & 0 & 0 & -1 \\ \hline\end{array} \qquad \begin{array}{|ccccc|}\hline 0 & +1 & -1 & 0 & 0 \\ 0 & 0 & +1 & -1 & 0 \\ 0 & -1 & 0 & +1 & 0 \\ \hline\end{array} \qquad \begin{array}{|ccccc|}\hline +1 & -1 & 0 & 0 & 0 \\ 0 & 0 & 0 & +1 & -1 \\ -1 & +1 & 0 & -1 & +1 \\ \hline\end{array}$$

- $3 \times 4 \times 4$ move of degree 10 with slice degree $\{3,3,4\} \times \{2,2,3,3\} \times \{2,2,3,3\}$
  (not fundamental, circuit)
  $((3,4,4),(10),((3,3,4),(2,2,3,3),(2,2,3,3)),(Fcs),(333,344),((113,131,144,224,233,$ $242,314,323,332,341),(114,133,141,223,232,244,313,324,331,342)))$

$$\begin{array}{|cccc|}\hline 0 & 0 & +1 & -1 \\ 0 & 0 & 0 & 0 \\ +1 & 0 & -1 & 0 \\ -1 & 0 & 0 & +1 \\ \hline\end{array} \qquad \begin{array}{|cccc|}\hline 0 & 0 & 0 & 0 \\ 0 & 0 & -1 & +1 \\ 0 & -1 & +1 & 0 \\ 0 & +1 & 0 & -1 \\ \hline\end{array} \qquad \begin{array}{|cccc|}\hline 0 & 0 & -1 & +1 \\ 0 & 0 & +1 & -1 \\ -1 & +1 & (0) & 0 \\ +1 & -1 & 0 & (0) \\ \hline\end{array}$$

- $3 \times 4 \times 5$ move of degree 10 with slice degree $\{2,4,4\} \times \{2,2,3,3\} \times \{2,2,2,2,2\}$
  $((3,4,5),(10),((2,4,4),(2,2,3,3),(2,2,2,2,2)),(fcs),\emptyset,((131,142,213,225,234,241,$ $314,323,332,345),(132,141,214,223,231,245,313,325,334,342)))$

$$\begin{array}{|ccccc|}\hline 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \\ +1 & -1 & 0 & 0 & 0 \\ -1 & +1 & 0 & 0 & 0 \\ \hline\end{array} \qquad \begin{array}{|ccccc|}\hline 0 & 0 & +1 & -1 & 0 \\ 0 & 0 & -1 & 0 & +1 \\ -1 & 0 & 0 & +1 & 0 \\ +1 & 0 & 0 & 0 & -1 \\ \hline\end{array} \qquad \begin{array}{|ccccc|}\hline 0 & 0 & -1 & +1 & 0 \\ 0 & 0 & +1 & 0 & -1 \\ 0 & +1 & 0 & -1 & 0 \\ 0 & -1 & 0 & 0 & +1 \\ \hline\end{array}$$

- $3 \times 4 \times 5$ move of degree 10 with slice degree $\{3,3,4\} \times \{2,2,3,3\} \times \{2,2,2,2,2\}$
$((3,4,5),(10),((3,3,4),(2,2,3,3),(2,2,2,2,2)),(fcs),\emptyset,((111,133,142,224,235,243,$
$312,325,331,344),(112,131,143,225,233,244,311,324,335,342)))$

$$\begin{array}{|ccccc|}\hline +1 & -1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \\ -1 & 0 & +1 & 0 & 0 \\ 0 & +1 & -1 & 0 & 0 \\ \hline \end{array} \quad \begin{array}{|ccccc|}\hline 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & +1 & -1 \\ 0 & 0 & -1 & 0 & +1 \\ 0 & 0 & +1 & -1 & 0 \\ \hline \end{array} \quad \begin{array}{|ccccc|}\hline -1 & +1 & 0 & 0 & 0 \\ 0 & 0 & 0 & -1 & +1 \\ +1 & 0 & 0 & 0 & -1 \\ 0 & -1 & 0 & +1 & 0 \\ \hline \end{array}$$

- $3 \times 4 \times 5$ move of degree 12 with slice degree $\{4,4,4\} \times \{3,3,3,3\} \times \{2,2,2,2,4\}$
$((3,4,5),(12),((4,4,4),(3,3,3,3),(2,2,2,2,4)),(fcs),\emptyset,$
$((111,123,132,144,215,221,234,245,312,325,335,343),$
$(112,121,134,143,211,225,235,244,315,323,332,345)))$

$$\begin{array}{|ccccc|}\hline +1 & -1 & 0 & 0 & 0 \\ -1 & 0 & +1 & 0 & 0 \\ 0 & +1 & 0 & -1 & 0 \\ 0 & 0 & -1 & +1 & 0 \\ \hline \end{array} \quad \begin{array}{|ccccc|}\hline -1 & 0 & 0 & 0 & +1 \\ +1 & 0 & 0 & 0 & -1 \\ 0 & 0 & 0 & +1 & -1 \\ 0 & 0 & 0 & -1 & +1 \\ \hline \end{array} \quad \begin{array}{|ccccc|}\hline 0 & +1 & 0 & 0 & -1 \\ 0 & 0 & -1 & 0 & +1 \\ 0 & -1 & 0 & 0 & +1 \\ 0 & 0 & +1 & 0 & -1 \\ \hline \end{array}$$

- $3 \times 4 \times 6$ move of degree 12 with slice degree $\{3,4,5\} \times \{2,3,3,4\} \times \{2,2,2,2,2,2\}$
$((3,4,6),(12),((3,4,5),(2,3,3,4),(2,2,2,2,2,2)),(fcs),\emptyset,$
$((121,133,142,214,226,231,245,315,322,334,343,346),$
$(122,131,143,215,221,234,246,314,326,333,342,345)))$

$$\begin{array}{|cccccc|}\hline 0 & 0 & 0 & 0 & 0 & 0 \\ +1 & -1 & 0 & 0 & 0 & 0 \\ -1 & 0 & +1 & 0 & 0 & 0 \\ 0 & +1 & -1 & 0 & 0 & 0 \\ \hline \end{array} \quad \begin{array}{|cccccc|}\hline 0 & 0 & 0 & +1 & -1 & 0 \\ -1 & 0 & 0 & 0 & 0 & +1 \\ +1 & 0 & 0 & -1 & 0 & 0 \\ 0 & 0 & 0 & 0 & +1 & -1 \\ \hline \end{array} \quad \begin{array}{|cccccc|}\hline 0 & 0 & 0 & -1 & +1 & 0 \\ 0 & +1 & 0 & 0 & 0 & -1 \\ 0 & 0 & -1 & +1 & 0 & 0 \\ 0 & -1 & +1 & 0 & -1 & +1 \\ \hline \end{array}$$

- $3 \times 4 \times 6$ move of degree 12 with slice degree $\{4,4,4\} \times \{2,3,3,4\} \times \{2,2,2,2,2,2\}$
$((3,4,6),(12),((4,4,4),(2,3,3,4),(2,2,2,2,2,2)),(fcs),\emptyset,$
$((111,123,132,144,212,221,236,245,325,334,343,346),$
$(112,121,134,143,211,225,232,246,323,336,344,345)))$

$$\begin{array}{|cccccc|}\hline +1 & -1 & 0 & 0 & 0 & 0 \\ -1 & 0 & +1 & 0 & 0 & 0 \\ 0 & +1 & 0 & -1 & 0 & 0 \\ 0 & 0 & -1 & +1 & 0 & 0 \\ \hline \end{array} \quad \begin{array}{|cccccc|}\hline -1 & +1 & 0 & 0 & 0 & 0 \\ +1 & 0 & 0 & 0 & -1 & 0 \\ 0 & -1 & 0 & 0 & 0 & +1 \\ 0 & 0 & 0 & 0 & +1 & -1 \\ \hline \end{array} \quad \begin{array}{|cccccc|}\hline 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & -1 & 0 & +1 & 0 \\ 0 & 0 & 0 & +1 & 0 & -1 \\ 0 & 0 & +1 & -1 & -1 & +1 \\ \hline \end{array}$$

- $3 \times 4 \times 6$ move of degree 12 with slice degree $\{4,4,4\} \times \{3,3,3,3\} \times \{2,2,2,2,2,2\}$
$((3,4,6),(12),((4,4,4),(3,3,3,3),(2,2,2,2,2,2)),(fcs),\emptyset,$
$((111,123,132,144,215,221,234,246,312,326,335,343),$
$(112,121,134,143,211,226,235,244,315,323,332,336)))$

$$\begin{array}{|cccccc|}\hline +1 & -1 & 0 & 0 & 0 & 0 \\ -1 & 0 & +1 & 0 & 0 & 0 \\ 0 & +1 & 0 & -1 & 0 & 0 \\ 0 & 0 & -1 & +1 & 0 & 0 \\ \hline \end{array} \quad \begin{array}{|cccccc|}\hline -1 & 0 & 0 & 0 & +1 & 0 \\ +1 & 0 & 0 & 0 & 0 & -1 \\ 0 & 0 & 0 & +1 & -1 & 0 \\ 0 & 0 & 0 & -1 & 0 & +1 \\ \hline \end{array} \quad \begin{array}{|cccccc|}\hline 0 & +1 & 0 & 0 & -1 & 0 \\ 0 & 0 & -1 & 0 & 0 & +1 \\ 0 & -1 & 0 & 0 & +1 & 0 \\ 0 & 0 & +1 & 0 & 0 & -1 \\ \hline \end{array}$$

- $3 \times 4 \times 6$ move of degree 14 with slice degree $\{4,4,6\} \times \{3,3,4,4\} \times \{2,2,2,2,2,4\}$
  $((3,4,6),(14),((4,4,6),(3,3,4,4),(2,2,2,2,2,4)),(fcS),\emptyset,$
  $((111,122,133,146,212,225,234,246,314,323,336,336,341,345),$
  $(112,123,136,141,214,222,236,245,311,325,333,334,346,346)))$

$$\begin{array}{|cccccc|}\hline +1 & -1 & 0 & 0 & 0 & 0 \\ 0 & +1 & -1 & 0 & 0 & 0 \\ 0 & 0 & +1 & 0 & 0 & -1 \\ -1 & 0 & 0 & 0 & 0 & +1 \\ \hline \end{array} \quad \begin{array}{|cccccc|}\hline 0 & +1 & 0 & -1 & 0 & 0 \\ 0 & -1 & 0 & 0 & +1 & 0 \\ 0 & 0 & 0 & +1 & 0 & -1 \\ 0 & 0 & 0 & 0 & -1 & +1 \\ \hline \end{array} \quad \begin{array}{|cccccc|}\hline -1 & 0 & 0 & +1 & 0 & 0 \\ 0 & 0 & +1 & 0 & -1 & 0 \\ 0 & 0 & -1 & -1 & 0 & +2 \\ +1 & 0 & 0 & 0 & +1 & -2 \\ \hline \end{array}$$

- $3 \times 4 \times 6$ move of degree 14 with slice degree $\{4,5,5\} \times \{3,3,3,5\} \times \{2,2,2,2,2,4\}$
  $((3,4,6),(14),((4,5,5),(3,3,3,5),(2,2,2,2,2,4)),(fcS),\emptyset,$
  $((111,122,133,144,216,223,236,241,245,312,325,334,346,346),$
  $(112,123,134,141,211,225,233,246,246,316,322,336,344,345)))$

$$\begin{array}{|cccccc|}\hline +1 & -1 & 0 & 0 & 0 & 0 \\ 0 & +1 & -1 & 0 & 0 & 0 \\ 0 & 0 & +1 & -1 & 0 & 0 \\ -1 & 0 & 0 & +1 & 0 & 0 \\ \hline \end{array} \quad \begin{array}{|cccccc|}\hline -1 & 0 & 0 & 0 & 0 & +1 \\ 0 & 0 & +1 & 0 & -1 & 0 \\ 0 & 0 & -1 & 0 & 0 & +1 \\ +1 & 0 & 0 & 0 & +1 & -2 \\ \hline \end{array} \quad \begin{array}{|cccccc|}\hline 0 & +1 & 0 & 0 & 0 & -1 \\ 0 & -1 & 0 & 0 & +1 & 0 \\ 0 & 0 & 0 & +1 & 0 & -1 \\ 0 & 0 & 0 & -1 & -1 & +2 \\ \hline \end{array}$$

- $3 \times 4 \times 7$ move(1) of degree 14 with slice degree $\{4,4,6\} \times \{3,3,4,4\} \times \{2,2,2,2,2,2,2\}$
  $((3,4,7),(14),((4,4,6),(3,3,4,4),(2,2,2,2,2,2,2)),(fcs),\emptyset,$
  $((111,123,132,144,215,221,237,246,312,327,334,336,343,345),$
  $(112,121,134,143,211,227,236,245,315,323,332,337,344,346)))$

$$\begin{array}{|ccccccc|}\hline +1 & -1 & 0 & 0 & 0 & 0 & 0 \\ -1 & 0 & +1 & 0 & 0 & 0 & 0 \\ 0 & +1 & 0 & -1 & 0 & 0 & 0 \\ 0 & 0 & -1 & +1 & 0 & 0 & 0 \\ \hline \end{array} \quad \begin{array}{|ccccccc|}\hline -1 & 0 & 0 & 0 & +1 & 0 & 0 \\ +1 & 0 & 0 & 0 & 0 & 0 & -1 \\ 0 & 0 & 0 & 0 & 0 & -1 & +1 \\ 0 & 0 & 0 & 0 & -1 & +1 & 0 \\ \hline \end{array} \quad \begin{array}{|ccccccc|}\hline 0 & +1 & 0 & 0 & -1 & 0 & 0 \\ 0 & 0 & -1 & 0 & 0 & 0 & +1 \\ 0 & -1 & 0 & +1 & 0 & +1 & -1 \\ 0 & 0 & +1 & -1 & +1 & -1 & 0 \\ \hline \end{array}$$

- $3 \times 4 \times 7$ move(2) of degree 14 with slice degree $\{4,4,6\} \times \{3,3,4,4\} \times \{2,2,2,2,2,2,2\}$
  $((3,4,7),(14),((4,4,6),(3,3,4,4),(2,2,2,2,2,2,2)),(fcs),\emptyset,$
  $((111,123,132,144,215,221,236,247,312,327,334,335,343,346),$
  $(112,121,134,143,211,227,235,246,315,323,332,336,344,347)))$

$$\begin{array}{|ccccccc|}\hline +1 & -1 & 0 & 0 & 0 & 0 & 0 \\ -1 & 0 & +1 & 0 & 0 & 0 & 0 \\ 0 & +1 & 0 & -1 & 0 & 0 & 0 \\ 0 & 0 & -1 & +1 & 0 & 0 & 0 \\ \hline \end{array} \quad \begin{array}{|ccccccc|}\hline -1 & 0 & 0 & 0 & +1 & 0 & 0 \\ +1 & 0 & 0 & 0 & 0 & 0 & -1 \\ 0 & 0 & 0 & 0 & -1 & +1 & 0 \\ 0 & 0 & 0 & 0 & 0 & -1 & +1 \\ \hline \end{array} \quad \begin{array}{|ccccccc|}\hline 0 & +1 & 0 & 0 & -1 & 0 & 0 \\ 0 & 0 & -1 & 0 & 0 & 0 & +1 \\ 0 & -1 & 0 & +1 & +1 & -1 & 0 \\ 0 & 0 & +1 & -1 & 0 & +1 & -1 \\ \hline \end{array}$$

- $3 \times 4 \times 7$ move of degree 14 with slice degree $\{4,5,5\} \times \{3,3,3,5\} \times \{2,2,2,2,2,2,2\}$
  $((3,4,7),(14),((4,5,5),(3,3,3,5),(2,2,2,2,2,2,2)),(fcs),\emptyset,$
  $((111,122,133,144,215,226,232,241,247,313,324,337,345,346),$
  $(113,124,132,141,211,222,237,245,246,315,326,333,344,347)))$

$$\begin{array}{|ccccccc|}\hline +1 & 0 & -1 & 0 & 0 & 0 & 0 \\ 0 & +1 & 0 & -1 & 0 & 0 & 0 \\ 0 & -1 & +1 & 0 & 0 & 0 & 0 \\ -1 & 0 & 0 & +1 & 0 & 0 & 0 \\ \hline \end{array} \quad \begin{array}{|ccccccc|}\hline -1 & 0 & 0 & 0 & +1 & 0 & 0 \\ 0 & -1 & 0 & 0 & 0 & +1 & 0 \\ 0 & +1 & 0 & 0 & 0 & 0 & -1 \\ +1 & 0 & 0 & 0 & -1 & -1 & +1 \\ \hline \end{array} \quad \begin{array}{|ccccccc|}\hline 0 & 0 & +1 & 0 & -1 & 0 & 0 \\ 0 & 0 & 0 & +1 & 0 & -1 & 0 \\ 0 & 0 & -1 & 0 & 0 & 0 & +1 \\ 0 & 0 & 0 & -1 & +1 & +1 & -1 \\ \hline \end{array}$$

- $3 \times 4 \times 7$ move of degree 14 with slice degree $\{4,5,5\} \times \{3,3,4,4\} \times \{2,2,2,2,2,2,2\}$
  $((3,4,7),(14),((4,5,5),(3,3,4,4),(2,2,2,2,2,2,2)),(fcs),\emptyset,$
  $((111,122,133,144,215,224,237,241,246,313,326,332,335,347),$
  $(113,124,132,141,211,226,235,244,247,315,322,333,337,346)))$

$$\begin{array}{|ccccccc|}\hline +1 & 0 & -1 & 0 & 0 & 0 & 0 \\ 0 & +1 & 0 & -1 & 0 & 0 & 0 \\ 0 & -1 & +1 & 0 & 0 & 0 & 0 \\ -1 & 0 & 0 & +1 & 0 & 0 & 0 \\ \hline \end{array} \quad \begin{array}{|ccccccc|}\hline -1 & 0 & 0 & 0 & +1 & 0 & 0 \\ 0 & 0 & 0 & +1 & 0 & -1 & 0 \\ 0 & 0 & 0 & 0 & -1 & 0 & +1 \\ +1 & 0 & 0 & -1 & 0 & +1 & -1 \\ \hline \end{array} \quad \begin{array}{|ccccccc|}\hline 0 & 0 & +1 & 0 & -1 & 0 & 0 \\ 0 & -1 & 0 & 0 & 0 & +1 & 0 \\ 0 & +1 & -1 & 0 & +1 & 0 & -1 \\ 0 & 0 & 0 & 0 & 0 & -1 & +1 \\ \hline \end{array}$$

- $3 \times 4 \times 7$ move of degree 16 with slice degree $\{4,6,6\} \times \{3,3,5,5\} \times \{2,2,2,2,2,2,4\}$
  $((3,4,7),(16),((4,6,6),(3,3,5,5),(2,2,2,2,2,2,4)),(fcS),\emptyset,$
  $((111,123,132,144,215,221,234,236,247,247,312,326,337,337,343,345),$
  $(112,121,134,143,211,226,237,237,244,245,315,323,332,336,347,347)))$

$$\begin{array}{|ccccccc|}\hline +1 & -1 & 0 & 0 & 0 & 0 & 0 \\ -1 & 0 & +1 & 0 & 0 & 0 & 0 \\ 0 & +1 & 0 & -1 & 0 & 0 & 0 \\ 0 & 0 & -1 & +1 & 0 & 0 & 0 \\ \hline \end{array} \quad \begin{array}{|ccccccc|}\hline -1 & 0 & 0 & 0 & +1 & 0 & 0 \\ +1 & 0 & 0 & 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & +1 & 0 & +1 & -2 \\ 0 & 0 & 0 & -1 & -1 & 0 & +2 \\ \hline \end{array} \quad \begin{array}{|ccccccc|}\hline 0 & +1 & 0 & 0 & -1 & 0 & 0 \\ 0 & 0 & -1 & 0 & 0 & +1 & 0 \\ 0 & -1 & 0 & 0 & 0 & -1 & +2 \\ 0 & 0 & +1 & 0 & +1 & 0 & -2 \\ \hline \end{array}$$

- $3 \times 4 \times 8$ move of degree 16 with slice degree $\{4,6,6\} \times \{3,3,5,5\} \times \{2,2,2,2,2,2,2,2\}$
  (not fundamental, not circuit)
  $((3,4,8),(16),((4,6,6),(3,3,5,5),(2,2,2,2,2,2,2,2)),(FCs),\emptyset,$
  $((111,123,132,144,218,221,234,237,245,246,312,327,335,336,343,348),$
  $(112,121,134,143,211,227,235,236,244,248,318,323,332,337,345,346)))$

$$\begin{array}{|cccccccc|}\hline +1 & -1 & 0 & 0 & 0 & 0 & 0 & 0 \\ -1 & 0 & +1 & 0 & 0 & 0 & 0 & 0 \\ 0 & +1 & 0 & -1 & 0 & 0 & 0 & 0 \\ 0 & 0 & -1 & +1 & 0 & 0 & 0 & 0 \\ \hline \end{array} \quad \begin{array}{|cccccccc|}\hline -1 & 0 & 0 & 0 & 0 & 0 & 0 & +1 \\ +1 & 0 & 0 & 0 & 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & +1 & -1 & -1 & +1 & 0 \\ 0 & 0 & 0 & -1 & +1 & +1 & 0 & -1 \\ \hline \end{array} \quad \begin{array}{|cccccccc|}\hline 0 & +1 & 0 & 0 & 0 & 0 & 0 & -1 \\ 0 & 0 & -1 & 0 & 0 & 0 & +1 & 0 \\ 0 & -1 & 0 & 0 & +1 & +1 & -1 & 0 \\ 0 & 0 & +1 & 0 & -1 & -1 & 0 & +1 \\ \hline \end{array}$$

List of indispensable moves for $4 \times 4 \times 4$ tables

- $4 \times 4 \times 4$ move(1) of degree 10 with slice degree $\{2,2,3,3\} \times \{2,2,3,3\} \times \{2,2,3,3\}$
  $((4,4,4),(10),((2,2,3,3),(2,2,3,3),(2,2,3,3)),(fcs),\emptyset,((113,124,231,242,314,333,341,$
  $423,432,444),(114,123,232,241,313,331,344,424,433,442)))$

$$\begin{array}{|cccc|}\hline 0 & 0 & +1 & -1 \\ 0 & 0 & -1 & +1 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ \hline \end{array} \quad \begin{array}{|cccc|}\hline 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ +1 & -1 & 0 & 0 \\ -1 & +1 & 0 & 0 \\ \hline \end{array} \quad \begin{array}{|cccc|}\hline 0 & 0 & -1 & +1 \\ 0 & 0 & 0 & 0 \\ -1 & 0 & +1 & 0 \\ +1 & 0 & 0 & -1 \\ \hline \end{array} \quad \begin{array}{|cccc|}\hline 0 & 0 & 0 & 0 \\ 0 & 0 & +1 & -1 \\ 0 & +1 & -1 & 0 \\ 0 & -1 & 0 & +1 \\ \hline \end{array}$$

- $4 \times 4 \times 4$ move(2) of degree 10 with slice degree $\{2,2,3,3\} \times \{2,2,3,3\} \times \{2,2,3,3\}$
  $((4,4,4),(10),((2,2,3,3),(2,2,3,3),(2,2,3,3)),(fcs),\emptyset,((114,133,231,243,313,324,342,$
  $422,434,441),(113,134,233,241,314,322,343,424,431,442)))$

$$\begin{array}{|cccc|}\hline 0 & 0 & -1 & +1 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & +1 & -1 \\ 0 & 0 & 0 & 0 \\ \hline \end{array} \quad \begin{array}{|cccc|}\hline 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ +1 & 0 & -1 & 0 \\ -1 & 0 & +1 & 0 \\ \hline \end{array} \quad \begin{array}{|cccc|}\hline 0 & 0 & +1 & -1 \\ 0 & -1 & 0 & +1 \\ 0 & 0 & 0 & 0 \\ 0 & +1 & -1 & 0 \\ \hline \end{array} \quad \begin{array}{|cccc|}\hline 0 & 0 & 0 & 0 \\ 0 & +1 & 0 & -1 \\ -1 & 0 & 0 & +1 \\ +1 & -1 & 0 & 0 \\ \hline \end{array}$$

- $4 \times 4 \times 4$ move of degree 12 with slice degree $\{2,2,4,4\} \times \{2,2,4,4\} \times \{3,3,3,3\}$
  $((4,4,4),(12),((2,2,4,4),(2,2,4,4),(3,3,3,3)),(fcs),\emptyset,$
  $((131,142,234,243,311,324,332,333,413,422,441,444),$
  $(132,141,233,244,313,322,331,334,411,424,442,443)))$

$$\begin{array}{|cccc|}\hline 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ +1 & -1 & 0 & 0 \\ -1 & +1 & 0 & 0 \\ \hline\end{array} \quad \begin{array}{|cccc|}\hline 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & -1 & +1 \\ 0 & 0 & +1 & -1 \\ \hline\end{array} \quad \begin{array}{|cccc|}\hline +1 & 0 & -1 & 0 \\ 0 & -1 & 0 & +1 \\ -1 & +1 & +1 & -1 \\ 0 & 0 & 0 & 0 \\ \hline\end{array} \quad \begin{array}{|cccc|}\hline -1 & 0 & +1 & 0 \\ 0 & +1 & 0 & -1 \\ 0 & 0 & 0 & 0 \\ +1 & -1 & -1 & +1 \\ \hline\end{array}$$

- $4 \times 4 \times 4$ move of degree 12 with slice degree $\{2,3,3,4\} \times \{2,3,3,4\} \times \{3,3,3,3\}$
  (not fundamental, circuit)
  $((4,4,4),(12),((2,3,3,4),(2,3,3,4),(3,3,3,3)),(Fcs),(242,421),$
  $((134,142,221,232,243,311,324,333,413,422,441,444),$
  $(132,144,222,233,241,313,321,334,411,424,442,443)))$

$$\begin{array}{|cccc|}\hline 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & -1 & 0 & +1 \\ 0 & +1 & 0 & -1 \\ \hline\end{array} \quad \begin{array}{|cccc|}\hline 0 & 0 & 0 & 0 \\ +1 & -1 & 0 & 0 \\ 0 & +1 & -1 & 0 \\ -1 & (0) & +1 & 0 \\ \hline\end{array} \quad \begin{array}{|cccc|}\hline +1 & 0 & -1 & 0 \\ -1 & 0 & 0 & +1 \\ 0 & 0 & +1 & -1 \\ 0 & 0 & 0 & 0 \\ \hline\end{array} \quad \begin{array}{|cccc|}\hline -1 & 0 & +1 & 0 \\ (0) & +1 & 0 & -1 \\ 0 & 0 & 0 & 0 \\ +1 & -1 & -1 & +1 \\ \hline\end{array}$$

- $4 \times 4 \times 4$ move(1) of degree 12 with slice degree $\{3,3,3,3\} \times \{3,3,3,3\} \times \{3,3,3,3\}$
  (not fundamental, circuit)
  $((4,4,4),(12),((3,3,3,3),(3,3,3,3),(3,3,3,3)),(Fcs),(122,244,311,433),$
  $((111,123,132,214,233,241,312,321,344,422,434,443),$
  $(112,121,133,211,234,243,314,322,341,423,432,444)))$

$$\begin{array}{|cccc|}\hline +1 & -1 & 0 & 0 \\ -1 & (0) & +1 & 0 \\ 0 & +1 & -1 & 0 \\ 0 & 0 & 0 & 0 \\ \hline\end{array} \quad \begin{array}{|cccc|}\hline -1 & 0 & 0 & +1 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & +1 & -1 \\ +1 & 0 & -1 & (0) \\ \hline\end{array} \quad \begin{array}{|cccc|}\hline (0) & +1 & 0 & -1 \\ +1 & -1 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ -1 & 0 & 0 & +1 \\ \hline\end{array} \quad \begin{array}{|cccc|}\hline 0 & 0 & 0 & 0 \\ 0 & +1 & -1 & 0 \\ 0 & -1 & (0) & +1 \\ 0 & 0 & +1 & -1 \\ \hline\end{array}$$

- $4 \times 4 \times 4$ move(2) of degree 12 with slice degree $\{3,3,3,3\} \times \{3,3,3,3\} \times \{3,3,3,3\}$
  $((4,4,4),(12),((3,3,3,3),(3,3,3,3),(3,3,3,3)),(fcs),\emptyset,$
  $((111,123,132,214,233,241,312,324,343,421,434,442),$
  $(112,121,133,211,234,243,314,323,342,424,432,441)))$

$$\begin{array}{|cccc|}\hline +1 & -1 & 0 & 0 \\ -1 & 0 & +1 & 0 \\ 0 & +1 & -1 & 0 \\ 0 & 0 & 0 & 0 \\ \hline\end{array} \quad \begin{array}{|cccc|}\hline -1 & 0 & 0 & +1 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & +1 & -1 \\ +1 & 0 & -1 & 0 \\ \hline\end{array} \quad \begin{array}{|cccc|}\hline 0 & +1 & 0 & -1 \\ 0 & 0 & -1 & +1 \\ 0 & 0 & 0 & 0 \\ 0 & -1 & +1 & 0 \\ \hline\end{array} \quad \begin{array}{|cccc|}\hline 0 & 0 & 0 & 0 \\ +1 & 0 & 0 & -1 \\ 0 & -1 & 0 & +1 \\ -1 & +1 & 0 & 0 \\ \hline\end{array}$$

- $4 \times 4 \times 4$ move(1) of degree 14 with slice degree $\{3,3,3,5\} \times \{3,3,3,5\} \times \{3,3,4,4\}$ (not fundamental, circuit)
$((4,4,4),(14),((3,3,3,5),(3,3,3,5),(3,3,4,4)),(FcS),(113,234,442),$
$((111,123,142,221,232,244,313,331,344,412,424,434,443,443),$
$(112,121,143,224,231,242,311,334,343,413,423,432,444,444)))$

$$\begin{array}{|cccc|}\hline +1 & -1 & (0) & 0 \\ -1 & 0 & +1 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & +1 & -1 & 0 \\ \hline\end{array}\quad \begin{array}{|cccc|}\hline 0 & 0 & 0 & 0 \\ +1 & 0 & 0 & -1 \\ -1 & +1 & 0 & (0) \\ 0 & -1 & 0 & +1 \\ \hline\end{array}\quad \begin{array}{|cccc|}\hline -1 & 0 & +1 & 0 \\ 0 & 0 & 0 & 0 \\ +1 & 0 & 0 & -1 \\ 0 & 0 & -1 & +1 \\ \hline\end{array}\quad \begin{array}{|cccc|}\hline 0 & +1 & -1 & 0 \\ 0 & 0 & -1 & +1 \\ 0 & -1 & 0 & +1 \\ 0 & (0) & +2 & -2 \\ \hline\end{array}$$

- $4 \times 4 \times 4$ move(2) of degree 14 with slice degree $\{3,3,3,5\} \times \{3,3,3,5\} \times \{3,3,4,4\}$ (not fundamental, circuit)
$((4,4,4),(14),((3,3,3,5),(3,3,3,5),(3,3,4,4)),(FcS),(342,421),$
$((111,123,142,221,232,244,312,333,344,414,424,431,443,443),$
$(112,121,143,224,231,242,314,332,343,411,423,433,444,444)))$

$$\begin{array}{|cccc|}\hline +1 & -1 & 0 & 0 \\ -1 & 0 & +1 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & +1 & -1 & 0 \\ \hline\end{array}\quad \begin{array}{|cccc|}\hline 0 & 0 & 0 & 0 \\ +1 & 0 & 0 & -1 \\ -1 & +1 & 0 & 0 \\ 0 & -1 & 0 & +1 \\ \hline\end{array}\quad \begin{array}{|cccc|}\hline 0 & +1 & 0 & -1 \\ 0 & 0 & 0 & 0 \\ 0 & -1 & +1 & 0 \\ 0 & (0) & -1 & +1 \\ \hline\end{array}\quad \begin{array}{|cccc|}\hline -1 & 0 & 0 & +1 \\ (0) & 0 & -1 & +1 \\ +1 & 0 & -1 & 0 \\ 0 & 0 & +2 & -2 \\ \hline\end{array}$$

3.3.2 Sufficient condition for type-2 combination of indispensable moves which preserves the indispensability

As is stated, it is important to find the indispensable moves especially when the unique minimal Markov basis exists. However, our approach seems to be difficult to generalize to larger tables. Then, how can we find indispensable moves of larger sizes, i.e., $3 \times 5 \times 5, 4 \times 4 \times 5$ and so on? In Section 3.3.2 and Section 3.3.3, we give some basic features of indispensable moves, which we can make use of for finding larger indispensable moves.

As the first basic feature of the indispensable moves, in Section 3.3.2 we consider indispensable moves having the structure that they are separated to two indispensable moves. Important findings are obtained by comparing $2 \times 3 \times 3$ indispensable move of degree 6 with slice degree $\{3,3\} \times \{2,2,2\} \times \{2,2,2\}$,

$$\begin{array}{|ccc|}\hline +1 & -1 & 0 \\ -1 & 0 & +1 \\ 0 & +1 & -1 \\ \hline\end{array}\quad \begin{array}{|ccc|}\hline -1 & +1 & 0 \\ +1 & 0 & -1 \\ 0 & -1 & +1 \\ \hline\end{array}$$

and the following $3 \times 3 \times 3$ move of degree 7 with slice degree $\{2,2,3\} \times \{2,2,3\} \times \{2,2,3\}$,

$$\begin{array}{|ccc|}\hline +1 & -1 & 0 \\ -1 & +1 & 0 \\ 0 & 0 & 0 \\ \hline\end{array}\quad \begin{array}{|ccc|}\hline -1 & +1 & 0 \\ +1 & 0 & -1 \\ 0 & -1 & +1 \\ \hline\end{array}\quad \begin{array}{|ccc|}\hline 0 & 0 & 0 \\ 0 & -1 & +1 \\ 0 & +1 & -1 \\ \hline\end{array}.$$

These two moves have the common structure that they are represented as a combination of two basic moves. The difference between these two moves lies in the number of overlapping cells, i.e., the move of degree 6 is made from two basic moves that overlap at two non-zero entries, while the move of degree 7 is made from two basic moves that overlap at one non-zero entry. In Section 3.2.1, we called the former combination as a *type-2 combination* and the latter combination as a *type-1 combination*. In Section 3.2.1, it is shown that the move of degree 7 is dispensable because two basic moves can be applied one by one in an appropriate order without causing negative entries on the way instead of applying the move of degree 7. On the other hand, because the type-2 combination has two overlapped cells, one of these cells necessarily becomes negative in adding two basic moves one by one. For this reason, the type-2 combination is essential. In fact, all indispensable moves of the $3 \times 3 \times K$ case are made by the type-2 combinations of some basic moves (see Section 3.2.1).

From these considerations, we are interested in a relationship between the type-2 combination and the indispensability. We give a sufficient condition for type-2 combination of indispensable moves which preserves the indispensability in Theorem 3.3.1 below. Note that this is only a *sufficient condition* for obtaining an indispensable move from combining some smaller indispensable moves. We discuss this point in Section 3.3.4.

Before stating the theorem, we consider some additional constraints to the type-2 combination and consider a simple situation. Let $\boldsymbol{z}$ and $\boldsymbol{z}'$ be moves satisfying $R(\boldsymbol{z}), R(\boldsymbol{z}') \subset [I] \times [J] \times [K]$. We assume that $R(\boldsymbol{z}) \cap R(\boldsymbol{z}') (\neq \emptyset)$ is included in a one-dimensional line. Without loss of generality, we write $R(\boldsymbol{z}) \cap R(\boldsymbol{z}') \subset \{(i_0, j_0, k) \mid k \in [K]\}$. The two nonzero elements of $\boldsymbol{z}$ or $\boldsymbol{z}'$ where they overlap and cancel signs are on this line. We write the $i = i_0, j = j_0$-line of $\boldsymbol{z}, \boldsymbol{z}'$ as

$$z_{i_0 j_0 k} = \begin{cases} +1, & \text{if } k = k_2 \\ -1, & \text{if } k = k_1 \\ 0, & \text{otherwise,} \end{cases} \qquad z'_{i_0 j_0 k} = \begin{cases} +1, & \text{if } k = k_1 \\ -1, & \text{if } k = k_2 \\ 0, & \text{otherwise,} \end{cases}$$

without loss of generality. It should be noted that the following five lines

$$\begin{array}{ll} \{(i_0, j_0, k) \mid k \in [K]\}, & \\ \{(i, j_0, k_1) \mid i \in [I]\}, & \{(i, j_0, k_2) \mid i \in [I]\}, \\ \{(i_0, j, k_1) \mid j \in [J]\}, & \{(i_0, j, k_2) \mid j \in [J]\} \end{array} \tag{3.10}$$

intersect both $R(\boldsymbol{z})$ and $R(\boldsymbol{z}')$. We assume that there does not exist one-dimensional line other than the above five lines that intersect both $R(\boldsymbol{z})$ and $R(\boldsymbol{z}')$. In addition, we assume that the (i_0, k_1)-,(i_0, k_2)-,(j_0, k_1)-,(j_0, k_2)-marginals of $\boldsymbol{z}^+, \boldsymbol{z}^-, \boldsymbol{z}'^+, \boldsymbol{z}'^-$ are all one, i.e.,

$$\begin{aligned} 1 &= z^+_{i_0 \cdot k_1} = z^-_{i_0 \cdot k_1} = z'^+_{i_0 \cdot k_1} = z'^-_{i_0 \cdot k_1} = z^+_{i_0 \cdot k_2} = z^-_{i_0 \cdot k_2} = z'^+_{i_0 \cdot k_2} = z'^-_{i_0 \cdot k_2} \\ &= z^+_{\cdot j_0 k_1} = z^-_{\cdot j_0 k_1} = z'^+_{\cdot j_0 k_1} = z'^-_{\cdot j_0 k_1} = z^+_{\cdot j_0 k_2} = z^-_{\cdot j_0 k_2} = z'^+_{\cdot j_0 k_2} = z'^-_{\cdot j_0 k_2}. \end{aligned}$$

Now we present a theorem.

Theorem 3.3.1 *Let $\boldsymbol{z}$ and $\boldsymbol{z}'$ be indispensable moves satisfying the above conditions then $\boldsymbol{z}^* = \boldsymbol{z} + \boldsymbol{z}'$ is an indispensable move with its positive part*

$$\boldsymbol{z}^{*+} = \boldsymbol{z}^+ + \boldsymbol{z}'^+ - (\boldsymbol{\delta}_{i_0 j_0 k_1} + \boldsymbol{\delta}_{i_0 j_0 k_2})$$

and its negative part

$$\boldsymbol{z}^{*-} = \boldsymbol{z}^- + \boldsymbol{z}'^- - (\boldsymbol{\delta}_{i_0 j_0 k_1} + \boldsymbol{\delta}_{i_0 j_0 k_2}),$$

where $\boldsymbol{\delta}_{ijk}$ is a table with the element $+1$ only at the cell (i, j, k), and 0 otherwise.

For example, let $\boldsymbol{z}$ be a $2 \times 3 \times 3$ indispensable move of degree 6 with slice degree $\{3,3\} \times \{2,2,2\} \times \{2,2,2\}$ and $\boldsymbol{z}'$ be a $3 \times 3 \times 4$ indispensable move of degree 8 with slice degree $\{2,3,3\} \times \{2,3,3\} \times \{2,2,2,2\}$. Then the following $4 \times 5 \times 5$ move is made by the type-2 combination of $\boldsymbol{z}$ and $\boldsymbol{z}'$ satisfying the conditions and is an indispensable move. In this case, $R(\boldsymbol{z}) \cap R(\boldsymbol{z}') \subset \{(2,3,k) \mid k \in [K]\}$ and $k_1 = 2, k_2 = 3$.

+1	−1	0	0	0
−1	0	+1	0	0
0	+1	−1	0	0
0	0	0	0	0
0	0	0	0	0

−1	+1	0	0	0
+1	0	−1	0	0
0	0	0	0	0
0	−1	+1	0	0
0	0	0	0	0

0	0	0	0	0
0	0	0	0	0
0	−1	0	+1	0
0	+1	0	0	−1
0	0	0	−1	+1

0	0	0	0	0
0	0	0	0	0
0	0	+1	−1	0
0	0	−1	0	+1
0	0	0	+1	−1

Proof It is seen that $\boldsymbol{z}^{*+}$ and $\boldsymbol{z}^{*-}$ have the same marginal totals by definition. We write the reference set of the tables that have the same marginal totals to $\boldsymbol{z}^{*+}$ and $\boldsymbol{z}^{*-}$ as $\mathcal{F}^*$. We want to show that $\mathcal{F}^*$ is a two-element set, i.e., if $\boldsymbol{x} \in \mathcal{F}^*$ then $\boldsymbol{x} = \boldsymbol{z}^{*+}$ or $\boldsymbol{x} = \boldsymbol{z}^{*-}$. We consider the cells in the support of $\boldsymbol{x}$. Let $(i,j,k) \in \mathrm{supp}(\boldsymbol{x})$.

First we consider the case that $(i,j,k) \notin R(\boldsymbol{z}) \cup R(\boldsymbol{z}')$. In this case, (i,j,k) lies on at least one two-dimensional slice which is zero slice in $\boldsymbol{z}$ since $(i,j,k) \notin R(\boldsymbol{z})$. Similarly, (i,j,k) also lies on at least one two-dimensional slice which is zero slice in $\boldsymbol{z}'$ since $(i,j,k) \notin R(\boldsymbol{z}')$. These two slices have at least one line in common, and corresponding line sum of $\boldsymbol{x}$ must be zero, which contradicts that $(i,j,k) \in \mathrm{supp}(\boldsymbol{x})$. Next we consider the case that $(i,j,k) \in R(\boldsymbol{z}) \cap R(\boldsymbol{z}')$. In this case, (i,j,k) is in the line $\{(i_0,j_0,k) \mid k \in [K]\}$ by definition. However, $x_{i_0 j_0 \cdot}$ must be zero by definition and therefore this case is also contradiction. From these considerations, it is seen that each cell in the support of $\boldsymbol{x}$ belongs to exactly one of $R(\boldsymbol{z})$ or $R(\boldsymbol{z}')$. We write $\boldsymbol{x} = \boldsymbol{y} + \boldsymbol{y}'$ where

$$y_{ijk} = \begin{cases} x_{ijk}, & \text{if } (i,j,k) \in R(\boldsymbol{z}), \\ 0, & \text{otherwise,} \end{cases}$$

$$y'_{ijk} = \begin{cases} x_{ijk}, & \text{if } (i,j,k) \in R(\boldsymbol{z}'), \\ 0, & \text{otherwise.} \end{cases}$$

Let $n = \sum_{i,j,k} y_{ijk}$ and $n' = \sum_{i,j,k} y'_{ijk}$.

Here we consider the marginal totals of $\boldsymbol{y}$. By definition, only the five line sums described as (3.10) can differ between $\boldsymbol{y}$ and $\boldsymbol{z}^+, \boldsymbol{z}^-$. First we consider the line sums along the k-axis. It follows that

$$\begin{aligned} & y_{ij\cdot} = z^+_{ij\cdot} = z^-_{ij\cdot}, \quad \text{for } (i,j) \neq (i_0,j_0), \\ & y_{i_0 j_0 \cdot} = 0, \\ & z^+_{i_0 j_0 \cdot} = z^-_{i_0 j_0 \cdot} = 1. \end{aligned}$$

Therefore $n = \sum_{i,j} y_{ij\cdot} = \deg(\boldsymbol{z}) - 1$. Similarly $n' = \sum_{i,j} y'_{ij\cdot} = \deg(\boldsymbol{z}') - 1$ holds. Next we consider the line sums along the j-axis. It follows that

$$y_{i\cdot k} = z^+_{i\cdot k} = z^-_{i\cdot k}, \quad \text{for } (i,k) \neq (i_0,k_1), (i_0,k_2).$$

Since

$$\begin{aligned} z^+_{i_0\cdot k_1} = z^-_{i_0\cdot k_1} = z^+_{i_0\cdot k_2} = z^-_{i_0\cdot k_2} = 1, \\ z^{*+}_{i_0\cdot k_1} = z^{*-}_{i_0\cdot k_1} = z^{*+}_{i_0\cdot k_2} = z^{*-}_{i_0\cdot k_2} = 1 \end{aligned}$$

and $n+1 = \deg(\boldsymbol{z})$, it follows that

$$(y_{i_0 \cdot k_1}, y_{i_0 \cdot k_2}) = (1,0) \text{ or } (0,1).$$

Similarly, by considering the line sums along the i-axis, it follows that

$$(y_{\cdot j_0 k_1}, y_{\cdot j_0 k_2}) = (1,0) \text{ or } (0,1).$$

Moreover, since

$$\begin{aligned} z^+_{\cdot\cdot k_1} &= \sum_i z^+_{i\cdot k_1} = \sum_{i \neq i_0} z^+_{i\cdot k_1} + z^+_{i_0 \cdot k_1} = \sum_{i \neq i_0} y_{i\cdot k_1} + 1 \\ &= \sum_j z^+_{\cdot j k_1} = \sum_{j \neq j_0} z^+_{\cdot j k_1} + z^+_{\cdot j_0 k_1} = \sum_{j \neq j_0} y_{\cdot j k_1} + 1 \end{aligned}$$

and

$$y_{\cdot\cdot k_1} = \sum_i y_{i\cdot k_1} = \sum_j y_{\cdot j k_1},$$

we have

$$0 = \left(\sum_i y_{i\cdot k_1} - \sum_j y_{\cdot j k_1} \right) - \left(\sum_{i \neq i_0} y_{i\cdot k_1} - \sum_{j \neq j_0} y_{\cdot j k_1} \right) = y_{i_0 \cdot k_1} - y_{\cdot j_0 k_1}.$$

Similarly we have $y_{i_0 \cdot k_2} = y_{\cdot j_0 k_2}$. From these considerations, only possible patterns are

$$(a) : (y_{i_0 \cdot k_1}, y_{i_0 \cdot k_2}, y_{\cdot j_0 k_1}, y_{\cdot j_0 k_2}) = (1,0,1,0)$$

or

$$(b) : (y_{i_0 \cdot k_1}, y_{i_0 \cdot k_2}, y_{\cdot j_0 k_1}, y_{\cdot j_0 k_2}) = (0,1,0,1).$$

In the case of (a), it follows that $\boldsymbol{y} = \boldsymbol{z}^+ - \boldsymbol{\delta}_{i_0 j_0 k_2}$ since $\boldsymbol{z}$ is an indispensable move. In this case, it also follows that $\boldsymbol{y}' = \boldsymbol{z}^{'+} - \boldsymbol{\delta}_{i_0 j_0 k_1}$ by definition, and therefore $\boldsymbol{x} = \boldsymbol{y} + \boldsymbol{y}' = \boldsymbol{z}^{*+}$. Similarly, in the case of (b), it is shown that $\boldsymbol{x}$ must be $\boldsymbol{z}^{*-}$ and Theorem 3.3.1 is proved. Q.E.D.

3.3.3 Separation and combination of two-dimensional slices

In Section 3.3.3 we consider separation and combination of two-dimensional slices preserving the indispensability. First we provide a sufficient condition that a move created by separation of a two-dimensional slice of an indispensable move is again an indispensable move. Next, conversely, we also consider combination of two-dimensional slices of an indispensable move. Using these results, we can produce many larger indispensable moves from a set of indispensable moves that we have. In Appendix, we give a list of indispensable moves for larger tables produced by the separations and combinations of two-dimensional slices of $3 \times 4 \times K$ and $4 \times 4 \times 4$ indispensable moves presented in Section 3.3.1.

Sufficient condition for indispensability in separations of a two-dimensional slice

First we consider separation of a two-dimensional slice of an indispensable move. To illustrate our result on separation, we consider two examples. First example is the following $3 \times 4 \times 4$

move of degree 10 with slice degree $\{3,3,4\} \times \{2,2,3,3\} \times \{2,2,3,3\}$:

$$\begin{array}{|cccc|}\hline 0 & 0 & +1 & -1 \\ 0 & 0 & 0 & 0 \\ +1 & 0 & -1 & 0 \\ -1 & 0 & 0 & +1 \\ \hline\end{array} \quad \begin{array}{|cccc|}\hline 0 & 0 & 0 & 0 \\ 0 & 0 & -1 & +1 \\ 0 & -1 & +1 & 0 \\ 0 & +1 & 0 & -1 \\ \hline\end{array} \quad \begin{array}{|cccc|}\hline 0 & 0 & -1 & +1 \\ 0 & 0 & +1 & -1 \\ -1 & +1 & 0 & 0 \\ +1 & -1 & 0 & 0 \\ \hline\end{array}.$$

The $i = 3$-slice of this indispensable move seems to contain two *loops*, i.e., the following decomposition is observed.

$$\begin{array}{|cccc|}\hline 0 & 0 & -1 & +1 \\ 0 & 0 & +1 & -1 \\ -1 & +1 & 0 & 0 \\ +1 & -1 & 0 & 0 \\ \hline\end{array} = \begin{array}{|cccc|}\hline 0 & 0 & -1 & +1 \\ 0 & 0 & +1 & -1 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ \hline\end{array} + \begin{array}{|cccc|}\hline 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ -1 & +1 & 0 & 0 \\ +1 & -1 & 0 & 0 \\ \hline\end{array}$$

In fact, the above separation of the $i = 3$-slice creates another indispensable move ($4 \times 4 \times 4$ move(1) of degree 10 with slice degree$\{2,2,3,3\} \times \{2,2,3,3\} \times \{2,2,3,3\}$).

Next example is the following $3 \times 3 \times 5$ move of degree 10 with slice degree $\{3,3,4\} \times \{3,3,4\} \times \{2,2,2,2,2\}$

$$\begin{array}{|ccccc|}\hline -1 & 0 & +1 & 0 & 0 \\ 0 & 0 & -1 & 0 & +1 \\ +1 & 0 & 0 & 0 & -1 \\ \hline\end{array} \quad \begin{array}{|ccccc|}\hline 0 & +1 & -1 & 0 & 0 \\ 0 & 0 & +1 & -1 & 0 \\ 0 & -1 & 0 & +1 & 0 \\ \hline\end{array} \quad \begin{array}{|ccccc|}\hline +1 & -1 & 0 & 0 & 0 \\ 0 & 0 & 0 & +1 & -1 \\ -1 & +1 & 0 & -1 & +1 \\ \hline\end{array}.$$

We consider the $i = 3$-slice of this indispensable move. It is seen that this slice is again decomposed to two loops as follows:

$$\begin{array}{|ccccc|}\hline +1 & -1 & 0 & 0 & 0 \\ 0 & 0 & 0 & +1 & -1 \\ -1 & +1 & 0 & -1 & +1 \\ \hline\end{array} = \begin{array}{|ccccc|}\hline +1 & -1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \\ -1 & +1 & 0 & 0 & 0 \\ \hline\end{array} + \begin{array}{|ccccc|}\hline 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & +1 & -1 \\ 0 & 0 & 0 & -1 & +1 \\ \hline\end{array}.$$

In fact, the above separation of the $i = 3$-slice creates a $4 \times 3 \times 5$ move. After permuting the axes and the indices, we see that the move is a $3 \times 4 \times 5$ indispensable move of degree 10 with slice degree $\{3,3,4\} \times \{2,2,3,3\} \times \{2,2,2,2,2\}$, which is included in our list. These two examples suggest the possibility that we can create a new indispensable move by separations of a two-dimensional slice of an already obtained indispensable move under some conditions.

Now we provide some definitions. Let $\boldsymbol{z} = \boldsymbol{z}^+ - \boldsymbol{z}^-$ be a move of the size $I \times J \times K$ with the positive part $\boldsymbol{z}^+$ and the negative part $\boldsymbol{z}^-$. Without loss of generality, we consider the separation of $\boldsymbol{z}_{k=k_0}$, i.e., $k = k_0$-slice of $\boldsymbol{z}$. Note that $\boldsymbol{z}_{k=k_0}$ is an $I \times J$ two-dimensional integer array with zero row sums and zero column sums. In the following, we assume that the level indices $i_1, i_2, \ldots \in [I], j_1, j_2, \ldots \in [J]$ are all distinct, i.e.,

$$i_m \neq i_n \text{ and } j_m \neq j_n \text{ for all } m \neq n. \tag{3.11}$$

The following definition gives a fundamental tool.

Definition 3.3.2 *A loop of degree r is an $I \times J$ integer array $\boldsymbol{L}_r$, where $\boldsymbol{L}_r$ has the elements*

$$\begin{array}{l} L_{i_1 j_1} = L_{i_2 j_2} = \cdots = L_{i_{r-1} j_{r-1}} = L_{i_r j_r} = 1, \\ L_{i_1 j_2} = L_{i_2 j_3} = \cdots = L_{i_{r-1} j_r} = L_{i_r j_1} = -1, \end{array}$$

for some $i_1, \ldots, i_r \in [I], j_1, \ldots, j_r \in [J]$ and all the other elements in the two-way subarray $\{i_1, \ldots, i_r\} \times \{j_1, \ldots, j_r\}$ are zero.

Note that there is at most one $+1$ and -1 in each row and column of a loop. We call $\{i_1, \dots, i_r\} \times \{j_1, \dots, j_r\}$ the supporting rectangle of the loop $\boldsymbol{L}_r$. Now we clarify the separation of the two-dimensional slice of moves which we have seen in the above examples.

Lemma 3.3.1 *Let $\boldsymbol{z}_{k=k_0}$ be an $I \times J$ two-dimensional slice of a move $\boldsymbol{z}$. Then $\boldsymbol{z}_{k=k_0}$ can be expressed as a sum*

$$\boldsymbol{z} = a_1 \boldsymbol{L}_{r(1)} + \cdots + a_n \boldsymbol{L}_{r(n)}, \tag{3.12}$$

where $a_1, \dots, a_n$ are positive integers, $r(1), \dots, r(n) \le \min(I, J)$, $\boldsymbol{L}_{r(1)}, \dots, \boldsymbol{L}_{r(n)}$ are all distinct and there is no cancellation of signs in any cell.

Proof of this lemma is postponed to Section 3.4.4. In Section 3.4.4, we give more detailed descriptions of the loops and the above lemma.

The separations of slices in the examples above correspond to the cases that the expression (3.12) is uniquely determined. Note that there are cases of unique separation of a slice even when the supporting rectangles of the loops in (3.12) have common cells. The following is an example of such a case:

$$\boxed{\begin{array}{ccc} +1 & -1 & 0 \\ +1 & +1 & -2 \\ -2 & 0 & +2 \end{array}} = \boxed{\begin{array}{ccc} +1 & -1 & 0 \\ 0 & +1 & -1 \\ -1 & 0 & +1 \end{array}} + \boxed{\begin{array}{ccc} 0 & 0 & 0 \\ +1 & 0 & -1 \\ -1 & 0 & +1 \end{array}}.$$

Conversely, there are cases of non-unique separation of a slice even when the supporting rectangles of the loops in (3.12) are disjoint. The following is an example of such a case:

$$\begin{aligned} \boxed{\begin{array}{cccc} +1 & +1 & -1 & -1 \\ -1 & -1 & +1 & +1 \end{array}} &= \boxed{\begin{array}{cccc} +1 & 0 & -1 & 0 \\ -1 & 0 & +1 & 0 \end{array}} + \boxed{\begin{array}{cccc} 0 & +1 & 0 & -1 \\ 0 & -1 & 0 & +1 \end{array}} \\ &= \boxed{\begin{array}{cccc} +1 & 0 & 0 & -1 \\ -1 & 0 & 0 & +1 \end{array}} + \boxed{\begin{array}{cccc} 0 & +1 & -1 & 0 \\ 0 & -1 & +1 & 0 \end{array}}. \end{aligned}$$

Now we give the main theorem related to the separation of two-dimensional slices.

Theorem 3.3.2 *Let $\boldsymbol{z}$ be an $I \times J \times K$ indispensable move. Suppose that a slice $\boldsymbol{z}_{k=k_0}$ is expressed uniquely as (3.12) and $a_1 + \cdots + a_n \ge 2$. Then*

(i) $I \times J \times (K+n-1)$ move $\boldsymbol{z}^*$ that is created from $\boldsymbol{z}$ by the separation of $\boldsymbol{z}_{k=k_0}$ with respect to the loops of (3.12) and

(ii) $I \times J \times (K + a_1 + \cdots + a_n - 1)$ move $\boldsymbol{z}^{**}$ that is created from $\boldsymbol{z}^*$ such that the each k-slice that is created from the $\boldsymbol{z}_{k=k_0}$ is a single loop
are indispensable moves, respectively.

Proof. We only show a proof of (i) since (ii) is obvious when (i) is shown. The positive part and the negative part of $\boldsymbol{z}^*$ are in the same reference set of $I \times J \times (K+n-1)$ contingency tables. We write this reference set as $\mathcal{F}^*$. Let $\widetilde{\boldsymbol{z}}^+$ and $\widetilde{\boldsymbol{z}}^-$ be the $I \times J \times (K+n-1)$ contingency tables created from $\boldsymbol{z}^+$ and $\boldsymbol{z}^-$ by the separation (3.12), respectively. Since $\widetilde{\boldsymbol{z}}^+, \widetilde{\boldsymbol{z}}^- \in \mathcal{F}^*$, all we have to show is that $\boldsymbol{x} = \widetilde{\boldsymbol{z}}^+$ or $\boldsymbol{x} = \widetilde{\boldsymbol{z}}^-$ holds for any $\boldsymbol{x} \in \mathcal{F}^*$. Let κ denote the set of slice indices which are the separation of $\boldsymbol{z}_{k=k_0}$. We have $|\kappa| = n$ by definition. Let $\widehat{\boldsymbol{x}}$ be the

$I \times J \times K$ contingency table which is made from $\boldsymbol{x}$ by the addition of the k-slices for $k \in \kappa$. Since $\widehat{\boldsymbol{x}}$ has the same marginal totals to $\boldsymbol{z}^+$ and $\boldsymbol{z}^-$, $\widehat{\boldsymbol{x}} = \boldsymbol{z}^+$ or $\widehat{\boldsymbol{x}} = \boldsymbol{z}^-$ holds. We assume $\widehat{\boldsymbol{x}} = \boldsymbol{z}^+$ without loss of generality. Note that

$$x_{ijk} = \widetilde{z}^+_{ijk} \text{ for } i \in [I], j \in [J], k \notin \kappa. \tag{3.13}$$

Therefore we only have to show that $x_{ijk} = \widetilde{z}^+_{ijk}$ for $k \in \kappa$. Here consider $I \times J \times n$ subarrays of $\boldsymbol{x}$ and $\widetilde{\boldsymbol{z}}^+$ for $k \in \kappa$. From (3.13), we see that $\boldsymbol{x}$ and $\widetilde{\boldsymbol{z}}^+$ have the same two-dimensional marginals in these subarrays. Note that $\sum_{k\in\kappa} x_{ijk} = \sum_{k\in\kappa} \widetilde{z}^+_{ijk}$ in particular. From this, it is seen that

$$\{(i,j) \mid x_{ijk} > 0, \exists k \in \kappa\} = \{(i,j) \mid \widetilde{z}^+_{ijk} > 0, \exists k \in \kappa\}.$$

Moreover, since there is no cancellation of signs in (3.12), it is also seen that

$$\{(i,j) \mid \widetilde{z}^+_{ijk} > 0, \exists k \in \kappa\} \cap \{(i,j) \mid \widetilde{z}^-_{ijk} > 0, \exists k \in \kappa\} = \emptyset.$$

Therefore, if $\boldsymbol{x} \neq \widetilde{\boldsymbol{z}}^+$, $\boldsymbol{x}$ and $\widetilde{\boldsymbol{z}}^-$ have disjoint supports, then $\boldsymbol{x} - \widetilde{\boldsymbol{z}}^- \neq \boldsymbol{z}^*$ is another separation of $\boldsymbol{z}$, which contradicts the assumption that the separation is unique. Q.E.D.

Combinations of two-dimensional slices

Next we consider combinations of two-dimensional slices of indispensable moves. It should be noted that the converse of the statement in Theorem 3.3.2 is not always true. To see this, consider again the following $3 \times 3 \times 5$ indispensable move of degree 10 with slice degree $\{3,3,4\} \times \{3,3,4\} \times \{2,2,2,2,2\}$

$$\boxed{\begin{array}{ccccc} -1 & 0 & +1 & 0 & 0 \\ 0 & 0 & -1 & 0 & +1 \\ +1 & 0 & 0 & 0 & -1 \end{array}} \quad \boxed{\begin{array}{ccccc} 0 & +1 & -1 & 0 & 0 \\ 0 & 0 & +1 & -1 & 0 \\ 0 & -1 & 0 & +1 & 0 \end{array}} \quad \boxed{\begin{array}{ccccc} +1 & -1 & 0 & 0 & 0 \\ 0 & 0 & 0 & +1 & -1 \\ -1 & +1 & 0 & -1 & +1 \end{array}}. \tag{3.14}$$

Combining $k=1$-slice and $k=4$-slice of this move makes the following $3 \times 3 \times 4$ move.

$$\begin{array}{cccc} 1+4 & 2 & 3 & 5 \\ \hline -1 & 0 & +1 & 0 \\ 0 & 0 & -1 & +1 \\ +1 & 0 & 0 & -1 \end{array} \quad \begin{array}{cccc} 1+4 & 2 & 3 & 5 \\ \hline 0 & +1 & -1 & 0 \\ -1 & 0 & +1 & 0 \\ +1 & -1 & 0 & 0 \end{array} \quad \begin{array}{cccc} 1+4 & 2 & 3 & 5 \\ \hline +1 & -1 & 0 & 0 \\ +1 & 0 & 0 & -1 \\ -2 & +1 & 0 & +1 \end{array} \tag{3.15}$$

It is seen that this is a dispensable move, although [k = 1-slice] + [k = 4-slice] is a unique decomposition of the form (3.12). This example implies that we have to consider some additional conditions to assure that moves made by combining two-dimensional slices of indispensable moves are again indispensable moves.

Unfortunately, it seems difficult to derive a necessary and sufficient condition for this problem. We give a sufficient condition similar as Theorem 3.3.1 for this problem.

Let $\boldsymbol{z} = \boldsymbol{z}^+ - \boldsymbol{z}^-$ be an indispensable move of the size $I \times J \times K$ with the positive part $\boldsymbol{z}^+$ and the negative part $\boldsymbol{z}^-$. Without loss of generality, we consider the combination of $k = K-1$-slice and $k = K$-slice of $\boldsymbol{z}$. Let $\boldsymbol{z}^* = \boldsymbol{z}^{*+} - \boldsymbol{z}^{*-}$ be a move of the size $I \times J \times (K-1)$ with the positive part $\boldsymbol{z}^{*+}$ and the negative part $\boldsymbol{z}^{*-}$, which is made by the combination of $\boldsymbol{z}_{k=K-1}$ and $\boldsymbol{z}_{k=K}$ from $\boldsymbol{z}$, i.e., the elements of $\boldsymbol{z}^{*}$ are given by

$$z^{*}_{ijk} = \begin{cases} z_{ijk}, & \text{for } k \in [K-2], \\ z_{ijK-1} + z_{ijK}, & \text{for } k = K-1, \end{cases} \tag{3.16}$$

for $i \in [I], j \in [J]$. We also assume that there is no cancellation of signs in any cell of $\boldsymbol{z}_{k=K-1}$ and $\boldsymbol{z}_{k=K}$. Hence we only consider the case of $\deg(\boldsymbol{z}) = \deg(\boldsymbol{z}^{*})$. $\boldsymbol{z}^{*+}$ and $\boldsymbol{z}^{*-}$ are obtained by combining $k = K-1$- and $k = K$-slices of $\boldsymbol{z}^{+}$ and $\boldsymbol{z}^{-}$, respectively, and have the same two-dimensional marginal totals, which are calculated as

$$\begin{aligned} z^{*+}_{ij\cdot} &= z^{+}_{ij\cdot}, \\ z^{*+}_{i\cdot k} &= \begin{cases} z^{+}_{i\cdot k}, & \text{for } k \in [K-2], \\ z^{+}_{i\cdot K-1} + z^{+}_{i\cdot K}, & \text{for } k = K-1, \end{cases} \\ z^{*+}_{\cdot jk} &= \begin{cases} z^{+}_{\cdot jk}, & \text{for } k \in [K-2], \\ z^{+}_{\cdot jK-1} + z^{+}_{\cdot jK}, & \text{for } k = K-1, \end{cases} \end{aligned}$$

for $i \in [I], j \in [J]$. Our aim is to derive a sufficient condition that $\boldsymbol{z}^{*} = \boldsymbol{z}^{*+} - \boldsymbol{z}^{*-}$ is an indispensable move, i.e.,

$$\mathcal{F}(\{z^{*+}_{ij\cdot}\}, \{z^{*+}_{i\cdot k}\}, \{z^{*+}_{\cdot jk}\}) = \{\boldsymbol{z}^{*+}, \boldsymbol{z}^{*-}\}.$$

Here we consider a separation of the one-dimensional marginal totals of the two-dimensional slice $\boldsymbol{z}^{*+}_{k=K-1}$, which is expressed as integer vectors $\boldsymbol{p}_1 = \{p_{1i}\}, \boldsymbol{p}_2 = \{p_{2i}\}, i \in [I]$, and $\boldsymbol{q}_1 = \{q_{1j}\}, \boldsymbol{q}_2 = \{q_{2j}\}, j \in [J]$, satisfying

$$\begin{cases} z^{*+}_{i\cdot K-1} = p_{1i} + p_{2i}, \ \text{for } i \in [I], \\ z^{*+}_{\cdot jK-1} = q_{1j} + q_{2j}, \ \text{for } j \in [J], \\ \displaystyle\sum_{i=1}^{I} p_{1i} = \sum_{j=1}^{J} q_{1j} \geq 2, \ \sum_{i=1}^{I} p_{2i} = \sum_{j=1}^{J} q_{2j} \geq 2. \end{cases} \tag{3.17}$$

Then, for given $\{z^{*+}_{ij\cdot}\}, \{z^{*+}_{i\cdot k}\}, \{z^{*+}_{\cdot jk}\}, i \in [I], j \in [J], k \in [K-1]$ and $\boldsymbol{p}_1, \boldsymbol{p}_2, \boldsymbol{q}_1, \boldsymbol{q}_2$, we consider the following simultaneous equation (for cell frequencies $\boldsymbol{y} = \{y_{ijk}\}$ of the size $I \times J \times K$).

$$\begin{cases} y_{ij\cdot} = z^{*+}_{ij\cdot}, \\ y_{i\cdot k} = z^{*+}_{i\cdot k}, \ y_{i\cdot K-1} = p_{1i}, \ y_{i\cdot K} = p_{2i}, \\ y_{\cdot jk} = z^{*+}_{\cdot jk}, \ y_{\cdot jK-1} = q_{1i}, \ y_{\cdot jK} = q_{2i}, \\ \qquad i \in [I], \ j \in [J], \ k \in [K-2]. \end{cases} \tag{3.18}$$

By definition, Equation (3.18) has solutions $\boldsymbol{y} = \boldsymbol{z}^{+}$ and $\boldsymbol{y} = \boldsymbol{z}^{-}$ when

$$\begin{cases} p_{1i} = z^{+}_{i\cdot K-1}, \ p_{2i} = z^{+}_{i\cdot K}, \ i \in [I], \\ q_{1j} = z^{+}_{\cdot jK-1}, \ q_{2j} = z^{+}_{\cdot jK}, \ j \in [J] \end{cases} \tag{3.19}$$

or

$$\begin{cases} p_{1i} = z^{+}_{i\cdot K}, \ p_{2i} = z^{+}_{i\cdot K-1}, \ i \in [I], \\ q_{1j} = z^{+}_{\cdot jK}, \ q_{2j} = z^{+}_{\cdot jK-1}, \ j \in [J]. \end{cases} \tag{3.20}$$

Our sufficient concerns the situation that (3.18) has solutions only when the condition (3.19) or (3.20) holds.

Theorem 3.3.3 *Let $\boldsymbol{z}$ be an $I \times J \times K$ indispensable move and let $\boldsymbol{z}^*$ be an $I \times J \times (K-1)$ move satisfying* $\deg(\boldsymbol{z}) = \deg(\boldsymbol{z}^*)$*, which is made from $\boldsymbol{z}$ by combining $k = K-1$- and $k = K$-slices of $\boldsymbol{z}$ as (3.16). Then $\boldsymbol{z}^*$ is an indispensable move when the following two conditions are satisfied.*

(a) The simultaneous equations (3.18) has solutions only when the condition (3.19) or (3.20) holds.

(b) $\max(z^{*+}_{1 \cdot K-1}, \dots, z^{*+}_{I \cdot K-1}, z^{*+}_{\cdot 1 K-1}, \dots, z^{*+}_{\cdot J K-1}) \geq 2.$

Proof. We argue by contradiction. Suppose $\boldsymbol{z}^*$ is a dispensable move. Then there is some $\boldsymbol{x} \in \mathcal{F}(\{z^{*+}_{ij\cdot}\}, \{z^{*+}_{i\cdot k}\}, \{z^{*+}_{\cdot jk}\})$ where $\boldsymbol{x} \neq \boldsymbol{z}^{*+}$ and $\boldsymbol{x} \neq \boldsymbol{z}^{*-}$. If $\boldsymbol{x}_{k=K-1} = \boldsymbol{z}^{*+}_{k=K-1}$ or $\boldsymbol{x}_{k=K-1} = \boldsymbol{z}^{*-}_{k=K-1}$ holds, we can make an $I \times J \times K$ table $\widetilde{\boldsymbol{x}}$ by the separation of $\boldsymbol{x}_{k=K-1}$ satisfying $\widetilde{\boldsymbol{x}} \in \mathcal{F}(\{z^{+}_{ij\cdot}\}, \{z^{+}_{i\cdot k}\}, \{z^{+}_{\cdot jk}\})$, which contradicts the assumption $\boldsymbol{x} \neq \boldsymbol{z}^{*+}$ and $\boldsymbol{x} \neq \boldsymbol{z}^{*-}$ since $\boldsymbol{z}$ is an indispensable move. Hence we only have to consider the case that $\boldsymbol{x}_{k=K-1} \neq \boldsymbol{z}^{*+}_{k=K-1}$ and $\boldsymbol{x}_{k=K-1} \neq \boldsymbol{z}^{*-}_{k=K-1}$. Define an $I \times J \times (K-1)$ move $\boldsymbol{v}$ as $\boldsymbol{v} = \boldsymbol{z}^{*+} - \boldsymbol{x}$ and an $I \times J \times (K-1)$ table $\boldsymbol{u} = \{u_{ijk}\}$ as $u_{ijk} = \min(z^{*+}_{ijk},\ x_{ijk})$ for $i \in [I], j \in [J], k \in [K-1]$.

Case 1. First we consider the case that there is some $i \in [I], j \in [J]$ such that $u_{ijK-1} > 0$. Note that $\boldsymbol{z}^{*+} = \boldsymbol{v}^+ + \boldsymbol{u}$ and $\boldsymbol{x} = \boldsymbol{v}^- + \boldsymbol{u}$ hold. Separation of the $k = K-1$-slice of $\boldsymbol{z}^{*+}$ to $\boldsymbol{v}^+_{k=K-1}$ and $\boldsymbol{u}_{k=K-1}$ makes a solution for (3.18) where

$$
\begin{aligned}
p_{1i} &= v^{+}_{i\cdot K-1},\ p_{2i} = u_{i\cdot K-1},\ i \in [I], \\
q_{1i} &= v^{+}_{\cdot jK-1},\ q_{2i} = u_{\cdot jK-1},\ j \in [J].
\end{aligned}
\tag{3.21}
$$

Similarly, separation of the $k = K-1$-slice of $\boldsymbol{x}$ to $\boldsymbol{v}^-_{k=K-1}$ and $\boldsymbol{u}_{k=K-1}$ makes another solution for (3.18) where $\boldsymbol{p}_1, \boldsymbol{p}_2, \boldsymbol{q}_1, \boldsymbol{q}_2$ are defined as (3.21). From the condition *(a)* and the assumption that $\boldsymbol{z}$ is an indispensable move, it follows that $\boldsymbol{x} = \boldsymbol{z}^{*+}$ or $\boldsymbol{x} = \boldsymbol{z}^{*-}$, which is a contradiction.

Case 2. Next we consider the case that $u_{ijK-1} = 0$ for all $i \in [I], j \in [J]$. In this case, $\boldsymbol{z}^{*+}$ and $\boldsymbol{x}$ do not have positive elements at common cells in the $k = K-1$-slice. In addition, an $I \times J$ two-dimensional $k = K-1$-slice of $\boldsymbol{z}^{*+} - \boldsymbol{x}$ has zero marginal totals. Hence $(\boldsymbol{z}^{*+} - \boldsymbol{x})_{k=K-1}$ can be expressed as a finite sum of loops with the form (3.12). Furthermore, $(\boldsymbol{z}^{*+} - \boldsymbol{x})_{k=K-1}$ is expressed as at least two loops, i.e., $a_1 + \cdots + a_n \geq 2$ in the expression (3.12), because otherwise it contradicts the condition *(b)*. According to this expression, we can write $(\boldsymbol{z}^{*+} - \boldsymbol{x})_{k=K-1} = \boldsymbol{L} + \widetilde{\boldsymbol{L}}$, where $\boldsymbol{L}$ and $\widetilde{\boldsymbol{L}}$ are (possibly sum of) $I \times J$ loops such that there is no cancellation of signs in any cell. Here, separation of the $k = K-1$-slice of $\boldsymbol{z}^{*+}$ to $\boldsymbol{L}^+$ and $\widetilde{\boldsymbol{L}}^+$ makes a solution for (3.18) where

$$
\begin{aligned}
p_{1i} &= L^{+}_{i\cdot},\ p_{2i} = \widetilde{L_{i\cdot}}^{+},\ i \in [I], \\
q_{1i} &= L^{+}_{\cdot j},\ q_{2i} = \widetilde{L_{\cdot j}}^{+},\ j \in [J].
\end{aligned}
\tag{3.22}
$$

Similarly, separation of the $k = K-1$-slice of $\boldsymbol{x}$ to $\boldsymbol{L}^-$ and $\widetilde{\boldsymbol{L}}^-$ makes another solution for (3.18) where $\boldsymbol{p}_1, \boldsymbol{p}_2, \boldsymbol{q}_1, \boldsymbol{q}_2$ are defined as (3.22). Then we see that Case 2 is also a contradiction for the same reason as Case 1. Q.E.D.

To see whether a move $\boldsymbol{z}^*$ is an indispensable move or not according to Theorem 3.3.3, we have to consider all the possible patterns of $\boldsymbol{p}_1, \boldsymbol{p}_2, \boldsymbol{q}_1, \boldsymbol{q}_2$ satisfying the condition (3.17).

However, it is usually a much more complicated task than simply investigating $\boldsymbol{z}^*$ itself. For example, consider the $3 \times 3 \times 5$ indispensable move of degree 10 with slice degree $\{3, 3, 4\} \times \{3, 3, 4\} \times \{2, 2, 2, 2, 2\}$ displayed as (3.14) again. Considering the move (3.15) which is made by the combination of the $k = 1$- and $k = 4$-slices of (3.14), possible patterns of $\boldsymbol{p}_1, \boldsymbol{p}_2, \boldsymbol{q}_1, \boldsymbol{q}_2$ include

$$\boldsymbol{p}_1 = (1, 1, 0),\ \boldsymbol{p}_2 = (0, 0, 2),\ \boldsymbol{q}_1 = (1, 1, 0),\ \boldsymbol{q}_2 = (0, 0, 2)$$

and

$$\boldsymbol{p}_1 = (1, 0, 1),\ \boldsymbol{p}_2 = (0, 1, 1),\ \boldsymbol{q}_1 = (0, 1, 1),\ \boldsymbol{q}_2 = (1, 0, 1).$$

Note that these two patterns permit solutions for (3.18), while the original indispensable move (3.14) is the difference of the two solutions for (3.18) when

$$\boldsymbol{p}_1 = (1, 0, 1),\ \boldsymbol{p}_2 = (0, 1, 1),\ \boldsymbol{q}_1 = (1, 0, 1),\ \boldsymbol{q}_2 = (0, 1, 1).$$

3.3.4 Discussion

In this section, we provide an explicit form of the unique minimal Markov basis for $3 \times 4 \times K$ and $4 \times 4 \times 4$ contingency tables by considering all the sign patterns. Our approach is an elementary one and similar to Section 3.2.

Our results in this section enable us to construct a connected Markov chain over $3 \times 4 \times K$ and $4 \times 4 \times 4$ contingency tables. Adjusting this chain to have a given stationary distribution by the Metropolis procedure, we can perform various tests by the Monte Carlo method. It should be noted that, for some data sets, construction of a connected Markov chain over three-dimensional contingency tables with the given two-dimensional marginals is a difficult problem. Moreover, it is also difficult to determine whether a simple-minded Markov chain described in Section 3.1, i.e., a Markov chain constructed from the $2 \times 2 \times 2$ basic moves described in (3.2) alone, is connected or not for given marginal totals. Therefore our results are valuable since our definition of Markov basis takes into account *arbitrary* patterns of the marginal totals. In addition, our result of the unique minimal Markov basis for $3 \times 4 \times K$ contingency tables shows that it is sufficient to consider the moves with sizes up to $3 \times 4 \times 8$ to construct a connected Markov chain over $3 \times 4 \times K$ tables for any $K \geq 8$. This result is attractive since it cannot be derived by performing algebraic algorithms.

There are still many open problems on the Markov basis for three-way contingency tables with fixed two-dimensional marginals. One of the most interesting problems may be a problem concerning the existence of unique minimal Markov basis.

> **Problem** For any positive integers I, J and K, does there exist a unique minimal Markov basis for the three-dimensional $I \times J \times K$ contingency tables with fixed two-dimensional marginals?

As we show in Section 3.5 and Section 3.6, a minimal Markov basis is not unique for many problems that we usually consider. For example, a minimal Markov basis for the model of complete independence in the log-linear model in the three-dimensional contingency tables, $p_{ijk} = \alpha_i \beta_j \gamma_k$, is shown to be not unique in Section 3.5. It is also shown in Section 3.6 that minimal Markov bases for many models of the hierarchical $2 \times 2 \times 2 \times 2$ log-linear models are not unique. Clearly the uniqueness of a minimal Markov basis depends on the models, i.e., the sufficient statistics that we fix. However, it seems very difficult to determine whether the given model has unique minimal Markov basis or not.

The list of indispensable moves in Section 3.3.1 gives some further informations.

(i) An importance of the type-2 combination of indispensable moves are suggested in Section 3.3.2. However, $3 \times 4 \times 4$ move of degree 9 with slice degree $\{3,3,3\} \times \{2,2,2,3\} \times \{2,2,2,3\}$ suggests another possibility of forming larger indispensable moves. In Section 3.2.4, it is pointed out that this move of degree 9 has a structure that three $2 \times 2 \times 2$ basic moves combine *all at once* in such a way that any two of the three basic moves forms a type-1 combination, and this move suggests the difficulty in forming a conjecture on a minimal Markov basis for larger tables. In fact, our list in Appendix contains many moves of odd degrees.

(ii) We found that some indispensable moves have entries ± 2, which leads to a next general problem.

> **Problem** What is the value $U_{I,J,K}$ depending on I, J and K, such that for each element $\boldsymbol{z}$ of a minimal Markov basis for the three-dimensional $I \times J \times K$ contingency tables with fixed two-dimensional marginals, $U_{I,J,K} = \max_{i,j,k} |z_{ijk}|$?

We see that $U_{3,4,K} = 1$ when $K \leq 5$, $U_{3,4,K} = 2$ when $K \geq 6$ and $U_{4,4,4} = 2$.

(iii) We found that some indispensable moves are asymmetric, where we define a symmetric move as a move $\boldsymbol{z}$ which can be transformed to $-\boldsymbol{z}$ by the permutations of indices for each axis of the move. We consider this symmetry in Section 3.6. In our list of indispensable moves in Section 3.3.1,

$$3 \times 4 \times 6 \text{ move of degree 12 with slice degree } \{3,4,5\} \times \{2,3,3,4\} \times \{2,2,2,2,2,2\} \text{ and}$$

$$4 \times 4 \times 4 \text{ move of degree 12 with slice degree } \{2,3,3,4\} \times \{2,3,3,4\} \times \{3,3,3,3\}$$

are asymmetric, while all the other indispensable moves are symmetric. Furthermore, we found another indispensable move of size $3 \times 5 \times 6$ that has only one of $+2$ or -2:

$$\begin{array}{|cccccc|}\hline +1 & 0 & 0 & 0 & 0 & -1 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & +1 & -1 & 0 & 0 & 0 \\ -1 & 0 & +1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 & 0 & +1 \\ \hline \end{array} \quad \begin{array}{|cccccc|}\hline 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & +1 & 0 & -1 \\ 0 & 0 & +1 & -1 & 0 & 0 \\ 0 & 0 & -1 & 0 & +1 & 0 \\ 0 & 0 & 0 & 0 & -1 & +1 \\ \hline \end{array} \quad \begin{array}{|cccccc|}\hline -1 & 0 & 0 & 0 & 0 & +1 \\ 0 & 0 & 0 & -1 & 0 & +1 \\ 0 & -1 & 0 & +1 & 0 & 0 \\ +1 & 0 & 0 & 0 & -1 & 0 \\ 0 & +1 & 0 & 0 & +1 & -2 \\ \hline \end{array}\ .$$

This is an example of obvious asymmetric indispensable moves.

(iv) In Section 3.3.1, we label each indispensable move by three invariants for the permutations of indices for each axis and the permutations of axes of moves: size, degree and slice degree. However, we cannot completely distinguish all indispensable moves by these invariants. As is seen in Section 3.3.1, the following four pairs of indispensable moves have these three invariants in common:

$$3 \times 4 \times 7 \text{ moves of degree 14 with slice degree } \{4,4,6\} \times \{3,3,4,4\} \times \{2,2,2,2,2,2,2\},$$

$$4 \times 4 \times 4 \text{ moves of degree 10 with slice degree } \{2,2,3,3\} \times \{2,2,3,3\} \times \{2,2,3,3\},$$

$4 \times 4 \times 4$ moves of degree 12 with slice degree $\{3,3,3,3\} \times \{3,3,3,3\} \times \{3,3,3,3\}$,

$4 \times 4 \times 4$ moves of degree 14 with slice degree $\{3,3,3,5\} \times \{3,3,3,5\} \times \{3,3,4,4\}$.

To distinguish these indispensable moves, other invariants can be considered. For example, consider a set of values $\{c_0, c_1, c_2, \ldots\}$ which we define as

$$c_n = \left| \left\{ (i,j,k) \;\middle|\; \sum_i z_{ijk}^+ + \sum_j z_{ijk}^+ + \sum_k z_{ijk}^+ = n \right\} \right|.$$

It is seen that $\{c_0, c_1, c_2, \ldots\}$ is an invariant. We can distinguish two $4 \times 4 \times 4$ moves of degree 12 with slice degree $\{3,3,3,3\} \times \{3,3,3,3\} \times \{3,3,3,3\}$ by this invariant. In fact the values for the two indispensable moves are $\{0, 12, 24, 28\}$ and $\{4, 0, 36, 24\}$, respectively. We can also distinguish two $4 \times 4 \times 4$ moves of degree 14 with slice degree $\{3,3,3,5\} \times \{3,3,3,5\} \times \{3,3,4,4\}$ by this invariant ($\{1,6,24,22,9,0,2\}$ and $\{2,4,24,24,8,0,2\}$, respectively). Unfortunately, however, we cannot distinguish two $3 \times 4 \times 7$ moves of degree 14 with slice degree $\{4,4,6\} \times \{3,3,4,4\} \times \{2,2,2,2,2,2,2\}$ and two $4 \times 4 \times 4$ moves of degree 10 with slice degree $\{2,2,3,3\} \times \{2,2,3,3\} \times \{2,2,3,3\}$ even when we consider the above invariant. To distinguish these indispensable moves, we have to consider other invariants. In this study, however, we do not consider the identification of indispensable moves by invariants furthermore.

We found that substantial number of non-fundamental indispensable moves. We also found the following rare examples of non-circuit indispensable moves in Section 3.3.1 and Appendix:

- $((3,4,8),(16),((4,6,6),(3,3,5,5),(2,2,2,2,2,2,2,2)),(FCs),\emptyset,$
  $((111,123,132,144,218,221,234,237,245,246,312,327,335,336,343,348),$
  $(112,121,134,143,211,227,235,236,244,248,318,323,332,337,345,346)))$
- $((3,5,7),(16),((4,6,6),(2,3,3,3,5),(2,2,2,2,2,2,4)),(FCs),\emptyset,$
  $((121,133,142,154,216,222,237,247,253,255,317,325,331,344,356,357),$
  $(122,131,144,153,217,225,233,242,256,257,316,321,337,347,354,355)))$

3.4 Construction of a connected Markov chain over incomplete two-way contingency tables with fixed marginals

3.4.1 Structural zero and sampling zero cells

Researchers often encounter the problem of analyzing incomplete contingency tables, i.e., tables containing some structural, or *a priori*, zeros. Structural zeros arise in situations where it is theoretically impossible for some cells to contain observations. For example, when a secondary infection can occur only if a primary infection occurs, the cell in the contingency table that corresponds to the secondary infection without the primary infection would necessarily contain a structural zero. Such cells can occur naturally as a feature of the data and can be distinguished from sampling zeros, which occur due to the sampling variability and the relative smallness of the cell probabilities. It is noted that if probabilities of some cells are free from models, i.e., if the probabilities of some cells are regarded as nuisance parameters, these cells can also be treated as if they are structural zero cells.

For analyzing two-way incomplete contingency tables, one of the most familiar models is the quasi-independence model (see Bishop *et al.*, 1975, for example). To perform the exact test of quasi-independence, the null distribution of an appropriate test statistic is required. However, a complete enumeration of this distribution is often computationally infeasible and a Monte Carlo exact test is used.

As we have seen in Section 3.1, a Markov chain Monte Carlo approach is extensively used in various settings of contingency tables, including Smith *et al.* (1996) for tests of independence, quasi-independence and quasi-symmetry for square contingency tables. This section gives an extension of the work of Smith *et al.* (1996), which considers the situation that the contingency table is square and the diagonal cells are structural zeros. In this section, we consider more general situation; the contingency table is not necessarily square and there is no constraint on the configuration of structural zero cells. In addition, our approach provides more concise and explicit expressions of a Markov basis than the general algorithms by Diaconis and Sturmfels (1998), and subsequent work by Rapallo (2003). As is stated in Section 3.1, Gröbner basis computation produces large number of redundant basis elements due to the lack of symmetry and minimality inherent in Gröbner basis. In this section, we give the closed form expression of the unique minimal basis for two-way contingency tables with arbitrary configuration of structural zeros. Though Rapallo (2003) considered the same problem to us, he does not produce the closed form expression of the basis by his Gröbner basis approach and does not refer the minimality of a basis.

The construction of this section is as follows. Section 3.4.2 and Section 3.4.3 describe the problem. Section 3.4.4 gives an explicit characterization a minimal basis. We also prove its uniqueness. Section 3.4.5 describes the algorithms for enumerating elements of the unique minimal basis. In this section, an explicit forms of minimal bases for some typical situations are also given. Computational example is given in Section 3.4.6. In Section 3.4.7 we discuss further basis reduction for the case of positive sufficient statistics. Finally in Section 3.4.8 we give a corresponding result on quasi-symmetry for square two-way tables.

3.4.2 Exact tests for quasi-independence

Let $\boldsymbol{x} = \{x_{ij}\} \in \mathbb{Z}_{\geq 0}^{IJ}$ be an $I \times J$ contingency table. Let $S \subset \{(i,j) \mid i \in [I], j \in [J]\}$ be the set of cells that are not structural zeros. We consider models for the cell probability in incomplete contingency tables in the (natural) logarithmic scale as

$$\log p_{ij} = \mu + \alpha_i + \beta_j + \gamma_{ij} \tag{3.23}$$

for $(i,j) \in S$ and $p_{ij} \equiv 0$ for $(i,j) \notin S$. We then define the model of quasi-independence for the subtable S by setting

$$\mathrm{H}_0 : \gamma_{ij} = 0$$

for $(i,j) \in S$. This is a natural extension of the familiar model of independence of the variables corresponding to rows and columns in the ordinary two-way contingency tables. An interpretation of this model and restrictions on the parameters are discussed in detail in Bishop *et al.* (1975).

According to the general theory of similar tests described in Chapter 1, our approach is to base the inference on the conditional distribution given a sufficient statistic for the nuisance parameters. Under the null hypothesis of quasi-independence, the row sums, $x_{i\cdot}$, and the column sums, $x_{\cdot j}$, are the sufficient statistics for the nuisance parameters μ, α_i, β_j. The conditional distribution is then written as

$$f(\boldsymbol{x} \mid \{x_{i\cdot}\}, \{x_{\cdot j}\}, S) = C \prod_{(i,j)\in S} \frac{1}{x_{ij}!}, \tag{3.24}$$

where C is the normalizing constant determined from $\{x_{i\cdot}\}, \{x_{\cdot j}\}, S$ and written as

$$C^{-1} = \sum_{\boldsymbol{x}\in\mathcal{F}(\{x_{i\cdot}\},\{x_{\cdot j}\},S)} \left(\prod_{(i,j)\in S} \frac{1}{x_{ij}!} \right),$$

where

$$\mathcal{F}(\{x_{i\cdot}\}, \{x_{\cdot j}\}, S) = \left\{ \boldsymbol{Y} \;\middle|\; \sum_{j=1}^{J} y_{ij} = x_{i\cdot}, \sum_{i=1}^{I} y_{ij} = x_{\cdot j},\ y_{ij} \in \mathbb{Z},\ \text{and } y_{ij} = 0 \text{ for } (i,j) \notin S \right\}.$$

Hereafter, for simplicity we omit S in $\mathcal{F}(\{x_{i\cdot}\}, \{x_{\cdot j}\}, S)$, when $S = [I] \times [J]$, i.e., there is no structural zero cell. The discrepancy from the null hypothesis H_0 is measured by an appropriate test statistic. For each element in $\mathcal{F}(\{x_{i\cdot}\}, \{x_{\cdot j}\}, S)$, the value of this test statistic is calculated. The exact conditional p value is the sum of the conditional probabilities for the elements in $\mathcal{F}(\{x_{i\cdot}\}, \{x_{\cdot j}\}, S)$ which are at least as discrepant from the null hypothesis as the observed data. To calculate the p values, we use a Markov chain Monte Carlo method in this section, supposing the situations that a complete enumeration of all the elements in $\mathcal{F}(\{x_{i\cdot}\}, \{x_{\cdot j}\}, S)$, and hence the calculation of the normalizing constant C, is computationally infeasible.

3.4.3 Metropolis-Hastings sampling

To perform the exact tests of quasi-independence, our approach is to generate samples from $f(\boldsymbol{X} \mid \{x_{i\cdot}\}, \{x_{\cdot j}\}, S)$ and calculate the null distribution of various test statistics. If a connected Markov chain over $\mathcal{F}(\{x_{i\cdot}\}, \{x_{\cdot j}\}, S)$ is constructed, the chain can be modified to give a connected and aperiodic Markov chain with stationary distribution $f(\boldsymbol{X} \mid \{x_{i\cdot}\}, \{x_{\cdot j}\}, S)$ by the usual Metropolis procedure (Hastings, 1970, for example).

As we have seen in Section 3.1, if there is no structural zero cell, a connected Markov chain over $\mathcal{F}(\{x_{i\cdot}\}, \{x_{\cdot j}\})$ is easily constructed. Recall that the rectangular moves described in (3.1) form a Markov basis for this problem. On the other hand, if there are structural zero cells, a chain constructed from this type of moves might not be connected. As the simplest example, consider 3×3 contingency tables having structural zero cells as the diagonal elements, i.e., $S = \{(i,j),\ i \neq j\}$. If the marginal totals are $x_{i\cdot} = x_{\cdot j} = 1$ for all $1 \le i, j \le 3$, there are two states in $\mathcal{F}(\{x_{i\cdot}\}, \{x_{\cdot j}\}, S)$ displayed as

$$\boxed{\begin{array}{ccc} [0] & 1 & 0 \\ 0 & [0] & 1 \\ 1 & 0 & [0] \end{array}} \quad \text{and} \quad \boxed{\begin{array}{ccc} [0] & 0 & 1 \\ 1 & [0] & 0 \\ 0 & 1 & [0] \end{array}}\,.$$

Here and hereafter we denote a structural zero cell by [0], in order to distinguish it from a sampling zero cell. To connect these two states, moves such as

$$\begin{array}{|ccc|} \hline 0 & -1 & +1 \\ +1 & 0 & -1 \\ -1 & +1 & 0 \\ \hline \end{array}$$

are needed. In Smith *et al.* (1996), it is remarked without proofs that a connected chain can be constructed only by the moves such as (3.1) for $I \times I$ contingency tables with structural zeros as diagonal cells, when $I > 3$. In Section 3.4.7 we show that this statement is true when all the marginal totals are positive. But our concern in this section is to list a common minimal set of moves that is needed to construct a connected chain for *arbitrary* values of the marginal totals, depending only on the size of the contingency tables and S, the configuration of the structural zero cells.

To describe the problem precisely, we give a definition of a Markov basis and its minimality as described in Section 3.1, which adapt to this section. Let $\mathcal{F}_0(S)$ be the set of $I \times J$ integer arrays with non-structural zero cells as S and zero marginal totals

$$\mathcal{F}_0(S) = \{\, \boldsymbol{y} \mid y_{i\cdot} = y_{\cdot j} = 0,\ y_{ij} \in \mathbb{Z},\ \text{and } y_{ij} = 0 \text{ for } (i,j) \notin S \,\},$$

The elements of $\mathcal{F}_0(S)$ are *moves* on S.

Definition 3.4.1 *A Markov basis is a set $\mathcal{B} = \{\boldsymbol{z}_1, \ldots, \boldsymbol{z}_L\}$ of $I \times J$ integer arrays $\boldsymbol{z}_i \in \mathcal{F}_0(S)$, $i \in [L]$, such that, for any $\{x_{i\cdot}\}, \{x_{\cdot j}\}$ and $\boldsymbol{x}, \boldsymbol{x}' \in \mathcal{F}(\{x_{i\cdot}\}, \{x_{\cdot j}\}, S)$, there exist $A > 0$, $(\varepsilon_1, \boldsymbol{B}_{t_1}), \ldots, (\varepsilon_A, \boldsymbol{B}_{t_A})$ with $\varepsilon_s = \pm 1$, such that*

$$\boldsymbol{x}' = \boldsymbol{x} + \sum_{s=1}^{A} \varepsilon_s \boldsymbol{z}_{t_s} \quad \text{and} \quad \boldsymbol{x} + \sum_{s=1}^{a} \varepsilon_s \boldsymbol{z}_{t_s} \in \mathcal{F}(\{x_{i\cdot}\}, \{x_{\cdot j}\}, S) \text{ for } 1 \le a \le A.$$

A Markov basis $\mathcal{B}$ is minimal if no proper subset of $\mathcal{B}$ is a Markov basis.

3.4.4 Unique minimal basis for quasi-independence in two-way incomplete contingency tables

In this section, we derive a minimal Markov basis for $I \times J$ contingency tables with structural zeros. We assume the condition (3.11) again, i.e., that the level indices $i_1, i_2, \ldots$ and $j_1, j_2, \ldots$ are all distinct.

In this section, a loop described in Definition 3.3.2 again plays an important role. Though it is slightly redundant, we give the definition again in more precise form to use in the proofs of theorems afterward.

Definition 3.4.2 *A loop of degree r on S is an $I \times J$ integer array*

$$\boldsymbol{L}_r(i_1, \ldots, i_r; j_1, \ldots, j_r) \in \mathcal{F}_0(S), \quad i_1, \ldots, i_r \in [I],\ j_1, \ldots, j_r \in [J],$$

where $\boldsymbol{L}_r(i_1, \ldots, i_r; j_1, \ldots, j_r)$ has the elements

$$\begin{array}{l} L_{i_1 j_1} = L_{i_2 j_2} = \cdots = L_{i_{r-1} j_{r-1}} = L_{i_r j_r} = 1, \\ L_{i_1 j_2} = L_{i_2 j_3} = \cdots = L_{i_{r-1} j_r} = L_{i_r j_1} = -1, \end{array}$$

and all the other elements are zero. Specifically degree 2 loop $\boldsymbol{L}_2(i_1, i_2; j_1, j_2)$ is called a basic move. The support of $\boldsymbol{L}_r(i_1, \ldots, i_r; j_1, \ldots, j_r)$ is the set of its non-zero cells $\{(i_1, j_1), (i_1, j_2), \ldots, (i_r, j_1)\}$.

Note that because of the condition (3.11), there is at most one $+1$ and -1 in each row and each column of a degree r loop. Loops constitute an essential subset of $\mathcal{F}_0(S)$. We have already seen the role of the loops as Lemma 3.3.1 in Section 3.3.3, i.e., any $\boldsymbol{y} \in \mathcal{F}_0(S)$ can be expressed as a finite sum

$$\boldsymbol{y} = \sum_k a_k \boldsymbol{L}_{r(k)}(i_{1(k)}, \ldots, i_{r(k)}; j_{1(k)}, \ldots, j_{r(k)}), \tag{3.25}$$

where a_k is a positive integer, $r(k) \le \min\{I, J\}$ and there is no cancellation of signs in any cell. Here we give a proof of Lemma 3.3.1.

Proof of Lemma 3.3.1. Let $\boldsymbol{y} \in \mathcal{F}_0(S)$ have some nonzero elements and write $|\boldsymbol{y}| = \sum_{i=1}^{I} \sum_{j=1}^{J} |y_{ij}| < \infty$. Since all the row and column sums of $\boldsymbol{y}$ are zero, there exists at least one sequence $\{(i_1, j_1), (i_1, j_2), (i_2, j_2), (i_2, j_3), \ldots, (i_{p-1}, j_{p-1}), (i_{p-1}, j_p), (i_p, j_p), (i_p, j_1)\}$ satisfying

$$\begin{cases} y_{i_1 j_1}, y_{i_2 j_2}, \ldots, y_{i_{p-1} j_{p-1}}, y_{i_p j_p} > 0, \\ y_{i_1 j_2}, y_{i_2 j_3}, \ldots, y_{i_{p-1} j_p}, y_{i_p j_1} < 0. \end{cases} \tag{3.26}$$

We call the above sequence satisfying (3.26) a cycle $C(i_1, \ldots, i_p; j_1, \ldots, j_p)$ of the length p. Note that the condition (3.11) does not necessarily hold for cycles here. Our argument in this proof is to consider the shortest cycles, i.e., cycles which have the smallest length. We claim that the condition (3.11) holds for the shortest cycles for the following reason. Let $C(i_1, \ldots, i_r; j_1, \ldots, j_r)$ be one of the shortest cycles in $\boldsymbol{y}$ and suppose $i_n = i_m$ for $1 \le n < m \le r$. In this case, we see another cycle $C(i_n, i_{n+1}, \ldots, i_{m-1}; j_m, j_{n+1}, \ldots, j_{m-1})$ of the length $m - n < r$, which contradicts that $C(i_1, \ldots, i_r; j_1, \ldots, j_r)$ is a shortest cycle. Corresponding to this shortest cycle $C(i_1, \ldots, i_r; j_1, \ldots, j_r)$, let $0 < a \le \min\{y_{i_1 j_1}, \ldots, y_{i_r j_r}, -y_{i_1 j_2}, \ldots, -y_{i_r j_1}\}$ and $\boldsymbol{y}' = \boldsymbol{y} - a\boldsymbol{L}_r(i_1, \ldots, i_r; j_1, \ldots, j_r)$. Then we see that there is no cancellation of signs in any cell of the right hand side, and $\boldsymbol{y}'$ is again in $\mathcal{F}_0(S)$. Moreover it follows that $|\boldsymbol{y}'| = |\boldsymbol{y}| - 2ar < |\boldsymbol{y}|$. Similarly, we can subtract loops corresponding to the shortest cycles one by one, and make a finite sequence $\boldsymbol{y}'', \boldsymbol{y}''', \ldots$ satisfying $|\boldsymbol{y}| > |\boldsymbol{y}'| > |\boldsymbol{y}''| > |\boldsymbol{y}'''| > \cdots > |\boldsymbol{y}''^{\cdots}''| = 0$ since $|\boldsymbol{y}|$ is finite, which gives the expression (3.25). $r(k) \le \min\{I, J\}$ also holds from (3.11). Q.E.D.

We show an example to clarify the meaning of Lemma 3.3.1. Let $\boldsymbol{y} \in \mathcal{F}_0(S)$ be 4×5 integer array expressed as follows.

3	−2	0	−2	1
−2	3	0	0	−1
−1	−1	2	0	0
0	0	−2	2	0

In this example, the shortest cycle is $C(1, 2; 1, 2)$, which corresponds to the basic move $\boldsymbol{L}_2(1, 2; 1, 2)$.

Then we can subtract (twice) this basic move from $\boldsymbol{y}$ as follows.

$$\begin{array}{ccccc} \boldsymbol{y} & = & \begin{array}{|rrrrr|} \hline 2 & -2 & 0 & 0 & 0 \\ -2 & 2 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \\ \hline \end{array} & + & \begin{array}{|rrrrr|} \hline 1 & 0 & 0 & -2 & 1 \\ 0 & 1 & 0 & 0 & -1 \\ -1 & -1 & 2 & 0 & 0 \\ 0 & 0 & -2 & 2 & 0 \\ \hline \end{array} \\ & & & & \\ & = & 2\boldsymbol{L}_2(1,2;1,2) & + & \boldsymbol{y}' \end{array}$$

Note that there is no cancellation of signs in any cell and the remaining pattern, $\boldsymbol{y}' = \boldsymbol{y} - 2\boldsymbol{L}_2(1,2;1,2)$, is again in $\mathcal{F}_0(S)$. Hence we can consider a further decomposition of $\boldsymbol{y}'$. We observe that one of the shortest cycles in $\boldsymbol{y}'$ is $C(1,4,3;1,4,3)$, which corresponds to the degree 3 loop $\boldsymbol{L}_3(1,4,3;1,4,3)$, and the remaining pattern is $\boldsymbol{L}_4(1,4,3,2;5,4,3,2)$. Now the following decomposition of $\boldsymbol{y}$ is obtained.

$$\begin{array}{ccccccc} \boldsymbol{y} & = & \begin{array}{|rrrrr|} \hline 2 & -2 & 0 & 0 & 0 \\ -2 & 2 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \\ \hline \end{array} & + & \begin{array}{|rrrrr|} \hline 1 & 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & 0 & 0 \\ -1 & 0 & 1 & 0 & 0 \\ 0 & 0 & -1 & 1 & 0 \\ \hline \end{array} & + & \begin{array}{|rrrrr|} \hline 0 & 0 & 0 & -1 & 1 \\ 0 & 1 & 0 & 0 & -1 \\ 0 & -1 & 1 & 0 & 0 \\ 0 & 0 & -1 & 1 & 0 \\ \hline \end{array} \\ & & & & & & \\ & = & 2\boldsymbol{L}_2(1,2;1,2) & + & \boldsymbol{L}_3(1,4,3;1,4,3) & + & \boldsymbol{L}_4(1,4,3,2;5,4,3,2) \end{array}$$

It should be noted that this is not the only decomposition of $\boldsymbol{y}$.

$$\boldsymbol{y} = \boldsymbol{L}_2(1,2;1,2) + \boldsymbol{L}_2(1,2;5,2) + \boldsymbol{L}_3(1,4,3;1,4,3) + \boldsymbol{L}_4(1,4,3,2;1,4,3,2)$$

is another decomposition of $\boldsymbol{y}$, satisfying the condition of Lemma 3.3.1. Lemma 3.3.1 describes the relation between Definition 3.4.2 and a Markov chain over $\mathcal{F}(\{x_{i\cdot}\},\{x_{\cdot j}\},S)$. Suppose $\boldsymbol{x},\boldsymbol{x}' \in \mathcal{F}(\{x_{i\cdot}\},\{x_{\cdot j}\},S)$. Then the difference $\boldsymbol{y} = \boldsymbol{x} - \boldsymbol{x}'$ is in $\mathcal{F}_0(S)$. Hence to move from $\boldsymbol{x}$ to $\boldsymbol{x}'$, we can add a sequence of loops in Definition 3.4.2 to $\boldsymbol{x}$, without forcing negative entries on the way. In other words, a set of all the loops of degree $2,\ldots,\min\{I,J\}$ constitute a trivial Markov basis.

From the definition, we have the relations

$$\begin{aligned} \boldsymbol{L}_r(i_1,\ldots,i_r;j_1,\ldots,j_r) &= \boldsymbol{L}_r(i_2,\ldots,i_r,i_1;j_2,\ldots,j_r,j_1) \\ &= -\boldsymbol{L}_r(i_{r-1},i_{r-2},\ldots,i_2,i_1,i_r;j_r,j_{r-1},\ldots,j_2,j_1). \end{aligned}$$

Using these relations, we have $2r$ equivalent representations for a degree r loop. For example, a degree 4 loop used above

$$\begin{array}{|rrrrr|} \hline 0 & 0 & 0 & -1 & 1 \\ 0 & 1 & 0 & 0 & -1 \\ 0 & -1 & 1 & 0 & 0 \\ 0 & 0 & -1 & 1 & 0 \\ \hline \end{array}$$

is expressed as either as

$$\begin{array}{lll} \boldsymbol{L}_4(1,4,3,2;5,4,3,2), & \boldsymbol{L}_4(4,3,2,1;4,3,2,5), & \boldsymbol{L}_4(3,2,1,4;3,2,5,4), \\ \boldsymbol{L}_4(2,1,4,3;2,5,4,3), & -\boldsymbol{L}_4(3,4,1,2;2,3,4,5), & -\boldsymbol{L}_4(4,1,2,3;3,4,5,2), \\ -\boldsymbol{L}_4(1,2,3,4;4,5,2,3), & -\boldsymbol{L}_4(2,3,4,1;5,2,3,4). & \end{array}$$

Then if there is no structural zero cells, there are

$$\sum_{r=2}^{\min\{I,J\}} \binom{I}{r}\binom{J}{r}\frac{(r!)^2}{2r}$$

distinct loops in $I \times J$ contingency tables.

It is well known that the set of all basic moves constitutes a Markov basis for the case of no structural zero cells. Moreover, it is shown in Section 3.5 that this is the unique minimal Markov basis. In the presence of structural zeros, the set of loops is generally not a minimal basis. In this section, we give an explicit characterization of the unique minimal Markov basis for an arbitrary configuration of structural zero cells. The next definition provides a key tool.

Definition 3.4.3 *A loop $\boldsymbol{L}_r(i_1,\dots,i_r;j_1,\dots,j_r)$ is called df 1 if $R(i_1,\dots,i_r;j_1,\dots,j_r)$ does not contain support of any loop on S of degree $2,\dots,r-1$, where*

$$R(i_1,\dots,i_r;j_1,\dots,j_r) = R(\boldsymbol{L}_r(i_1,\dots,i_r;j_1,\dots,j_r)) = \{(i,j) \mid i \in \{i_1,\dots,i_r\}, j \in \{j_1,\dots,j_r\}\}$$

is the supporting rectangle of $\boldsymbol{L}_r(i_1,\dots,i_r;j_1,\dots,j_r)$ described in Section 3.3.1.

Here the term *df* is intended as "degree of freedom". To clarify the meaning of this definition, we give an equivalent condition to Definition 3.4.3 in the following lemma.

Lemma 3.4.1 *$\boldsymbol{L}_r(i_1,\dots,i_r;j_1,\dots,j_r)$ is df 1 if and only if $R(i_1,\dots,i_r;j_1,\dots,j_r)$ contains exactly two elements in S in every row and column.*

Proof. The case $r = 2$ is obvious. Consider $r \geq 3$.

(Sufficiency) We argue by contradiction. By permuting the rows and columns, without loss of generality suppose that $\boldsymbol{L}_r(1,\dots,r;1,\dots,r)$ is a degree r loop which does not satisfy the statement of the lemma. We also suppose $(1,a) \in S,\ 3 \leq \exists a \leq r$, without loss of generality. Then this loop is decomposed as

$$\begin{aligned}\boldsymbol{L}_r(1,\dots,r;1,\dots,r) &= \boldsymbol{L}_{r-a+2}(1,a,a+1,\dots,r;1,a,a+1,\dots,r)\\ &\qquad + \boldsymbol{L}_{a-1}(1,2,\dots,a-1;a,2,3,\dots,a-1). \qquad (3.27)\end{aligned}$$

An example of $r = 5, a = 4$ is displayed as follows.

$$\begin{array}{|ccccc|}\hline +1 & -1 & [0] & 0 & [0]\\ [0] & +1 & -1 & [0] & [0]\\ [0] & [0] & +1 & -1 & [0]\\ [0] & [0] & [0] & +1 & -1\\ -1 & [0] & [0] & [0] & +1\\ \hline\end{array} = \begin{array}{|ccccc|}\hline +1 & 0 & [0] & -1 & [0]\\ [0] & 0 & 0 & [0] & [0]\\ [0] & [0] & 0 & 0 & [0]\\ [0] & [0] & [0] & +1 & -1\\ -1 & [0] & [0] & [0] & +1\\ \hline\end{array} + \begin{array}{|ccccc|}\hline 0 & -1 & [0] & +1 & [0]\\ [0] & +1 & -1 & [0] & [0]\\ [0] & [0] & +1 & -1 & [0]\\ [0] & [0] & [0] & 0 & 0\\ 0 & [0] & [0] & [0] & 0\\ \hline\end{array}$$

Here, the nonzero cells of the two loops, $\boldsymbol{L}_{r-a+2}(1,a,a+1,\dots,r;1,a,a+1,\dots,r)$ and $\boldsymbol{L}_{a-1}(1,2,\dots,a-1;a,2,3,\dots,a-1)$ overlap at $(1,a) \in S$ only. Therefore $R(1,\dots,r;1,\dots,r)$ contains the supports of $\boldsymbol{L}_{r-a+2}(1,a,a+1,\dots,r;1,a,a+1,\dots,r)$ and $\boldsymbol{L}_{a-1}(1,2,\dots,a-1;a,2,3,\dots,a-1)$, which are loops on S. Hence $\boldsymbol{L}_r(1,\dots,r;1,\dots,r)$ is not df 1.

(Necessity) Suppose that $\boldsymbol{L}_r(1,\dots,r;1,\dots,r)$ is a degree r loop such that $R(1,\dots,r;1,\dots,r)$ contains exactly two elements in S in every row and column. Without loss of generality, it is sufficient to show that $R(1,\dots,r-1;1,\dots,r)$ does not contain support of any loop of degree $2,\dots,r-1$ on S. An example of $R(1,2,3,4;1,2,3,4,5)$ is displayed as follows.

$$\begin{array}{|ccccc|}\hline L_{11} & L_{12} & [0] & [0] & [0] \\ [0] & L_{22} & L_{23} & [0] & [0] \\ [0] & [0] & L_{33} & L_{34} & [0] \\ [0] & [0] & [0] & L_{44} & L_{45} \\ \hline\end{array}$$

From the assumption, $(1,1)$ is the only cell in S in $R(1,\dots,r-1;1)$, since $\boldsymbol{L}_r(1,\dots,r;1,\dots,r)$ has exactly two nonzero elements there, i.e., $L_{11}=+1$ and $L_{r1}=-1$. Hence L_{11} is zero in any loop in $R(1,\dots,r-1;1,\dots,r)$. Moreover, by using the constraints $L_{1\cdot}=L_{\cdot 2}=L_{2\cdot}=\cdots=L_{r-1\cdot}=0$, it is shown that only the element of $\mathcal{F}_0(S)$ that can be contained in $R(1,\dots,r-1;1,\dots,r)$ is the zero contingency table. Q.E.D.

Lemma 3.4.1 describes the forms of the df 1 loops. The displays below are examples of df 1 loops of degree 2,3,4 in 4×5 integer arrays.

$$\begin{array}{|ccccc|}\hline +1 & -1 & 0 & 0 & 0 \\ -1 & +1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \\ \hline\end{array} \quad \begin{array}{|ccccc|}\hline +1 & -1 & [0] & 0 & 0 \\ -1 & [0] & +1 & 0 & 0 \\ [0] & +1 & -1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \\ \hline\end{array} \quad \begin{array}{|ccccc|}\hline +1 & -1 & [0] & [0] & 0 \\ -1 & [0] & +1 & [0] & 0 \\ [0] & +1 & [0] & -1 & 0 \\ [0] & [0] & -1 & +1 & 0 \\ \hline\end{array}$$

Obviously, every basic move is df 1. The term df 1 is motivated by the following consideration. Denote the positive and the negative part of a df 1 loop $\boldsymbol{L}_r(i_1,\dots,i_r;j_1,\dots,j_r)$ as $\boldsymbol{L}_r^+(i_1,\dots,i_r;j_1,\dots,j_r)$ and $\boldsymbol{L}_r^-(i_1,\dots,i_r;j_1,\dots,j_r)$, respectively, i.e.,

$$L_{ij}^+=\max(L_{ij},0),\ \ L_{ij}^-=\max(-L_{ij},0).$$

Then

$$\boldsymbol{L}_r(i_1,\dots,i_r;j_1,\dots,j_r)=\boldsymbol{L}_r^+(i_1,\dots,i_r;j_1,\dots,j_r)-\boldsymbol{L}_r^-(i_1,\dots,i_r;j_1,\dots,j_r). \tag{3.28}$$

Here, consider the set of contingency tables which have the same marginal totals and the configuration of S as $\boldsymbol{L}_r^+(i_1,\dots,i_r;j_1,\dots,j_r)$ or $\boldsymbol{L}_r^-(i_1,\dots,i_r;j_1,\dots,j_r)$, in other words,

$$\mathcal{F}(\{L_{i\cdot}^+\},\{L_{\cdot j}^+\},S)=\mathcal{F}(\{L_{i\cdot}^-\},\{L_{\cdot j}^-\},S).$$

Then we see that this set is a two-elements set with $\boldsymbol{L}_r^+(i_1,\dots,i_r;j_1,\dots,j_r)$ and $\boldsymbol{L}_r^-(i_1,\dots,i_r;j_1,\dots,j_r)$ being the only members.

Here we give our main theorem.

Theorem 3.4.1 *The set of df* 1 *loops of degree* $2,\dots,\min\{I,J\}$ *constitutes a unique minimal Markov basis for* $I\times J$ *contingency tables.*

Proof. We have already seen that the set of loops forms a Markov basis. We also note that every minimal Markov basis has to contain all loops of degrees $2, \ldots, \min\{I, J\}$ on S. This is because, as we have seen in (3.28), df 1 loop is written as the difference of the two elements of $\mathcal{F}(\{x_{i\cdot}\}, \{x_{\cdot j}\}, S)$, which is exactly the two-elements set. Following the arguments of indispensable moves in Section 3.5, we only need to verify that the set of the df 1 loops is itself a Markov basis. In order to show this, we argue by induction. We start from the trivial Markov basis consisting of all loops. We look at a non-df-1 loop of the highest degree. Below we show that this loop can be replaced by a combination of loops of smaller degrees, so that the resulting set is still a Markov basis. Then by induction on the highest degree of non-df-1 loops, it follows that the set of df 1 loops is a Markov basis.

In order to show that a non-df-1 loop of the highest degree can be replaced by combination of loops of lower degrees we again use the decomposition of loops that we have already seen. Suppose a Markov basis contains non-df-1 loops. Without loss of generality let $\boldsymbol{L}_r(1, \ldots, r; 1, \ldots, r)$ be a non-df-1 loop of the highest degree and $(1, a) \in S, 3 \le \exists a \le r$. Then this loop is decomposed as (3.27). Here, the two loops, $\boldsymbol{L}_{r-a+2}(1, a, a+1, \ldots, r; 1, a, a+1, \ldots, r)$ and $\boldsymbol{L}_{a-1}(1, 2, \ldots, a-1; a, 2, 3, \ldots, a-1)$, overlap, i.e., have nonzero element in common position, only at $(1, a) \in S$. Since $(1, a)$ elements of these loops are -1 and $+1$, respectively, we can add or subtract these loops in an appropriate order to $\boldsymbol{x} \in \mathcal{F}(\{x_{i\cdot}\}, \{x_{\cdot j}\}, S)$ without forcing negative entries on the way, instead of adding or subtracting $\boldsymbol{L}_r(1, \ldots, r; 1, \ldots, r)$ to $\boldsymbol{x}$. Therefore $\boldsymbol{L}_r(1, \ldots, r; 1, \ldots, r)$ can be removed from the Markov basis and the remaining set is still a Markov basis. Q.E.D.

We clarify the last step of the above proof by an example. Let $\boldsymbol{x}$ and $\boldsymbol{x}'$ be

$$
\boldsymbol{x} = \begin{array}{|ccccc|}\hline 0 & 1 & [0] & 0 & [0] \\ [0] & 0 & 1 & [0] & [0] \\ [0] & [0] & 0 & 1 & [0] \\ [0] & [0] & [0] & 0 & 1 \\ 1 & [0] & [0] & [0] & 0 \\ \hline \end{array}\,, \qquad \boldsymbol{x}' = \begin{array}{|ccccc|}\hline 1 & 0 & [0] & 0 & [0] \\ [0] & 1 & 0 & [0] & [0] \\ [0] & [0] & 1 & 0 & [0] \\ [0] & [0] & [0] & 1 & 0 \\ 0 & [0] & [0] & [0] & 1 \\ \hline \end{array}\,.
$$

$\boldsymbol{x}$ and $\boldsymbol{x}'$ are in the same $\mathcal{F}(\{x_{i\cdot}\}, \{x_{\cdot j}\}, S)$ and the difference $\boldsymbol{x}' - \boldsymbol{x}$ is expressed as a non-df-1 loop,

$$
\boldsymbol{L}_5(1,2,3,4,5;1,2,3,4,5) = \begin{array}{|ccccc|}\hline +1 & -1 & [0] & 0 & [0] \\ [0] & +1 & -1 & [0] & [0] \\ [0] & [0] & +1 & -1 & [0] \\ [0] & [0] & [0] & +1 & -1 \\ -1 & [0] & [0] & [0] & +1 \\ \hline \end{array}\,.
$$

However we have already seen the decomposition

$$
\begin{aligned}
\boldsymbol{L}_5(1,2,3,4,5;1,2,3,4,5) &= \begin{array}{|ccccc|}\hline +1 & 0 & [0] & -1 & [0] \\ [0] & 0 & 0 & [0] & [0] \\ [0] & [0] & 0 & 0 & [0] \\ [0] & [0] & [0] & +1 & -1 \\ -1 & [0] & [0] & [0] & +1 \\ \hline \end{array} + \begin{array}{|ccccc|}\hline 0 & -1 & [0] & +1 & [0] \\ [0] & +1 & -1 & [0] & [0] \\ [0] & [0] & +1 & -1 & [0] \\ [0] & [0] & [0] & 0 & 0 \\ 0 & [0] & [0] & [0] & 0 \\ \hline \end{array} \\
&= \qquad \boldsymbol{L}_3(1,4,5;1,4,5) \qquad + \qquad \boldsymbol{L}_3(1,2,3;4,2,3).
\end{aligned}
$$

Seeing that the $(1,4)$ element of $\boldsymbol{L}_3(1,2,3;4,2,3)$ is positive, it follows $\boldsymbol{x} + \boldsymbol{L}_3(1,2,3;4,2,3) \in \mathcal{F}(\{x_{i\cdot}\},\{x_{\cdot j}\},S)$ as

$$\boldsymbol{x} + \boldsymbol{L}_3(1,2,3;4,2,3) = \begin{array}{|ccccc|} \hline 0 & 0 & [0] & 1 & [0] \\ [0] & 1 & 0 & [0] & [0] \\ [0] & [0] & 1 & 0 & [0] \\ [0] & [0] & [0] & 0 & 1 \\ 1 & [0] & [0] & [0] & 0 \\ \hline \end{array}\,.$$

Now, seeing that $(1,4),(4,5),(5,1)$ elements are positive, we can add $\boldsymbol{L}_3(1,4,5;1,4,5)$ to $\boldsymbol{x} + \boldsymbol{L}_3(1,2,3;4,2,3)$ and obtain $\boldsymbol{x}'$. Hence it is shown that the non-df-1 loop $\boldsymbol{L}_5(1,2,3,4,5;1,2,3,4,5)$ is redundant. It should also be noted that the two loops, $\boldsymbol{L}_3(1,4,5;1,4,5)$ and $\boldsymbol{L}_3(1,2,3;4,2,3)$, are both df 1 and hence cannot be removed.

Remark. As is stated in Remark 3.4 of Diaconis and Sturmfels (1998), two-way contingency tables with structural zero cells are considered to be a subgraph G of K_{IJ}, where K_{IJ} is the complete bipartite graph on I and J nodes, and G is formed by deleting the edges (i,j) of K_{IJ} for $(i,j) \notin S$. In graph theoretic terms, a cycle in G corresponds to a move on S, and an induced cycle in G corresponds to a df 1 move on S. Theorem 3.4.1 states that the set of all induced cycles in G constitute a unique minimal Markov basis. See Ohsugi and Hibi (1999a) for further relations between bipartite graphs and Gröbner basis.

Example. Comparison of the minimal basis and the reduced Gröbner basis. Consider 6×6 contingency tables of the following form.

$$\begin{array}{|cccccc|} \hline [0] & x_{12} & x_{13} & [0] & [0] & x_{16} \\ x_{21} & [0] & x_{23} & x_{24} & [0] & [0] \\ x_{31} & x_{32} & [0] & [0] & x_{35} & [0] \\ [0] & [0] & x_{43} & [0] & x_{45} & x_{46} \\ x_{51} & [0] & [0] & x_{54} & [0] & x_{56} \\ [0] & x_{62} & [0] & x_{64} & x_{65} & [0] \\ \hline \end{array}$$

By the algebraic algorithm described in Diaconis and Sturmfels (1998), we calculated the reduced Gröbner basis using the degree reverse lexicographical ordering. The result was composed of 3 basic moves, 20 degree 3 loops, 10 degree 4 loops and 3 degree 5 loops. The following is a list of these loops.

$\boldsymbol{L}_2(1,4;6,3)$	$\boldsymbol{L}_2(2,5;4,1)$	$\boldsymbol{L}_2(3,6;5,2)$
$\boldsymbol{L}_3(1,2,3;2,3,1)$	$\boldsymbol{L}_3(1,2,5;6,3,1)$	$\boldsymbol{L}_3(1,2,5;6,3,4)$
$\boldsymbol{L}_3(1,3,4;6,2,5)$	$\boldsymbol{L}_3(1,3,5;6,2,1)$	$\boldsymbol{L}_3(1,4,3;2,3,5)$
$\boldsymbol{L}_3(1,6,2;3,2,4)$	$\boldsymbol{L}_3(1,6,4;3,2,5)$	$\boldsymbol{L}_3(1,6,4;6,2,5)$
$\boldsymbol{L}_3(1,6,5;6,2,4)$	$\boldsymbol{L}_3(2,3,6;4,1,2)$	$\boldsymbol{L}_3(2,4,3;1,3,5)$
$\boldsymbol{L}_3(2,5,4;3,1,6)$	$\boldsymbol{L}_3(2,5,4;3,4,6)$	$\boldsymbol{L}_3(2,6,3;1,4,5)$
$\boldsymbol{L}_3(2,6,4;3,4,5)$	$\boldsymbol{L}_3(3,5,4;5,1,6)$	$\boldsymbol{L}_3(3,5,6;5,1,4)$
$\boldsymbol{L}_3(3,6,5;1,2,4)$	$\boldsymbol{L}_3(4,5,6;5,6,4)$	
$\boldsymbol{L}_4(1,2,3,4;6,3,1,5)$	$\boldsymbol{L}_4(1,2,6,3;2,3,4,5)$	$\boldsymbol{L}_4(1,3,2,5;6,2,1,4)$
$\boldsymbol{L}_4(1,3,5,4;3,2,1,6)$	$\boldsymbol{L}_4(1,5,6,3;2,6,4,5)$	$\boldsymbol{L}_4(1,6,5,4;3,2,4,6)$
$\boldsymbol{L}_4(1,6,5,2;3,2,4,1)$	$\boldsymbol{L}_4(2,3,6,4;3,1,2,5)$	$\boldsymbol{L}_4(2,5,4,3;1,4,6,5)$
$\boldsymbol{L}_4(3,6,4,5;1,2,5,6)$		
$\boldsymbol{L}_5(1,3,2,5,4;3,2,1,4,6)$	$\boldsymbol{L}_5(1,3,2,6,4;3,2,1,4,5)$	$\boldsymbol{L}_5(1,3,5,6,4;3,2,1,4,5)$

This list is very confusing and we cannot recognize the structure of the basis at first sight. One reason for the difficulty is that the above list is not minimal. (Note that the reduced Gröbner basis may not be a minimal basis.) It can be easily checked that the loops of degree 4 and 5 are not df 1. On the other hand, all the 20 loops of degree 3 are df 1. Hence from Theorem 3.4.1, the above 3 basic moves and 20 degree 3 loops constitute the unique minimal Markov basis.

In Section 3.4.5, a simple algorithm to list all the elements of the unique minimal Markov basis is given.

3.4.5 Algorithms for enumerating elements of a minimal basis

In this section, we discuss how to list all the elements of the unique minimal basis. As we have seen, the elements of the unique minimal Markov basis have a simple structure described in Lemma 3.4.1. Considering this structure, we have an explicit form of a minimal basis for some typical situations, which play important roles in applications. We consider these special cases first and then consider general cases.

Separable tables Separability is one of the most important concepts for analyzing incomplete contingency tables. The definition of the separability is as follows (Mantel, 1970, Bishop *et al.*, 1975). In a two-way contingency table two cells are *associated* if they do not contain structural zeros and if they are either in the same row or the same column. A set of non-structural zero cells is *connected* if every pairs of cells can be linked by a chain of cells, any two consecutive members of which must be associated. Finally, an incomplete two-way table is connected if its non-structural zero cells form a connected set. An incomplete table that is not connected is said to be *separable*. Separable two-way contingency tables can be rearranged to a block diagonal form with connected subtables by permuting the rows and columns. Table 3.1 is an example of separable table from Harris (1910). By permuting the rows and columns, we see that this table is separable with exactly two connected subtables as displayed in Table 3.2.

We see easily that the minimal Markov basis for this example consists of basic moves only. This is obvious from the fact that the two connected subtables do not contain structural zero cells respectively. When the connected subtables contain some structural zero cells, the minimal

Table 3.1: An example of a separable table:
Relationship between radial asymmetry and locular
composition in *Staphylea* (Series A of Harris, 1910)

locular composition	coefficient of radial asymmetry 0.00	0.47	0.82	0.94	1.25	1.41	1.63	1.70	1.89
3 even, 0 odd	462	[0]	[0]	130	[0]	[0]	2	[0]	1
2 even, 1 odd	[0]	614	138	[0]	21	14	[0]	1	[0]
1 even, 2 odd	[0]	443	95	[0]	22	8	[0]	5	[0]
0 even, 3 odd	103	[0]	[0]	35	[0]	[0]	1	[0]	0

Table 3.2: Data from Table 3.1 after rearrangement of rows and columns

locular composition	coefficient of radial asymmetry 0.00	0.94	1.63	1.89	0.47	0.82	1.25	1.41	1.70
3 even, 0 odd	462	130	2	1	[0]	[0]	[0]	[0]	[0]
0 even, 3 odd	103	35	1	0	[0]	[0]	[0]	[0]	[0]
2 even, 1 odd	[0]	[0]	[0]	[0]	614	138	21	14	1
1 even, 2 odd	[0]	[0]	[0]	[0]	443	95	22	8	5

Markov basis for the whole table is a union of the minimal Markov bases for these subtables. For example, the minimal Markov basis for the following separable 6×7 contingency table

$$\begin{array}{|ccccccc|}\hline x_{11} & x_{12} & x_{13} & [0] & [0] & [0] & [0] \\ [0] & [0] & x_{23} & x_{24} & [0] & [0] & [0] \\ x_{31} & x_{32} & [0] & x_{34} & [0] & [0] & [0] \\ [0] & [0] & [0] & [0] & x_{45} & x_{46} & [0] \\ [0] & [0] & [0] & [0] & [0] & x_{56} & x_{57} \\ [0] & [0] & [0] & [0] & x_{65} & [0] & x_{67} \\ \hline \end{array}$$

is the union of the minimal Markov basis for two subtables,

$$\begin{array}{|cccc|}\hline x_{11} & x_{12} & x_{13} & [0] \\ [0] & [0] & x_{23} & x_{24} \\ x_{31} & x_{32} & [0] & x_{34} \\ \hline \end{array} \quad \text{and} \quad \begin{array}{|ccc|}\hline x_{45} & x_{46} & [0] \\ [0] & x_{56} & x_{57} \\ x_{65} & [0] & x_{67} \\ \hline \end{array}.$$

We see it is $\{\boldsymbol{L}_2(1,3;1,2), \boldsymbol{L}_3(1,2,3;1,3,4), \boldsymbol{L}_3(1,2,3;2,3,4), \boldsymbol{L}_3(4,5,6;5,6,7)\}$.

Block triangular tables Another typical situation is that an incomplete table is in *block triangular* form, i.e., after suitable permutation of rows and columns, $(i,j) \notin S$ implies $(k,l) \notin S$ for all $k \geq i$ and $l \geq j$ (Goodman, 1968, Bishop *et al.*, 1975). The following tables are examples of block triangular tables.

$$\begin{array}{|cccc|}\hline x_{11} & x_{12} & x_{13} & x_{14} \\ x_{21} & x_{22} & x_{23} & [0] \\ x_{31} & x_{32} & [0] & [0] \\ x_{41} & [0] & [0] & [0] \\ \hline \end{array} \quad \begin{array}{|cccc|}\hline [0] & [0] & x_{13} & x_{14} \\ [0] & [0] & x_{23} & x_{24} \\ x_{31} & x_{32} & x_{33} & x_{34} \\ x_{41} & x_{42} & x_{43} & x_{44} \\ \hline \end{array} \quad \begin{array}{|cccc|}\hline x_{11} & x_{12} & x_{13} & x_{14} \\ [0] & x_{22} & x_{23} & x_{24} \\ [0] & x_{32} & x_{33} & x_{34} \\ [0] & [0] & x_{43} & x_{44} \\ [0] & [0] & x_{53} & x_{54} \\ \hline \end{array}$$

Table 3.3 shows an example of a block triangle contingency table from Bishop and Fienberg (1969). The minimal Markov bases for these tables are simple, i.e., the set of basic moves

Table 3.3: An example of a block triangular table:
Initial and final ratings on disability of stroke patients

	final state				
initial state	A	B	C	D	E
E	11	23	12	15	8
D	9	10	4	1	[0]
C	6	4	4	[0]	[0]
B	4	5	[0]	[0]	[0]
A	5	[0]	[0]	[0]	[0]

Source: Bishop and Fienberg (1969).

constitutes the minimal Markov basis. Hence a Metropolis-Hasting sampling can be constructed simply by choosing pairs of rows and columns, which intersect at non-structural zero cells. McDonald and Smith (1995) also proposed Monte Carlo exact tests of quasi-independence for such types of tables.

Square tables with diagonal elements being structural zeros There are many situations that the contingency tables are square and all the diagonal elements are structural zero cells. Table 3.4 is an example of such tables. It is obvious that the minimal Markov basis for

Table 3.4: An example of a square table
with diagonal elements being structural zeros

	passive participant					
active participant	R	S	T	U	V	W
R	[0]	1	5	8	9	0
S	29	[0]	14	46	4	0
T	0	0	[0]	0	0	0
U	2	3	1	[0]	28	2
V	0	0	0	0	[0]	1
W	9	25	4	6	13	[0]

Source: Ploog (1967).

such tables contains degree 3 loops which correspond to every triplet of the structural zeros. For examples, degree 3 loops such as

$$\begin{array}{|cccccc|}\hline [0] & -1 & +1 & 0 & 0 & 0 \\ +1 & [0] & -1 & 0 & 0 & 0 \\ -1 & +1 & [0] & 0 & 0 & 0 \\ 0 & 0 & 0 & [0] & 0 & 0 \\ 0 & 0 & 0 & 0 & [0] & 0 \\ 0 & 0 & 0 & 0 & 0 & [0] \\ \hline \end{array} \quad \text{or} \quad \begin{array}{|cccccc|}\hline [0] & 0 & 0 & 0 & 0 & 0 \\ 0 & [0] & 0 & 0 & +1 & -1 \\ 0 & 0 & [0] & 0 & 0 & 0 \\ 0 & 0 & 0 & [0] & 0 & 0 \\ 0 & -1 & 0 & 0 & [0] & +1 \\ 0 & +1 & 0 & 0 & -1 & [0] \\ \hline \end{array}$$

are needed to construct a connected Markov chain. It is seen that for $I \times I$ contingency tables, there are $\binom{I}{2}\binom{I-2}{2}$ basic moves and $\binom{I}{3}$ df 1 degree 3 loops in the minimal Markov basis.

For such types of contingency tables, the hypothesis of quasi-symmetry is also of interest in many situations (Smith *et al.*, 1996). We also derive the unique minimal Markov basis for the case of a quasi-symmetry hypothesis in Section 3.4.8.

General incomplete tables We have seen some typical situations which frequently appear in applications. Now we give some rules and algorithms to list all the elements in the minimal Markov basis for arbitrary configuration of structural zeros. Table 3.5 is an example of incomplete tables which cannot be categorized as any type discussed above. In view of Lemma

Table 3.5: Classification of Purum marriages

	Sib of husband				
Sib of wife	Marrim	Makan	Parpa	Thao	Kheyang
Marrim	[0]	5	17	[0]	6
Makan	5	[0]	0	16	2
Parpa	[0]	2	[0]	10	11
Thao	10	[0]	[0]	[0]	9
Kheyang	6	20	8	0	1

Source: White (1963), based on data of Das (1945).

3.4.1, it may be easy to list all the elements of the unique minimal basis for many situations, especially when there are only a few structural zero cells.

It is also easy to obtain an upper bound of the degree of loops which is in the minimal basis, simply by counting the number of structural zero cells in each row and column. It should be noted that if the minimal Markov basis contains a degree r loop, then there are at least r rows and r columns which have $r-2$ structural zero cells. Hence for Table 3.5, we see that the degree of the loops contained in the minimal Markov basis is at most 3. For these types of contingency tables, simple enumeration algorithms may be effective. Indeed, for Table 3.5, we see that $\boldsymbol{L}_3(1,2,3;2,3,4)$ is the only degree 3 loop in the minimal basis by considering every triplet of structural zero cells located in distinct rows and columns.

In general, we can make use of the following recursive algorithm to list all the elements in the minimal basis. This algorithm works especially well in some situations that the contingency table is *near* separable, or *semi-separable* (Mantel, 1970), i.e., when the table can be made separable into two or more connected subtables by the removal of a single row or a single column. The following tables are examples of semi-separable tables.

$$(i)\qquad \begin{array}{|ccccc|}\hline x_{11} & x_{12} & [0] & [0] & [0] \\ x_{21} & x_{22} & [0] & [0] & x_{25} \\ [0] & [0] & x_{33} & x_{34} & x_{35} \\ [0] & [0] & x_{43} & x_{44} & [0] \\ [0] & [0] & x_{53} & x_{54} & x_{55} \\ \hline \end{array} \qquad (ii)\qquad \begin{array}{|ccccc|}\hline x_{11} & x_{12} & [0] & [0] & [0] \\ x_{21} & x_{22} & [0] & [0] & [0] \\ [0] & [0] & x_{33} & x_{34} & x_{35} \\ [0] & [0] & x_{43} & x_{44} & [0] \\ x_{51} & x_{52} & [0] & x_{54} & x_{55} \\ \hline \end{array}$$

We see that these tables are made to be separable by removal of *(i)* the row 2 or the column 5 and *(ii)* the row 5, respectively. Now we give a simple recursive algorithm.

```
Input:  I_0 = {1,...,I}, J_0 = {1,...,J}, S
Output:  elements of a minimal basis

ListMoves(I_0; J_0)
{
    Choose i* ∈ I_0 and J* = {j | (i*, j) ∈ S};
    List df 1 moves which have ±1 elements in R(i*; J*);
    ListMoves(I_0 − {i*}; J_0);
}
```

To illustrate the meanings of this algorithm, we reanalyze the 6×6 example discussed in Section 3.4.4, which is displayed below.

$$\begin{array}{c|cccccc|} & 1 & 2 & 3 & 4 & 5 & 6 \\ \hline 1 & [0] & x_{12} & x_{13} & [0] & [0] & x_{16} \\ 2 & x_{21} & [0] & x_{23} & x_{24} & [0] & [0] \\ 3 & x_{31} & x_{32} & [0] & [0] & x_{35} & [0] \\ 4 & [0] & [0] & x_{43} & [0] & x_{45} & x_{46} \\ 5 & x_{51} & [0] & [0] & x_{54} & [0] & x_{56} \\ 6 & [0] & x_{62} & [0] & x_{64} & x_{65} & [0] \\ \hline \end{array}$$

It has been already mentioned that the minimal Markov basis for this table is a set of basic moves and 20 degree 3 loops. To see this, first we choose $i^* = 1$ and hence $J^* = \{2, 3, 6\}$. We also denote $\widetilde{I} = I_0 - \{i^*\} = \{2, 3, 4, 5, 6\}$, $\widetilde{J} = J_0 - J^* = \{1, 4, 5\}$.

$$\begin{array}{cc|ccc|ccc|} & & & \widetilde{J} & & & J^* & \\ & & 1 & 4 & 5 & 2 & 3 & 6 \\ \hline i^* & 1 & [0] & [0] & [0] & x_{12} & x_{13} & x_{16} \\ \hline & 2 & x_{21} & x_{24} & [0] & [0] & x_{23} & [0] \\ & 3 & x_{31} & [0] & x_{35} & x_{32} & [0] & [0] \\ \widetilde{I} & 4 & [0] & [0] & x_{45} & [0] & x_{43} & x_{46} \\ & 5 & x_{51} & x_{54} & [0] & [0] & [0] & x_{56} \\ & 6 & [0] & x_{64} & x_{65} & x_{62} & [0] & [0] \\ \hline \end{array}$$

Next step of the algorithm is to list all df 1 loops which have ± 1 elements in $R(i^*; J^*)$. To perform this step, we can make use of the fact that such loop has exactly one $+1$ and one -1 both in $R(i^*; J^*)$ and $R(\widetilde{I}; J^*)$. For example, if we select $(2, 3)$ from J^* and $(2, 3)$ from $\widetilde{I}$, we can ignore the column 6, the rows 4 and 6. We can also ignore the column 5 because this column has only one cell in S when we ignore the rows 4 and 6. Then the table is reduced to the following.

$$
\begin{array}{cc|cc|cc|}
 & & \multicolumn{2}{c|}{\widetilde{J}} & \multicolumn{2}{c}{J^*} \\
 & & 1 & 4 & 2 & 3 \\
\cline{3-6}
i^* & 1 & [0] & [0] & x_{12} & x_{13} \\
\hline
 & 2 & x_{21} & x_{24} & [0] & x_{23} \\
\widetilde{I} & 3 & x_{31} & [0] & x_{32} & [0] \\
 & 5 & x_{51} & x_{54} & [0] & [0] \\
\cline{3-6}
\end{array}
$$

This subtable contains supports of $\boldsymbol{L}_3(1, 2, 3; 2, 3, 1)$ and $\boldsymbol{L}_4(1, 2, 4, 3; 3, 4, 2, 1)$. However, $\boldsymbol{L}_4(1, 2, 4, 3; 3, 4, 2, 1)$ is not df 1, and only $\boldsymbol{L}_3(1, 2, 3; 2, 3, 1)$ is listed in this case. Similarly we can list all loops which have exactly one $+1$ and one -1 both in $R(i^*; J^*)$ and $R(\widetilde{I}; J^*)$ by listing all pairs of columns in J^*. In this case,

- if select $(2, 3)$ from J^* then $\boldsymbol{L}_3(1, 2, 3; 2, 3, 1), \boldsymbol{L}_3(1, 6, 2; 3, 2, 4), \boldsymbol{L}_3(1, 4, 3; 2, 3, 5)$ and $\boldsymbol{L}_3(1, 6, 4; 3, 2, 5)$ are listed,
- if select $(2, 6)$ from J^* then $\boldsymbol{L}_3(1, 3, 4; 6, 2, 5), \boldsymbol{L}_3(1, 3, 5; 6, 2, 1), \boldsymbol{L}_3(1, 6, 4; 6, 2, 5)$ and $\boldsymbol{L}_3(1, 6, 5; 6, 2, 4)$ are listed,
- if select $(3, 6)$ from J^* then $\boldsymbol{L}_2(1, 4; 6, 3), \boldsymbol{L}_3(1, 2, 5; 6, 3, 1)$ and $\boldsymbol{L}_3(1, 2, 5; 6, 3, 4)$ are listed.

These are all the df 1 loops which have ± 1 in this $i^* = 1$-th row. Now all we have to consider is the subtable $R(\widetilde{I}; J_0)$, to which we can apply the similar procedure, and finally the solution described in Section 4 is given.

In general case, it is effective to select i^* so that there are as many structural zero cells in $R(i^*; J_0)$ as possible. Hence i^* should be chosen as

$$i^* = \arg\max_i \#\{j \mid (i^*, j) \notin S\}.$$

However, if the table is semi-separable, it is also effective to select i^* so that the remaining table $R(\widetilde{I}; J_0)$ becomes separable.

3.4.6 Computational examples

Using the Markov basis obtained above, we can perform various tests by the Monte Carlo method. In this section, we show an example of testing the hypothesis of quasi-independence for a given data set. Table 3.6 shows a data collected by Vidmar (1972) for discovering the possible effects on decision making of limiting the number of alternatives available to the members of a jury panel. This is a 4×7 contingency table which has 9 structural zero cells. The degrees of freedom for testing quasi-independence is 9. The maximum likelihood estimate under the hypothesis of quasi-independence is calculated by iterative method as displayed in Table 3.7. See Bishop *et al.*(1975) for maximum likelihood estimation of incomplete tables.

Table 3.6: Effects of decision alternatives on the verdicts and social perceptions of simulated jurors

	condition						
alternative	1	2	3	4	5	6	7
first-degree	11	[0]	[0]	2	7	[0]	2
second-degree	[0]	20	[0]	22	[0]	11	15
manslaughter	[0]	[0]	22	[0]	16	13	5
not guilty	13	4	2	0	1	0	2

Source: Vidmar (1972).

Table 3.7: Maximum likelihood estimate for Table 3.6

	condition						
alternative	1	2	3	4	5	6	7
first-degree	14.05	[0]	[0]	2.61	3.64	[0]	1.70
second-degree	[0]	21.93	[0]	19.55	[0]	13.75	12.77
manslaughter	[0]	[0]	20.95	[0]	17.78	8.95	8.32
not guilty	9.95	2.07	3.05	1.84	2.58	1.30	1.21

As the discrepancy measure from the hypothesis of quasi-independence, we use the likelihood-ratio statistic

$$G^2 = 2 \sum_S x_{ij} \log \frac{x_{ij}}{\hat{m}_{ij}},$$

where $\hat{m}_{ij}$ is the MLE of the expectation parameter m_{ij}. The observed value of G^2 is 18.816 and the corresponding asymptotic p value is 0.0268 from the asymptotic distribution χ^2_9.

To perform the Markov chain Monte Carlo method, first we obtain the minimal Markov basis. From the considerations in the above sections, we see easily that a set of basic moves and a degree 3 loop $\boldsymbol{L}_3(1, 2, 3; 5, 4, 6)$ constitute the unique minimal Markov basis. Using this basis, we construct a connected chain, which is modified so as to have the null distribution (3.24) as the stationary distribution by the Metropolis-Hasting procedure. The estimated exact p value is 0.0444, with estimated standard deviation 0.00052. (We use a batching method to obtain an estimate of variance. See Hastings, 1970, or Ripley, 1987.) Figure 3.11 shows a histogram of the Monte Carlo sampling generated from the exact distribution of the likelihood ratio statistic under the quasi-independence hypothesis, along with the corresponding asymptotic distribution χ^2_9. We see that the asymptotic distribution understates the probability that the test statistic is greater than the observed value, and overemphasize the significance.

3.4.7 Basis reduction for the case of positive marginals

The minimality of the basis considered in the previous sections is based on the condition that the values of the marginal totals are *arbitrary*. However, for performing exact conditional tests to a given data set, we can assume without loss of generality that $x_{i\cdot}, x_{\cdot j} > 0$ for all i, j because all cell values in rows or columns with zero marginals are necessarily zeros and such rows or

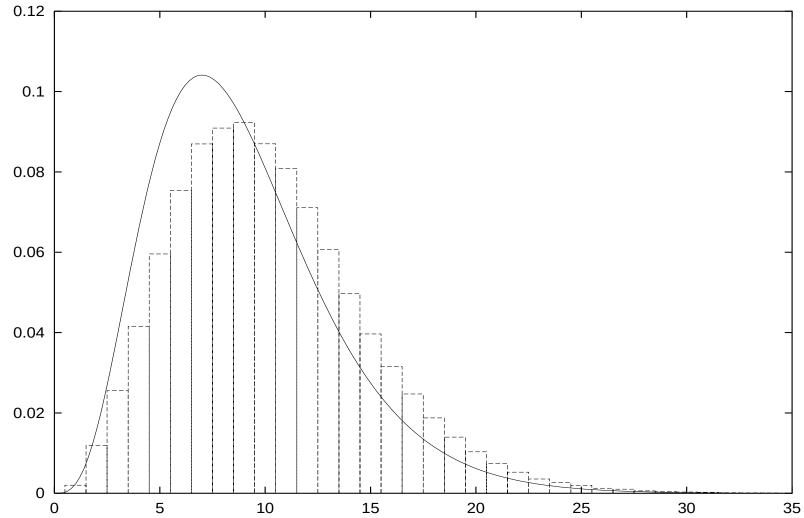

Figure 3.11: Asymptotic and Monte Carlo estimated exact distribution for the likelihood ratio statistic under the quasi-independence model

columns can be ignored in the conditional analysis.

Under the assumption of positive marginal totals, there may be cases, where some elements of the minimal basis obtained in Section 3.4.4 are not needed to construct a connected chain. Therefore it is worth investigating further reduction of the minimal basis to $\mathcal{F}(\{x_{i\cdot}\}, \{x_{\cdot j}\}, S)$ for fixed positive values of $x_{i\cdot}$ and $x_{\cdot j}$. From practical viewpoint it is important to give a sufficient condition on $x_{i\cdot}$ and $x_{\cdot j}$, such that a df 1 loop of degree $r \geq 3$ can be replaced by a series of basic moves. A simple example is the following 3×4 contingency table.

$$\begin{array}{|cccc|}\hline [0] & x_{12} & x_{13} & x_{14} \\ x_{21} & [0] & x_{23} & x_{24} \\ x_{31} & x_{32} & [0] & x_{34} \\ \hline \end{array}$$

From the considerations of Section 3.4.4, we know that the 4 loops, $\boldsymbol{L}_2(1,3;2,4), \boldsymbol{L}_2(1,2;3,4)$, $\boldsymbol{L}_2(2,3;1,4)$ and $\boldsymbol{L}_3(1,3,2;3,2,1)$, constitute the unique minimal Markov basis. They are displayed as follows.

$$\begin{array}{|cccc|}\hline 0 & +1 & 0 & -1 \\ 0 & 0 & 0 & 0 \\ 0 & -1 & 0 & +1 \\ \hline \end{array}, \begin{array}{|cccc|}\hline 0 & 0 & +1 & -1 \\ 0 & 0 & -1 & +1 \\ 0 & 0 & 0 & 0 \\ \hline \end{array}, \begin{array}{|cccc|}\hline 0 & 0 & 0 & 0 \\ +1 & 0 & 0 & -1 \\ -1 & 0 & 0 & +1 \\ \hline \end{array}, \begin{array}{|cccc|}\hline 0 & -1 & +1 & 0 \\ +1 & 0 & -1 & 0 \\ -1 & +1 & 0 & 0 \\ \hline \end{array}.$$

However, under the assumption that all the marginal totals are positive, it is shown that $\boldsymbol{L}_3(1,3,2;3,2,1)$ is not needed to construct a connected chain. To see this, suppose 3×4 tables $\boldsymbol{x}, \boldsymbol{x}'$ are in $\mathcal{F}(\{x_{i\cdot}\}, \{x_{\cdot j}\}, S = \{(1,1),(2,2),(3,3)\})$ and $\boldsymbol{x}' - \boldsymbol{x} = \boldsymbol{L}_3(1,3,2;3,2,1)$. In this case, two states $\boldsymbol{x}$ and $\boldsymbol{x}'$ are mutually reachable by adding or subtracting $\boldsymbol{L}_3(1,3,2;3,2,1)$. These two states can be written as

$$\boldsymbol{x} = \begin{array}{|cccc|}\hline [0] & a_1+1 & a_2 & a_3 \\ a_4 & [0] & a_5+1 & a_6 \\ a_7+1 & a_8 & [0] & a_9 \\ \hline \end{array} \quad \text{and} \quad \boldsymbol{x}' = \begin{array}{|cccc|}\hline [0] & a_1 & a_2+1 & a_3 \\ a_4+1 & [0] & a_5 & a_6 \\ a_7 & a_8+1 & [0] & a_9 \\ \hline \end{array}$$

where $a_1, \ldots, a_9 \in \mathbb{Z}_{\geq 0}$. Here an important point is that at least one of a_3, a_6, a_9 is positive because $x_{\cdot 4} > 0$. Then we can add or subtract the above three basic moves one by one in appropriate order to $\boldsymbol{x}$ to reach $\boldsymbol{x}'$. We show this procedure in the following when $a_3 \geq 1$.

$$\boldsymbol{x} = \begin{array}{|cccc|}\hline [0] & a_1+1 & a_2 & a_3(\geq 1) \\ a_4 & [0] & a_5+1 & a_6 \\ a_7+1 & a_8 & [0] & a_9 \\ \hline \end{array}$$

$$\underset{+\boldsymbol{L}_2(1,2;3,4)}{\longrightarrow} \begin{array}{|cccc|}\hline [0] & a_1+1 & a_2+1 & a_3-1 \\ a_4 & [0] & a_5 & a_6+1 \\ a_7+1 & a_8 & [0] & a_9 \\ \hline \end{array}$$

$$\underset{+\boldsymbol{L}_2(2,3;1,4)}{\longrightarrow} \begin{array}{|cccc|}\hline [0] & a_1+1 & a_2+1 & a_3-1 \\ a_4+1 & [0] & a_5 & a_6 \\ a_7 & a_8 & [0] & a_9+1 \\ \hline \end{array}$$

$$\underset{-\boldsymbol{L}_2(1,3;2,4)}{\longrightarrow} \begin{array}{|cccc|}\hline [0] & a_1 & a_2+1 & a_3 \\ a_4+1 & [0] & a_5 & a_6 \\ a_7 & a_8+1 & [0] & a_9 \\ \hline \end{array} = \boldsymbol{x}'$$

The above consideration gives a decomposition of a df 1 degree r loop into r basic moves, by using one additional row or column. If this row or column is known to contain at least one positive cell, a connected chain can simply be constructed by using basic moves, instead of using this degree r loop.

We summarize the above consideration in the following lemma.

Lemma 3.4.2 *Under the assumption of positive marginals, a df 1 loop $\boldsymbol{L}_r(i_1, \ldots, i_r; j_1, \ldots, j_r)$, $r \geq 3$, can be replaced by a series of basic moves, if one of the following conditions is satisfied.*

(a) There exists $i^* \neq i_k, 1 \leq k \leq r$, such that $(i^*, j_k) \in S$ for all $k = 1, \ldots, r$ and $x_{i^*\cdot} > \sum_{j \in A} x_{\cdot j}$ where $A = \{j \mid j \neq j_k, 1 \leq k \leq r \text{ and } (i^*, j) \in S\}$.

(b) There exists $j^* \neq j_k, 1 \leq k \leq r$, such that $(i_k, j^*) \in S$ for all $k = 1, \ldots, r$ and $x_{\cdot j^*} > \sum_{i \in A} x_{i\cdot}$ where $A = \{i \mid i \neq i_k, 1 \leq k \leq r \text{ and } (i, j^*) \in S\}$.

Proof. It is sufficient to show the lemma for the case (a). It holds that

$$\boldsymbol{L}_r(i_1, \ldots, i_r; j_1, \ldots, j_r) = \sum_{t=1}^{r-1} \boldsymbol{L}_2(i_t, i^*; i_t, i_{t+1}) + \boldsymbol{L}_2(i_r, i^*; i_r, 1). \tag{3.29}$$

It should be noted that the r basic moves of the right hand side constitute a cycle, of which the consecutive two basic moves have only one nonzero cell in common. Moreover, at least one of $x_{i^*j_1}, x_{i^*j_2}, \ldots, x_{i^*j_r}$ have to be positive for all the elements in $\mathcal{F}(\{x_{i\cdot}\}, \{x_{\cdot j}\}, S)$ from the positiveness of $x_{i^*\cdot}, x_{\cdot j}$. Hence we can add or subtract these r basic moves one by one to or from $\boldsymbol{x} \in \mathcal{F}(\{x_{i\cdot}\}, \{x_{\cdot j}\}, S)$ without forcing negative entries on the way, instead of using

$\boldsymbol{L}_r(i_1, \dots, i_r; j_1, \dots, j_r)$. Q.E.D.

To illustrate the argument of this lemma, let $\boldsymbol{L}_4(1,2,3,4;1,2,3,4)$ be df 1 loop and and for example let $i^* = 5$ satisfy the condition (a). Then the decomposition (3.29) is written as

$$\boldsymbol{L}_4(1,2,3,4;1,2,3,4) = \boldsymbol{L}_2(1,5;1,2) + \boldsymbol{L}_2(2,5;2,3) + \boldsymbol{L}_2(3,5;3,4) + \boldsymbol{L}_2(4,5;4,1). \quad (3.30)$$

In the case of $I = 5, J = 4$, this is displayed as

$$\begin{array}{|cccc|}\hline +1 & -1 & [0] & [0] \\ [0] & +1 & -1 & [0] \\ [0] & [0] & +1 & -1 \\ -1 & [0] & [0] & +1 \\ 0 & 0 & 0 & 0 \\ \hline \end{array} = \begin{array}{|cccc|}\hline +1 & -1 & [0] & [0] \\ [0] & 0 & 0 & [0] \\ [0] & [0] & 0 & 0 \\ 0 & [0] & [0] & 0 \\ -1 & +1 & 0 & 0 \\ \hline \end{array} + \begin{array}{|cccc|}\hline 0 & 0 & [0] & [0] \\ [0] & +1 & -1 & [0] \\ [0] & [0] & 0 & 0 \\ 0 & [0] & [0] & 0 \\ 0 & -1 & +1 & 0 \\ \hline \end{array}$$

$$+ \begin{array}{|cccc|}\hline 0 & 0 & [0] & [0] \\ [0] & 0 & 0 & [0] \\ [0] & [0] & +1 & -1 \\ 0 & [0] & [0] & 0 \\ 0 & 0 & -1 & +1 \\ \hline \end{array} + \begin{array}{|cccc|}\hline 0 & 0 & [0] & [0] \\ [0] & 0 & 0 & [0] \\ [0] & [0] & 0 & 0 \\ -1 & [0] & [0] & +1 \\ +1 & 0 & 0 & -1 \\ \hline \end{array}.$$

It should be noted that, in the above example, $A = \emptyset$ in the condition (a) and hence at least one of $x_{51}, \dots, x_{54}$ must be positive from $x_{5\cdot} > 0$. Now consider adding $\boldsymbol{L}_4(1,2,3,4;1,2,3,4)$ to some $\boldsymbol{x} \in \mathcal{F}(\{x_{i\cdot}\}, \{x_{\cdot j}\}, S)$. If $\boldsymbol{x} + \boldsymbol{L}_4(1,2,3,4;1,2,3,4)$ is again in $\mathcal{F}(\{x_{i\cdot}\}, \{x_{\cdot j}\}, S)$, at least 4 entries of $\boldsymbol{x}$, $x_{12}, x_{23}, x_{34}, x_{41}$, must be positive. Then if at least one of $x_{51}, \dots, x_{54}$ is positive, we can add some basic moves in the right hand side of (3.30). Suppose $x_{52} > 0$, for example, then $\boldsymbol{x} + \boldsymbol{L}_2(2,5;2,3) \in \mathcal{F}(\{x_{i\cdot}\}, \{x_{\cdot j}\}, S)$ holds. Now the $(5,3)$ element of $\boldsymbol{x} + \boldsymbol{L}_2(2,5;2,3)$ is positive, hence next basic move, $\boldsymbol{L}_2(3,5;3,4)$, can be added without forcing negative entries. In the similar way, we can add all the basic moves in the right hand side of (3.29) without forcing negative entries and df 1 loop $\boldsymbol{L}_r(i_1, \dots, i_r; j_1, \dots, j_r)$ is shown to be redundant.

We now consider another case not covered by Lemma 3.4.2. The following display is df 1 degree 3 loop $\boldsymbol{L}_3(1,2,3,2,3,1)$ in 5×5 square contingency table with diagonal elements being structural zeros.

$$\begin{array}{|ccccc|}\hline [0] & +1 & -1 & 0 & 0 \\ -1 & [0] & +1 & 0 & 0 \\ +1 & -1 & [0] & 0 & 0 \\ 0 & 0 & 0 & [0] & 0 \\ 0 & 0 & 0 & 0 & [0] \\ \hline \end{array}$$

Of course, we can decompose this loop to 3 basic moves as directed in Lemma 3.4.2 as

$$\boldsymbol{L}_3(1,2,3;2,3,1) = \begin{array}{|ccccc|}\hline [0] & +1 & -1 & 0 & 0 \\ 0 & [0] & 0 & 0 & 0 \\ 0 & 0 & [0] & 0 & 0 \\ 0 & -1 & +1 & [0] & 0 \\ 0 & 0 & 0 & 0 & [0] \\ \hline \end{array} + \begin{array}{|ccccc|}\hline [0] & 0 & 0 & 0 & 0 \\ -1 & [0] & +1 & 0 & 0 \\ 0 & 0 & [0] & 0 & 0 \\ +1 & 0 & -1 & [0] & 0 \\ 0 & 0 & 0 & 0 & [0] \\ \hline \end{array} + \begin{array}{|ccccc|}\hline [0] & 0 & 0 & 0 & 0 \\ 0 & [0] & 0 & 0 & 0 \\ +1 & -1 & [0] & 0 & 0 \\ -1 & +1 & 0 & [0] & 0 \\ 0 & 0 & 0 & 0 & [0] \\ \hline \end{array}.$$

However, it is not guaranteed that we can apply some of the above basic moves to every state which satisfies either of $x_{12}, x_{23}, x_{31} > 0$ or $x_{13}, x_{21}, x_{32} > 0$, because we cannot exclude the possibility that $x_{41} = x_{42} = x_{43} = 0$ even under the assumption of positive marginals. To deal with such cases, we give another decomposition of df 1 degree r loop into $r+1$ basic moves in the next lemma.

Lemma 3.4.3 *Under the assumption of positive marginals, a df 1 loop $\boldsymbol{L}_r(i_1, \ldots, i_r; j_1, \ldots, j_r)$, $r \geq 3$, can be replaced by a series of basic moves, if one of the following conditions is satisfied.*

(a) There exists $i^* \neq i_k, 1 \leq k \leq r$, such that $(i^*, j_k) \in S$ for all $k = 1, \ldots, r$ and for all j such that $(i^*, j) \in S, j \neq j_k, k = 1, \ldots, r$, there exists $i(j) \in \{i_1, \ldots, i_r\}$ such that $(i(j), j) \in S$.

(b) There exists $j^* \neq j_k, 1 \leq k \leq r$, such that $(i_k, j^*) \in S$ for all $k = 1, \ldots, r$ and for all i such that $(i, j^*) \in S, i \neq i_k, k = 1, \ldots, r$, there exists $j(i) \in \{j_1, \ldots, j_r\}$ such that $(i, j(i)) \in S$.

Proof. It is again sufficient to show the lemma for (a). Suppose that both $\boldsymbol{x}$ and $\boldsymbol{x} + \boldsymbol{L}_r(i_1, \ldots, i_r; j_1, \ldots, j_r)$ are in $\mathcal{F}(\{x_{i\cdot}\}, \{x_{\cdot j}\}, S)$. If this $\boldsymbol{x}$ has some positive entries at $(i^*, j_1), \ldots, (i^*, j_r)$, the decomposition in Lemma 3.4.2 can be applied and $\boldsymbol{L}_r(i_1, \ldots, i_r; j_1, \ldots, j_r)$ can be replaced by r basic moves. Hence it is sufficient to consider the case of $x_{i^* j_1} + \cdots + x_{i^* j_r} = 0$. In this case, there exists some $j \neq j_k, k = 1, \ldots, r$, such that $x_{i^* j} > 0, (i^*, j) \in S$ from $x_{i^* \cdot} > 0$. We denote this j by j^*. Now from the condition (a), there exists some $i \in \{i_1, \ldots, i_r\}$ such that $(i, j^*) \in S$. We assume that i_1 satisfies this condition without loss of generality. Here, consider the following decomposition

$$\boldsymbol{L}_r(i_1, \ldots, i_r; j_1, \ldots, j_r) = \boldsymbol{L}_2(i_1, i^*; j_1, j^*) + \boldsymbol{L}_2(i_1, i^*; j^*, j_2) + \sum_{t=2}^{r-1} \boldsymbol{L}_2(i_t, i^*; i_t, i_{t+1}) + \boldsymbol{L}_2(i_r, i^*; i_r, j_1).$$

It is again observed that the $r+1$ basic moves of the right hand side constitute a cycle, of which the consecutive two basic moves have only one nonzero cell in common. Moreover, since $x_{i^* j^*} > 0$, $\boldsymbol{x} + \boldsymbol{L}_2(i_1, i^*; j^*, j_2)$ is in $\mathcal{F}(\{x_{i\cdot}\}, \{x_{\cdot j}\}, S)$. From these considerations, we can add these $r+1$ basic moves one by one to $\boldsymbol{x}$ without forcing negative entries on the way, instead of adding $\boldsymbol{L}_r(i_1, \ldots, i_r; j_1, \ldots, j_r)$ to $\boldsymbol{x}$, and the lemma is proved. Q.E.D.

An example of the decomposition of $\boldsymbol{L}_4(1, 2, 3, 4; 1, 2, 3, 4)$ is displayed as follows.

$$\begin{array}{|ccccc|}\hline +1 & -1 & [0] & [0] & 0 \\ [0] & +1 & -1 & [0] & [0] \\ [0] & [0] & +1 & -1 & [0] \\ -1 & [0] & [0] & +1 & [0] \\ 0 & 0 & 0 & 0 & 0 \\ \hline \end{array} = \begin{array}{|ccccc|}\hline +1 & 0 & [0] & [0] & -1 \\ [0] & 0 & 0 & [0] & [0] \\ [0] & [0] & 0 & 0 & [0] \\ 0 & [0] & [0] & 0 & [0] \\ -1 & 0 & 0 & 0 & +1 \\ \hline \end{array} + \begin{array}{|ccccc|}\hline 0 & -1 & [0] & [0] & +1 \\ [0] & 0 & 0 & [0] & [0] \\ [0] & [0] & 0 & 0 & [0] \\ 0 & [0] & [0] & 0 & [0] \\ 0 & +1 & 0 & 0 & -1 \\ \hline \end{array}$$

$$+ \begin{array}{|ccccc|}\hline 0 & 0 & [0] & [0] & 0 \\ [0] & +1 & -1 & [0] & [0] \\ [0] & [0] & 0 & 0 & [0] \\ 0 & [0] & [0] & 0 & [0] \\ 0 & -1 & +1 & 0 & 0 \\ \hline \end{array} + \begin{array}{|ccccc|}\hline 0 & 0 & [0] & [0] & 0 \\ [0] & 0 & 0 & [0] & [0] \\ [0] & [0] & +1 & -1 & [0] \\ 0 & [0] & [0] & 0 & [0] \\ 0 & 0 & -1 & +1 & 0 \\ \hline \end{array} + \begin{array}{|ccccc|}\hline 0 & 0 & [0] & [0] & 0 \\ [0] & 0 & 0 & [0] & [0] \\ [0] & [0] & 0 & 0 & [0] \\ -1 & [0] & [0] & +1 & [0] \\ +1 & 0 & 0 & -1 & 0 \\ \hline \end{array}$$

Lemma 3.4.2 and 3.4.3 are concerned with replacing a particular degree r loop by a series of basic moves. We now consider the case, where all loops of degree $r \geq 3$ can be replaced by basic moves, so that a connected Markov chain over $\mathcal{F}(\{x_{i\cdot}\}, \{x_{\cdot j}\}, S)$ can be constructed by basic moves only.

Following Smith *et al.* (1996), consider the situation that the contingency table is $I \times I$ and the diagonal cells are structural zeros. By symmetry and as a direct consequence of Lemma 3.4.2, we see that the set of basic moves are sufficient to construct a connected chain under the assumption of positive marginals for 4×4 contingency tables with diagonal elements being structural zeros. For the case of $I \geq 5$, we see that the degree 3 loop $\boldsymbol{L}_3(1, 2, 3; 2, 3, 4)$ in Table 5 satisfies the condition of Lemma 3.4.3. Considering the symmetry again, we see the set of basic moves constitutes a connected Markov chain. Therefore we obtain the following corollary to Lemma 3.4.3.

Corollary 3.4.1 *A connected chain can be constructed by a set of basic moves for $I \times I$ contingency tables, $I \geq 4$, with only diagonal elements being structural zeros under the assumption of positive marginals.*

Lemma 3.4.2 and Lemma 3.4.3 give convenient sufficient conditions that a df 1 loop of degree $r \geq 3$ can be replaced by a series of basic moves. Hence for the situations that do not satisfy the conditions of Lemma 3.4.2 nor Lemma 3.4.3, we may have to use df 1 loops of degree $r \geq 3$, to ensure the connectivity of the chain. To demonstrate the importance of the minimal basis, we give an example where the set of the basic moves does not constitute a connected chain even if all the marginals are positive as follows.

$$\begin{array}{|cccc|c} \hline x_{11} & x_{12} & [0] & x_{14} & 1 \\ [0] & x_{22} & x_{23} & x_{24} & 1 \\ x_{31} & [0] & x_{33} & [0] & 1 \\ [0] & x_{42} & x_{43} & x_{44} & 1 \\ \hline 1 & 1 & 1 & 1 & \end{array}$$

In this case, there are 6 elements in $\mathcal{F}(\{x_{i\cdot}\}, \{x_{\cdot j}\}, S)$ displayed as

$$\mathcal{F}(\{x_{i\cdot}\}, \{x_{\cdot j}\}, S)$$

$$= \left\{ \begin{array}{|cccc|} \hline 1 & 0 & [0] & 0 \\ [0] & 1 & 0 & 0 \\ 0 & [0] & 1 & [0] \\ [0] & 0 & 0 & 1 \\ \hline \end{array}, \begin{array}{|cccc|} \hline 1 & 0 & [0] & 0 \\ [0] & 0 & 0 & 1 \\ 0 & [0] & 1 & [0] \\ [0] & 1 & 0 & 0 \\ \hline \end{array}, \begin{array}{|cccc|} \hline 0 & 1 & [0] & 0 \\ [0] & 0 & 1 & 0 \\ 1 & [0] & 0 & [0] \\ [0] & 0 & 0 & 1 \\ \hline \end{array}, \right.$$

$$\left. \begin{array}{|cccc|} \hline 0 & 1 & [0] & 0 \\ [0] & 0 & 0 & 1 \\ 1 & [0] & 0 & [0] \\ [0] & 0 & 1 & 0 \\ \hline \end{array}, \begin{array}{|cccc|} \hline 0 & 0 & [0] & 1 \\ [0] & 1 & 0 & 0 \\ 1 & [0] & 0 & [0] \\ [0] & 0 & 1 & 0 \\ \hline \end{array}, \begin{array}{|cccc|} \hline 0 & 0 & [0] & 1 \\ [0] & 0 & 1 & 0 \\ 1 & [0] & 0 & 0 \\ [0] & 1 & 0 & 0 \\ \hline \end{array} \right\}.$$

We see that these 6 elements are not mutually reachable simply by the basic moves. To connect all the elements, we have to use degree 3 loops.

Conversely, when some of the conditions of Lemma 3.4.2 or 3.4.3 are satisfied, there is a possibility that we do not have to consider all the elements of the minimal basis. For example, if we can permute rows and columns to $\{I_1, I_2\}, \{J_1, J_2\}$, where the elements of $R(I_1; J_2), R(I_2; J_1), R(I_2; J_2)$ are all in S and there are at least one cells of S in every row and column of $R(I_1; J_1)$, we know that a set of basic moves constitutes a connected Markov chain regardless of the remaining pattern of $R(I_1; J_1)$.

3.4.8 Minimal Markov basis for the hypothesis of quasi-symmetry

For some types of square contingency tables, the hypothesis of quasi-symmetry is of interest (Bishop *et al.*, 1975, for example). Quasi-symmetry corresponds to symmetric off-diagonal association, which implies that the interaction parameters in a log-linear model for symmetrically opposite cells are equal, but makes no assumption on the diagonal interaction parameters. Hence it is represented as $\mathrm{H}_1 : \gamma_{ij} = \gamma_{ji},\ i \neq j$ in the log-linear model (3.23). Quasi-symmetry model is also related to Bradley-Terry model.

For the quasi-symmetry hypothesis, an exact conditional test can also be constructed (Smith *et al.*, 1996). For this case, a sufficient statistic is $\{x_{i\cdot}\}, \{x_{\cdot j}\}, \{x_{ij} + x_{ji}\}$ and the conditional distribution is proportional to $\prod_{ij}(x_{ij}!)^{-1}$. See Smith *et al.* (1996) for detail.

To perform the exact tests of quasi-symmetry, the Markov chain Monte Carlo approach is also useful if a complete enumeration is infeasible. In this case, a connected Markov chain over the reference set

$$\mathcal{F}(\{x_{i\cdot}\}, \{x_{\cdot j}\}, \{x_{ij} + x_{ji}\}) = \{\ \boldsymbol{y}\ \mid y_{i\cdot} = x_{i\cdot}, y_{\cdot j} = x_{\cdot j}, y_{ij} + y_{ji} = x_{ij} + x_{ji},\ y_{ij} \in \mathbb{Z}_{\geq 0}\}$$

can be modified to give a connected and aperiodic Markov chain with stationary distribution as the conditional null distribution under the quasi-symmetry hypothesis by the Metropolis procedure. Similarly to the quasi-independence hypothesis, our interest is a minimal basis for a connected chain over $\mathcal{F}(\{x_{i\cdot}\}, \{x_{\cdot j}\}, \{x_{ij} + x_{ji}\})$. The result is summarized as follows.

Definition 3.4.4 *A loop of degree r is an $I \times I$ integer array $\boldsymbol{L}^*_r(i_1, \ldots, i_r), i_1, \ldots, i_r \in [I]$, where $\boldsymbol{L}^*_r(i_1, \ldots, i_r)$ has the elements*

$$\begin{aligned} L^*_{i_1 i_2} &= L^*_{i_2 i_3} = \cdots = L^*_{i_{r-1} i_r} = L^*_{i_r i_1} = +1, \\ L^*_{i_2 i_1} &= L^*_{i_3 i_2} = \cdots = L^*_{i_r i_{r-1}} = L^*_{i_1 i_r} = -1, \end{aligned}$$

and all the other elements are zero. Specifically, we call degree 3 loop $\boldsymbol{L}^*_3(i_1, i_2, i_3)$ a basic move.

Theorem 3.4.2 *The set of the loops described in Definition 3.4.4 of degree $r = 3, \ldots, I$ constitutes a unique minimal Markov basis for $I \times I$ contingency tables under the quasi-symmetry hypothesis.*

The set of all loops described above constitutes a Markov basis for the following reason. Suppose $\boldsymbol{x}, \boldsymbol{x}' \in \mathcal{F}(\{x_{i\cdot}\}, \{x_{\cdot j}\}, \{x_{ij} + x_{ji}\})$. Then the difference $\boldsymbol{x} - \boldsymbol{x}'$ can be expressed as a finite sum

$$\boldsymbol{x} - \boldsymbol{x}' = \sum_k a_k \boldsymbol{L}^*_{r(k)}(i_{1(k)}, \ldots, i_{r(k)}),$$

where a_k is a positive integer, $r(k) \leq I$ and there is no cancellation of signs in any cell. Hence to move from $\boldsymbol{x}$ to $\boldsymbol{x}'$, we can add a sequence of loops in Definition 3.4.4 to $\boldsymbol{x}$, without forcing negative entries on the way. Uniqueness and minimality is due to the fact that $\boldsymbol{L}_r^*(i_1,\ldots,i_r)$ can be written as the difference of the elements of $\mathcal{F}(\{x_{i\cdot}\},\{x_{\cdot j}\},\{x_{ij}+x_{ji}\})$ which is a two-elements set.

We have the relations

$$\boldsymbol{L}_r^*(i_1,\ldots,i_r)=\boldsymbol{L}_r^*(i_2,i_3,\ldots,i_r,i_1)=-\boldsymbol{L}_r^*(i_1,i_r,i_{r-1},\ldots,i_2)$$

and there are

$$\sum_{r=3}^{I}\frac{I(I-1)(I-2)\cdots(I-r+1)}{2r}$$

loops in the minimal Markov basis for $I\times I$ case. Hence the algorithm can be constructed simply by generating a sequence $i_1\cdots i_r,\ 3\le r\le I$ randomly.

Similarly as in Section 3.4.7, a basis reduction is also possible if all the sufficient statistics are positive.

Lemma 3.4.4 *If $x_{i\cdot},x_{\cdot j}>0$ for all i,j and $x_{ij}+x_{ji}>0$ for all $i\neq j$, the set of basic moves $\boldsymbol{L}_3^*(i_1,i_2,i_3)$ constitutes a connected chain.*

This lemma follows from the decomposition

$$\boldsymbol{L}_r^*(i_1,\ldots,i_r)=\boldsymbol{L}_a^*(i_1,\ldots,i_a)+\boldsymbol{L}_{r-a+2}^*(i_a,i_{a+1},\ldots,i_r,i_1),$$

because the two loops of the right hand side have only two nonzero cells $L_{i_a i_1}^*,L_{i_1 i_a}^*$ in common and at least one of $x_{i_1 i_a}$ and $x_{i_a i_1}$ is positive for every element in $\mathcal{F}(\{x_{i\cdot}\},\{x_{\cdot j}\},\{x_{ij}+x_{ji}\})$ since $x_{ij}+x_{ji}>0$.

3.4.9 Discussion

In our analysis of an example data displayed in Table 3.6, the asymptotic goodness-of-fit test overemphasizes the significance of the data and is misleading. Indeed, for many sparse tables where large-sample theory does not work well, a Markov chain Monte Carlo method is a valuable tool to calculate p values for various test statistics. To construct a connected chain, a concept of the Markov basis described in this thesis is essential. In this section, we give an explicit characterization of the elements of the unique minimal Markov basis for arbitrary configurations of structural zero cells. Using the algorithm described in Section 3.4.5, we can easily obtain all the elements of the minimal basis for various problems, and we can implement a Markov chain Monte Carlo program for calculating exact p values for various test statistics. Moreover, the basis reduction described in Section 3.4.7 makes the algorithm very brief for many problems. Our experience shows that there are many problems where the set of basic moves constitutes a connected chain. For these problems, a Markov chain Monte Carlo algorithm is simply implemented by choosing pairs of rows and columns randomly.

3.5 Characterizations of a minimal Markov basis and its uniqueness

In the previous sections, we have derived closed form expressions of minimal Markov bases for some problems, i.e., no three-factor interaction model for some three-way contingency tables and independence and quasi-independence models for two-way contingency tables. These results are important since, in general, the Gröbner basis computation proposed by Diaconis and Sturmfels (1998) produces large number of redundant basis elements due to the lack of symmetry and minimality in Gröbner basis. In this section, we give some basic characterizations of a minimal Markov basis in general settings. Our arguments are totally elementary. We also give a necessary and sufficient condition for the uniqueness of a minimal Markov basis. Our approach is basically constructive and it clarifies a partially ordered structure of a minimal Markov basis. At present our result is not powerful enough to completely characterize a minimal Markov basis for a given problem, but with further refinement it might be possible to implement an alternative algorithm for constructing a Markov basis for a connected Markov chain over a given sample space.

First we give necessary notations and definitions on a Markov basis in Section 3.5.1, and then derive our characterization of a minimal Markov basis in Section 3.5.2 and Section 3.5.3. Relevant examples of discrete exponential families are studied in Section 3.5.4.

3.5.1 Notations and definitions

Let $\mathcal{I}$ be a finite set. With contingency tables in mind, an element of $\mathcal{I}$ is called a *cell* and denoted by $\boldsymbol{i} \in \mathcal{I}$. $|\mathcal{I}|$ denotes the number of cells. In the case of $I_1 \times \cdots \times I_k$ k-way contingency tables, $\boldsymbol{i}$ represents a multi-index $\boldsymbol{i} = (i_1, \ldots, i_k)$ and $|\mathcal{I}| = I_1 \times \cdots \times I_k$. This typical situation is further considered in Section 3.6. A non-negative integer $x(\boldsymbol{i})$ denotes the frequency of cell $\boldsymbol{i}$. For the case of two-way or three-way contingency tables, we occasionally write x_{ij} or x_{ijk} instead of $x(\boldsymbol{i})$ for simplicity as we have seen in the previous sections. $n = \displaystyle\sum_{\boldsymbol{i} \in \mathcal{I}} x(\boldsymbol{i})$ denotes the sample size.

$\boldsymbol{a}(\boldsymbol{i}) \in \mathbb{Z}_{\geq 0}^{\nu}, \boldsymbol{i} \in \mathcal{I}$, denote ν-dimensional fixed column vectors consisting of non-negative integers. A ν-dimensional sufficient statistic $\boldsymbol{t}$ is given by

$$\boldsymbol{t} = \sum_{\boldsymbol{i} \in \mathcal{I}} \boldsymbol{a}(\boldsymbol{i}) x(\boldsymbol{i}).$$

In the case of hierarchical model for k-way contingency tables $\boldsymbol{t}$ consists of appropriate marginal totals.

Let the cells and the vectors $\boldsymbol{a}(\boldsymbol{i})$ be appropriately ordered. For k-way contingency tables, we may order the multi-indices lexicographically. Let

$$\boldsymbol{x} = \{x(\boldsymbol{i})\}_{\boldsymbol{i} \in \mathcal{I}} \in \mathbb{Z}_{\geq 0}^{|\mathcal{I}|}$$

denote an $|\mathcal{I}|$-dimensional column vector of cell frequencies and let

$$A = \{\boldsymbol{a}(\boldsymbol{i})\}_{\boldsymbol{i} \in \mathcal{I}}$$

denote a $\nu \times |\mathcal{I}|$ matrix. Then the sufficient statistic $\boldsymbol{t}$ is written as

$$\boldsymbol{t} = A\boldsymbol{x}.$$

We sometimes call $\boldsymbol{x}$ a *frequency vector*, while we call it a contingency table at the same time. We also use the notation $|\boldsymbol{x}| = n = \displaystyle\sum_{\boldsymbol{i} \in \mathcal{I}} x(\boldsymbol{i})$ to denote the sample size and the notation $\boldsymbol{x} \geq \boldsymbol{0}$

to denote that the elements of $\boldsymbol{x}$ are non-negative integers, i.e., $\boldsymbol{x} \in \mathbb{Z}_{\geq 0}^{|\mathcal{I}|}$. We write $\boldsymbol{x} \geq \boldsymbol{y}$ if $\boldsymbol{x} - \boldsymbol{y} \geq \boldsymbol{0}$. The reference set of $\boldsymbol{x}$'s for a given $\boldsymbol{t}$ is denoted by

$$\mathcal{F}_{\boldsymbol{t}} = \{\boldsymbol{x} \geq \boldsymbol{0} \mid A\boldsymbol{x} = \boldsymbol{t}\}.$$

Concerning the matrix A we make the following assumption.

Assumption 3.5.1 *The $|\mathcal{I}|$-dimensional row vector $(1, 1, \ldots, 1)$ is a linear combination of the rows of A.*

Assumption 3.5.1 is satisfied in all the examples in this thesis. Assumption 3.5.1 implies that the sample size n is determined from the sufficient statistic $\boldsymbol{t}$ and all elements of $\mathcal{F}_{\boldsymbol{t}}$ have the same sample size. Somewhat abusing the notation, we write $n = |\boldsymbol{t}|$ to denote the sample size of elements of $\mathcal{F}_{\boldsymbol{t}}$. Another consequence of this assumption is that each $\boldsymbol{a}(\boldsymbol{i})$, $\boldsymbol{i} \in \mathcal{I}$, is a non-zero vector, because otherwise each linear combination of the rows of A has 0 in the $\boldsymbol{i}$-th position.

For the case of $I \times J$ contingency tables with fixed one-dimensional marginals and with lexicographical ordering of cells, A is written as

$$A = \begin{bmatrix} 1_I' \otimes E_J \\ E_I \otimes 1_J' \end{bmatrix}, \tag{3.31}$$

where 1_I is the I-dimensional vector consisting of 1's, E_J is the $J \times J$ identity matrix and $\otimes$ denotes the Kronecker product. Similarly for $I \times J \times K$ contingency tables with fixed two-dimensional marginals and with lexicographical ordering of cells, A is written as

$$A = \begin{bmatrix} 1_I' \otimes E_J \otimes E_K \\ E_I \otimes 1_J' \otimes E_K \\ E_I \otimes E_J \otimes 1_K' \end{bmatrix}. \tag{3.32}$$

An $|\mathcal{I}|$-dimensional vector of integers $\boldsymbol{z} \in \mathbb{Z}^{|\mathcal{I}|}$ is called a *move* if it is in the kernel of A:

$$A\boldsymbol{z} = \boldsymbol{0}.$$

Adding a move $\boldsymbol{z}$ to $\boldsymbol{x}$ does not change the sufficient statistic

$$\boldsymbol{t} = A\boldsymbol{x} = A(\boldsymbol{x} + \boldsymbol{z}).$$

Therefore $\boldsymbol{z}$ can be interpreted as a move within $\mathcal{F}_{\boldsymbol{t}}$ for any $\boldsymbol{t}$. By definition the zero frequency vector $\boldsymbol{z} = \boldsymbol{0}$ is also a move, although it does not move anything. For a move $\boldsymbol{z} = \{z(\boldsymbol{i})\}_{\boldsymbol{i} \in \mathcal{I}}$, the positive part $\boldsymbol{z}^+ = \{z^+(\boldsymbol{i})\}_{\boldsymbol{i} \in \mathcal{I}}$ and the negative part $\boldsymbol{z}^- = \{z^-(\boldsymbol{i})\}_{\boldsymbol{i} \in \mathcal{I}}$ are defined by

$$z^+(\boldsymbol{i}) = \max(z(\boldsymbol{i}), 0), \qquad z^-(\boldsymbol{i}) = -\min(z(\boldsymbol{i}), 0),$$

respectively. Then $\boldsymbol{z} = \boldsymbol{z}^+ - \boldsymbol{z}^-$. Note that if $\boldsymbol{z}$ is a move, then $-\boldsymbol{z}$ is also a move with $(-\boldsymbol{z})^+ = \boldsymbol{z}^-$ and $(-\boldsymbol{z})^- = \boldsymbol{z}^+$. Note also that non-zero elements of $\boldsymbol{z}^+$ and $\boldsymbol{z}^-$ do not share a common cell. The positive part $\boldsymbol{z}^+$ and the negative part $\boldsymbol{z}^-$ have the same value of sufficient statistic $\boldsymbol{t} = A\boldsymbol{z}^+ = A\boldsymbol{z}^-$. The sample size of $\boldsymbol{z}^+$ (or $\boldsymbol{z}^-$) is called the *degree* of $\boldsymbol{z}$ and denoted by

$$\deg(\boldsymbol{z}) = |\boldsymbol{z}^+| = |\boldsymbol{z}^-|.$$

Occasionally we also write $|\boldsymbol{z}| = \sum_{\boldsymbol{i}\in\mathcal{I}} |z(\boldsymbol{i})| = 2\deg(\boldsymbol{z})$.

We say that a move $\boldsymbol{z}$ is *applicable* to $\boldsymbol{x} \in \mathcal{F}_{\boldsymbol{t}}$ if $\boldsymbol{x} + \boldsymbol{z} \in \mathcal{F}_{\boldsymbol{t}}$, i.e., adding $\boldsymbol{z}$ to $\boldsymbol{x}$ does not produce a negative cell. Since

$$\boldsymbol{x} + \boldsymbol{z} = \boldsymbol{x} + \boldsymbol{z}^+ - \boldsymbol{z}^-,$$

$\boldsymbol{z}$ is applicable to $\boldsymbol{x}$ if and only if

$$\boldsymbol{x} \geq \boldsymbol{z}^-. \tag{3.33}$$

Note also that $\boldsymbol{z}$ is applicable to $\boldsymbol{x}$ if and only if $-\boldsymbol{z}$ is applicable to $\boldsymbol{x} + \boldsymbol{z}$.

Let $\mathcal{B} = \{\boldsymbol{z}_1, \ldots, \boldsymbol{z}_L\}$ be a finite set of moves. Let $\boldsymbol{x}, \boldsymbol{y} \in \mathcal{F}_{\boldsymbol{t}}$. We say that $\boldsymbol{y}$ is *accessible* from $\boldsymbol{x}$ by $\mathcal{B}$ and denote it by

$$\boldsymbol{x} \sim \boldsymbol{y} \qquad (\mathrm{mod}\ \mathcal{B}),$$

if there exists a sequence of moves $\boldsymbol{z}_{i_1}, \ldots, \boldsymbol{z}_{i_k}$ from $\mathcal{B}$ and $\varepsilon_j = \pm 1,\ j = 1, \ldots, k$, such that $\boldsymbol{y} = \boldsymbol{x} + \sum_{j=1}^{k} \varepsilon_j \boldsymbol{z}_{i_j}$ and

$$\boldsymbol{x} + \sum_{j=1}^{h} \varepsilon_j \boldsymbol{z}_{i_j} \in \mathcal{F}_{\boldsymbol{t}}, \qquad h = 1, \ldots, k-1, \tag{3.34}$$

i.e., we can move from $\boldsymbol{x}$ to $\boldsymbol{y}$ by moves from $\mathcal{B}$ without causing negative cells on the way. Obviously the notion of accessibility is symmetric and transitive:

$$\begin{aligned} &\boldsymbol{x} \sim \boldsymbol{y} \quad \Rightarrow \quad \boldsymbol{y} \sim \boldsymbol{x} \qquad (\mathrm{mod}\ \mathcal{B}), \\ &\boldsymbol{x}_1 \sim \boldsymbol{x}_2, \quad \boldsymbol{x}_2 \sim \boldsymbol{x}_3 \quad \Rightarrow \quad \boldsymbol{x}_1 \sim \boldsymbol{x}_3 \qquad (\mathrm{mod}\ \mathcal{B}). \end{aligned}$$

Therefore accessibility by $\mathcal{B}$ is an equivalence relation and each $\mathcal{F}_{\boldsymbol{t}}$ is partitioned into disjoint equivalence classes by moves of $\mathcal{B}$. We call these equivalence classes $\mathcal{B}$-equivalence classes of $\mathcal{F}_{\boldsymbol{t}}$. Since the notion of accessibility is symmetric, we also say that $\boldsymbol{x}$ and $\boldsymbol{y}$ are mutually accessible by $\mathcal{B}$ if $\boldsymbol{x} \sim \boldsymbol{y}$ (mod $\mathcal{B}$). Let $\boldsymbol{x}$ and $\boldsymbol{y}$ be elements from two different $\mathcal{B}$-equivalence classes of $\mathcal{F}_{\boldsymbol{t}}$. We say that a move

$$\boldsymbol{z} = \boldsymbol{x} - \boldsymbol{y}$$

connects these two equivalence classes. Diaconis, Eisenbud and Sturmfels (1998) gives results on properties of a $\mathcal{B}$-equivalence class from algebraic viewpoint.

Particular sets of moves we consider below are

$$\mathcal{B}_{\boldsymbol{t}} = \{\boldsymbol{z} \mid \boldsymbol{t} = A\boldsymbol{z}^+ = A\boldsymbol{z}^-\},$$

which is a set of moves $\boldsymbol{z}$ with the same value of the sufficient statistic $\boldsymbol{t} = A\boldsymbol{z}^+$, and

$$\mathcal{B}_n = \{\boldsymbol{z} \mid \deg(\boldsymbol{z}) \leq n\},$$

which is a set of moves with degree less than or equal to n.

A set of finite moves $\mathcal{B} = \{\boldsymbol{z}_1, \ldots, \boldsymbol{z}_L\}$ is a *Markov basis* if for all $\boldsymbol{t}$, $\mathcal{F}_{\boldsymbol{t}}$ itself constitutes one $\mathcal{B}$-equivalence class, i.e., for every $\boldsymbol{t}$ and for every $\boldsymbol{x}, \boldsymbol{y} \in \mathcal{F}_{\boldsymbol{t}}$, $\boldsymbol{y}$ and $\boldsymbol{x}$ are mutually accessible by $\mathcal{B}$. Logically important point here is the existence of a finite Markov basis, which is guaranteed by the Hilbert basis theorem (see Section 3.1 of Diaconis and Sturmfels, 1998). In fact Diaconis and Sturmfels (1998) gave an algorithm to produce a finite Markov basis. A Markov basis $\mathcal{B}$ is *minimal* if no proper subset of $\mathcal{B}$ is a Markov basis. A minimal Markov basis always exists, because from any Markov basis, we can remove redundant elements one by one, until none of the remaining elements can be removed any further. From the definition, a minimal Markov basis is not symmetric, i.e. for each $\boldsymbol{z} \in \mathcal{B}$, $-\boldsymbol{z}$ is not a member of $\mathcal{B}$ when $\mathcal{B}$ is a minimal Markov basis.

It should be noted that a Markov basis $\mathcal{B}$ is common for all $\boldsymbol{t}$. Suppose that a data frequency vector $\boldsymbol{x}$ is given and we are concerned only with connecting frequency vectors of $\mathcal{F}_{\boldsymbol{t}}$ for the given $\boldsymbol{t} = A\boldsymbol{x}$. Then we may not need all of the moves from $\mathcal{B}$. It is a subtle problem to determine which moves of $\mathcal{B}$ are needed for connecting $\mathcal{F}_{\boldsymbol{t}}$ for a given $\boldsymbol{t}$ from the viewpoint of minimality. We discuss this point further in Section 3.5.5. We have also investigated this problem for the case of two-way contingency tables with structural zeros in Section 3.4.7.

Having prepared adequate notations and definitions, we now proceed to characterize structure of the minimal Markov basis.

3.5.2 Characterization of a minimal Markov basis

For each $\boldsymbol{t}$, let $n = |\boldsymbol{t}|$ be the sample size of elements of $\mathcal{F}_{\boldsymbol{t}}$ and let $\mathcal{B}_{n-1}$ be the set of moves with degree less than n. Write the $\mathcal{B}_{n-1}$-equivalence classes of $\mathcal{F}_{\boldsymbol{t}}$ as

$$\mathcal{F}_{\boldsymbol{t}} = \mathcal{F}_{\boldsymbol{t},1} \cup \cdots \cup \mathcal{F}_{\boldsymbol{t},K_{\boldsymbol{t}}}. \tag{3.35}$$

Let $\boldsymbol{x}_j \in \mathcal{F}_{\boldsymbol{t},j},\ j = 1, \ldots, K_{\boldsymbol{t}}$, be representative elements of the equivalence classes and

$$\boldsymbol{z}_{j_1,j_2} = \boldsymbol{x}_{j_1} - \boldsymbol{x}_{j_2}, \quad j_1 \neq j_2$$

be a move connecting $\mathcal{F}_{\boldsymbol{t},j_1}$ and $\mathcal{F}_{\boldsymbol{t},j_2}$. Note that we can connect all equivalence classes with $K_{\boldsymbol{t}} - 1$ moves of this type, by forming a tree, where the equivalence classes are interpreted as vertices and connecting moves are interpreted as edges of an undirected graph. Now we state our main theorem. The following result is already known to algebraists. See Theorem 2.5 of Briales et al. (1998).

Theorem 3.5.1 *Let $\mathcal{B}$ be a minimal Markov basis. For each $\boldsymbol{t}$, $\mathcal{B} \cap \mathcal{B}_{\boldsymbol{t}}$ consists of $K_{\boldsymbol{t}} - 1$ moves connecting different $\mathcal{B}_{|\boldsymbol{t}|-1}$-equivalence classes of $\mathcal{F}_{\boldsymbol{t}}$, in such a way that the equivalence classes are connected into a tree by these moves.*

Conversely choose any $K_{\boldsymbol{t}} - 1$ moves $z_{\boldsymbol{t},1}, \ldots, z_{\boldsymbol{t},K_{\boldsymbol{t}}-1}$ connecting different $\mathcal{B}_{|\boldsymbol{t}|-1}$-equivalence classes of $\mathcal{F}_{\boldsymbol{t}}$, in such a way that the equivalence classes are connected into a tree by these moves. Then

$$\mathcal{B} = \bigcup_{\boldsymbol{t}:K_{\boldsymbol{t}}\geq 2} \{z_{\boldsymbol{t},1}, \ldots, z_{\boldsymbol{t},K_{\boldsymbol{t}}-1}\} \tag{3.36}$$

is a minimal Markov basis.

Note that no move is needed from $\mathcal{F}_{\boldsymbol{t}}$ with $K_{\boldsymbol{t}} = 1$, including the case where $\mathcal{F}_{\boldsymbol{t}}$ is a one-element set. If $\mathcal{F}_{\boldsymbol{t}} = \{\boldsymbol{x}\}$ is a one-element set, no non-zero move is applicable to $\boldsymbol{x}$, but at the same time we do not need to move from $\boldsymbol{x}$ at all for such a $\boldsymbol{t}$.

In principle this theorem can be used to construct a minimal Markov basis from below as follows. As the initial step we consider $\boldsymbol{t}$ with the sample size $n = |\boldsymbol{t}| = 1$. Because $\mathcal{B}_0$ consists only of the zero move $\mathcal{B}_0 = \{0\}$, each point $\boldsymbol{x} \in \mathcal{F}_{\boldsymbol{t}},\ |\boldsymbol{t}| = 1$, is isolated and forms an equivalence class by itself. For each $\boldsymbol{t}$ with $|\boldsymbol{t}| = 1$, we choose $K_{\boldsymbol{t}} - 1$ degree 1 moves to connect $K_{\boldsymbol{t}}$ points of $\mathcal{F}_{\boldsymbol{t}}$ into a tree. Let $\tilde{\mathcal{B}}_1$ be the set of chosen moves. $\tilde{\mathcal{B}}_1$ is a subset of the set $\mathcal{B}_1$ of all degree 1 moves. Since every degree 1 move can be expressed by non-negative integer combination of chosen degree 1 moves, it follows that $\tilde{\mathcal{B}}_1$ and $\mathcal{B}_1$ induce same equivalence classes for each $\mathcal{F}_{\boldsymbol{t}}$ with $|\boldsymbol{t}| = 2$. Therefore as the second step we consider $\tilde{\mathcal{B}}_1$-equivalence classes of $\mathcal{F}_{\boldsymbol{t}}$ for each $\boldsymbol{t}$ with $|\boldsymbol{t}| = 2$ and choose representative elements from each equivalence class to form degree 2 moves connecting the equivalence classes into a tree. We add the chosen moves to $\tilde{\mathcal{B}}_1$ and form a set $\tilde{\mathcal{B}}_2$. We can repeat this process for $n = |\boldsymbol{t}| = 3, 4, \ldots$. By the Hilbert basis theorem there exists some n_0 such that for $n \geq n_0$ no new moves need to be added. Then a minimal Markov basis $\mathcal{B}$ of (3.36) is written as $\mathcal{B} = \tilde{\mathcal{B}}_{n_0}$. Obviously there is a considerable difficulty in implementing this procedure. We will discuss this point further in Section 3.5.5.

Theorem 3.5.1 clarifies to what extent minimal Markov basis is unique. If an equivalence class consists of more than one element, then any element can be chosen as the representative element of the equivalence class. Another indeterminacy is how to form a tree of the equivalence classes. In addition there exists a trivial indeterminacy of a Markov basis $\mathcal{B}$ in changing the signs of its elements. We say that a minimal basis is *unique* if all minimal bases differ only by sign changes of the elements. Considering the indeterminacies except for the sign changes and in view of Lemma 3.5.3 below, we have the following corollary to Theorem 3.5.1.

Corollary 3.5.1 *Minimal Markov basis is unique if and only if for each $\boldsymbol{t}$, $\mathcal{F}_{\boldsymbol{t}}$ itself constitutes one $\mathcal{B}_{|\boldsymbol{t}|-1}$-equivalence class or $\mathcal{F}_{\boldsymbol{t}}$ is a two element set.*

In this corollary, the two cases are not necessarily exclusive, namely, there are cases where $\mathcal{F}_{\boldsymbol{t}}$ is a two element set forming a single $\mathcal{B}_{|\boldsymbol{t}|-1}$-equivalence class. In this corollary the importance of two element set $\mathcal{F}_{\boldsymbol{t}} = \{\boldsymbol{x}, \boldsymbol{y}\}$ is suggested. When $\mathcal{F}_{\boldsymbol{t}} = \{\boldsymbol{x}, \boldsymbol{y}\}$ is a two element set, then we call $\boldsymbol{z} = \boldsymbol{x} - \boldsymbol{y}$ an *indispensable move.* Now we state another corollary, which is more convenient to use.

Corollary 3.5.2 *The unique minimal Markov basis exists if and only if the set of indispensable moves forms a Markov basis. In this case, the set of indispensable moves is the unique Markov basis.*

From these corollaries it seems that minimal Markov basis is unique only under special conditions. It is therefore of great interest that minimal Markov basis is unique for some standard problems in k-way ($k \geq 2$) contingency tables with fixed marginals. On the other hand for the simplest case of one-way contingency tables, minimal Markov basis is not unique. These facts will be confirmed in Section 3.5.4.

3.5.3 Proofs and some additional facts

Here we give a proof of Theorem 3.5.1 and its corollaries. We also state some lemmas, which is of some independent interest.

Lemma 3.5.1 *If a move $\boldsymbol{z}$ is applicable to at least one element of $\mathcal{F}_{\boldsymbol{t}}$, then*

$$\deg \boldsymbol{z} \le |\boldsymbol{t}|, \tag{3.37}$$

where the equality holds if and only if $\boldsymbol{t} = A\boldsymbol{z}^+ = A\boldsymbol{z}^-$.

Proof. Let $\boldsymbol{z}$ be applicable to $\boldsymbol{x} \in \mathcal{F}_{\boldsymbol{t}}$. Then by (3.33) $x(\boldsymbol{i}) \ge z^-(\boldsymbol{i}),\ \forall \boldsymbol{i} \in \mathcal{I}$. Summing over $\mathcal{I}$ yields (3.37).

Concerning the equality, if $\boldsymbol{z}$ be applicable to $\boldsymbol{x} \in \mathcal{F}_{\boldsymbol{t}}$ and the equality holds in (3.37), then $x(\boldsymbol{i}) = z^-(\boldsymbol{i}),\ \forall \boldsymbol{i} \in \mathcal{I}$ and

$$\boldsymbol{t} = A\boldsymbol{x} = \sum_{\boldsymbol{i}\in\mathcal{I}} \boldsymbol{a}(\boldsymbol{i})x(\boldsymbol{i}) = \sum_{\boldsymbol{i}\in\mathcal{I}} \boldsymbol{a}(\boldsymbol{i})z^-(\boldsymbol{i}) = A\boldsymbol{z}^-.$$

Conversely if $\boldsymbol{t} = A\boldsymbol{z}^+ = A\boldsymbol{z}^-$, then $\deg \boldsymbol{z} = |\boldsymbol{t}|$ by definition of $\deg \boldsymbol{z}$ and $|\boldsymbol{t}|$. Q.E.D.

Lemma 3.5.1 implies that in considering mutual accessibility between $\boldsymbol{x}, \boldsymbol{y} \in \mathcal{F}_{\boldsymbol{t}}$, we only need to consider moves of degree smaller than $|\boldsymbol{t}|$ or moves $\boldsymbol{z}$ with $\boldsymbol{t} = A\boldsymbol{z}^+ = A\boldsymbol{z}^-$.

Recall that, for a frequency vector $\boldsymbol{x} = \{x(\boldsymbol{i})\}_{\boldsymbol{i}\in\mathcal{I}}$, its support is defined by

$$\mathrm{supp}(\boldsymbol{x}) = \{\boldsymbol{i} \mid x(\boldsymbol{i}) > 0\},$$

which is the set of positive cells of $\boldsymbol{x}$. Lemma 3.5.1 also implies the following simple but useful fact.

Lemma 3.5.2 *Suppose that $\mathcal{F}_{\boldsymbol{t}} = \{\boldsymbol{x}, \boldsymbol{y}\}$ is a two-element set and suppose that the supports of $\boldsymbol{x}$ and $\boldsymbol{y}$ are disjoint. Then $K_{\boldsymbol{t}} = 2$ and $\boldsymbol{x}, \boldsymbol{y}$ are $\mathcal{B}_{|\boldsymbol{t}|-1}$-equivalence classes by themselves. Furthermore $\boldsymbol{z} = \boldsymbol{y} - \boldsymbol{x}$ belongs to each Markov basis.*

Proof. Suppose that $\boldsymbol{y}$ is accessible from $\boldsymbol{x}$ by $\mathcal{B}_{|\boldsymbol{t}|-1}$. Then there exists a non-zero move $\boldsymbol{z}$ with $\deg \boldsymbol{z} \le |\boldsymbol{t}| - 1$ such that $\boldsymbol{z}$ is applicable to $\boldsymbol{x}$. If $\boldsymbol{x} + \boldsymbol{z} = \boldsymbol{y}$, then $\boldsymbol{z} = \boldsymbol{y} - \boldsymbol{x}$ and $\deg \boldsymbol{z} = |\boldsymbol{t}|$ because the supports of $\boldsymbol{x}$ and $\boldsymbol{y}$ are disjoint. Therefore $\boldsymbol{x} + \boldsymbol{z} \ne \boldsymbol{y}$ and $\mathcal{F}_{\boldsymbol{t}}$ contains a third element $\boldsymbol{x} + \boldsymbol{z}$, which is a contradiction. Therefore $\boldsymbol{y}$ and $\boldsymbol{x}$ are in different $\mathcal{B}_{|\boldsymbol{t}|-1}$-equivalence classes, implying that $\boldsymbol{y}$ and $\boldsymbol{x}$ are $\mathcal{B}_{|\boldsymbol{t}|-1}$-equivalence classes by themselves.

Now consider moving from $\boldsymbol{x}$ to $\boldsymbol{y}$. Since they are $\mathcal{B}_{|\boldsymbol{t}|-1}$-equivalence classes by themselves, no non-zero move $\boldsymbol{z}$ of degree $\deg \boldsymbol{z} < |\boldsymbol{t}|$ is applicable to $\boldsymbol{x}$. By Lemma 3.5.1, only moves $\boldsymbol{z}$ with $\boldsymbol{t} = A\boldsymbol{z}^+ = A\boldsymbol{z}^-$ are applicable to $\boldsymbol{x}$. If any such move is different from $\boldsymbol{y} - \boldsymbol{x}$, then as above $\mathcal{F}_{\boldsymbol{t}}$ contains a third element. It follows that in order to move from $\boldsymbol{x}$ to $\boldsymbol{y}$, we have to move by exactly one step using the move $\boldsymbol{z} = \boldsymbol{y} - \boldsymbol{x}$. Therefore $\boldsymbol{z}$ has to belong to any Markov basis. Q.E.D.

Define $\min(\boldsymbol{x}, \boldsymbol{y})$, the minimum of $\boldsymbol{x}$ and $\boldsymbol{y}$, elementwise

$$\min(\boldsymbol{x}, \boldsymbol{y})(\boldsymbol{i}) = \min(x(\boldsymbol{i}), y(\boldsymbol{i})).$$

Lemma 3.5.2 can be slightly modified to yield the following result for the case, where supports of $\boldsymbol{x}$ and $\boldsymbol{y}$ are not necessarily disjoint.

Lemma 3.5.3 *Suppose that $\mathcal{F}_{\boldsymbol{t}} = \{\boldsymbol{x}, \boldsymbol{y}\}$ is a two-element set. Then $\boldsymbol{z} = \boldsymbol{y} - \boldsymbol{x}$ belongs to each Markov basis.*

Proof. If the supports of $\boldsymbol{x}$ and $\boldsymbol{y}$ are disjoint, then the result is already contained in Lemma 3.5.2. Otherwise let $\boldsymbol{v} = \min(\boldsymbol{x}, \boldsymbol{y})$ and consider $\boldsymbol{y} - \boldsymbol{v}$ and $\boldsymbol{x} - \boldsymbol{v}$. Then the supports of $\boldsymbol{y} - \boldsymbol{v}$ and $\boldsymbol{x} - \boldsymbol{v}$ are disjoint and by Lemma 3.5.2 again

$$\boldsymbol{z} = (\boldsymbol{y} - \boldsymbol{v}) - (\boldsymbol{x} - \boldsymbol{v}) = \boldsymbol{y} - \boldsymbol{x}$$

belongs to each Markov basis. Q.E.D.

The following lemma concerns replacing a move by series of moves.

Lemma 3.5.4 *Let $\mathcal{B}$ be a set of moves and let $\boldsymbol{z}_0 \notin \mathcal{B}$ be another non-zero move. Assume that $\boldsymbol{z}_0^+$ is accessible from $\boldsymbol{z}_0^-$ by $\mathcal{B}$. Then for each $\boldsymbol{x}$, to which $\boldsymbol{z}_0$ is applicable, $\boldsymbol{x} + \boldsymbol{z}_0$ is accessible from $\boldsymbol{x}$ by $\mathcal{B}$.*

This lemma shows that if $\boldsymbol{z}_0^+$ is accessible from $\boldsymbol{z}_0^-$ by $\mathcal{B}$, then we can always replace $\boldsymbol{z}_0$ by a series of moves from $\mathcal{B}$.

Proof. Suppose that $\boldsymbol{z}_0$ is applicable to $\boldsymbol{x}$. Then $\boldsymbol{x} - \boldsymbol{z}_0^- \geq 0$ by (3.33). By the definition of accessibility (cf. (3.34)), we can move from $\boldsymbol{z}_0^-$ to $\boldsymbol{z}_0^+$ by moves from $\mathcal{B}$ without causing negative cells on the way. Then the same sequence of moves can be applied to $\boldsymbol{x}$ without causing negative cells on the way, leading from $\boldsymbol{x}$ to $\boldsymbol{x} + \boldsymbol{z}_0$. Q.E.D.

Now we are ready to prove Theorem 3.5.1 and is corollaries.

Proof of Theorem 3.5.1. Let $\mathcal{B}$ be a minimal Markov basis. For each $\boldsymbol{z} \in \mathcal{B}_n \setminus (\mathcal{B} \cap \mathcal{B}_n)$, $\boldsymbol{z}^+$ is accessible from $\boldsymbol{z}^-$ by $\mathcal{B} \cap \mathcal{B}_n$, because no move of degree greater than n is applicable to $\boldsymbol{z}^+$ as stated in Lemma 1. Considering this fact and Lemma 5, it follows that $\mathcal{B}_n$ and $\mathcal{B} \cap \mathcal{B}_n$ induces the same equivalence classes in $\mathcal{F}_{\boldsymbol{t}}$, $|\boldsymbol{t}| = n + 1$. Fix a particular $\boldsymbol{t}$. Write

$$\{\boldsymbol{z}_1, \ldots, \boldsymbol{z}_L\} = \mathcal{B} \cap \mathcal{B}_{\boldsymbol{t}}.$$

For any $j = 1, \ldots, L$, let

$$\boldsymbol{x} = \boldsymbol{z}_j^+, \ \boldsymbol{y} = \boldsymbol{z}_j^-.$$

If $\boldsymbol{x}$ and $\boldsymbol{y}$ are in the same $\mathcal{B}_{|\boldsymbol{t}|-1}$-equivalence class, then by Lemma 3.5.4, $\boldsymbol{z}_j$ can be replaced by a series of moves of lower degree from $\mathcal{B}$ and $\mathcal{B} \setminus \{\boldsymbol{z}_j\}$ remains to be a Markov basis. This contradicts the minimality of $\mathcal{B}$. Therefore $\boldsymbol{z}_j^+$ and $\boldsymbol{z}_j^-$ are in two different $\mathcal{B}_{|\boldsymbol{t}|-1}$-equivalence classes connecting them. Now we consider an undirected graph, whose vertices are $\mathcal{B}_{|\boldsymbol{t}|-1}$-equivalence classes of $\mathcal{F}_{\boldsymbol{t}}$ and whose edges are moves $\boldsymbol{z}_1, \ldots, \boldsymbol{z}_L$. Considering that $\mathcal{B}$ is a Markov basis, and no move of degree greater than $|\boldsymbol{t}|$ is applicable to each element of $\mathcal{F}_{\boldsymbol{t}}$ as stated in Lemma 1, this graph is connected. On the other hand if the graph contains a cycle, then there exits $\boldsymbol{z}_j$, such that $\boldsymbol{z}_j^+$ and $\boldsymbol{z}_j^-$ are mutually accessible by $\mathcal{B} \setminus \{\boldsymbol{z}_j\}$. By Lemma 3.5.4 again, this contradicts the minimality of $\mathcal{B}$. It follows that the graph is a tree. Since any tree with $K_{\boldsymbol{t}}$ vertices has $K_{\boldsymbol{t}} - 1$ edges, $L = K_{\boldsymbol{t}} - 1$.

Reversing the above argument, it is now easy to see that if $K_{\boldsymbol{t}} - 1$ moves $z_{\boldsymbol{t},1}, \ldots, z_{\boldsymbol{t},K_{\boldsymbol{t}}-1}$ connecting different $\mathcal{B}_{|\boldsymbol{t}|-1}$-equivalence classes of $\mathcal{F}_{\boldsymbol{t}}$ are chosen in such a way that the equivalence classes are connected into a tree by these moves, then

$$\mathcal{B} = \bigcup_{\boldsymbol{t}:K_{\boldsymbol{t}}\geq 2} \{z_{\boldsymbol{t},1}, \ldots, z_{\boldsymbol{t},K_{\boldsymbol{t}}-1}\}$$

is a minimal Markov basis. Q.E.D.

Proof of Corollary 3.5.1. From our argument preceding Corollary 3.5.1, it follows that if minimal Markov basis is unique then for each $\boldsymbol{t}$, $\mathcal{F}_{\boldsymbol{t}}$ itself constitutes one $\mathcal{B}_{|\boldsymbol{t}|-1}$-equivalence class or $\mathcal{F}_{\boldsymbol{t}}$ is a two element set $\{\boldsymbol{x}_{\boldsymbol{t},1}, \boldsymbol{x}_{\boldsymbol{t},2}\}$, such that $\boldsymbol{x}_{\boldsymbol{t},1} \not\sim \boldsymbol{x}_{\boldsymbol{t},2} \pmod{\mathcal{B}_{|\boldsymbol{t}|-1}}$. Therefore we only need to prove the converse. Suppose that for each $\boldsymbol{t}$, $\mathcal{F}_{\boldsymbol{t}}$ itself constitutes one $\mathcal{B}_{|\boldsymbol{t}|-1}$-equivalence class or $\mathcal{F}_{\boldsymbol{t}}$ is a two element set. By Lemma 3.5.3, for each two-element set $\mathcal{F}_{\boldsymbol{t}} = \{\boldsymbol{x}, \boldsymbol{y}\}$ the move $\boldsymbol{z} = \boldsymbol{y} - \boldsymbol{x}$ belongs to each Markov basis. However by Theorem 3.5.1 each minimal Markov basis consists only of these moves. Therefore minimal Markov basis is unique. Q.E.D.

Proof of Corollary 3.5.2. By Lemma 3.5.3, indispensable moves belong to each Markov basis. Therefore if the set of indispensable moves forms a Markov basis, then it is the unique Markov basis.

On the other hand if the set of indispensable moves do not constitute a Markov basis, then there is a term with $K_{\boldsymbol{t}} \geq 3$ in (3.36) and in this case a minimal Markov basis $\mathcal{B}$ is not unique as discussed after Theorem 3.5.1.

From these considerations it is obvious that if the unique Markov basis exists, it coincides with the set of indispensable moves. Q.E.D.

Finally we derive an additional lemma, which is of some independent interest. For some set $\mathcal{F}$ of frequency vectors, define its support by

$$\mathrm{supp}(\mathcal{F}) = \bigcup_{\boldsymbol{x}\in\mathcal{F}} \mathrm{supp}(\boldsymbol{x}) = \{\boldsymbol{i} \mid x(\boldsymbol{i}) > 0 \text{ for some } \boldsymbol{x} \in \mathcal{F}\}.$$

Then we have the following lemma.

Lemma 3.5.5 *Consider the $\mathcal{B}_{|\boldsymbol{t}|-1}$-equivalence classes of (3.35). The supports of the equivalence classes* $\mathrm{supp}(\mathcal{F}_{\boldsymbol{t},1}), \ldots, \mathrm{supp}(\mathcal{F}_{\boldsymbol{t},K_{\boldsymbol{t}}})$ *are disjoint.*

Proof. Suppose that there exist $\boldsymbol{x} \in \mathcal{F}_{\boldsymbol{t},j_1}$, $\boldsymbol{y} \in \mathcal{F}_{\boldsymbol{t},j_2}$, $j_1 \neq j_2$, such that the supports of $\boldsymbol{x}$ and $\boldsymbol{y}$ are not disjoint. Let $\boldsymbol{v} = \min(\boldsymbol{x}, \boldsymbol{y})$ and consider $\boldsymbol{y} - \boldsymbol{v}$ and $\boldsymbol{x} - \boldsymbol{v}$. Because $\boldsymbol{v}$ is a non-zero vector, the sample size becomes smaller

$$|\boldsymbol{x} - \boldsymbol{v}| = |\boldsymbol{y} - \boldsymbol{v}| < n = |\boldsymbol{x}| = |\boldsymbol{y}|.$$

Then

$$\boldsymbol{z} = \boldsymbol{y} - \boldsymbol{x} = (\boldsymbol{y} - \boldsymbol{v}) - (\boldsymbol{x} - \boldsymbol{v})$$

has degree $\deg \boldsymbol{z} = |\boldsymbol{x} - \boldsymbol{v}| < n$. Now $\boldsymbol{y} = \boldsymbol{x} + \boldsymbol{z}$ is accessible from $\boldsymbol{x}$ by a single move $\boldsymbol{z}$. This is a contradiction, because $\boldsymbol{x}$ and $\boldsymbol{y}$ belong to different $\mathcal{B}_{n-1}$-equivalence classes. Q.E.D.

3.5.4 Some examples of minimal Markov bases

In this section we verify Theorem 3.5.1 for various problems. First we investigate standard contingency tables with fixed marginals. Then we investigate some other models including a simple case of Poisson regression model and the Hardy-Weinberg model.

One-way contingency tables. We start with the simplest case of one-way contingency tables. Let $\boldsymbol{x} = \{x_i\}_{i\in[I]}$ be an I dimensional frequency vector and $A = 1_I'$. In this case, $\boldsymbol{t}$ is the sample size n. This situation corresponds to testing the homogeneity of mean parameters for I independent Poisson variables conditional on the total sample size n. See also the example of Poisson regression below. In this case, a minimal Markov basis is formed as a set of $I-1$ degree 1 moves, but is not unique. A minimal Markov basis is constructed as follows. First consider the case of $n = |\boldsymbol{t}| = 1$. There are I elements in $\mathcal{F}_{\boldsymbol{t}}$ as

$$\mathcal{F}_{\boldsymbol{t}} = \{(1,0,\ldots,0)', (0,1,0,\ldots,0)', \ldots, (0,\ldots,0,1)'\}.$$

Each element $\boldsymbol{x} \in \mathcal{F}_{\boldsymbol{t}}$ forms an equivalence class by itself. To connect these points into a tree, there are I^{I-2} ways of choosing $I-1$ degree 1 moves by Cayley's theorem (see e.g. Chapter 4 of Wilson, 1985). One example is

$$\mathcal{B} = \{(1,-1,0,\ldots,0)', (0,1,-1,0,\ldots,0)', \ldots, (0,\ldots,0,1,-1)'\}.$$

It is easily verified that no move of degree larger than 1 is needed.

Two-way contingency tables. Next example is a standard two-way contingency table with fixed row and column sums. As is already seen, $\boldsymbol{x} = \{x_{ij}\}_{i\in[I],j\in[J]}$ and

$$A = \begin{bmatrix} 1_I' \otimes E_J \\ E_I \otimes 1_J' \end{bmatrix}.$$

This is an elementary example of testing the hypothesis that the rows and the columns are independent. In this case, it is well known that the set of degree 2 moves displayed as

$$\boxed{\begin{array}{cc} +1 & -1 \\ -1 & +1 \end{array}}$$

is a Markov basis. In addition, this is the unique minimal Markov basis from the discussion in the previous section. Indeed, for every $\boldsymbol{t}$ with $|\boldsymbol{t}| = 2$, except for a trivial case of one-element set $\#\mathcal{F}_{\boldsymbol{t}} = 1$, there are only two elements in $\mathcal{F}_{\boldsymbol{t}}$ and the above move is the difference of these two elements.

Three-way contingency tables with fixed two-dimensional marginals. Next we consider three-way contingency tables with fixed two-dimensional marginals. As we have seen in Section 3.5.1, $\boldsymbol{x} = \{x_{ijk}\}_{i\in[I],j\in[J],k\in[K]}$ is the frequency vector of $I \times J \times K$ contingency table with lexicographical ordering of cells and A is written as

$$A = \begin{bmatrix} 1_I' \otimes E_J \otimes E_K \\ E_I \otimes 1_J' \otimes E_K \\ E_I \otimes E_J \otimes 1_K' \end{bmatrix}.$$

This corresponds to testing no three-way interactions of the log-linear model. As is already stated, it is surprisingly difficult to construct a connected Markov chain. Although an algebraic algorithm to calculate a Markov basis is given by Diaconis and Sturmfels (1998), any explicit characterization of a Markov basis is not known at present, except for some special cases. For the case of $2 \times J \times K$ tables, an explicit form of a Markov basis is given in Diaconis and Sturmfels (1998). Their basis is a set of degree $4, 6, \dots, \min\{J, K\}$ moves, where a typical degree $2n$ move is the following $2 \times n \times n$ move displayed as

$$\begin{array}{|cccccc|}\hline +1 & -1 & 0 & 0 & \cdots & 0 \\ 0 & +1 & -1 & 0 & \cdots & 0 \\ \vdots & & \ddots & \ddots & & \vdots \\ 0 & & & +1 & -1 & 0 \\ 0 & 0 & \cdots & 0 & +1 & -1 \\ -1 & 0 & \cdots & 0 & 0 & +1 \\ \hline \end{array} \quad \begin{array}{|cccccc|}\hline -1 & +1 & 0 & 0 & \cdots & 0 \\ 0 & -1 & +1 & 0 & \cdots & 0 \\ \vdots & & \ddots & \ddots & & \vdots \\ 0 & & & -1 & +1 & 0 \\ 0 & 0 & \cdots & 0 & -1 & +1 \\ +1 & 0 & \cdots & 0 & 0 & -1 \\ \hline \end{array}.$$

All the other degree $2n$ moves are obtained from this by permutations of indices or axes.

For the case of $3 \times 3 \times K$ tables, we proves in Section 3.2 that a Markov basis is given as a set of the following four types of moves (and permutation of their indices and axes).

$$\text{degree 4 move :} \quad \begin{array}{|ccccc|}\hline +1 & -1 & 0 & 0 & 0 \\ -1 & +1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \\ \hline \end{array} \quad \begin{array}{|ccccc|}\hline -1 & +1 & 0 & 0 & 0 \\ +1 & -1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \\ \hline \end{array} \quad \begin{array}{|ccccc|}\hline 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \\ \hline \end{array}$$

$$\text{degree 6 move :} \quad \begin{array}{|ccccc|}\hline +1 & -1 & 0 & 0 & 0 \\ -1 & 0 & +1 & 0 & 0 \\ 0 & +1 & -1 & 0 & 0 \\ \hline \end{array} \quad \begin{array}{|ccccc|}\hline -1 & +1 & 0 & 0 & 0 \\ +1 & 0 & -1 & 0 & 0 \\ 0 & -1 & +1 & 0 & 0 \\ \hline \end{array} \quad \begin{array}{|ccccc|}\hline 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \\ \hline \end{array}$$

$$\text{degree 8 move :} \quad \begin{array}{|ccccc|}\hline +1 & -1 & 0 & 0 & 0 \\ -1 & +1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \\ \hline \end{array} \quad \begin{array}{|ccccc|}\hline -1 & 0 & +1 & 0 & 0 \\ +1 & 0 & 0 & -1 & 0 \\ 0 & 0 & -1 & +1 & 0 \\ \hline \end{array} \quad \begin{array}{|ccccc|}\hline 0 & +1 & -1 & 0 & 0 \\ 0 & -1 & 0 & +1 & 0 \\ 0 & 0 & +1 & -1 & 0 \\ \hline \end{array}$$

$$\text{degree 10 move :} \quad \begin{array}{|ccccc|}\hline +1 & -1 & 0 & 0 & 0 \\ -1 & +1 & 0 & -1 & +1 \\ 0 & 0 & 0 & +1 & -1 \\ \hline \end{array} \quad \begin{array}{|ccccc|}\hline -1 & 0 & +1 & 0 & 0 \\ +1 & 0 & 0 & 0 & -1 \\ 0 & 0 & -1 & 0 & +1 \\ \hline \end{array} \quad \begin{array}{|ccccc|}\hline 0 & +1 & -1 & 0 & 0 \\ 0 & -1 & 0 & +1 & 0 \\ 0 & 0 & +1 & -1 & 0 \\ \hline \end{array}$$

It is observed that $\mathcal{F}_{\boldsymbol{t}}$ is a two element set for each $\boldsymbol{t} = A\boldsymbol{z}$ of the above moves $\boldsymbol{z}$ for the $2 \times J \times K$ case and for the $3 \times 3 \times K$ case. Hence these moves constitute the unique minimal basis for respective cases. In addition, for the cases of $3 \times 4 \times K$ and $4 \times 4 \times 4$, we proves that the set of indispensable moves listed in Section 3.3 constitutes the unique minimal Markov basis for each cases. However, for general $I \times J \times K$ case, we do not know whether a unique minimal Markov basis exists or not. This is one of very attractive open problems.

Three-way contingency tables with fixed one-dimensional marginals. We now consider general three-way tables with fixed one-dimensional marginals. This corresponds to testing the independence model for three-way tables. Recently Dobra and Sullivant (2002) gave a general construction of Markov basis for decomposable and reducible models. The three-way independence model is a special case of decomposable models and can be treated in the framework of Dobra and Sullivant (2002). However our main concern here is the question of minimality of the Markov basis given in Proposition 3.5.1 below.

With lexicographic ordering of indices, the matrix A is written as

$$A = \begin{bmatrix} 1'_I \otimes 1'_J \otimes E_K \\ 1'_I \otimes E_J \otimes 1'_K \\ E_I \otimes 1'_J \otimes 1'_K \end{bmatrix}.$$

In this case, we construct a minimal Markov basis as follows.

There are two obvious patterns of moves of degree 2. An example of moves of type I is

$$z_{111} = z_{222} = 1, \ z_{211} = z_{122} = -1,$$

with other elements being 0. For the case of $2 \times 2 \times 2$ table, this move can be displayed as follows

$$\boxed{\begin{array}{cc} +1 & 0 \\ 0 & -1 \end{array}} \quad \boxed{\begin{array}{cc} -1 & 0 \\ 0 & +1 \end{array}}\ .$$

All the other moves of type I are obtained by permutation of indices or the axes.

An example of moves of type II is

$$z_{111} = z_{122} = 1, \ z_{112} = z_{121} = -1,$$

with other elements being 0. For the case of $2 \times 2 \times 2$ table, this move can be displayed as follows

$$\boxed{\begin{array}{cc} +1 & -1 \\ -1 & +1 \end{array}} \quad \boxed{\begin{array}{cc} 0 & 0 \\ 0 & 0 \end{array}}\ .$$

All the other moves of type II are obtained by permutation of indices or the axes. Let $\mathcal{B}^*$ be the set of type I and type II degree 2 moves. Then we have the following proposition.

Proposition 3.5.1 *$\mathcal{B}^*$ is a Markov basis for three-way contingency tables with fixed one-dimensional marginals.*

Proof. In this problem it is obvious that no degree 1 move is applicable to any frequency vector. Furthermore it is easy to verify that every degree 2 move is either of type I or type II. It remains to verify that for $|\boldsymbol{t}| \geq 3$, $\mathcal{F}_{\boldsymbol{t}}$ itself constitutes one $\mathcal{B}^*$-equivalence class. We can now apply the same argument used for $3 \times 3 \times K$ tables with fixed two-dimensional marginals in

Section 3.2. Suppose that for some $\boldsymbol{t}$, $\mathcal{F}_{\boldsymbol{t}}$ consists of more than one $\mathcal{B}^*$-equivalence classes. Let $\mathcal{F}_1, \mathcal{F}_2$ denote two different $\mathcal{B}^*$-equivalence classes. Choose $\boldsymbol{x} \in \mathcal{F}_1, \boldsymbol{y} \in \mathcal{F}_2$ such that

$$|\boldsymbol{z}| = |\boldsymbol{x} - \boldsymbol{y}| = \sum_{i,j,k} |x_{ijk} - y_{ijk}|$$

is minimized. Because $\boldsymbol{x}$ and $\boldsymbol{y}$ are chosen from different $\mathcal{B}^*$-equivalence classes, this minimum has to be positive. In the following we let $z_{111} > 0$ without loss of generality.

Case 1: Suppose that there exists a negative cell $z_{i_0 11} < 0, i_0 \geq 2$. Then because $\sum_{j,k} z_{i_0 jk} = 0$, there exists $(j,k), j+k > 2$, with $z_{i_0 jk} > 0$. Then the four cells

$$(1,1,1),\ (i_0,1,1),\ (i_0,j,k),\ (1,j,k)$$

are in the positions of either type I move or type II move. In either case we can apply a type I move or a type II move to $\boldsymbol{x}$ or $\boldsymbol{y}$ and make $|\boldsymbol{z}| = |\boldsymbol{x} - \boldsymbol{y}|$ smaller, which is a contradiction. This argument shows that $\boldsymbol{z}$ can not contain both positive and negative elements in any one-dimensional slice.

Case 2: Now we consider the remaining case, where no one-dimensional slice of $\boldsymbol{z}$ contains both positive and negative elements. Since $\sum_{j,k} z_{1jk} = 0$, there exists (j_1, k_1), $j_1, k_1 \geq 2$, such that $z_{1j_1k_1} < 0$. Similarly there exists (i_1, k_2), $i_1, k_2 \geq 2$, such that $z_{i_1 1 k_2} < 0$. Then the four cells

$$(1, j_1, k_1), (1, 1, k_1), (i_1, 1, k_2), (i_1, j_1, k_2)$$

are in the positions of a type II move (if $k_1 = k_2$) or a type I move (if $k_1 \neq k_2$) and we can apply a degree 2 move. By doing this $|\boldsymbol{z}| = |\boldsymbol{x} - \boldsymbol{y}|$ may remain the same, but now z_{11k_1} becomes negative and this case reduces to Case 1. Therefore Case 2 itself is a contradiction. Q.E.D.

We show in the following that $\mathcal{B}^*$ is not a minimal Markov basis. Let $\boldsymbol{z}$ be a degree 2 move and let $\boldsymbol{t} = A\boldsymbol{z}^+$. If $\boldsymbol{z}$ is a type II move, it is easy to verify that $\mathcal{F}_{\boldsymbol{t}}$ is a two-element set $\{\boldsymbol{z}^+, \boldsymbol{z}^-\}$. Therefore degree 2 moves of type II belong to each Markov basis. On the other hand, if $\boldsymbol{z}$ is a type I move, $\mathcal{F}_{\boldsymbol{t}}$ is a four-element set. For the $2 \times 2 \times 2$ case, let $\boldsymbol{t} = (z_{1\cdot\cdot}, z_{2\cdot\cdot}, z_{\cdot 1\cdot}, z_{\cdot 2\cdot}, z_{\cdot\cdot 1}, z_{\cdot\cdot 2})' = (1,1,1,1,1,1)'$. Then it follows

$$\mathcal{F}_{(1,1,1,1,1,1)'} = \left\{ \boxed{\begin{matrix} 1 & 0 \\ 0 & 0 \end{matrix}}\ \boxed{\begin{matrix} 0 & 0 \\ 0 & 1 \end{matrix}}\ ,\ \boxed{\begin{matrix} 0 & 1 \\ 0 & 0 \end{matrix}}\ \boxed{\begin{matrix} 0 & 0 \\ 1 & 0 \end{matrix}}\ ,\ \boxed{\begin{matrix} 0 & 0 \\ 1 & 0 \end{matrix}}\ \boxed{\begin{matrix} 0 & 1 \\ 0 & 0 \end{matrix}}\ ,\ \boxed{\begin{matrix} 0 & 0 \\ 0 & 1 \end{matrix}}\ \boxed{\begin{matrix} 1 & 0 \\ 0 & 0 \end{matrix}} \right\}.$$

To connect these elements to a tree, only three moves of type I are needed. In the $2 \times 2 \times 2$ case, there are $4^{4-2} = 16$ possibilities, such as

$$\boxed{\begin{matrix} +1 & -1 \\ 0 & 0 \end{matrix}}\ \boxed{\begin{matrix} 0 & 0 \\ -1 & +1 \end{matrix}}\ ,\ \boxed{\begin{matrix} 0 & +1 \\ -1 & 0 \end{matrix}}\ \boxed{\begin{matrix} 0 & -1 \\ +1 & 0 \end{matrix}}\ ,\ \boxed{\begin{matrix} 0 & 0 \\ +1 & -1 \end{matrix}}\ \boxed{\begin{matrix} -1 & +1 \\ 0 & 0 \end{matrix}}$$

or

$$\boxed{\begin{matrix} +1 & -1 \\ 0 & 0 \end{matrix}}\ \boxed{\begin{matrix} 0 & 0 \\ -1 & +1 \end{matrix}}\ ,\ \boxed{\begin{matrix} +1 & 0 \\ -1 & 0 \end{matrix}}\ \boxed{\begin{matrix} 0 & -1 \\ 0 & +1 \end{matrix}}\ ,\ \boxed{\begin{matrix} +1 & 0 \\ 0 & -1 \end{matrix}}\ \boxed{\begin{matrix} -1 & 0 \\ 0 & +1 \end{matrix}}$$

and so on. From these considerations, a minimal Markov basis for $I \times J \times K$ tables consists of

$$3 \binom{I}{2} \binom{J}{2} \binom{K}{2}$$

degree 2 moves of type I and

$$I\binom{J}{2}\binom{K}{2}+J\binom{I}{2}\binom{K}{2}+K\binom{I}{2}\binom{J}{2}$$

degree 2 moves of type II.

Poisson regression. Here we consider a simple example of Poisson regression discussed in Diaconis, Eisenbud and Sturmfels (1998). Let $\boldsymbol{x} = (x_0, x_1, \ldots, x_4)'$ and

$$A = \begin{bmatrix} 1 & 1 & 1 & 1 & 1 \\ 0 & 1 & 2 & 3 & 4 \end{bmatrix}.$$

Diaconis, Eisenbud and Sturmfels (1998) states that the set of degree 2 moves,

$$\begin{aligned}\mathcal{B} \;=\; & \{(1,-1,-1,1,0)', (1,-1,0,-1,1)', (0,1,-1,-1,1)', \\ & (1,-2,1,0,0)', (0,1,-2,1,0)', (0,0,1,-2,1)'\}\end{aligned}$$

enables a connected chain. Indeed, the above basis is a minimal Markov basis but is not unique. To see this, consider $\mathcal{F}_{\boldsymbol{t}}$ with $|\boldsymbol{t}| = 2$. There are 9 possible values of $\boldsymbol{t}$ as

$$\boldsymbol{t}' = (2,0), (2,1), \ldots, (2,8).$$

For the case of $\boldsymbol{t}' = (2,0), (2,1), (2,7), (2,8)$, there is only one element in $\mathcal{F}_{\boldsymbol{t}}$ and we need not any move. For the case of $\boldsymbol{t}' = (2,2), (2,3), (2,5), (2,6)$, there are two elements in $\mathcal{F}_{\boldsymbol{t}}$, but for the case of $\boldsymbol{t}' = (2,4)$ there are three elements in $\mathcal{F}_{\boldsymbol{t}}$ as

$$\mathcal{F}_{(2,4)'} = \{(1,0,0,0,1)', (0,1,0,1,0)', (0,0,2,0,0)'\}.$$

The elements of the above $\mathcal{B}$ corresponds to the difference of the two elements in $\mathcal{F}_{\boldsymbol{t}}$, $\boldsymbol{t}' = (2,2), (2,3), (2,5), (2,6)$, and $\{(1,-1,0,-1,1)', (0,1,-2,1,0)'\}$, which connects the three elements in $\mathcal{F}_{(2,4)'}$ into a tree. This is not the only pair of moves to connect the three elements in $\mathcal{F}_{(2,4)'}$ to form a tree. There are three possibilities, i.e.,

$$\begin{aligned}\mathcal{B}^* \;=\; & \{(1,-1,-1,1,0)', (1,-1,0,-1,1)', (0,1,-1,-1,1)', \\ & (1,-2,1,0,0)', (1,0,-2,0,1)', (0,0,1,-2,1)'\}\end{aligned}$$

and

$$\begin{aligned}\mathcal{B}^{**} \;=\; & \{(1,-1,-1,1,0)', (1,0,2,0,1)', (0,1,-1,-1,1)', \\ & (1,-2,1,0,0)', (0,1,-2,1,0)', (0,0,1,-2,1)'\}\end{aligned}$$

are also minimal Markov bases.

Hardy-Weinberg model. Consider the case of

$$\boldsymbol{x} = (x_{11}, x_{12}, \ldots, x_{1I}, x_{22}, x_{23}, \ldots, x_{2I}, x_{33}, \ldots, x_{II})'$$

and $\boldsymbol{t} = (t_1, \ldots, t_I)'$ defined as

$$t_i = 2x_{ii} + \sum_{j \neq i} x_{ij}, \qquad i = 1, \ldots, I,$$

where $x_{ij} = x_{ji}$ for $i > j$. In this case, A is written as

$$A = (A_I \ A_{I-1} \ \cdots \ A_1), \quad A_k = \left(O_{k \times (I-k)} \ B_k'\right)',$$

where B_k is the following $k \times k$ square matrix

$$B_k = \begin{bmatrix} 2 & 1 & 1 & \cdots & 1 \\ 0 & 1 & 0 & \cdots & 0 \\ 0 & 0 & 1 & & 0 \\ \vdots & \vdots & & \ddots & \vdots \\ 0 & 0 & \cdots & 0 & 1 \end{bmatrix}.$$

This corresponds to the conditional test of the Hardy-Weinberg proportion. For this problem, Guo and Thompson (1992) construct a connected Markov chain. Their basis consists of three types of degree 2 moves, namely, type 0, type 1 and type 2. Here the term type refers to the number of nonzero diagonal cells in the move. The examples of the moves are displayed as

$$\text{type 0: } \begin{array}{|cccc|} \hline 0 & +1 & -1 & 0 \\ & 0 & 0 & -1 \\ & & 0 & +1 \\ & & & 0 \\ \hline \end{array}, \quad \text{type 1: } \begin{array}{|cccc|} \hline +1 & -1 & -1 & 0 \\ & 0 & +1 & 0 \\ & & 0 & 0 \\ & & & 0 \\ \hline \end{array}, \quad \text{type 2: } \begin{array}{|cccc|} \hline +1 & 0 & -2 & 0 \\ & 0 & 0 & 0 \\ & & +1 & 0 \\ & & & 0 \\ \hline \end{array}.$$

We show in the following that their basis is not minimal, and a minimal basis is not unique. Consider $\mathcal{F}_{\boldsymbol{t}}$ with $|\boldsymbol{t}| = 2$ for the above three types of moves. If $\boldsymbol{t} = A\boldsymbol{z}^+ = A\boldsymbol{z}^-$ for moves $\boldsymbol{z}$ of type 1 or type 2, there are two elements in $\mathcal{F}_{\boldsymbol{t}}$ and the move of type 1 or type 2 is the difference of these two elements. But if $\boldsymbol{t} = A\boldsymbol{z}^+ = A\boldsymbol{z}^-$ for a move $\boldsymbol{z}$ of type 0, there are three elements in $\mathcal{F}_{\boldsymbol{t}}$. Then to connect these three elements to form a tree, we can chose two moves to construct a minimal Markov basis. (There are three ways of doing this.) For example, consider the case of $I = 4$ and $\boldsymbol{t} = (1, 1, 1, 1)'$. $\mathcal{F}_{(1,1,1,1)'}$ is written as

$$\mathcal{F}_{(1,1,1,1)'} = \left\{ \begin{array}{|cccc|} \hline 0 & 1 & 0 & 0 \\ & 0 & 0 & 0 \\ & & 0 & 1 \\ & & & 0 \\ \hline \end{array}, \begin{array}{|cccc|} \hline 0 & 0 & 1 & 0 \\ & 0 & 0 & 1 \\ & & 0 & 0 \\ & & & 0 \\ \hline \end{array}, \begin{array}{|cccc|} \hline 0 & 0 & 0 & 1 \\ & 0 & 1 & 0 \\ & & 0 & 0 \\ & & & 0 \\ \hline \end{array} \right\}.$$

To connect these three elements to a tree, any two of the following type 0 moves of degree 2,

$$\begin{array}{|cccc|} \hline 0 & +1 & -1 & 0 \\ & 0 & 0 & -1 \\ & & 0 & +1 \\ & & & 0 \\ \hline \end{array}, \begin{array}{|cccc|} \hline 0 & +1 & 0 & -1 \\ & 0 & -1 & 0 \\ & & 0 & +1 \\ & & & 0 \\ \hline \end{array}, \begin{array}{|cccc|} \hline 0 & 0 & -1 & +1 \\ & 0 & +1 & -1 \\ & & 0 & 0 \\ & & & 0 \\ \hline \end{array}$$

can be included in a minimal Markov basis. Accordingly, $I(I-1)(I-2)(I-3)/12$ moves of type 0, $I(I-1)(I-2)/2$ moves of type 1 and $I(I-1)/2$ moves of type 2 constitute a minimal Markov basis. The basis by Guo and Thompson (1992) is not minimal in the sense that all of $I(I-1)(I-2)(I-3)/8$ moves of type 0 are used in the algorithm proposed by them.

3.5.5 Discussion

In the examples above we saw that for some problems minimal Markov basis is unique and for other problems it is not unique. Clearly this depends only on the properties of matrix A. But it seems very difficult to give a simple necessary and sufficient condition on A such that minimal Markov basis is unique. In integer programming literature (e.g. Schrijver, 1986), an important condition is the total unimodularity of the matrix A. We have seen that in the case of two-way contingency tables minimal Markov basis is unique and it is well known that A in (3.31) is totally unimodular. However in the simplest case of one-way tables minimal Markov basis is not unique and yet $A = (1, \ldots, 1)$ is obviously totally unimodular. This shows that total unimodularity is not directly related to uniqueness of minimal Markov basis. We should also mention that A for three-way tables with fixed two-dimensional marginals in (3.32) is not totally unimodular in general. In fact we have found a submatrix of A in (3.32) with determinant 2 by simple computer search.

As mentioned in Section 3.5.2, Theorem 3.5.1 is conceptually constructive, building up a minimal Markov basis from below. However it is computationally difficult to characterize the $\mathcal{B}_{|\boldsymbol{t}|-1}$-equivalence classes of $\mathcal{F}_{\boldsymbol{t}}$ for large $|\boldsymbol{t}|$ as discussed in Diaconis, Eisenbud and Sturmfels (1998). If we could easily select representative elements from $\mathcal{B}_{|\boldsymbol{t}|-1}$-equivalence classes $\mathcal{F}_{\boldsymbol{t}}$ for each $\boldsymbol{t}$, then a minimal Markov basis could be constructed as described in Theorem 3.5.1. Another question is to find a theoretical upper bound for n_0 such that $\mathcal{F}_{\boldsymbol{t}}$ itself constitutes one $\mathcal{B}_{|\boldsymbol{t}|-1}$-equivalence class for all $\boldsymbol{t}$ with $|\boldsymbol{t}| \geq n_0$. By the Hilbert basis theorem existence of such an n_0 is guaranteed, but if we do not know some upper bound for n_0 we can not actually stop forming $\mathcal{B}_{|\boldsymbol{t}|-1}$-equivalence classes of $\mathcal{F}_{\boldsymbol{t}}$.

As mentioned at the end of Section 3.5.1, it is a subtle question to determine which moves of a minimal Markov basis $\mathcal{B}$ are needed for connecting $\mathcal{F}_{\boldsymbol{t}}$ for a given $\boldsymbol{t}$. Obviously we only need those elements of $\mathcal{B}$, that are applicable to at least one frequency vector of $\mathcal{F}_{\boldsymbol{t}}$. However the set of these move may not be minimal for connecting $\mathcal{F}_{\boldsymbol{t}}$ for a given $\boldsymbol{t}$. See the discussion on corner minors for two-way tables in Section 3 of Diaconis, Eisenbud and Sturmfels (1998). We study this question on two-way tables with structural zeros in Section 3.4.7.

3.6 Characterizations of an invariant minimal Markov basis and its uniqueness

In this section we define an invariant Markov basis for a connected Markov chain over the set of contingency tables with fixed marginals and derive some characterizations of minimality of the invariant basis. We also give a necessary and sufficient condition for uniqueness of invariant minimal Markov basis. The invariance here refers to permutation of indices of each axis of the contingency tables. If the categories of each axis do not have any order relations among them, it is natural to consider the action of the symmetric group on each axis of the contingency table. Logically important point is that if a unique minimal Markov basis exists then it is also the unique invariant Markov basis. On the other hand, if a minimal Markov basis is not unique, an invariant minimal Markov basis is important, since a minimal Markov basis is usually not symmetric (see Section 3.5). In Section 3.5, we derived some characterizations of a minimal Markov basis and gave a necessary and sufficient condition for uniqueness of a minimal Markov basis. We combine this approach with the theory of transformation groups to study minimality of invariant Markov bases and give some characterizations of invariant Markov basis and its minimality. We also give a necessary and sufficient condition for uniqueness of invariant minimal Markov basis.

The construction of this section is as follows. Definitions and notations of contingency tables and invariant Markov basis are given in Section 3.6.1. Structures of an invariant minimal Markov basis are derived in Section 3.6.2. Examples of all hierarchical $2 \times 2 \times 2 \times 2$ models are studied in Section 3.6.3.

3.6.1 Preliminaries

Notations and definitions

First we give some additional notations and definitions on contingency tables to the notations given in Section 3.5.1. In Section 3.6 we focus our attention on the ordinary k-way contingency tables. Then we consider an $I_1 \times \cdots \times I_k$ k-way contingency table $\boldsymbol{x}$. We denote a cell of the contingency table by $\boldsymbol{i} = (i_1, \ldots, i_k)$ or $\boldsymbol{i} = (i_1 \ldots i_k)$. The set of cells is denoted by $\mathcal{I} = \mathcal{I}^1 \times \cdots \times \mathcal{I}^k$, where $\mathcal{I}^\ell = [I_\ell],\ \ell \in [k]$. We write $\boldsymbol{x} = \{x(\boldsymbol{i})\}_{\boldsymbol{i} \in \mathcal{I}}$ where $x(\boldsymbol{i})$ is a frequency of cell $\boldsymbol{i}$. Let X denote the set of all k-way contingency tables given by

$$X = \left\{ \boldsymbol{x} = \{x(\boldsymbol{i})\}_{\boldsymbol{i} \in \mathcal{I}} \mid x(\boldsymbol{i}) \in \mathbb{Z}_{\geq 0} \text{ for } \boldsymbol{i} \in \mathcal{I} \right\} .$$

X is partitioned as

$$X = \bigcup_{n=0}^{\infty} X_n, \quad X_n = \{\boldsymbol{x} \in X \mid |\boldsymbol{x}| = n\},$$

where we have already defined as $|\boldsymbol{x}| = \sum_{\boldsymbol{i} \in \mathcal{I}} x(\boldsymbol{i})$.

Let $K = [k]$ and let D denote a subset of K. The *D-marginal* $\boldsymbol{x}_D = \{x_D(\boldsymbol{i}_D)\}_{\boldsymbol{i}_D \in \mathcal{I}_D}$ of $\boldsymbol{x}$ is the contingency table with *marginal cells* $\boldsymbol{i}_D \in \prod_{\ell \in D} \mathcal{I}^\ell$ and entries given by

$$x_D(\boldsymbol{i}_D) = \sum_{\boldsymbol{j}_{K \setminus D} \in \mathcal{I}_{K \setminus D}} x(\boldsymbol{i}_D, \boldsymbol{j}_{K \setminus D}) .$$

Note that $\boldsymbol{x}_D$ is an m-way contingency table if $D = \{i_1, \ldots, i_m\}$.

Let $D_1, \ldots, D_r \subset K$. Throughout this section we assume that $D_1 \cup \cdots \cup D_r = K$ and there does not exist $i \neq j$ such that $D_i \subseteq D_j$. Note that $\{D_1, \ldots, D_r\}$ corresponds to the generating class of a hierarchical log-linear model for the contingency table. The set of D-marginal frequencies

$$\boldsymbol{t} = \boldsymbol{t}(\boldsymbol{x}) = (\boldsymbol{x}_{D_1}, \ldots, \boldsymbol{x}_{D_r})$$

is the sufficient statistic under the hierarchical log-linear model. Note that if the cells and the elements of the sufficient statistic are ordered appropriately, we can write $\boldsymbol{t}$ in matrix form as $\boldsymbol{t} = A\boldsymbol{x}$ as in Section 3.5.1. We prefer the D-marginal expressions rather than the matrix expressions in this section, to represent the hierarchical models that we consider clearly. We also write the reference set of all the contingency tables having the same $(D_1, \ldots, D_r)$-marginals as

$$\mathcal{F}_{\boldsymbol{t}} = \mathcal{F}_{\boldsymbol{t}}(D_1, \ldots, D_r) = \{\boldsymbol{x} \in X \mid \boldsymbol{t}(\boldsymbol{x}) = \boldsymbol{t}\} \ .$$

Recall that we have defined the sample size of $\boldsymbol{t}$ by the sample size of $\boldsymbol{x}$ in $\mathcal{F}_{\boldsymbol{t}}$ since all the contingency tables in the same reference set have the same sample size. Then the set T of possible values of the sufficient statistic $\boldsymbol{t}$, i.e., $T = \{\boldsymbol{t}(\boldsymbol{x}) \mid \boldsymbol{x} \in X\}$, is partitioned as

$$T = \bigcup_{n=0}^{\infty} T_n, \quad T_n = \{\boldsymbol{t} \mid |\boldsymbol{t}| = n\} \ .$$

Let $Z \supset X$ be the set of k-way arrays $\boldsymbol{z} = \{z(\boldsymbol{i})\}_{\boldsymbol{i} \in \mathcal{I}}$ containing integer entries

$$Z = \left\{\boldsymbol{z} = \{z(\boldsymbol{i})\}_{\boldsymbol{i} \in \mathcal{I}} \mid z(\boldsymbol{i}) \in \mathbb{Z} \text{ for } \boldsymbol{i} \in \mathcal{I}\right\} \ .$$

The set of moves is an important subset of Z defined as

$$M(D_1, \ldots, D_r) = \{\boldsymbol{z} \in Z \mid \boldsymbol{z}_{D_j} = \boldsymbol{0}, \quad j \in [r]\} \subset Z,$$

where $\boldsymbol{z}_D$ is the D-marginal of $\boldsymbol{z}$. $\boldsymbol{z} \in M(D_1, \ldots, D_r)$ is sometimes called as a *move for* $D_1, \ldots, D_r$. We also define a set of moves with degree less than or equal to n as

$$M_n(D_1, \ldots, D_r) = \{\boldsymbol{z} \in M(D_1, \ldots, D_r) \mid \ \deg(\boldsymbol{z}) \leq n\}, \tag{3.38}$$

where $\deg(\boldsymbol{z})$ is defined as the sample size of the positive or negative part of $\boldsymbol{z}$ as we have defined in Section 3.5.1. We occasionally write simply M_n for convenience.

As we have defined in Section 3.5.1, a finite set $\mathcal{B} \subset M(D_1, \ldots, D_r)$ is called a Markov basis for $D_1, \ldots, D_r$ if for all $\boldsymbol{t} \in T$, $\mathcal{F}_{\boldsymbol{t}}(D_1, \ldots, D_r)$ itself constitutes one $\mathcal{B}$-equivalence class. Note that, in this definition, if $\mathcal{B}$ is a Markov basis and $\boldsymbol{z}, -\boldsymbol{z} \in \mathcal{B}$, then $\mathcal{B} \setminus \{\boldsymbol{z}\}$ and $\mathcal{B} \setminus \{-\boldsymbol{z}\}$ are also Markov bases, respectively. Moreover, if we replace any element $\boldsymbol{z}$ of a Markov basis $\mathcal{B}$ with $-\boldsymbol{z}$, the remaining set is still a Markov basis. In other words, there is a freedom of the signs of the elements of a Markov basis. In this section, we identify an element $\boldsymbol{z}$ of a Markov basis with its sign change $-\boldsymbol{z}$ for convenience.

Our moves contain many zero cells. Furthermore often the non-zero cells of a move contain either 1 or -1. Therefore a move can be concisely denoted by locations of its non-zero cells. We express a move $\boldsymbol{z}$ of degree n as

$$\boldsymbol{z} = [\{\boldsymbol{i}_1, \ldots, \boldsymbol{i}_n\} \parallel \{\boldsymbol{j}_1, \ldots, \boldsymbol{j}_n\}],$$

where $\boldsymbol{i}_1, \ldots, \boldsymbol{i}_n$ are the cells of positive frequencies of $\boldsymbol{z}$ and $\boldsymbol{j}_1, \ldots, \boldsymbol{j}_n$ are the cells of negative frequencies of $\boldsymbol{z}$. In the case $z(\boldsymbol{i}) > 1$, $\boldsymbol{i}$ is repeated $z(\boldsymbol{i})$ times. Similarly $\boldsymbol{j}$ is repeated $-z(\boldsymbol{j})$ times if $z(\boldsymbol{j}) < -1$. We use similar notation for contingency tables as well. $\boldsymbol{x} \in X_n$ is simply denoted as

$$\boldsymbol{x} = [\{\boldsymbol{i}_1, \ldots, \boldsymbol{i}_n\}] = [\boldsymbol{i}_1, \ldots, \boldsymbol{i}_n] \ .$$

Symmetric group and its action

Here we define an action of a direct product of symmetric groups on cells. From the action on cells, further actions are induced on contingency tables, marginal cells, marginal frequencies and moves.

First we give a brief list of definitions and notations of group action. Let a group G act on a set $\mathcal{X}$. $G(x) = \{gx \mid g \in G\}$ is the orbit through x. For a subset A of $\mathcal{X}$, $G(A) = \{gx \mid x \in A,\ g \in G\}$. $\mathcal{X}/G$ denotes the orbit space, i.e. the set of orbits. $G_x = \{g \mid gx = x\}$ denotes the isotropy subgroup of x in G. If G acts on $\mathcal{X}$, the action of G on the set of functions f on $\mathcal{X}$ is induced by $gf(x) = f(g^{-1}x)$. Let $h : \mathcal{X} \to \mathcal{Y}$ be a surjection. If $h(x) = h(x') \Rightarrow h(gx') = h(gx), \forall g \in G$, then the action of G on $\mathcal{Y}$ is induced by defining $gy = h(gx)$, where $y = h(x)$. Throughout the rest of this paper, the number of elements of a finite set A is denoted by $|A|$.

In our problem G is the direct product of symmetric groups, which acts on the index set $\mathcal{I}$. Let G^ℓ denote the symmetric group of order I_ℓ for $\ell \in [k]$ and let

$$G = G^1 \times G^2 \times \cdots \times G^k$$

be the direct product. We write an element of $g \in G$ as

$$g = g_1 \times \cdots \times g_k = \begin{pmatrix} 1 & \cdots & I_1 \\ \sigma_1(1) & \cdots & \sigma_1(I_1) \end{pmatrix} \times \cdots \times \begin{pmatrix} 1 & \cdots & I_k \\ \sigma_k(1) & \cdots & \sigma_k(I_k) \end{pmatrix}.$$

G acts on $\mathcal{I}$ by

$$\begin{aligned} \boldsymbol{i}' &= g\boldsymbol{i} \\ &= (g_1 i_1, \ldots, g_k i_k) \\ &= (\sigma_1(i_1), \ldots, \sigma_k(i_k)) . \end{aligned}$$

Then the action of G on X is induced by

$$\begin{aligned} \boldsymbol{x}' &= g\boldsymbol{x} \\ &= \{x(g^{-1}\boldsymbol{i})\}_{\boldsymbol{i}\in\mathcal{I}}. \end{aligned}$$

G also acts on the marginal cells by

$$\begin{aligned} \boldsymbol{i}'_D &= g\boldsymbol{i}_D \\ &= (g_{s_1} i_{s_1}, \ldots, g_{s_m} i_{s_m}) \\ &= (\sigma_{s_1}(i_{s_1}), \ldots, \sigma_{s_m}(i_{s_m})), \end{aligned}$$

where $D = \{s_1, \ldots, s_m\}$. Hence G acts on marginal tables by

$$\begin{aligned} \boldsymbol{x}'_D &= g\boldsymbol{x}_D \\ &= \{x_D(g^{-1}\boldsymbol{i}_D)\}_{\boldsymbol{i}_D\in\mathcal{I}_D}. \end{aligned}$$

Considering this action simultaneously for $D_1, \ldots, D_r$, the action of G on the sufficient statistic $\boldsymbol{t} = (\boldsymbol{x}_{D_1}, \ldots, \boldsymbol{x}_{D_r})$ is defined by

$$g\boldsymbol{t} = (g\boldsymbol{x}_{D_1}, \ldots, g\boldsymbol{x}_{D_r}).$$

An important point here is that the action of G on $\boldsymbol{t}$ is induced from the action of G on $\boldsymbol{x}$, because the the calculation of D-marginals and the action of G on X are commutative. Although this is intuitively clear, we state this as a lemma and give a proof.

Lemma 3.6.1 *$(g\boldsymbol{x})_D = g\boldsymbol{x}_D$ for all $g \in G$ and $\boldsymbol{x} \in X$.*

Proof. Write $\tilde{\boldsymbol{x}} = g\boldsymbol{x}$. From the definitions, it follows that

$$
\begin{aligned}
\tilde{x}_D(\boldsymbol{i}_D) &= \sum_{\boldsymbol{j}_{K\setminus D}\in\mathcal{I}_{K\setminus D}} \tilde{x}(\boldsymbol{i}_D, \boldsymbol{j}_{K\setminus D}) \\
&= \sum_{\boldsymbol{j}_{K\setminus D}\in\mathcal{I}_{K\setminus D}} x(g^{-1}(\boldsymbol{i}_D, \boldsymbol{j}_{K\setminus D})) \\
&= \sum_{\boldsymbol{j}_{K\setminus D}\in\mathcal{I}_{K\setminus D}} x(g^{-1}\boldsymbol{i}_D, g^{-1}\boldsymbol{j}_{K\setminus D}) \\
&= x_D(g^{-1}\boldsymbol{i}_D) \\
&= (g\boldsymbol{x}_D)(\boldsymbol{i}_D)\ .
\end{aligned}
$$

Q.E.D.

By this lemma, if $\boldsymbol{x}_{D_i} = \boldsymbol{y}_{D_i}$, $i \in [r]$, then $(g\boldsymbol{x})_{D_i} = (g\boldsymbol{y})_{D_i}$, $i \in [r]$, $\forall g \in G$. In terms of the sufficient statistic this can be equivalently written as $\boldsymbol{t}(\boldsymbol{x}) = \boldsymbol{t}(\boldsymbol{y}) \Rightarrow \boldsymbol{t}(g\boldsymbol{x}) = \boldsymbol{t}(g\boldsymbol{y})$, $\forall g \in G$. Therefore the action of G on T is induced from the action of G on X. Also it is important to note that the isotropy subgroup $G_{\boldsymbol{t}}$ of $\boldsymbol{t}$ acts on the reference set $\mathcal{F}_{\boldsymbol{t}}$.

So far we have only considered non-negative frequencies. However clearly the above consideration can also be applied to the set Z of integer arrays. In particular, Lemma 3.6.1 holds for the action of G on Z, i.e., taking marginals of integer arrays commutes with the action of G. Therefore if $\boldsymbol{z}$ is a move, then $g\boldsymbol{z}$ is a move as well. Therefore

$$G(M(D_1, \ldots, D_r)) = M(D_1, \ldots, D_r).$$

and G acts on $M(D_1, \ldots, D_r)$. More concretely, in terms of the positive part and the negative part we can write

$$
\begin{aligned}
\boldsymbol{z}' &= g\boldsymbol{z} \\
&= g\boldsymbol{z}^+ - g\boldsymbol{z}^-\ .
\end{aligned}
$$

We also define that a move $\boldsymbol{z} = \boldsymbol{z}^+ - \boldsymbol{z}^-$ is *symmetric* if $\boldsymbol{z}^+ = g\boldsymbol{z}^-$ for some $g \in G$. Conversely, a move $\boldsymbol{z}$ is *asymmetric* if $G(\boldsymbol{z}^+) \neq G(\boldsymbol{z}^-)$.

Now we can define an invariant set of moves. $\mathcal{B} \subset M(D_1, \ldots, D_r)$ is *G-invariant* if $G(\mathcal{B}) = \mathcal{B}$. Note that here we are identifying a move $\boldsymbol{z} \in \mathcal{B}$ with its sign change $-\boldsymbol{z}$. Therefore $\mathcal{B}$ is G-invariant if and only if

$$\forall g \in G, \forall \boldsymbol{z} \in \mathcal{B} \implies g\boldsymbol{z} \in \mathcal{B} \text{ or } -g\boldsymbol{z} \in \mathcal{B}\ .$$

In other words, $\mathcal{B}$ is G-invariant if and only if it is a union of orbits $\mathcal{B} = \bigcup_{\boldsymbol{z}\in A} G(\boldsymbol{z})$ for some subset $A \subset M(D_1, \ldots, D_r)$ of moves.

A finite set $\mathcal{B} \subset M(D_1, \ldots, D_r)$ is an *invariant Markov basis* for $D_1, \ldots, D_r$ if it is a Markov basis and it is G-invariant. An invariant Markov basis is minimal if no proper G-invariant subset of $\mathcal{B}$ is a Markov basis. A minimal invariant Markov basis always exists, because from any invariant Markov basis, we can remove orbits one by one, until none of the remaining orbits can be removed any further.

3.6.2 Characterizations of an invariant Markov basis and its uniqueness

In this section, we first study the relationships between the orbits and $M_{n-1}(D_1, ..., D_r)$-equivalence classes of X_n and then derive some characterizations of an invariant minimal Markov basis and its uniqueness.

Some properties of orbits of contingency tables and marginal frequencies

Here we derive some basic properties of orbits of G acting on X and T. First we note that $|\boldsymbol{x}| = |g\boldsymbol{x}|$, $\forall g \in G$, and hence $G(X_n) = X_n$. Therefore we consider the action of G on each X_n separately. Similarly we consider the action of G on each T_n separately.

Consider a particular sufficient statistic $\boldsymbol{t} \in T_n$. Let $G(\boldsymbol{t}) \in T_n/G$ be the orbit through $\boldsymbol{t}$. Let

$$\mathcal{F}_{G(\boldsymbol{t})} = \bigcup_{\boldsymbol{t}' \in G(\boldsymbol{t})} F_{\boldsymbol{t}'}$$

denote the union of reference sets over the orbit $G(\boldsymbol{t})$ through $\boldsymbol{t}$. Let $\boldsymbol{x} \in \mathcal{F}_{\boldsymbol{t}}$. Because $\boldsymbol{t}(g\boldsymbol{x}) = g\boldsymbol{t}$, it follows that

$$g\boldsymbol{x} \in \mathcal{F}_{g\boldsymbol{t}} \subset \mathcal{F}_{G(\boldsymbol{t})}.$$

Therefore $G(\mathcal{F}_{G(\boldsymbol{t})}) = \mathcal{F}_{G(\boldsymbol{t})}$. This implies that X_n is partitioned as

$$X_n = \bigcup_{\alpha \in T_n/G} \mathcal{F}_\alpha, \tag{3.39}$$

where α runs over the set of different orbits and we can consider the action of G on each $\mathcal{F}_{G(\boldsymbol{t})}$ separately.

Example 3.6.1 *Consider the case of $k = 3$ and $D_1 = \{1\}, D_2 = \{2\}, D_3 = \{3\}$. This is the complete independence model of the three-way tables. The decomposition (3.39) of X_1 for this case is trivial since T_1 itself is one G-orbit. We consider the decomposition of X_2. For this case there are eight G-orbits in T_2 as*

$$\begin{array}{l} T_2/G = \{G(\boldsymbol{t}_1), \ldots, G(\boldsymbol{t}_8)\}, \\ \boldsymbol{t}_i = \boldsymbol{t}(\boldsymbol{x}_i), \ i = 1, \ldots, 8, \\ \boldsymbol{x}_1 = [(111), (111)], \ \boldsymbol{x}_2 = [(111), (112)], \\ \boldsymbol{x}_3 = [(111), (121)], \ \boldsymbol{x}_4 = [(111), (211)], \\ \boldsymbol{x}_5 = [(111), (122)], \ \boldsymbol{x}_6 = [(111), (212)], \\ \boldsymbol{x}_7 = [(111), (221)], \ \boldsymbol{x}_8 = [(111), (222)] \end{array} \tag{3.40}$$

and we have

$$X_2 = \mathcal{F}_{G(\boldsymbol{t}_1)} \cup \cdots \cup \mathcal{F}_{G(\boldsymbol{t}_8)}. \tag{3.41}$$

The numbers of elements of the orbits $G(\boldsymbol{t}_1),\dots,G(\boldsymbol{t}_8)$ are calculated as follows.

$$
\begin{aligned}
&|G(\boldsymbol{t}_1)| = I_1 I_2 I_3, && |G(\boldsymbol{t}_2)| = I_1 I_2 \binom{I_3}{2},\\
&|G(\boldsymbol{t}_3)| = I_1 \binom{I_2}{2} I_3, && |G(\boldsymbol{t}_4)| = \binom{I_1}{2} I_2 I_3,\\
&|G(\boldsymbol{t}_5)| = I_1 \binom{I_2}{2}\binom{I_3}{2}, && |G(\boldsymbol{t}_6)| = \binom{I_1}{2} I_2 \binom{I_3}{2},\\
&|G(\boldsymbol{t}_7)| = \binom{I_1}{2}\binom{I_2}{2} I_3, && |G(\boldsymbol{t}_8)| = \binom{I_1}{2}\binom{I_2}{2}\binom{I_3}{2}.
\end{aligned}
\tag{3.42}
$$

Furthermore we have

$$
|\mathcal{F}_{\boldsymbol{t}}| = \begin{cases} 1 & \textit{for} \ \ \boldsymbol{t} \in G(\boldsymbol{t}_1)\cup G(\boldsymbol{t}_2)\cup G(\boldsymbol{t}_3)\cup G(\boldsymbol{t}_4),\\ 2 & \textit{for} \ \ \boldsymbol{t} \in G(\boldsymbol{t}_5)\cup G(\boldsymbol{t}_6)\cup G(\boldsymbol{t}_7),\\ 4 & \textit{for} \ \ \boldsymbol{t} \in G(\boldsymbol{t}_8). \end{cases} \tag{3.43}
$$

Consider a particular $\mathcal{F}_{G(\boldsymbol{t})}$. An important observation is that there is a direct product structure in $\mathcal{F}_{G(\boldsymbol{t})}$. Write

$$
G(\boldsymbol{t}) = \{\boldsymbol{t}_1,\dots,\boldsymbol{t}_a\},
$$

where $a = a(\boldsymbol{t}) = |G(\boldsymbol{t})|$ is the number of elements of the orbit $G(\boldsymbol{t}) \subset T_n$. Let $b = b(\boldsymbol{t}) = |\mathcal{F}_{G(\boldsymbol{t})}/G|$ be the number of orbits of G acting on $\mathcal{F}_{G(\boldsymbol{t})}$ and let $\boldsymbol{x}_1,\dots,\boldsymbol{x}_b$ be representative elements of different orbits, i.e., $\mathcal{F}_{G(\boldsymbol{t})} = G(\boldsymbol{x}_1)\cup\cdots\cup G(\boldsymbol{x}_b)$ gives a partition of $\mathcal{F}_{G(\boldsymbol{t})}$. Then we have the following lemma.

Lemma 3.6.2 *$\mathcal{F}_{G(\boldsymbol{t})}$ is partitioned as*

$$
\mathcal{F}_{G(\boldsymbol{t})} = \bigcup_{i=1}^{a}\bigcup_{j=1}^{b} \mathcal{F}_{\boldsymbol{t}_i}\cap G(\boldsymbol{x}_j), \tag{3.44}
$$

where each $\mathcal{F}_{\boldsymbol{t}_i}\cap G(\boldsymbol{x}_j)$ is non-empty. Furthermore if $\boldsymbol{t}'_i = g\boldsymbol{t}_i$, then $\boldsymbol{x}\in\mathcal{F}_{\boldsymbol{t}_i}\mapsto g\boldsymbol{x}\in\mathcal{F}_{\boldsymbol{t}'_i}$ gives a bijection between $\mathcal{F}_{\boldsymbol{t}_i}\cap G(\boldsymbol{x})$ and $\mathcal{F}_{\boldsymbol{t}'_i}\cap G(\boldsymbol{x})$.

Proof. $\mathcal{F}_{G(\boldsymbol{t})} = \mathcal{F}_{\boldsymbol{t}_1}\cup\cdots\cup\mathcal{F}_{\boldsymbol{t}_a}$ is a partition. Intersecting this partition with $\mathcal{F}_{G(\boldsymbol{t})} = \bigcup_{j=1}^{b} G(\boldsymbol{x}_j)$ gives the partition (3.44). Let $\boldsymbol{x}\in\mathcal{F}_{\boldsymbol{t}}$. Then the orbit $G(\boldsymbol{x})$ intersects each reference set, i.e. $G(\boldsymbol{x})\cap\mathcal{F}_{\boldsymbol{t}_i}\neq\emptyset$ for $i\in[a]$.

Since every $g\in G$ is a bijection of $\mathcal{F}_{G(\boldsymbol{t})}$ to itself and

$$
g(\mathcal{F}_{\boldsymbol{t}}\cap G(\boldsymbol{x})) = \mathcal{F}_{g\boldsymbol{t}}\cap G(\boldsymbol{x}),
$$

g gives a bijection between $\mathcal{F}_{\boldsymbol{t}_i}\cap G(\boldsymbol{x})$ and $\mathcal{F}_{\boldsymbol{t}'_i}\cap G(\boldsymbol{x})$. Q.E.D.

In particular for each j, $\mathcal{F}_{\boldsymbol{t}_i}\cap G(\boldsymbol{x}_j)$, $i\in[a]$, have the same number of elements

$$
|\mathcal{F}_{\boldsymbol{t}_1}\cap G(\boldsymbol{x}_j)| = \cdots = |\mathcal{F}_{\boldsymbol{t}_a}\cap G(\boldsymbol{x}_j)|.
$$

In addition, for $\boldsymbol{t}_i,\boldsymbol{t}'_i\in G(\boldsymbol{t})$ such that $\boldsymbol{t}'_i = g\boldsymbol{t}_i$, the map $g: G_{\boldsymbol{t}_i}\to gG_{\boldsymbol{t}_i}g^{-1}$ gives an isomorphism between $G_{\boldsymbol{t}_i}$ and $G_{\boldsymbol{t}'_i} = gG_{\boldsymbol{t}_i}g^{-1}$, where $G_{\boldsymbol{t}_i}$ and $G_{\boldsymbol{t}'_i}$ are the the isotropy subgroup of $\boldsymbol{t}_i$ and $\boldsymbol{t}'_i$ in G, respectively. Therefore there are the following isomorphic structures in $\mathcal{F}_{\boldsymbol{t}_i}$,

$$
(G_{\boldsymbol{t}_i},\mathcal{F}_{\boldsymbol{t}_i}) \simeq (G_{\boldsymbol{t}'_i},\mathcal{F}_{\boldsymbol{t}'_i}). \tag{3.45}
$$

Example 3.6.2 *(Example 3.6.1 continued.) In the decomposition (3.41), we have* $|\mathcal{F}_{G(\boldsymbol{t}_i)}/G| = b(\boldsymbol{t}_i) = 1$ *and* $\mathcal{F}_{G(\boldsymbol{t}_i)} = G(\boldsymbol{x}_i)$ *for* $i = 1, \ldots, 8$*. Therefore the right hand side of (3.44) is simply* $\bigcup_{i=1}^{a} \mathcal{F}_{\boldsymbol{t}_i}$ *in this case. To see the isomorphic structure (3.45), consider* $\mathcal{F}_{G(\boldsymbol{t}_8)}$*, for example. The isotropy subgroup of* $\boldsymbol{t}_8$ *is given by*

$$G_{\boldsymbol{t}_8} = \widetilde{G}^1_{12,12} \times \widetilde{G}^2_{12,12} \times \widetilde{G}^3_{12,12},$$

where we define

$$\widetilde{G}^{\ell}_{i_1 i_2, j_1 j_2} = \{g \in G^{\ell} \mid (\sigma_\ell(i_1), \sigma_\ell(i_2)) \in \{(j_1, j_2), (j_2, j_1)\}\},\ i_1 \neq i_2, j_1 \neq j_2.$$

We also define

$$G^{\ell}_{i_1 i_2, j_1 j_2} = \{g \in G^{\ell} \mid (\sigma_\ell(i_1), \sigma_\ell(i_2)) = (j_1, j_2)\} \subset \widetilde{G}^{\ell}_{i_1 i_2, j_1 j_2}$$

for later use. Since G^ℓ *is the symmetric group of order* I_ℓ*, we have* $|\widetilde{G}^{\ell}_{i_1 i_2, j_1 j_2}| = 2(I_\ell - 2)!$ *and* $|G^{\ell}_{i_1 i_2, j_1 j_2}| = (I_\ell - 2)!$*. The reference set* $\mathcal{F}_{\boldsymbol{t}_8}$ *is written as*

$$\mathcal{F}_{\boldsymbol{t}_8} = \{[(111), (222)], [(112), (221)], [(121), (212)], [(122), (211)]\}.$$

Consider another element $\boldsymbol{x}' = [(111), (223)] \in \mathcal{F}_{G(\boldsymbol{t}_8)}$ *and write* $\boldsymbol{t}' = \boldsymbol{t}(\boldsymbol{x}')$*. The isotropy subgroup of* $\boldsymbol{t}'$ *is given by*

$$G_{\boldsymbol{t}'} = \widetilde{G}^1_{12,12} \times \widetilde{G}^2_{12,12} \times \widetilde{G}^3_{13,13}$$

and the reference set $\mathcal{F}_{\boldsymbol{t}'}$ *is written as*

$$\mathcal{F}_{\boldsymbol{t}'} = \{[(111), (223)], [(113), (221)], [(121), (213)], [(123), (211)]\}.$$

We see the relations $\boldsymbol{t}' = g\boldsymbol{t}_8$ *and* $gG_{\boldsymbol{t}_8}g^{-1} = G_{\boldsymbol{t}'}$ *for* $g \in \widetilde{G}^1_{12,12} \times \widetilde{G}^2_{12,12} \times \widetilde{G}^3_{12,13}$*. In particular* $\boldsymbol{x}' = g\boldsymbol{x}_8$ *holds if* $g \in G^1_{12,12} \times G^2_{12,12} \times G^3_{12,13} \cup G^1_{12,21} \times G^2_{12,21} \times G^3_{12,31}$*.*

Next we present examples of $b = 2$ and $b = 3$.

Example 3.6.3 *Consider the case of* $k = 4$ *and* $D_1 = \{1, 2\}, D_2 = \{1, 3\}, D_3 = \{2, 3\}, D_4 = \{3, 4\}$*. This is an example of reducible models. Consider a particular* $\boldsymbol{t} \in T_4$ *such that*

$$\boldsymbol{t} = (\boldsymbol{x}_{D_1}, \boldsymbol{x}_{D_2}, \boldsymbol{x}_{D_3}, \boldsymbol{x}_{D_4}),$$

where

$$\begin{aligned}
\boldsymbol{x}_{D_1} &= [(i_1 i_2), (i_1 i_2'), (i_1' i_2), (i_1' i_2')],\\
\boldsymbol{x}_{D_2} &= [(i_1 i_3), (i_1 i_3'), (i_1' i_3), (i_1' i_3')],\\
\boldsymbol{x}_{D_3} &= [(i_2 i_3), (i_2 i_3'), (i_2' i_3), (i_2' i_3')],\\
\boldsymbol{x}_{D_4} &= [(i_3 i_4), (i_3 i_4'), (i_3' i_4), (i_3' i_4')].
\end{aligned}$$

For each $i_m \neq i_m', m = 1, \ldots, 4$*, there are eights elements in* $\mathcal{F}_{\boldsymbol{t}}$ *as*

$$\begin{aligned}
\mathcal{F}_{\boldsymbol{t}} &= \{\boldsymbol{x}_1, \ldots, \boldsymbol{x}_8\},\\
\boldsymbol{x}_1 &= [(i_1 i_2 i_3 i_4), (i_1 i_2' i_3' i_4), (i_1' i_2 i_3' i_4'), (i_1' i_2' i_3 i_4')],\\
\boldsymbol{x}_2 &= [(i_1 i_2 i_3 i_4), (i_1 i_2' i_3' i_4'), (i_1' i_2 i_3' i_4), (i_1' i_2' i_3 i_4')],\\
\boldsymbol{x}_3 &= [(i_1 i_2 i_3 i_4'), (i_1 i_2' i_3' i_4), (i_1' i_2 i_3' i_4'), (i_1' i_2' i_3 i_4)],\\
\boldsymbol{x}_4 &= [(i_1 i_2 i_3 i_4'), (i_1 i_2' i_3' i_4'), (i_1' i_2 i_3' i_4), (i_1' i_2' i_3 i_4)],\\
\boldsymbol{x}_5 &= [(i_1 i_2 i_3' i_4), (i_1 i_2' i_3 i_4), (i_1' i_2 i_3 i_4'), (i_1' i_2' i_3' i_4')],\\
\boldsymbol{x}_6 &= [(i_1 i_2 i_3' i_4), (i_1 i_2' i_3 i_4'), (i_1' i_2 i_3 i_4), (i_1' i_2' i_3' i_4')],\\
\boldsymbol{x}_7 &= [(i_1 i_2 i_3' i_4'), (i_1 i_2' i_3 i_4), (i_1' i_2 i_3 i_4'), (i_1' i_2' i_3' i_4)],\\
\boldsymbol{x}_8 &= [(i_1 i_2 i_3' i_4'), (i_1 i_2' i_3 i_4'), (i_1' i_2 i_3 i_4), (i_1' i_2' i_3' i_4)].
\end{aligned}$$

We see that

$$G_{\boldsymbol{t}} = \widetilde{G}^1_{i_1i'_1,i_1i'_1} \times \widetilde{G}^2_{i_2i'_2,i_2i'_2} \times \widetilde{G}^3_{i_3i'_3,i_3i'_3} \times \widetilde{G}^4_{i_4i'_4,i_4i'_4} \tag{3.46}$$

for this case, and each $\mathcal{F}_{\boldsymbol{t}}$ contains two $G_{\boldsymbol{t}}$-orbits, i.e.,

$$\mathcal{F}_{\boldsymbol{t}} = \{\boldsymbol{x}_1, \boldsymbol{x}_4, \boldsymbol{x}_5, \boldsymbol{x}_8\} \cup \{\boldsymbol{x}_2, \boldsymbol{x}_3, \boldsymbol{x}_6, \boldsymbol{x}_7\} = G_{\boldsymbol{t}}(\boldsymbol{x}_1) \cup G_{\boldsymbol{t}}(\boldsymbol{x}_2).$$

Extending $\boldsymbol{t}$ to $G(\boldsymbol{t})$, we see the direct product structure (3.44) of $\mathcal{F}_{G(\boldsymbol{t})}$, where $b = |\mathcal{F}_{G(\boldsymbol{t})}/G| = |\mathcal{F}_{\boldsymbol{t}}/G_{\boldsymbol{t}}| = 2$,

$$a = |G(\boldsymbol{t})| = \binom{I_1}{2}\binom{I_2}{2}\binom{I_3}{2}\binom{I_4}{2}$$

and

$$|\mathcal{F}_{\boldsymbol{t}'} \cap G(\boldsymbol{x}_1)| = |\mathcal{F}_{\boldsymbol{t}'} \cap G(\boldsymbol{x}_2)| = 4$$

for each $\boldsymbol{t}' \in G(\boldsymbol{t})$.

Example 3.6.4 *Consider the case of $k = 4$ and $D_1 = \{1, 2\}, D_2 = \{1, 3\}, D_3 = \{2, 3\}, D_4 = \{4\}$. Again this is an example of reducible models. Consider a particular $\boldsymbol{t} \in T_4$ such that*

$$\boldsymbol{t} = (\boldsymbol{x}_{D_1}, \boldsymbol{x}_{D_2}, \boldsymbol{x}_{D_3}, \boldsymbol{x}_{D_4}),$$

where $\boldsymbol{x}_{D_1}, \boldsymbol{x}_{D_2}, \boldsymbol{x}_{D_3}$ are the same as in Example 3.6.3, and $\boldsymbol{x}_{D_4} = [(i_4), (i_4), (i'_4), (i'_4)]$. For each $i_m \neq i'_m, m = 1, \ldots, 4$, there are twelve elements in $\mathcal{F}_{\boldsymbol{t}}$ as

$$\begin{aligned} \mathcal{F}_{\boldsymbol{t}} &= \{\boldsymbol{x}_1, \ldots, \boldsymbol{x}_{12}\}, \\ \boldsymbol{x}_9 &= [(i_1i_2i_3i_4), (i_1i'_2i'_3i'_4), (i'_1i_2i'_3i'_4), (i'_1i'_2i_3i_4)], \\ \boldsymbol{x}_{10} &= [(i_1i_2i_3i'_4), (i_1i'_2i'_3i_4), (i'_1i_2i'_3i_4), (i'_1i'_2i_3i'_4)], \\ \boldsymbol{x}_{11} &= [(i_1i_2i'_3i_4), (i_1i'_2i_3i'_4), (i'_1i_2i_3i'_4), (i'_1i'_2i'_3i_4)], \\ \boldsymbol{x}_{12} &= [(i_1i_2i'_3i'_4), (i_1i'_2i_3i_4), (i'_1i_2i_3i_4), (i'_1i'_2i'_3i'_4)] \end{aligned}$$

and $\boldsymbol{x}_1, \ldots, \boldsymbol{x}_8$ are the same as in Example 3.6.3. We see that $G_{\boldsymbol{t}}$ is defined by (3.46) again, and each $\mathcal{F}_{\boldsymbol{t}}$ contains three $G_{\boldsymbol{t}}$-orbits, i.e.,

$$\mathcal{F}_{\boldsymbol{t}} = \{\boldsymbol{x}_1, \boldsymbol{x}_4, \boldsymbol{x}_5, \boldsymbol{x}_8\} \cup \{\boldsymbol{x}_2, \boldsymbol{x}_3, \boldsymbol{x}_6, \boldsymbol{x}_7\} \cup \{\boldsymbol{x}_9, \boldsymbol{x}_{10}, \boldsymbol{x}_{11}, \boldsymbol{x}_{12}\} = G_{\boldsymbol{t}}(\boldsymbol{x}_1) \cup G_{\boldsymbol{t}}(\boldsymbol{x}_2) \cup G_{\boldsymbol{t}}(\boldsymbol{x}_9).$$

Extending $\boldsymbol{t}$ to $G(\boldsymbol{t})$, we see the direct product structure (3.44) of $\mathcal{F}_{G(\boldsymbol{t})}$, where $b = |\mathcal{F}_{G(\boldsymbol{t})}/G| = |\mathcal{F}_{\boldsymbol{t}}/G_{\boldsymbol{t}}| = 3$,

$$a = |G(\boldsymbol{t})| = \binom{I_1}{2}\binom{I_2}{2}\binom{I_3}{2}\binom{I_4}{2}$$

and

$$|\mathcal{F}_{\boldsymbol{t}'} \cap G(\boldsymbol{x}_1)| = |\mathcal{F}_{\boldsymbol{t}'} \cap G(\boldsymbol{x}_2)| = |\mathcal{F}_{\boldsymbol{t}'} \cap G(\boldsymbol{x}_9)| = 4$$

for each $\boldsymbol{t}' \in G(\boldsymbol{t})$.

The following example of $b = 2$ is somewhat complicated but it is important in showing an asymmetric indispensable move.

Example 3.6.5 *Consider the case of $k = 3$ and $D_1 = \{1,2\}, D_2 = \{1,3\}, D_3 = \{2,3\}$. This model is considered extensively for $I_1 = I_2 = 3$ in Section 3.2 and Section 3.3. Here we study the case of $I_1 = 3, I_2 = 5, I_3 = 6$ and a sufficient statistic $\boldsymbol{t} = (\boldsymbol{x}_{D_1}, \boldsymbol{x}_{D_2}, \boldsymbol{x}_{D_3}) \in T_{14}$, where*

$$\begin{aligned}
\boldsymbol{x}_{D_1} &= [(11),(13),(14),(15),(22),(23),(24),(25),(31),(32),(33),(34),(35),(35)],\\
\boldsymbol{x}_{D_2} &= [(11),(12),(13),(16),(23),(24),(25),(26),(31),(32),(34),(35),(36),(36)],\\
\boldsymbol{x}_{D_3} &= [(11),(16),(24),(26),(32),(33),(34),(41),(43),(45),(52),(55),(56),(56)].
\end{aligned}$$

In this case, $\mathcal{F}_{\boldsymbol{t}} = \{\boldsymbol{x}_1, \boldsymbol{x}_2\}$, where

$$\begin{aligned}
\boldsymbol{x}_1 &= [(111),(132),(143),(156),(224),(233),(245),(256),(316),(326),(334),(341),(352),(355)],\\
\boldsymbol{x}_2 &= [(116),(133),(141),(152),(226),(234),(243),(255),(311),(324),(332),(345),(356),(356)].
\end{aligned}$$

Furthermore, there is no $g \in G$ satisfying $\boldsymbol{x}_1 = g\boldsymbol{x}_2$, i.e., $G(\boldsymbol{x}_1) \cap G(\boldsymbol{x}_2) = \emptyset$. (This is obvious since only $\boldsymbol{x}_2$ contains 2 as a cell frequency.) Therefore $\boldsymbol{x}_1 - \boldsymbol{x}_2$ is an asymmetric indispensable move. Extending $\boldsymbol{t}$ to $G(\boldsymbol{t})$, we see that

$$|\mathcal{F}_{\boldsymbol{t}'} \cap G(\boldsymbol{x}_1)| = |\mathcal{F}_{\boldsymbol{t}'} \cap G(\boldsymbol{x}_2)| = 1$$

for each $\boldsymbol{t}' \in G(\boldsymbol{t})$.

A direct product structure of each reference set

Considering the isomorphic structures of (3.45), now we can focus our attention on each reference set. Consider a particular reference set $\mathcal{F}_{\boldsymbol{t}}$. Here we can restrict our attention to the action of $G_{\boldsymbol{t}}$ on $\mathcal{F}_{\boldsymbol{t}}$. In characterizing a Markov basis and its minimality, we showed in Section 3.5 that it is essential to consider $M_{|\boldsymbol{t}|-1}(D_1,\ldots,D_r)$-equivalence classes of $\mathcal{F}_{\boldsymbol{t}}$, where $M_{n-1}(D_1,\ldots,D_r)$ is given in (3.38). Therefore we have to confirm the relation between the action of $G_{\boldsymbol{t}}$ and $M_{n-1}(D_1,\ldots,D_r)$-equivalence classes of $\mathcal{F}_{\boldsymbol{t}}$, $|\boldsymbol{t}| = n$.

Let $K_{\boldsymbol{t}}$ denote the number of $M_{n-1}(D_1,\ldots,D_r)$-equivalence classes of $\mathcal{F}_{\boldsymbol{t}}$ as in Theorem 3.5.1. In this section, we write the set of $M_{n-1}(D_1,\ldots,D_r)$-equivalence classes of $\mathcal{F}_{\boldsymbol{t}}$ as $\mathcal{H}_{\boldsymbol{t}}$ for simplicity, i.e.,

$$\mathcal{H}_{\boldsymbol{t}} = \mathcal{F}_{\boldsymbol{t}}/M_{n-1}(D_1,\ldots,D_r) = \{X_1,\ldots,X_{K_{\boldsymbol{t}}}\}, \quad K_{\boldsymbol{t}} = |\mathcal{H}_{\boldsymbol{t}}|,\ |\boldsymbol{t}| = n,$$

in the notation of Theorem 3.5.1. In the sequel let $X_\gamma \in \mathcal{H}_{\boldsymbol{t}}$ denote each equivalence class.

Example 3.6.6 *(Example 3.6.3 continued.) Consider the model considered in Example 3.6.3. Now we can restrict our attention to $I_1 = I_2 = I_3 = I_4 = 2$ case, i.e., $i_m = 1, i'_m = 2$ for $m = 1,\ldots,4$ and consider $M_3(D_1,\ldots,D_4)$-equivalence classes of $\mathcal{F}_{\boldsymbol{t}}$. In this case, we see that $|\mathcal{H}_{\boldsymbol{t}}| = 2$ and*

$$\mathcal{H}_{\boldsymbol{t}} = \mathcal{F}_{\boldsymbol{t}}/M_{n-1}(D_1,\ldots,D_r) = \{\{\boldsymbol{x}_1,\boldsymbol{x}_2,\boldsymbol{x}_3,\boldsymbol{x}_4\},\{\boldsymbol{x}_5,\boldsymbol{x}_6,\boldsymbol{x}_7,\boldsymbol{x}_8\}\}$$

since

$$\begin{aligned}
\boldsymbol{x}_1 - \boldsymbol{x}_2 &= [(1111),(1221),(2122),(2212)] - [(1111),(1222),(2121),(2212)]\\
&= [\{(1221),(2122)\} \parallel \{(1222),(2121)\}] \in M_2(D_1,\ldots,D_4),
\end{aligned}$$

for example.

Example 3.6.7 *(Example 3.6.4 continued.) Similar result to Example 3.6.6 is derived for the model in Example 3.6.4. Again we can restrict our attention to $I_1 = I_2 = I_3 = I_4 = 2$ case and consider $M_3(D_1, \ldots, D_4)$-equivalence classes of $\mathcal{F}_{\boldsymbol{t}}$. In this case, we see that $|\mathcal{H}_{\boldsymbol{t}}| = 2$ and*

$$\mathcal{H}_{\boldsymbol{t}} = \mathcal{F}_{\boldsymbol{t}}/M_{n-1}(D_1, \ldots, D_r) = \{\{\boldsymbol{x}_1, \boldsymbol{x}_2, \boldsymbol{x}_3, \boldsymbol{x}_4, \boldsymbol{x}_9, \boldsymbol{x}_{10}\}, \{\boldsymbol{x}_5, \boldsymbol{x}_6, \boldsymbol{x}_7, \boldsymbol{x}_8, \boldsymbol{x}_{11}, \boldsymbol{x}_{12}\}\}.$$

We now have the following important lemma.

Lemma 3.6.3 *If $\boldsymbol{x}'$ is accessible from $\boldsymbol{x}$ by $M_{n-1}(D_1, \ldots, D_r)$, then $g\boldsymbol{x}'$ is accessible from $g\boldsymbol{x}$ by $M_{n-1}(D_1, \ldots, D_r)$.*

Proof. Note that $\deg(\boldsymbol{z}) \leq n-1$ if and only if $\deg(g\boldsymbol{z}) \leq n-1$. If $\boldsymbol{x}'$ is accessible from $\boldsymbol{x}$, then by (3.34)

$$\boldsymbol{x}' = \boldsymbol{x} + \sum_{s=1}^{A} \varepsilon_s \boldsymbol{z}_s,$$

$$\boldsymbol{x} + \sum_{s=1}^{a} \varepsilon_s \boldsymbol{z}_s \in \mathcal{F}_{\boldsymbol{t}}(D_1, \ldots, D_r) \text{ for } 1 \leq a \leq A\ .$$

Applying g to the both sides of the equations we get

$$g\boldsymbol{x}' = g\boldsymbol{x} + \sum_{s=1}^{A} \varepsilon_s g\boldsymbol{z}_s,$$

$$g\boldsymbol{x} + \sum_{s=1}^{a} \varepsilon_s g\boldsymbol{z}_s \in \mathcal{F}_{g\boldsymbol{t}}(D_1, \ldots, D_r) \text{ for } 1 \leq a \leq A\ .$$

Q.E.D.

This lemma holds for all $g \in G$. In particular, $g\boldsymbol{x} \in \mathcal{F}_{\boldsymbol{t}(\boldsymbol{x})}$ if $g \in G_{\boldsymbol{t}}$. This implies that an action of $G_{\boldsymbol{t}}$ is induced on $\mathcal{H}_{\boldsymbol{t}}$. In fact if $\pi : \boldsymbol{x} \mapsto X_\gamma$ denotes the natural projection of $\boldsymbol{x}$ to its equivalence class, then Lemma 3.6.3 states

$$\pi(\boldsymbol{x}) = \pi(\boldsymbol{x}') \Rightarrow \pi(g\boldsymbol{x}) = \pi(g\boldsymbol{x}').$$

Let $\boldsymbol{x} \in X_\gamma$ and $g \in G_{\boldsymbol{t}}$. Then $g\boldsymbol{x}$ belongs to some $M_{n-1}(D_1, \ldots, D_r)$-equivalence class $X_{\gamma'}$. By Lemma 3.6.3, this γ' does not depend on the choice of $\boldsymbol{x} \in X_\gamma$ and we may write $\gamma' = g\gamma$. Since by definition a group action is bijective we have the following lemma.

Lemma 3.6.4

$$g \in G_{\boldsymbol{t}} : X_\gamma \mapsto X_{\gamma'}$$

is a bijection of $\mathcal{H}_{\boldsymbol{t}}$ to itself.

Combining this result and the isomorphic structure of (3.45), we see that the structure of $\mathcal{H}_{\boldsymbol{t}'}$ and in particular $|\mathcal{H}_{\boldsymbol{t}'}|$ are common for all $\boldsymbol{t}' \in G(\boldsymbol{t})$.

Now consider the orbit space $\mathcal{H}_{\boldsymbol{t}}/G_{\boldsymbol{t}}$. Write each element of $\mathcal{H}_{\boldsymbol{t}}/G_{\boldsymbol{t}}$ as Γ, and write

$$X_\Gamma = \bigcup_{X_\gamma \in \Gamma} X_\gamma. \tag{3.47}$$

Then we have the decomposition

$$\mathcal{F}_{\boldsymbol{t}} = \bigcup_{\Gamma \in \mathcal{H}_{\boldsymbol{t}}/G_{\boldsymbol{t}}} X_\Gamma.$$

By definition, X_Γ is $G_{\boldsymbol{t}}$-invariant for each Γ and $G_{\boldsymbol{t}}$ acts on X_Γ. Therefore we consider each X_Γ separately. An important observation is that there is a direct product structure in X_Γ, which is similar to Lemma 3.6.2. Let $\Delta = \Delta(\Gamma) = X_\Gamma/G_{\boldsymbol{t}}$ be the $G_{\boldsymbol{t}}$-orbit space of X_Γ and $\boldsymbol{x}_\delta \in X_\Gamma, \delta \in \Delta$, be the representative elements of different orbits. Then we have the following lemma.

Lemma 3.6.5 *$\mathcal{F}_{\boldsymbol{t}}$ is partitioned as*

$$\begin{aligned}
\mathcal{F}_{\boldsymbol{t}} &= \bigcup_{\Gamma \in \mathcal{H}_{\boldsymbol{t}}/G_{\boldsymbol{t}}} X_\Gamma \\
&= \bigcup_{\Gamma \in \mathcal{H}_{\boldsymbol{t}}/G_{\boldsymbol{t}}} \left(\bigcup_{X_\gamma \in \Gamma} \bigcup_{\delta \in \Delta} X_\gamma \cap G_{\boldsymbol{t}}(\boldsymbol{x}_\delta) \right),
\end{aligned} \tag{3.48}$$

where each $X_\gamma \cap G_{\boldsymbol{t}}(\boldsymbol{x}_\delta)$ is non-empty. Furthermore if $\gamma' = g\gamma, g \in G_{\boldsymbol{t}}$, then $\boldsymbol{x} \in X_\gamma \mapsto g\boldsymbol{x} \in X_{g\gamma}$ gives a bijection between $X_\gamma \cap G_{\boldsymbol{t}}(\boldsymbol{x})$ and $X_{\gamma'} \cap G_{\boldsymbol{t}}(\boldsymbol{x})$.

Proof. Similarly to the proof of Lemma 3.6.2, intersecting the partition (3.47) with $X_\Gamma = \bigcup_{\delta \in \Delta} G_{\boldsymbol{t}}(\boldsymbol{x}_\delta)$ gives the partition (3.48). For each $\boldsymbol{x} \in X_\Gamma$, the orbit $G_{\boldsymbol{t}}(\boldsymbol{x})$ intersects each equivalence class X_γ, i.e. $G_{\boldsymbol{t}}(\boldsymbol{x}) \cap X_\gamma \neq \emptyset$ for all $X_\gamma \in \Gamma$.

From Lemma 3.6.4 and the definition of X_Γ, every $g \in G_{\boldsymbol{t}}$ is a bijection of X_Γ to itself and

$$g(X_\gamma \cap G_{\boldsymbol{t}}(\boldsymbol{x})) = X_{g\gamma} \cap G_{\boldsymbol{t}}(\boldsymbol{x}).$$

Therefore $g \in G_{\boldsymbol{t}}$ gives a bijection between $X_\gamma \cap G_{\boldsymbol{t}}(\boldsymbol{x})$ and $X_{\gamma'} \cap G_{\boldsymbol{t}}(\boldsymbol{x})$. Q.E.D.

Example 3.6.8 *(Examples 3.6.3, 3.6.6 continued.) Combining the results of Example 3.6.3 and Example 3.6.6, a direct product structure for this model is obtained. We see that $|\Gamma| = |\Delta| = 2$ and $|X_\gamma \cap G_{\boldsymbol{t}}(\boldsymbol{x})| = 2$ for each $X_\gamma \in \Gamma$. Since $G_{\boldsymbol{t}}(X_\gamma) = \mathcal{F}_{\boldsymbol{t}}$, $|\mathcal{H}_{\boldsymbol{t}}/G_{\boldsymbol{t}}| = 1$ for this model.*

Example 3.6.9 *(Examples 3.6.4, 3.6.7 continued.) Similarly, combining the results of Example 3.6.4 and Example 3.6.7 yields a direct product structure for this model. We see that $|\Gamma| = 2, |\Delta| = 3$ and $|X_\gamma \cap G_{\boldsymbol{t}}(\boldsymbol{x})| = 2$ for each $X_\gamma \in \Gamma$. Since $G_{\boldsymbol{t}}(X_\gamma) = \mathcal{F}_{\boldsymbol{t}}$, $|\mathcal{H}_{\boldsymbol{t}}/G_{\boldsymbol{t}}| = 1$ for this model.*

We see that $|\mathcal{H}_{\boldsymbol{t}}/G_{\boldsymbol{t}}| = 1$ in the above two examples. We present an example of $|\mathcal{H}_{\boldsymbol{t}}/G_{\boldsymbol{t}}| = 2$ by considering the asymmetric indispensable move of Example 3.6.5.

Example 3.6.10 *(Extension of Example 3.6.5.) Consider the case of $k = 6$ and $D_1 = \{1, 2\}, D_2 = \{1, 3\}, D_3 = \{2, 3\}, D_4 = \{4, 5\}, D_5 = \{4, 6\}, D_6 = \{5, 6\}$. This is a direct product model of two three-way models with all two-dimensional marginals fixed. As for the $1, 2, 3$ axes,* *we consider* $I_1 = 3, I_2 = 5, I_3 = 6$ *and define* $\boldsymbol{x}_{D_1}, \boldsymbol{x}_{D_2}, \boldsymbol{x}_{D_3}$ *in the same way as Example 3.6.5. Therefore the possible patterns of* $\boldsymbol{x}_{\{1,2,3\}}$ *are either* $\boldsymbol{x}_1$ *or* $\boldsymbol{x}_2$ *of Example 3.6.5. As for the* $4, 5, 6$ *axes, we consider* $I_1 = 2, I_2 = 7, I_3 = 7$ *and define* $\boldsymbol{x}_{D_4}, \boldsymbol{x}_{D_5}, \boldsymbol{x}_{D_6}$ *as*

$$\boldsymbol{x}_{D_4} = \boldsymbol{x}_{D_5} = [(11),(12),(13),(14),(15),(16),(17),(21),(22),(23),(24),(25),(26),(27)],$$
$$\boldsymbol{x}_{D_6} = [(11),(12),(21),(23),(32),(34),(43),(45),(54),(56),(65),(67),(76),(77)].$$

In this case, again there are two possible patterns of $\boldsymbol{x}_{\{4,5,6\}}$ *as*

$$\boldsymbol{x}'_1 = [(111),(123),(132),(145),(154),(167),(176),(212),(221),(234),(243),(256),(265),(277)],$$
$$\boldsymbol{x}'_2 = [(112),(121),(134),(143),(156),(165),(177),(211),(223),(232),(245),(254),(267),(276)].$$

$\boldsymbol{x}'_1 - \boldsymbol{x}'_2$ *is a symmetric indispensable move in* $(4, 5, 6)$*-marginal tables.*

For the sufficient statistic $\boldsymbol{t}$ *defined above, consider the structure of* $\mathcal{F}_{\boldsymbol{t}}$*.* $\mathcal{F}_{\boldsymbol{t}}$ *is written as*

$$\mathcal{F}_{\boldsymbol{t}} = \{\boldsymbol{x} \mid \boldsymbol{x}_{\{1,2,3\}} = \boldsymbol{x}_1 \text{ or } \boldsymbol{x}_2 \text{ and } \boldsymbol{x}_{\{4,5,6\}} = \boldsymbol{x}'_1 \text{ or } \boldsymbol{x}'_2\}.$$

We have $|\mathcal{F}_{\boldsymbol{t}}| = 3 \cdot 14!$ *since*

$$|\{\boldsymbol{x} \mid \boldsymbol{x}_{\{1,2,3\}} = \boldsymbol{x}_1,\ \boldsymbol{x}_{\{4,5,6\}} = \boldsymbol{x}'_1\}| = 14!,$$
$$|\{\boldsymbol{x} \mid \boldsymbol{x}_{\{1,2,3\}} = \boldsymbol{x}_1,\ \boldsymbol{x}_{\{4,5,6\}} = \boldsymbol{x}'_2\}| = 14!,$$
$$|\{\boldsymbol{x} \mid \boldsymbol{x}_{\{1,2,3\}} = \boldsymbol{x}_2,\ \boldsymbol{x}_{\{4,5,6\}} = \boldsymbol{x}'_1\}| = 14!/2,$$
$$|\{\boldsymbol{x} \mid \boldsymbol{x}_{\{1,2,3\}} = \boldsymbol{x}_2,\ \boldsymbol{x}_{\{4,5,6\}} = \boldsymbol{x}'_2\}| = 14!/2.$$

Consider the M_{13}*-equivalence classes of* $\mathcal{F}_{\boldsymbol{t}}$*. Note that the above four sets are* M_2*-equivalence classes of* $\mathcal{F}_{\boldsymbol{t}}$ *since each set contains all combinations of permutations of* $(1, 2, 3)$*- and* $(4, 5, 6)$*-marginal patterns. Furthermore any two elements in the different sets are not accessible each other by* M_{13} *since* $\boldsymbol{x}_1 - \boldsymbol{x}_2$ *and* $\boldsymbol{x}'_1 - \boldsymbol{x}'_2$ *are indispensable moves in* $(1, 2, 3)$*- and* $(4, 5, 6)$*-marginal tables, respectively. From these considerations, we see that* $|\mathcal{H}_{\boldsymbol{t}}| = 4$*. Write* $\mathcal{H}_{\boldsymbol{t}} = \{X_{11}, X_{12}, X_{21}, X_{22}\}$*, where*

$$X_{ij} = \{\boldsymbol{x} \mid \boldsymbol{x}_{\{1,2,3\}} = \boldsymbol{x}_i,\ \boldsymbol{x}_{\{4,5,6\}} = \boldsymbol{x}'_j\}.$$

Considering the $G_{\boldsymbol{t}}$*-orbit space of* $\mathcal{H}_{\boldsymbol{t}}$*, we have*

$$\mathcal{H}_{\boldsymbol{t}}/G_{\boldsymbol{t}} = \{\{X_{11}, X_{12}\}, \{X_{21}, X_{22}\}\}$$

since $\boldsymbol{x}_1 - \boldsymbol{x}_2$ *is an asymmetric move in* $(1, 2, 3)$*-marginal tables, whereas* $\boldsymbol{x}'_1 - \boldsymbol{x}'_2$ *is a symmetric move in* $(4, 5, 6)$*-marginal tables. Therefore* $|\mathcal{H}_{\boldsymbol{t}}/G_{\boldsymbol{t}}| = 2$ *and* $|\Gamma| = 2$ *for each* $\Gamma \in \mathcal{H}_{\boldsymbol{t}}/G_{\boldsymbol{t}}$*, and we have the union of direct product structure in (3.48).*

Structure of an invariant minimal Markov basis and conditions for its uniqueness

Here we investigate the action of G on the moves. Let $\boldsymbol{z} = \boldsymbol{z}^+ - \boldsymbol{z}^- \in M(D_1, \ldots, D_r)$ be a move. By the identification

$$\boldsymbol{z} \leftrightarrow (\boldsymbol{z}^+, \boldsymbol{z}^-) \tag{3.49}$$

we can regard $\boldsymbol{z}$ as an element of $\mathcal{F}_{\boldsymbol{t}} \times \mathcal{F}_{\boldsymbol{t}}$, where $\boldsymbol{t} = \boldsymbol{t}(\boldsymbol{z}^+) = \boldsymbol{t}(\boldsymbol{z}^-)$. Let $M^{\boldsymbol{t}}(D_1, \ldots, D_r)$ denote the set of moves $\boldsymbol{z}$ such that $\boldsymbol{t} = \boldsymbol{t}(\boldsymbol{z}^+) = \boldsymbol{t}(\boldsymbol{z}^-)$.

In order to be more precise, we define

$$\mathcal{F}_{\boldsymbol{t},\boldsymbol{t}} = \{(\boldsymbol{x}_1, \boldsymbol{x}_2) \mid \boldsymbol{x}_1, \boldsymbol{x}_2 \in \mathcal{F}_{\boldsymbol{t}},\ \mathrm{supp}(\boldsymbol{x}_1) \cap \mathrm{supp}(\boldsymbol{x}_2) = \emptyset\},$$

where $\mathrm{supp}(\boldsymbol{x})$ denotes the set of positive cells of $\boldsymbol{x}$. Then by the identification (3.49), $M^{\boldsymbol{t}}(D_1, \ldots, D_r)$ and $\mathcal{F}_{\boldsymbol{t},\boldsymbol{t}}$ are in 1-to-1 correspondence. We identify $M^{\boldsymbol{t}}(D_1, \ldots, D_r)$ and $\mathcal{F}_{\boldsymbol{t},\boldsymbol{t}}$ hereafter. For $\alpha \in T_n/G$ we define

$$\mathcal{F}_{\alpha,\alpha} = \cup_{\boldsymbol{t}\in\alpha}\mathcal{F}_{\boldsymbol{t},\boldsymbol{t}}.$$

Then $G(\mathcal{F}_{\alpha,\alpha}) = \mathcal{F}_{\alpha,\alpha}$ and we can consider action of G on each $\mathcal{F}_{\alpha,\alpha}$ separately. It is then clear that Lemma 3.6.2 holds also for the moves, i.e.

$$\mathcal{F}_{G(\boldsymbol{t}),G(\boldsymbol{t})} = \bigcup_{i=1}^{a}\bigcup_{j=1}^{b'} \mathcal{F}_{\boldsymbol{t}_i,\boldsymbol{t}_i} \cap G(\boldsymbol{z}_j),$$

where $\boldsymbol{z}_1, \ldots, \boldsymbol{z}_{b'}$ are representative moves of the orbits $\mathcal{F}_{G(\boldsymbol{t}),G(\boldsymbol{t})}/G$.

Let $\mathcal{B} \subset M(D_1, \ldots, D_r)$ be a finite set of moves and define

$$\mathcal{B}_{n,\alpha} = \mathcal{B} \cap \mathcal{F}_{\alpha,\alpha}, \quad \alpha \in T_n/G.$$

Then $\mathcal{B}$ is partitioned as

$$\mathcal{B} = \bigcup_{n} \bigcup_{\alpha\in T_n/G} \mathcal{B}_{n,\alpha}. \tag{3.50}$$

Since $\mathcal{B}$ is invariant if and only if it is a union of orbits $G(\boldsymbol{z})$, the following lemma holds.

Lemma 3.6.6 *$\mathcal{B}$ is invariant if and only if $\mathcal{B}_{n,\alpha}$ is invariant for each n and $\alpha \in T_n/G$.*

This lemma shows that we can restrict our attention to a particular $\mathcal{F}_{\alpha,\alpha}$ in studying the invariance of a Markov basis.

We now use our argument in Section 3.5 to construct an invariant minimal Markov basis. Fix n and $\alpha \in T_n/G$. We shows in Section 3.5 that the essential ingredient in the construction of a minimal Markov basis is the $M_{n-1}(D_1, \ldots, D_r)$-equivalence classes of $\mathcal{F}_{\boldsymbol{t}}$, $\boldsymbol{t} \in \alpha$.

Let $\mathcal{B}$ be an invariant set of moves and consider the partition (3.50). Let $\boldsymbol{z} = \boldsymbol{z}^+ - \boldsymbol{z}^- \in \mathcal{B}_{n,\alpha}$ be a move connecting $X_\gamma \in \mathcal{H}_{\boldsymbol{t}}$ and $X_{\gamma'} \in \mathcal{H}_{\boldsymbol{t}}$, i.e., $\boldsymbol{z}^+ \in X_\gamma$ and $\boldsymbol{z}^- \in X_{\gamma'}$. Then $g\boldsymbol{z} = g\boldsymbol{z}^+ - g\boldsymbol{z}^-$ is a move connecting $X_{g\gamma}$ and $X_{g\gamma'}$. Applying g^{-1} the converse is also true. This implies that the way $\mathcal{B}_{n,\alpha} \cap F_{\boldsymbol{t},\boldsymbol{t}}$ connects the $M_{n-1}(D_1, \ldots, D_r)$-equivalence classes $\mathcal{H}_{\boldsymbol{t}}$ is the same for all $\boldsymbol{t} \in \alpha$.

Now we are in a position to state the following theorem

Theorem 3.6.1 *Let $\mathcal{B}$ be a G-invariant minimal Markov basis and Let $\mathcal{B} = \bigcup_n \bigcup_{\alpha\in T_n/G} \mathcal{B}_{n,\alpha}$ be the partition in (3.50). Then each $\mathcal{B}_{n,\alpha} \cap F_{\boldsymbol{t},\boldsymbol{t}}$, $\boldsymbol{t} \in \alpha, \alpha \in T_n/G$, is a minimal invariant set of moves, which connects $M_{|\boldsymbol{t}|-1}(D_1, \ldots, D_r)$-equivalence classes of $\mathcal{F}_{\boldsymbol{t}}$*

Conversely, from each $\alpha \in T_n/G$ with $|\mathcal{H}_\alpha| \geq 2$ choose a representative sufficient statistic $\boldsymbol{t} \in \alpha$ and choose a $G_{\boldsymbol{t}}$-invariant minimal set of moves $\mathcal{B}_{\boldsymbol{t}}$ connecting $M_{|\boldsymbol{t}|-1}(D_1, \ldots, D_r)$-equivalence classes of $\mathcal{F}_{\boldsymbol{t}}$, where $G_{\boldsymbol{t}} \subset G$ is the isotropy subgroup of $\boldsymbol{t}$, and extend $\mathcal{B}_{\boldsymbol{t}}$ to $G(\mathcal{B}_{\boldsymbol{t}})$. Then

$$\mathcal{B} = \bigcup_{n} \bigcup_{\substack{\boldsymbol{t}\in T_n/G \\ |\mathcal{H}_{\boldsymbol{t}}|\geq 2}} G(\mathcal{B}_{\boldsymbol{t}})$$

is a G-invariant minimal Markov basis.

This theorem only adds a statement of minimal G-invariance to the structure of a minimal Markov basis considered in Theorem 3.5.1. The reason why $\mathcal{B}$ is minimal G-invariant is stated above, and the reason why $\mathcal{B}$ is a Markov basis is included in the proof of Theorem 3.5.1.

In principle this theorem can be used to construct an invariant minimal Markov basis by considering $\bigcup_{\alpha \in T_n/G} \mathcal{B}_{n,\alpha}, n = 1, 2, 3, \ldots$ step by step. By the Hilbert basis theorem, there exists some n_0 such that for $n \geq n_0$ no new moves need to be added. Then an invariant minimal Markov basis is written as $\bigcup_{n=1}^{n_0} \bigcup_{\alpha \in T_n/G} \mathcal{B}_{n,\alpha}$. Obviously, there is a considerable difficulty in implementing this procedure directly. To see this, we apply Theorem 3.6.1 directly to the complete independence model of the three-way contingency tables.

Example 3.6.11 *(Examples 3.6.1, 3.6.2 continued.) Consider the complete independence model of the three-way contingency tables, i.e., $k = 3, D_1 = \{1\}, D_2 = \{2\}, D_3 = \{3\}$. We apply Theorem 3.6.1 directly to this case and derive an invariant minimal Markov basis.*

First consider the case $n = 1$. As is stated in Example 3.6.1, T_1 itself is one G-orbit. Further, $\mathcal{F}_{\boldsymbol{t}}$ is one element set for each $\boldsymbol{t} \in T_1$ and is itself an M_0-equivalence class. Therefore we can conclude that no degree 1 move is needed for Markov basis.

Next consider the case $n = 2$. As we derived in Example 3.6.1, the orbit space T_2/G is written as (3.40). Considering (3.43), we need not consider the case $\boldsymbol{t} \in G(\boldsymbol{t}_1) \cup G(\boldsymbol{t}_2) \cup G(\boldsymbol{t}_3) \cup G(\boldsymbol{t}_4)$ since $\mathcal{F}_{\boldsymbol{t}}$ is one element set (and is itself an M_1-equivalence class). We have to consider all $\boldsymbol{t}$ such that $\boldsymbol{t} \in G(\boldsymbol{t}_5) \cup G(\boldsymbol{t}_6) \cup G(\boldsymbol{t}_7) \cup G(\boldsymbol{t}_8)$. Consider the case $\boldsymbol{t} \in G(\boldsymbol{t}_5) \cup G(\boldsymbol{t}_6) \cup G(\boldsymbol{t}_7)$. We know that $|\mathcal{F}_{\boldsymbol{t}}| = 2$ for these $\boldsymbol{t}$. Representative reference sets are written as

$$
\begin{aligned}
\mathcal{F}_{\boldsymbol{t}_5} &= \{\boldsymbol{x}_5, \boldsymbol{x}'_5\},\ \boldsymbol{x}'_5 = [(112), (121)], \\
\mathcal{F}_{\boldsymbol{t}_6} &= \{\boldsymbol{x}_6, \boldsymbol{x}'_6\},\ \boldsymbol{x}'_6 = [(112), (211)], \\
\mathcal{F}_{\boldsymbol{t}_7} &= \{\boldsymbol{x}_7, \boldsymbol{x}'_7\},\ \boldsymbol{x}'_7 = [(121), (211)].
\end{aligned}
$$

Since each element of $\mathcal{F}_{\boldsymbol{t}}$ is itself an M_1-equivalence class of $\mathcal{F}_{\boldsymbol{t}}$, we have to connect these elements to construct a Markov basis. Obviously, the move that connects two elements of $\mathcal{F}_{\boldsymbol{t}}$ has to be the difference of these, and is an indispensable move. It is also shown that such move is $G_{\boldsymbol{t}}$-invariant. Therefore we have

$$
\mathcal{B}_{\boldsymbol{t}_j} = \{\boldsymbol{z}_j\} = \{\boldsymbol{x}_j - \boldsymbol{x}'_j\},\ j = 5, 6, 7 \tag{3.51}
$$

and $G(\mathcal{B}_{\boldsymbol{t}_5}) \cup G(\mathcal{B}_{\boldsymbol{t}_6}) \cup G(\mathcal{B}_{\boldsymbol{t}_7})$ is included in all G-invariant minimal Markov basis. Finally consider the case $\boldsymbol{t} \in G(\boldsymbol{t}_8)$. The representative reference set is written as

$$
\begin{gathered}
\mathcal{F}_{\boldsymbol{t}_8} = \{\boldsymbol{x}_8, \boldsymbol{x}'_8, \boldsymbol{x}''_8, \boldsymbol{x}'''_8\}, \\
\boldsymbol{x}'_8 = [(112), (221)],\ \boldsymbol{x}''_8 = [(121), (212)],\ \boldsymbol{x}'''_8 = [(211), (122)].
\end{gathered}
$$

and each element of $\mathcal{F}_{\boldsymbol{t}_8}$ is itself an M_1-equivalence class. We have to construct a set of moves which is $G_{\boldsymbol{t}_8}$-invariance and connects these four equivalence classes. Here we have the following proposition.

Proposition 3.6.1 *$G_{\boldsymbol{t}_8}$-invariant minimal set of moves $\mathcal{B}_{\boldsymbol{t}_8}$ which connects the four elements of $\mathcal{F}_{\boldsymbol{t}_8}$ is either of the following three sets.*

$$\begin{array}{l}\{\boldsymbol{x}_8 - \boldsymbol{x}'_8, \boldsymbol{x}''_8 - \boldsymbol{x}'''_8, \boldsymbol{x}_8 - \boldsymbol{x}''_8, \boldsymbol{x}'_8 - \boldsymbol{x}'''_8\}, \\ \{\boldsymbol{x}_8 - \boldsymbol{x}'_8, \boldsymbol{x}''_8 - \boldsymbol{x}'''_8, \boldsymbol{x}_8 - \boldsymbol{x}'''_8, \boldsymbol{x}'_8 - \boldsymbol{x}''_8\}, \\ \{\boldsymbol{x}_8 - \boldsymbol{x}''_8, \boldsymbol{x}'_8 - \boldsymbol{x}'''_8, \boldsymbol{x}_8 - \boldsymbol{x}'''_8, \boldsymbol{x}'_8 - \boldsymbol{x}''_8\}.\end{array} \tag{3.52}$$

Proof. *This proposition is directly shown from the fact that the following three sets of moves,*

$$\{\boldsymbol{x}_8 - \boldsymbol{x}'_8, \boldsymbol{x}''_8 - \boldsymbol{x}'''_8\},\ \{\boldsymbol{x}_8 - \boldsymbol{x}''_8, \boldsymbol{x}'_8 - \boldsymbol{x}'''_8\},\ \{\boldsymbol{x}_8 - \boldsymbol{x}'''_8, \boldsymbol{x}'_8 - \boldsymbol{x}''_8\} \tag{3.53}$$

are $G_{\boldsymbol{t}_8}$-orbits in $M(D_1, D_2, D_3)$, respectively. *Q.E.D.*

We consider the action of group $G_{\boldsymbol{t}_8}$ to the reference set $\mathcal{F}_{\boldsymbol{t}_8}$ in detail. We have shown in Example 3.6.2 that $G_{\boldsymbol{t}_8} = \widetilde{G}^1_{12,12} \times \widetilde{G}^2_{12,12} \times \widetilde{G}^3_{12,12}$. Let $g^1 \in G^1_{12,12} \times G^2_{12,12} \times G^3_{12,12} \subset G_{\boldsymbol{t}_8}$. Then it follows that $\{e, g^1\}$ is an isotropy subgroup either of $\boldsymbol{x}_8, \boldsymbol{x}'_8, \boldsymbol{x}''_8, \boldsymbol{x}'''_8$. The pair of $(G_{\boldsymbol{t}_8}, \mathcal{F}_{\boldsymbol{t}_8})$ is isomorphic to $(G_{\boldsymbol{t}_8}, G_{\boldsymbol{t}_8}/\{e, g^1\})$, and $G_{\boldsymbol{t}_8}/\{e, g^1\}$ is isomorphic to Klein four-group.

Next consider the case $n = 3$. But in this case, it is observed that no move of degree 3 is needed. In fact, no move of degree $n \geq 3$ is needed in this model as shown in Proposition 3.5.1. From these considerations, an invariant minimal Markov basis for this model is summarized as follows.

Proposition 3.6.2 *A G-invariant minimal Markov basis for the complete independent model of the three-way contingency tables is written as*

$$\mathcal{B} = G(\mathcal{B}_{\boldsymbol{t}_5}) \cup G(\mathcal{B}_{\boldsymbol{t}_6}) \cup G(\mathcal{B}_{\boldsymbol{t}_7}) \cup G(\mathcal{B}_{\boldsymbol{t}_8}),$$

where $\mathcal{B}_{\boldsymbol{t}_5}, \mathcal{B}_{\boldsymbol{t}_6}, \mathcal{B}_{\boldsymbol{t}_7}$ are sets of indispensable moves given in (3.51) and $\mathcal{B}_{\boldsymbol{t}_8}$ is either of the three sets of dispensable moves in (3.52).

The number of the G-invariant minimal Markov basis elements is derived as

$$|\mathcal{B}| = \sum_{j=5}^{8} |G(\mathcal{B}_{\boldsymbol{t}_j})| = \sum_{j=5}^{8} |G(\boldsymbol{t}_j)| \cdot |\mathcal{B}_{\boldsymbol{t}_j}| = \sum_{j=5}^{7} |G(\boldsymbol{t}_j)| + 2|G(\boldsymbol{t}_8)|$$

where $|G(\boldsymbol{t}_j)|$ is given in (3.42).

In this example, we see that an invariant minimal Markov basis for this model is not unique. It should be noted that a minimal Markov basis is not unique either for this model as is shown in Section 3.5.4. Since the set of the indispensable moves is G-invariant, an invariant minimal Markov basis and a minimal Markov basis differ only in dispensable moves. This is always true and here we also state the following obvious fact.

Lemma 3.6.7 *If there exists a unique minimal Markov basis, then it is a unique invariant minimal Markov basis.*

Now we derive a necessary and sufficient condition for the existence of a unique invariant minimal Markov basis. As a direct consequence of Theorem 3.6.1, first we give the following corollary to Theorem 3.6.1 without a proof.

Corollary 3.6.1 *An invariant minimal Markov basis is unique if and only if for each* n *and* $\alpha \in T_n/G$ *with* $|\mathcal{H}_\alpha| \geq 2$ $\mathcal{B}_{\boldsymbol{t}}, \boldsymbol{t} \in \alpha$*, is a unique minimal* $G_{\boldsymbol{t}}$*-invariant set of moves connecting* $M_{|\boldsymbol{t}|-1}(D_1, \ldots, D_r)$*-equivalence classes of* $\mathcal{F}_{\boldsymbol{t}}$*.*

Therefore we consider $\mathcal{F}_{\boldsymbol{t}}$ for each $\boldsymbol{t}$ separately. Recall that there is an union of direct products structure in $\mathcal{F}_{\boldsymbol{t}}$ as shown in (3.48). Since each X_Γ is $G_{\boldsymbol{t}}$-invariant, first we summarize the structure of a minimal invariant set of moves connecting different X_Γ's, $\Gamma \in \mathcal{H}_{\boldsymbol{t}}/G_{\boldsymbol{t}}$.

Lemma 3.6.8 $\mathcal{B}$ *is a* $G_{\boldsymbol{t}}$*-invariant minimal set of moves that connects* $X_\Gamma, \Gamma \in \mathcal{H}_{\boldsymbol{t}}/G_{\boldsymbol{t}}$ *if and only if* $\mathcal{B}$ *is written as*

$$\mathcal{B} = G_{\boldsymbol{t}}(\boldsymbol{z}_1) \cup \cdots \cup G_{\boldsymbol{t}}(\boldsymbol{z}_{|\mathcal{H}_{\boldsymbol{t}}/G_{\boldsymbol{t}}|-1}), \tag{3.54}$$

where the set of the representative moves $\boldsymbol{z}_1, \ldots, \boldsymbol{z}_{|\mathcal{H}_{\boldsymbol{t}}/G_{\boldsymbol{t}}|-1}$ *connects* $X_\Gamma, \Gamma \in \mathcal{H}_{\boldsymbol{t}}/G_{\boldsymbol{t}}$ *into a tree.*

Proof. Let $\boldsymbol{z} = \boldsymbol{z}^+ - \boldsymbol{z}^-$ is a move that connects X_Γ and $X_{\Gamma'}, \Gamma \neq \Gamma'$, i.e., $\boldsymbol{z}^+ \in X_\Gamma$ and $\boldsymbol{z}^- \in X_{\Gamma'}$. Then $g\boldsymbol{z}$ also connects X_Γ and $X_{\Gamma'}$ for any $g \in G_{\boldsymbol{t}}$, since $g\boldsymbol{z}^+ \in X_\Gamma, g\boldsymbol{z}^- \in X_{\Gamma'}$. Q.E.D.

This lemma implies the following necessarily condition for existing an unique invariant minimal Markov basis.

Corollary 3.6.2 *If an invariant minimal Markov basis is unique, then the following conditions hold for all* $\boldsymbol{t}$ *such that* $|\mathcal{H}_{\boldsymbol{t}}| \geq 2$*.*

- *(i)* $|\mathcal{H}_{\boldsymbol{t}}/G_{\boldsymbol{t}}|$ *is at most* 2*.*
- *(ii)* *For* $\mathcal{F}_{\boldsymbol{t}}$ *such that* $|\mathcal{H}_{\boldsymbol{t}}/G_{\boldsymbol{t}}| = 2, G_{\boldsymbol{t}}(\boldsymbol{z})$ *is the same for all* $\boldsymbol{z} = \boldsymbol{z}^+ - \boldsymbol{z}^-, \boldsymbol{z}^+ \in X_\gamma, \boldsymbol{z}^- \in X_{\gamma'}$*, where* $\mathcal{F}_{\boldsymbol{t}} = X_\gamma \cup X_{\gamma'}$*.*

Next we consider the structure of a minimal invariant set of moves connecting the equivalence classes in each X_Γ. Consider a move $\boldsymbol{z} = \boldsymbol{z}^+ - \boldsymbol{z}^-$ connecting different $X_\gamma \in X_\Gamma$, i.e., $\boldsymbol{z}^+ \in X_\gamma, \boldsymbol{z}^- \in X_{\gamma'}, X_\gamma \neq X_{\gamma'}$. Since the action of $G_{\boldsymbol{t}}$ on X_Γ is transitive, without loss of generality we fix X_γ to be a particular equivalence set X_{γ_0} and let $\boldsymbol{z}^+ \in X_{\gamma_0}$ when we consider $G_{\boldsymbol{t}}(\boldsymbol{z})$. For each $\gamma' \neq \gamma_0$, we define an *orbit graph* $\mathcal{G}_{\gamma'} = \mathcal{G}(X_\Gamma, E_{\gamma'})$, where the edge set $E_{\gamma'}$ is defined as

$$E_{\gamma'} = \{(X_{\gamma_1}, X_{\gamma_2}) \mid (g\boldsymbol{z}^+, g\boldsymbol{z}^-) \in (X_{\gamma_1}, X_{\gamma_2}) \text{ for some } g \in G_{\boldsymbol{t}} \text{ where } \boldsymbol{z}^+ \in X_{\gamma_0}, \boldsymbol{z}^- \in X_{\gamma'}\}.$$

It should be noted that $E_{\gamma'}$ (and hence $\mathcal{G}_{\gamma'}$) does not depend on the choice of $\boldsymbol{z}^+ \in X_{\gamma_0}$ and $\boldsymbol{z}^- \in X_{\gamma'}$, whereas the orbits $G_{\boldsymbol{t}}(\boldsymbol{z})$ differ for the different choice of (δ_1, δ_2), where $\boldsymbol{z}^+ \in X_{\gamma_0} \cap G_{\boldsymbol{t}}(\boldsymbol{x}_{\delta_1})$, $\boldsymbol{z}^- \in X_{\gamma'} \cap G_{\boldsymbol{t}}(\boldsymbol{x}_{\delta_2})$ when $|\Delta| = |X_\Gamma/G_{\boldsymbol{t}}| \geq 2$. Furthermore

$$E_{\gamma_1} \cap E_{\gamma_2} = \emptyset \text{ for all } \gamma_1 \neq \gamma_2$$

by definition. We also define that the orbit graph $\mathcal{G}_{\gamma'}$ is *indispensable* if the graph $\mathcal{G}(X_\Gamma, \bigcup_{\gamma\neq\gamma'} E_\gamma)$ is not connected. An important point here is that if the set of indispensable orbit graphs connects all the equivalence classes in X_Γ, then this corresponds to the unique minimal invariant set of moves for X_Γ. Combining this result and Corollary 3.6.2, we have the following result.

Theorem 3.6.2 *A minimal invariant Markov basis is unique if and only if the following conditions hold for all* $\boldsymbol{t}$ *such that* $|\mathcal{H}_{\boldsymbol{t}}| \geq 2$, *in addition to (i) and (ii) of Corollary 3.6.2.*

(*iii*) $|\Delta| = |X_\Gamma/G_{\boldsymbol{t}}| = 1$ *for all* Γ.
(*iv*) *The set of indispensable orbit graphs connects all* $X_\gamma \in X_\Gamma$ *for all* Γ.
(*v*) *For all indispensable orbit graphs of (iv), there is only one orbit* $G_{\boldsymbol{t}}(\boldsymbol{z})$ *that derives it.*

In Section 3.5.4, minimal Markov bases and their uniqueness are shown for some examples. We see that for some examples a minimal Markov basis is unique, and for other examples it is not unique. Since a unique minimal Markov basis is also the unique invariant minimal Markov basis, logically interesting case is that, an invariant minimal Markov basis is unique, nevertheless a minimal Markov basis is not unique. The Hardy-Weinberg model is such an example, if we define a symmetric group acting to the upper triangular tables appropriately. Except for this peculiar example, the only example that we have found so far is a one-way contingency tables.

Example 3.6.12 *Consider the case of* $k = 1$ *and* $D = \{1\}$. *As is stated in Section 3.5.4, a minimal Markov basis for this case is not unique, and consists of* $I_1 - 1$ *degree* 1 *moves that connect* I *elements in* X_1 *into a tree. By Cayley's theorem, there are* $I_1^{I_1-2}$ *ways of choosing a minimal Markov basis. On the other hand, the set of all degree* 1 *moves,*

$$\mathcal{B} = \{\boldsymbol{x} - \boldsymbol{x}' \mid \boldsymbol{x}, \boldsymbol{x}' \in X_1, \boldsymbol{x} \neq \boldsymbol{x}'\}$$

is a G-orbit in $M(D)$. *Therefore* $\mathcal{B}$ *is the unique invariant minimal Markov basis.* $\mathcal{B}$ *consists of* $\begin{pmatrix} I_1 \\ 2 \end{pmatrix}$ *degree* 1 *moves.*

We show that three examples considered so far do not have unique invariant minimal Markov basis.

Example 3.6.13 *(Examples 3.6.3, 3.6.6, 3.6.8 continued.) Consider* $\mathcal{B}_{4,\boldsymbol{t}}$ *where* $\boldsymbol{t} \in T_4/G$ *is given in Example 3.6.3. In this case, the conditions of Corollary 3.6.2 is satisfied since* $|\mathcal{H}_{\boldsymbol{t}}/G_{\boldsymbol{t}}| = 1$. *However, the ways of connecting two equivalence classes,* $\{\boldsymbol{x}_1, \boldsymbol{x}_2, \boldsymbol{x}_3, \boldsymbol{x}_4\}, \{\boldsymbol{x}_5, \boldsymbol{x}_6, \boldsymbol{x}_7, \boldsymbol{x}_8\}$ *are not unique. In fact, though the orbit graph (i.e., connected two vertices) is unique and indispensable, there are the following five* $G_{\boldsymbol{t}}$*-invariant minimal set of moves that derives it.*

$$\begin{aligned}
&\{\boldsymbol{x}_1 - \boldsymbol{x}_5, \boldsymbol{x}_4 - \boldsymbol{x}_8\}, \quad \{\boldsymbol{x}_1 - \boldsymbol{x}_8, \boldsymbol{x}_4 - \boldsymbol{x}_5\},\\
&\{\boldsymbol{x}_2 - \boldsymbol{x}_6, \boldsymbol{x}_3 - \boldsymbol{x}_7\}, \quad \{\boldsymbol{x}_2 - \boldsymbol{x}_7, \boldsymbol{x}_3 - \boldsymbol{x}_6\},\\
&\{\boldsymbol{x}_1 - \boldsymbol{x}_6, \boldsymbol{x}_1 - \boldsymbol{x}_7, \boldsymbol{x}_2 - \boldsymbol{x}_5, \boldsymbol{x}_2 - \boldsymbol{x}_8, \boldsymbol{x}_3 - \boldsymbol{x}_5, \boldsymbol{x}_3 - \boldsymbol{x}_8, \boldsymbol{x}_4 - \boldsymbol{x}_6, \boldsymbol{x}_4 - \boldsymbol{x}_7\}.
\end{aligned}$$

Example 3.6.14 *(Examples 3.6.4, 3.6.7, 3.6.9 continued.) Consider $\mathcal{B}_{4,\boldsymbol{t}}$ where $\boldsymbol{t} \in T_4/G$ is given in Example 3.6.4. Similarly to Example 3.6.13, the conditions of Corollary 3.6.2 is satisfied in this case since $|\mathcal{H}_{\boldsymbol{t}}/G_{\boldsymbol{t}}| = 1$. However, the ways of connecting two equivalence classes, $\{\boldsymbol{x}_1, \boldsymbol{x}_2, \boldsymbol{x}_3, \boldsymbol{x}_4, \boldsymbol{x}_9, \boldsymbol{x}_{10}\}$, $\{\boldsymbol{x}_5, \boldsymbol{x}_6, \boldsymbol{x}_7, \boldsymbol{x}_8, \boldsymbol{x}_{11}, \boldsymbol{x}_{12}\}$ are not unique. In this case, the orbit graph also consists of connected two vertices, and is unique and indispensable. However, there are the following nine $G_{\boldsymbol{t}}$-invariant minimal set of moves that derives it.*

$$
\begin{aligned}
&\{\boldsymbol{x}_1 - \boldsymbol{x}_5, \boldsymbol{x}_4 - \boldsymbol{x}_8\}, \quad \{\boldsymbol{x}_1 - \boldsymbol{x}_8, \boldsymbol{x}_4 - \boldsymbol{x}_5\},\\
&\{\boldsymbol{x}_2 - \boldsymbol{x}_6, \boldsymbol{x}_3 - \boldsymbol{x}_7\}, \quad \{\boldsymbol{x}_2 - \boldsymbol{x}_7, \boldsymbol{x}_3 - \boldsymbol{x}_6\},\\
&\{\boldsymbol{x}_9 - \boldsymbol{x}_{11}, \boldsymbol{x}_{10} - \boldsymbol{x}_{12}\}, \quad \{\boldsymbol{x}_9 - \boldsymbol{x}_{12}, \boldsymbol{x}_{10} - \boldsymbol{x}_{11}\},\\
&\{\boldsymbol{x}_1 - \boldsymbol{x}_6, \boldsymbol{x}_1 - \boldsymbol{x}_7, \boldsymbol{x}_2 - \boldsymbol{x}_5, \boldsymbol{x}_2 - \boldsymbol{x}_8, \boldsymbol{x}_3 - \boldsymbol{x}_5, \boldsymbol{x}_3 - \boldsymbol{x}_8, \boldsymbol{x}_4 - \boldsymbol{x}_7, \boldsymbol{x}_4 - \boldsymbol{x}_6\},\\
&\{\boldsymbol{x}_1 - \boldsymbol{x}_{11}, \boldsymbol{x}_1 - \boldsymbol{x}_{12}, \boldsymbol{x}_9 - \boldsymbol{x}_5, \boldsymbol{x}_9 - \boldsymbol{x}_8, \boldsymbol{x}_4 - \boldsymbol{x}_{11}, \boldsymbol{x}_4 - \boldsymbol{x}_{12}, \boldsymbol{x}_{10} - \boldsymbol{x}_5, \boldsymbol{x}_{10} - \boldsymbol{x}_8\},\\
&\{\boldsymbol{x}_2 - \boldsymbol{x}_{11}, \boldsymbol{x}_2 - \boldsymbol{x}_{12}, \boldsymbol{x}_9 - \boldsymbol{x}_6, \boldsymbol{x}_9 - \boldsymbol{x}_7, \boldsymbol{x}_3 - \boldsymbol{x}_{11}, \boldsymbol{x}_3 - \boldsymbol{x}_{12}, \boldsymbol{x}_{10} - \boldsymbol{x}_6, \boldsymbol{x}_{10} - \boldsymbol{x}_7\}.
\end{aligned}
$$

Example 3.6.15 *(Examples 3.6.1, 3.6.2, 3.6.11 continued.) We have seen that an invariant minimal Markov basis is not unique for the complete independence model of the three-way contingency tables. In fact, three sets of moves (3.53) in Proposition 3.6.1 correspond to different orbit graphs, respectively. Therefore in this case, each orbit graph is dispensable.*

3.6.3 Invariant minimal Markov basis for all hierarchical 2^4 models

In this section, we give a complete list of a minimal and an invariant minimal Markov basis for all hierarchical $2 \times 2 \times 2 \times 2$ models. Though our list is restricted to the case of $2 \times 2 \times 2 \times 2$, if a set of moves whose supports are contained in $2 \times 2 \times 2 \times 2$ array constitutes a Markov basis for a general $I_1 \times I_2 \times I_3 \times I_4$ case, we can derive a minimal and an invariant minimal Markov basis for the general case, by considering the orbits T_n/G. For example, a minimal and an invariant minimal Markov basis for the complete independence model of the three-way contingency tables are derived in Examples 3.6.1, 3.6.2 and 3.6.11. These results are extensions of the results for the $2 \times 2 \times 2$ case, since the moves with supports contained in $2 \times 2 \times 2$ arrays constitute a Markov basis for general case.

To derive the following list, we used several methods. If the model is decomposable, it is known that Markov bases consist of degree 2 moves only (Dobra, 2003). If the model is reducible, an algorithm proposed by Dobra and Sullivant (2002) can be used. We also perform a primitive consideration of the sign patterns, which is similar to Section 3.2.

What the list means is as follows. The models that we consider are hierarchical 2^4 models. There are 20 different models. Figure 3.12 is the list of independence graphs of these models.

We specify each model by their generating set. For example, a model 123/24/34 means $D_1 = \{1, 2, 3\}, D_2 = \{2, 4\}, D_3 = \{3, 4\}$. The **degree of freedom** is a number of independent cells in 2^4 tables under the models. For each model, we give a minimal and an invariant minimal Markov basis. As stated in Theorem 3.6.1, an invariant minimal Markov basis is written as

$$\mathcal{B} = \bigcup_{n=1}^{n_0} \bigcup_{\substack{\boldsymbol{t} \in T_n/G \\ |\mathcal{H}_{\boldsymbol{t}}| \geq 2}} G(\mathcal{B}_{\boldsymbol{t}}).$$

In our models, n_0 is at most 8. We give a list of $\mathcal{B}_{\boldsymbol{t}}$ for all $\boldsymbol{t} \in T_n/G, |\mathcal{H}_{\boldsymbol{t}}| \geq 2$. To specify each move, we use symbols $\boldsymbol{x}$ and $\boldsymbol{y}$ to denote representative elements $\boldsymbol{x} \in X_4$ and $\boldsymbol{y} \in X_2$

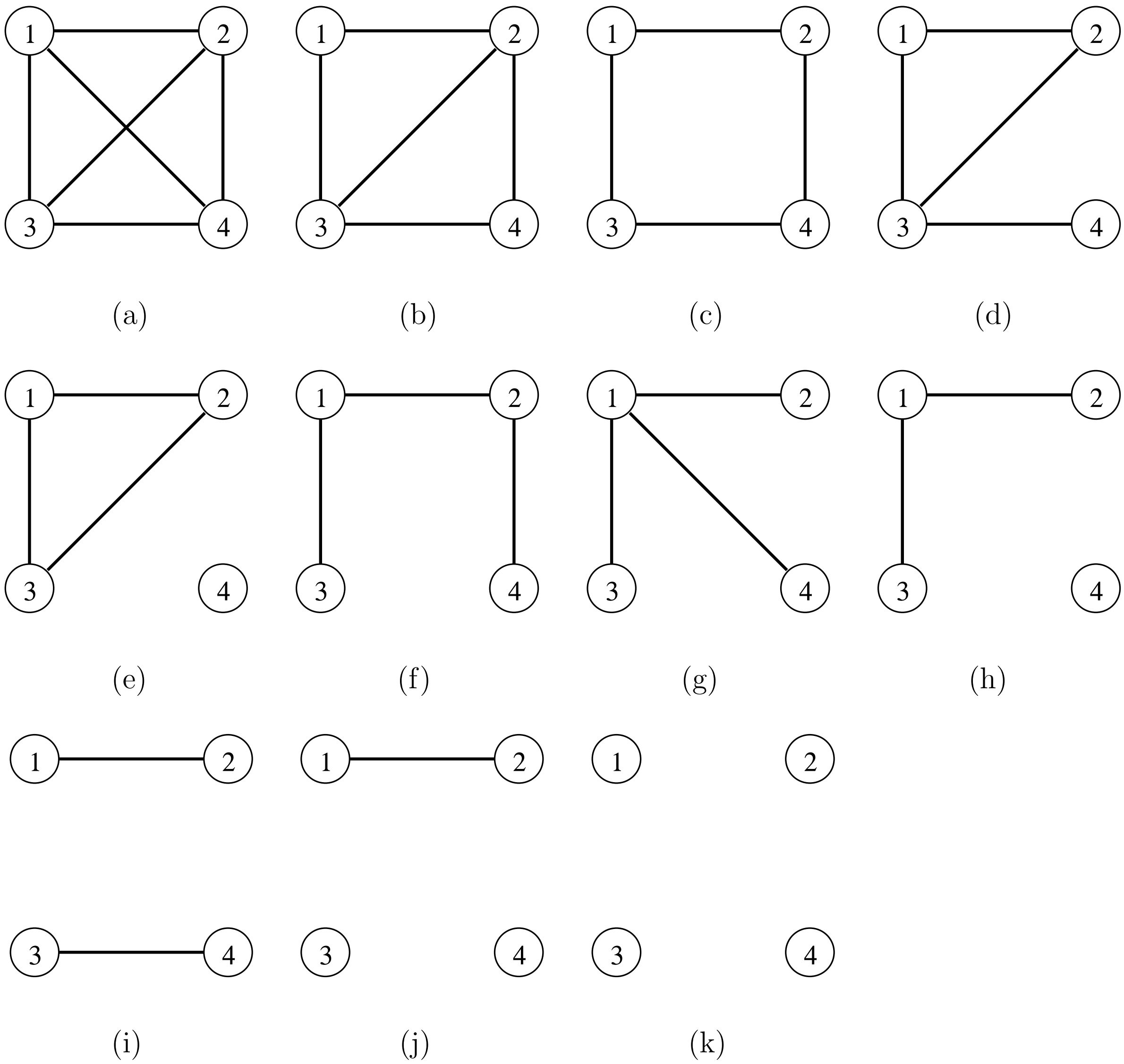

Figure 3.12: Independence graphs for four-way contingency tables

in this section. Though some of these representative elements are already used in Examples in the previous section, we newly number these elements to avoid confusion. We give sets of **indispensable moves**, i.e., $\mathcal{B}_{\boldsymbol{t}}$ such that $|\mathcal{H}_{\boldsymbol{t}}| = 2$, with their representative elements. For example, there are 6 indispensable moves of degree 4 with representative elements $\boldsymbol{x}_1, \boldsymbol{x}_2, \boldsymbol{x}_3$ for the model 123/124/34. This means that, for $i = 1, 2, 3$, each reference set with the same sufficient statistic $\boldsymbol{t}(\boldsymbol{x}_i)$ has two elements, i.e., $\mathcal{F}_{\boldsymbol{t}(\boldsymbol{x}_i)} = \{\boldsymbol{x}_{i,1}, \boldsymbol{x}_{i,2}\}$, and the representative move is written as $\mathcal{B}_{\boldsymbol{t}(\boldsymbol{x}_i)} = \{\boldsymbol{x}_{i,1} - \boldsymbol{x}_{i,2}\}$. A complete list of the indispensable moves is given by extending each $\mathcal{B}_{\boldsymbol{t}(\boldsymbol{x}_i)}$ to $G(\mathcal{B}_{\boldsymbol{t}(\boldsymbol{x}_i)})$, i.e.,

$$G(\mathcal{B}_{\boldsymbol{t}(\boldsymbol{x}_1)}) \cup G(\mathcal{B}_{\boldsymbol{t}(\boldsymbol{x}_2)}) \cup G(\mathcal{B}_{\boldsymbol{t}(\boldsymbol{x}_3)}),$$

and there are

$$6 = \sum_{i=1}^{3} |G(\mathcal{B}_{\boldsymbol{t}(\boldsymbol{x}_i)})| = \sum_{i=1}^{3} |\mathcal{B}_{\boldsymbol{t}(\boldsymbol{x}_i)}| \cdot |G(\boldsymbol{t}(\boldsymbol{x}_i))| = \sum_{i=1}^{3} |G(\boldsymbol{t}(\boldsymbol{x}_i))|$$

elements of indispensable moves. In our examples, $|G(\boldsymbol{t})|$ is equal for each n such that $\boldsymbol{t} \in T_n$ when $|\mathcal{H}_{\boldsymbol{t}}| = 2$ and given as

$$|G(\boldsymbol{t})| = \begin{cases} 1, & \boldsymbol{t} \in T_8, \\ 8, & \boldsymbol{t} \in T_6, \\ 2, & \boldsymbol{t} \in T_4, \\ 4, & \boldsymbol{t} \in T_2. \end{cases}$$

Uniqueness of a minimal Markov basis is also shown. As we have stated, if the set of indispensable moves constitutes a Markov basis, this is a unique (invariant) minimal Markov basis. On the other hand, if a minimal Markov basis is not unique, uniqueness of an invariant minimal Markov basis is important. In all of 2^4 hierarchical models, however, we found that an invariant minimal Markov basis is also not unique when a minimal Markov basis is not unique. We discuss this point in Section 3.6.4. When a minimal basis is not unique, there is at least one reference set which itself does not constitute one $\mathcal{B}$-equivalence class, where $\mathcal{B}$ is the set of indispensable moves. Furthermore, if $\mathcal{F}_{\boldsymbol{t}}$ is such a reference set, all the reference sets in $\mathcal{F}_{G(\boldsymbol{t})}$ have the isomorphic structures as stated in Lemma 3.6.2. We give this **isomorphic structures of reference sets** with representative elements, $|G(\boldsymbol{t})|, |\mathcal{F}_{G(\boldsymbol{t})}/G|$ and $|\mathcal{F}_{\boldsymbol{t}}|$. Then we give a **direct product structure for each reference set** $\mathcal{F}_{\boldsymbol{t}} \in \mathcal{F}_{G(\boldsymbol{t})}$ as shown in Lemma 3.6.5, with $|\Delta|$ and $|\Lambda|$. We omit $|\mathcal{H}_{\boldsymbol{t}}/G_{\boldsymbol{t}}|$ since for all our models $|\mathcal{H}_{\boldsymbol{t}}/G_{\boldsymbol{t}}| = 1$. Finally we give a **minimal basis**, **orbit graphs** and an **invariant minimal basis for each reference set**. As for a minimal basis, we only show the number of different set of dispensable moves and number of its elements, which are calculated from the number of equivalence classes and the number of their elements. As is stated in Section 3.5, if a reference set consists of t equivalence classes and each equivalence class has u elements, there are $u^{t^{t-2}}$ different set of $t-1$ moves for this reference set in a minimal basis. On the other hand, for an invariant minimal basis, we show the orbit graphs and the orbits of moves that derive them. Table 3.8 shows the numbers of elements in each minimal basis and invariant minimal basis.

Table 3.8: List of minimal basis and invariant minimal basis for 2^4 hierarchical models

graph	generating set	number of basis
(a)	1234	$\emptyset$
	123/124/134/234	unique minimal basis (1 move of deg 8)
	123/124/134	unique minimal basis (2 moves of deg 4)
	123/124/34	unique minimal basis (6 moves of deg 4)
	123/14/24/34	unique minimal basis (12 moves of deg 4 and 8 moves of deg 6)
	12/13/14/23/24/34	unique minimal basis (20 moves of deg 4 and 40 moves of deg 6)
(b)	123/234	unique minimal basis (4 moves of deg 2)
	123/24/34	unique minimal basis (4 moves of deg 2 and 16 moves of deg 4)
	12/13/23/24/34	indispensable moves: 4 moves of deg 2 and 28 moves of deg 4 dispensable moves of a minimal basis: 16 kinds of 3 moves of deg 4 dispensable moves of an invariant minimal basis: 3 kinds of 4 moves of deg 4
(c)	12/13/24/34	unique minimal basis (8 moves of deg 2 and 8 moves of deg 4)
(d)	123/34	unique minimal basis (12 moves of deg 2)
	12/13/23/34	indispensable moves: 12 moves of deg 2 and 4 moves of deg 4 dispensable moves of a minimal basis: 4096 kinds of 5 moves of deg 4 dispensable moves of an invariant minimal basis: 8 kinds of 10 moves of deg 4 or 2 kinds of 16 moves of deg 4
(e)	123/4	unique minimal basis (28 moves of deg 2)
	12/13/23/4	indispensable moves: 28 moves of deg 2 and 2 moves of deg 4 dispensable moves of a minimal basis: 9216 kinds of 3 moves of deg 4 dispensable moves of an invariant minimal basis: 24 kinds of 10 moves of deg 4 or 12 kinds of 16 moves of deg 4
(f)	12/13/24	unique minimal basis (20 moves of deg 2)
(g)	12/13/14	indispensable moves: 12 moves of deg 2 dispensable moves of a minimal basis: 256 kinds of 6 moves of deg 2 dispensable moves of an invariant minimal basis: 3 kinds of 8 moves of deg 2
(h)	12/13/4	indispensable moves: 28 moves of deg 2 dispensable moves of a minimal basis: 256 kinds of 6 moves of deg 2 dispensable moves of an invariant minimal basis: 3 kinds of 8 moves of deg 2
(i)	12/34	unique minimal basis (36 moves of deg 2)
(j)	12/3/4	indispensable moves: 28 moves of deg 2 dispensable moves of a minimal basis: $16^6 = 16777216$ kinds of 18 moves of deg 2 dispensable moves of an invariant minimal basis: 27 kinds of 24 moves of deg 2
(k)	1/2/3/4	indispensable moves: 24 moves of deg 2 dispensable moves of a minimal basis: $16^8 \times 8^6 = 1.1259 \times 10^{15}$ kinds of 31 moves of deg 2 dispensable moves of an invariant minimal basis: 2268 kinds of 44 moves of deg 2

Models with the independence graph (a)

- Model 1234 (saturated, graphical model)
  degree of freedom: 0

- Model 123/124/134/234
  degree of freedom: 1
  indispensable move: 1 move of degree 8 with representative element

$$[(1111)(1122)(1212)(1221)(2112)(2121)(2211)(2222)].$$

  uniqueness: unique minimal basis exists.

- Model 123/124/134
  degree of freedom: 2
  indispensable moves: 2 moves of degree 4 with representative element

$$\boldsymbol{x}_1 = [(1111)(1122)(1212)(1221)].$$

  uniqueness: unique minimal basis exists.

- Model 123/124/34
  degree of freedom: 3
  indispensable moves: 6 moves of degree 4 with representative elements

$$\boldsymbol{x}_1,\ \boldsymbol{x}_2 = [(1111)(1122)(2112)(2121)],\ \boldsymbol{x}_3 = [(1111)(1122)(2212)(2221)].$$

  uniqueness: unique minimal basis exists.

- Model 123/14/24/34
  degree of freedom: 4
  indispensable moves: 12 moves of degree 4 with representative elements

$$\begin{aligned}&\boldsymbol{x}_1,\ \boldsymbol{x}_2,\ \boldsymbol{x}_3,\ \boldsymbol{x}_4 = [(1111)(1212)(2112)(2211)],\\ &\boldsymbol{x}_5 = [(1111)(1212)(2122)(2221)],\ \boldsymbol{x}_6 = [(1111)(1222)(2112)(2221)]\end{aligned}$$

  and 8 moves of degree 6 with representative element

$$[(1111)(1111)(1122)(1212)(2112)(2221)].$$

  uniqueness: unique minimal basis exists.

- Model 12/13/14/23/24/34
  degree of freedom: 5
  indispensable moves: 20 moves of degree 4 with representative elements

$$\begin{aligned}&\boldsymbol{x}_1,\ \boldsymbol{x}_2,\ \boldsymbol{x}_3,\ \boldsymbol{x}_4,\ \boldsymbol{x}_5,\ \boldsymbol{x}_6,\\ &\boldsymbol{x}_7 = [(1111)(1221)(2121)(2211)],\ \boldsymbol{x}_8 = [(1111)(1221)(2122)(2212)],\\ &\boldsymbol{x}_9 = [(1111)(1222)(2121)(2212)],\ \boldsymbol{x}_{10} = [(1111)(1222)(2122)(2211)]\end{aligned}$$

and 40 moves of degree 6 with representative elements

$$\begin{gathered}[(1111)(1111)(1122)(1212)(2112)(2221)], \\ [(1111)(1111)(1222)(2122)(2212)(2221)], \\ [(1111)(1111)(1122)(1221)(2121)(2212)], \\ [(1111)(1111)(1212)(1221)(2122)(2211)], \\ [(1111)(1111)(1222)(2112)(2121)(2211)].\end{gathered}$$

uniqueness: unique minimal basis exists.

Models with the independence graph (b)

- Model 123/234 (graphical, decomposable model)
  degree of freedom: 4
  indispensable moves: 4 moves of degree 2 with representative element

  $$\boldsymbol{y}_1 = [(1111)(2112)].$$

  uniqueness: unique minimal basis exists.

- Model 123/24/34
  degree of freedom: 5
  indispensable moves: 4 moves of degree 2 with representative element $\boldsymbol{y}_1$, and 16 moves of degree 4 with representative elements

  $$\begin{aligned}&\boldsymbol{x}_1,\ \boldsymbol{x}_3, \\ &\boldsymbol{x}_{11} = [(1111)(1122)(1212)(2221)],\ \boldsymbol{x}_{12} = [(1111)(1122)(1221)(2212)], \\ &\boldsymbol{x}_{13} = [(1111)(1212)(1221)(2122)],\ \boldsymbol{x}_{14} = [(1111)(1212)(2122)(2221)], \\ &\boldsymbol{x}_{15} = [(1111)(1221)(2122)(2212)],\ \boldsymbol{x}_{16} = [(1111)(2122)(2212)(2221)].\end{aligned}$$

  uniqueness: unique minimal basis exists.

- Model 12/13/23/24/34
  degree of freedom: 6
  indispensable moves: 4 moves of degree 2 with representative element $\boldsymbol{y}_1$, and 28 moves of degree 4 with representative elements

  $$\begin{aligned}&\boldsymbol{x}_1,\ \boldsymbol{x}_3,\ \boldsymbol{x}_7,\ \boldsymbol{x}_9,\ \boldsymbol{x}_{11},\ \boldsymbol{x}_{12},\ \boldsymbol{x}_{13},\ \boldsymbol{x}_{14},\ \boldsymbol{x}_{16}, \\ &\boldsymbol{x}_{17} = [(1111)(1221)(2121)(2212)],\ \boldsymbol{x}_{18} = [(1111)(1221)(2122)(2211)], \\ &\boldsymbol{x}_{19} = [(1112)(1221)(2122)(2212)],\ \boldsymbol{x}_{20} = [(1111)(1222)(2122)(2212)], \\ &\boldsymbol{x}_{21} = [(1111)(1222)(2122)(2211)].\end{aligned}$$

  uniqueness: unique minimal basis does not exist.
  isomorphic structures of reference set:

  $$\mathcal{F}_{\boldsymbol{t}(\boldsymbol{x}_8)} = G(\boldsymbol{x}_8),\ |G(\boldsymbol{t}(\boldsymbol{x}_8))| = 1,\ |\mathcal{F}_{\boldsymbol{t}(\boldsymbol{x}_8)}| = 4.$$

direct product structure for $\mathcal{F}_{\boldsymbol{t}(\boldsymbol{x}_8)}$:

$$\begin{gathered}\mathcal{F}_{\boldsymbol{t}(\boldsymbol{x}_8)} = X_{\gamma_1} \cup X_{\gamma_2} \cup X_{\gamma_3} \cup X_{\gamma_4} = G(\boldsymbol{x}_8),\\ X_{\gamma_1} = \{\boldsymbol{x}_8\},\ X_{\gamma_2} = \{\boldsymbol{x}_{8,2}\},\ X_{\gamma_3} = \{\boldsymbol{x}_{8,3}\},\ X_{\gamma_4} = \{\boldsymbol{x}_{8,4}\},\\ |\Gamma| = 4,\ |\Lambda| = 1,\\ |X_{\gamma_1} \cap G(\boldsymbol{x}_8)| = |\{\boldsymbol{x}_8\}| = 1,\\ \boldsymbol{x}_{8,2} = [(1121)(1211)(2112)(2222)],\\ \boldsymbol{x}_{8,3} = [(1112)(1222)(2121)(2211)],\\ \boldsymbol{x}_{8,4} = [(1122)(1212)(2111)(2221)].\end{gathered}$$

minimal basis for $\mathcal{F}_{\boldsymbol{t}(\boldsymbol{x}_8)}$: 16 kinds of 3 moves.
orbit graphs for $\mathcal{F}_{\boldsymbol{t}(\boldsymbol{x}_8)}$: 3 kinds of dispensable orbit graphs,

$$\begin{aligned}E_{\gamma_2} &= \{(X_{\gamma_1}, X_{\gamma_2}), (X_{\gamma_3}, X_{\gamma_4})\},\\ E_{\gamma_3} &= \{(X_{\gamma_1}, X_{\gamma_3}), (X_{\gamma_2}, X_{\gamma_4})\},\\ E_{\gamma_4} &= \{(X_{\gamma_1}, X_{\gamma_4}), (X_{\gamma_2}, X_{\gamma_3})\},\end{aligned}$$

which correspond to

$$\begin{aligned}\mathcal{B}_{\gamma_2} &= \{\boldsymbol{x}_8 - \boldsymbol{x}_{8,2}, \boldsymbol{x}_{8,3} - \boldsymbol{x}_{8,4}\},\\ \mathcal{B}_{\gamma_3} &= \{\boldsymbol{x}_8 - \boldsymbol{x}_{8,3}, \boldsymbol{x}_{8,2} - \boldsymbol{x}_{8,4}\},\\ \mathcal{B}_{\gamma_4} &= \{\boldsymbol{x}_8 - \boldsymbol{x}_{8,4}, \boldsymbol{x}_{8,2} - \boldsymbol{x}_{8,3}\},\end{aligned}$$

respectively.
invariant minimal basis for $\mathcal{F}_{\boldsymbol{t}(\boldsymbol{x}_8)}$: 3 kinds of 4 moves,

$$\{\mathcal{B}_{\gamma_2}, \mathcal{B}_{\gamma_3}\},\ \{\mathcal{B}_{\gamma_2}, \mathcal{B}_{\gamma_4}\},\ \{\mathcal{B}_{\gamma_3}, \mathcal{B}_{\gamma_4}\}.$$

Models with the independence graph (c)

- Model 12/13/24/34 (graphical model)
  degree of freedom: 7
  indispensable moves: 8 moves of degree 2 with representative elements

  $$\boldsymbol{y}_1,\ \boldsymbol{y}_2 = [(1111)(1221)],$$

  and 8 moves of degree 4 with representative elements $\boldsymbol{x}_3, \boldsymbol{x}_5, \boldsymbol{x}_9, \boldsymbol{x}_{10}$.
  uniqueness: unique minimal basis exists.

Models with the independence graph (d)

- Model 123/34 (graphical, decomposable model)
  degree of freedom: 6
  indispensable moves: 12 moves of degree 2 with representative elements

  $$\boldsymbol{y}_1,\ \boldsymbol{y}_3 = [(1111)(1212)],\ \boldsymbol{y}_4 = [(1111)(2212)].$$

  uniqueness: unique minimal basis exists.

- Model 12/13/23/34

degree of freedom: 7

indispensable moves: 12 moves of degree 2 with representative elements $\boldsymbol{y}_1, \boldsymbol{y}_3, \boldsymbol{y}_4$, and 4 moves of degree 4 with representative elements $\boldsymbol{x}_7, \boldsymbol{x}_{10}$.

uniqueness: unique minimal basis does not exist.

isomorphic structures of reference sets:

$$\mathcal{F}_{G(\boldsymbol{t}(\boldsymbol{x}_{17}))} = \mathcal{F}_{\boldsymbol{t}(\boldsymbol{x}_{17})} \cup \mathcal{F}_{\boldsymbol{t}(\boldsymbol{x}_{18})} \cup \mathcal{F}_{\boldsymbol{t}(\boldsymbol{x}_{19})} \cup \mathcal{F}_{\boldsymbol{t}(\boldsymbol{x}_{20})} = G(\boldsymbol{x}_{17}),$$
$$|G(\boldsymbol{t}(\boldsymbol{x}_{17}))| = 4,\ |\mathcal{F}_{G(\boldsymbol{t}(\boldsymbol{x}_{17}))}/G| = 1,\ |\mathcal{F}_{\boldsymbol{t}(\boldsymbol{x}_{17})}| = 4,$$

$$\mathcal{F}_{\boldsymbol{t}(\boldsymbol{x}_8)} = G(\boldsymbol{x}_8) \cup G(\boldsymbol{x}_9),$$
$$|G(\boldsymbol{t}(\boldsymbol{x}_8))| = 1,\ |\mathcal{F}_{G(\boldsymbol{t}(\boldsymbol{x}_8))}/G| = 2,\ |\mathcal{F}_{\boldsymbol{t}(\boldsymbol{x}_8)}| = 8.$$

direct product structure for $\mathcal{F}_{\boldsymbol{t}(\boldsymbol{x}_{17})}$:

$$\mathcal{F}_{\boldsymbol{t}(\boldsymbol{x}_{17})} = X_{\gamma_1} \cup X_{\gamma_2} = G_{\boldsymbol{t}(\boldsymbol{x}_{17})}(\boldsymbol{x}_{17}),$$
$$X_{\gamma_1} = \{\boldsymbol{x}_{17}, \boldsymbol{x}_{20,3}\},\ X_{\gamma_2} = \{\boldsymbol{x}_{18,2}, \boldsymbol{x}_{19,4}\},$$
$$|\Gamma| = 2,\ |\Lambda| = 1,$$
$$|X_{\gamma_1} \cap G_{\boldsymbol{t}(\boldsymbol{x}_{17})}(\boldsymbol{x}_{17})| = |\{\boldsymbol{x}_{17}, \boldsymbol{x}_{20,3}\}| = 2,$$
$$\boldsymbol{x}_{18,2} = [(1121)(1211)(2112)(2221)],$$
$$\boldsymbol{x}_{19,4} = [(1121)(1212)(2111)(2221)],$$
$$\boldsymbol{x}_{20,3} = [(1112)(1221)(2121)(2211)].$$

direct product structure for $\mathcal{F}_{\boldsymbol{t}(\boldsymbol{x}_8)}$:

$$\mathcal{F}_{\boldsymbol{t}(\boldsymbol{x}_8)} = X_{\gamma_1} \cup X_{\gamma_2} = G_{\boldsymbol{t}(\boldsymbol{x}_8)}(\boldsymbol{x}_8) \cup G_{\boldsymbol{t}(\boldsymbol{x}_8)}(\boldsymbol{x}_9),$$
$$X_{\gamma_1} = \{\boldsymbol{x}_8, \boldsymbol{x}_{8,3}, \boldsymbol{x}_9, \boldsymbol{x}_{9,3}\},\ X_{\gamma_2} = \{\boldsymbol{x}_{8,2}, \boldsymbol{x}_{8,4}, \boldsymbol{x}_{9,2}, \boldsymbol{x}_{9,4}\},$$
$$|\Gamma| = 2,\ |\Lambda| = 2,$$
$$|X_{\gamma_1} \cap G_{\boldsymbol{t}(\boldsymbol{x}_8)}(\boldsymbol{x}_8)| = |\{\boldsymbol{x}_8, \boldsymbol{x}_{8,3}\}| = 2,$$
$$\boldsymbol{x}_{9,2} = [(1121)(1212)(2111)(2222)],$$
$$\boldsymbol{x}_{9,3} = [(1112)(1221)(2122)(2211)],$$
$$\boldsymbol{x}_{9,4} = [(1122)(1211)(2112)(2221)].$$

minimal basis for $\mathcal{F}_{\boldsymbol{t}(\boldsymbol{x}_{17})}$: 4 kinds of 1 move.

minimal basis for $\mathcal{F}_{\boldsymbol{t}(\boldsymbol{x}_8)}$: 16 kinds of 1 move.

orbit graph for $\mathcal{F}_{\boldsymbol{t}(\boldsymbol{x}_{17})}$: unique indispensable orbit graph,

$$\{(X_{\gamma_1}, X_{\gamma_2})\}$$

which either of

$$\mathcal{B}_1 = \{\boldsymbol{x}_{17} - \boldsymbol{x}_{18,2}, \boldsymbol{x}_{20,3} - \boldsymbol{x}_{19,4}\},$$
$$\mathcal{B}_2 = \{\boldsymbol{x}_{17} - \boldsymbol{x}_{19,4}, \boldsymbol{x}_{20,3} - \boldsymbol{x}_{18,2}\}$$

derives.

invariant minimal basis for $\mathcal{F}_{\boldsymbol{t}(\boldsymbol{x}_{17})}$: 2 kinds of 2 moves, $\mathcal{B}_1$ or $\mathcal{B}_2$.

orbit graph for $\mathcal{F}_{\boldsymbol{t}(\boldsymbol{x}_8)}$: unique indispensable orbit graph,

$$\{(X_{\gamma_1}, X_{\gamma_2})\}$$

which either of

$$\begin{gathered}\mathcal{B}_1 = \{\boldsymbol{x}_8 - \boldsymbol{x}_{8,2}, \boldsymbol{x}_{8,3} - \boldsymbol{x}_{8,4}\},\ \mathcal{B}_2 = \{\boldsymbol{x}_8 - \boldsymbol{x}_{8,4}, \boldsymbol{x}_{8,2} - \boldsymbol{x}_{8,3}\},\\ \mathcal{B}_3 = \{\boldsymbol{x}_9 - \boldsymbol{x}_{9,2}, \boldsymbol{x}_{9,3} - \boldsymbol{x}_{9,4}\},\ \mathcal{B}_4 = \{\boldsymbol{x}_9 - \boldsymbol{x}_{9,4}, \boldsymbol{x}_{9,2} - \boldsymbol{x}_{9,3}\},\\ \mathcal{B}_5 = \{\boldsymbol{x}_8 - \boldsymbol{x}_{9,2}, \boldsymbol{x}_8 - \boldsymbol{x}_{9,4}, \boldsymbol{x}_9 - \boldsymbol{x}_{8,2}, \boldsymbol{x}_9 - \boldsymbol{x}_{8,4}, \boldsymbol{x}_{9,3} - \boldsymbol{x}_{8,2}, \boldsymbol{x}_{9,3} - \boldsymbol{x}_{8,4}, \boldsymbol{x}_{8,3} - \boldsymbol{x}_{9,2}, \boldsymbol{x}_{8,3} - \boldsymbol{x}_{9,4}\}\end{gathered}$$

derives.
invariant minimal basis for $\mathcal{F}_{\boldsymbol{t}(\boldsymbol{x}_8)}$: 5 kinds, i.e., 4 kinds of 2 moves, $\mathcal{B}_1, \dots, \mathcal{B}_4$, or 1 kind of 8 moves, $\mathcal{B}_5$.

Models with the independence graph (e)

- Model 123/4 (graphical, decomposable model)
  degree of freedom: 7
  indispensable moves: 28 moves of degree 2 with representative elements

$$\begin{aligned}&\boldsymbol{y}_1,\ \boldsymbol{y}_3,\ \boldsymbol{y}_4,\\ &\boldsymbol{y}_5 = [(1111)(1122)],\ \boldsymbol{y}_6 = [(1111)(1222)],\\ &\boldsymbol{y}_7 = [(1111)(2122)],\ \boldsymbol{y}_8 = [(1111)(2222)].\end{aligned}$$

  uniqueness: unique minimal basis exists.

- Model 12/13/23/4
  degree of freedom: 8
  indispensable moves: 28 moves of degree 2 with representative elements

$$\boldsymbol{y}_1, \boldsymbol{y}_3, \boldsymbol{y}_4, \boldsymbol{y}_5, \boldsymbol{y}_6, \boldsymbol{y}_7, \boldsymbol{y}_8,$$

  and 2 moves of degree 4 with representative element $\boldsymbol{x}_7$.
  uniqueness: unique minimal basis does not exist.
  isomorphic structures of reference sets:

$$\begin{gathered}\mathcal{F}_{G(\boldsymbol{t}(\boldsymbol{x}_{17}))} = \mathcal{F}_{\boldsymbol{t}(\boldsymbol{x}_{17})} \cup \mathcal{F}_{\boldsymbol{t}(\boldsymbol{x}_{19})} = G(\boldsymbol{x}_{17}),\\ |G(\boldsymbol{t}(\boldsymbol{x}_{17}))| = 2,\ |\mathcal{F}_{G(\boldsymbol{t}(\boldsymbol{x}_{17}))}/G| = 1,\ |\mathcal{F}_{\boldsymbol{t}(\boldsymbol{x}_{17})}| = 8,\end{gathered}$$

$$\begin{gathered}\mathcal{F}_{\boldsymbol{t}(\boldsymbol{x}_8)} = G(\boldsymbol{x}_8) \cup G(\boldsymbol{x}_9) \cup G(\boldsymbol{x}_{10}),\\ |G(\boldsymbol{t}(\boldsymbol{x}_8))| = 1,\ |\mathcal{F}_{G(\boldsymbol{t}(\boldsymbol{x}_8))}/G| = 3,\ |\mathcal{F}_{\boldsymbol{t}(\boldsymbol{x}_8)}| = 12.\end{gathered}$$

  direct product structure for $\mathcal{F}_{\boldsymbol{t}(\boldsymbol{x}_{17})}$:

$$\begin{gathered}\mathcal{F}_{\boldsymbol{t}(\boldsymbol{x}_{17})} = X_{\gamma_1} \cup X_{\gamma_2} = G_{\boldsymbol{t}(\boldsymbol{x}_{17})}(\boldsymbol{x}_{17}),\\ X_{\gamma_1} = \{\boldsymbol{x}_{17}, \boldsymbol{x}_{18}, \boldsymbol{x}_{19,3}, \boldsymbol{x}_{20,3}\},\ X_{\gamma_2} = \{\boldsymbol{x}_{17,2}, \boldsymbol{x}_{18,2}, \boldsymbol{x}_{19,4}, \boldsymbol{x}_{20,4}\},\\ |\Gamma| = 2,\ |\Lambda| = 1,\\ |X_{\gamma_1} \cap G_{\boldsymbol{t}(\boldsymbol{x}_{17})}(\boldsymbol{x}_{17})| = |\{\boldsymbol{x}_{17}, \boldsymbol{x}_{18}, \boldsymbol{x}_{19,3}, \boldsymbol{x}_{20,3}\}| = 4,\\ \boldsymbol{x}_{17,2} = [(1121)(1211)(2111)(2222)],\\ \boldsymbol{x}_{19,3} = [(1111)(1222)(2121)(2211)],\\ \boldsymbol{x}_{20,4} = [(1122)(1211)(2111)(2221)].\end{gathered}$$

direct product structure for $\mathcal{F}_{\boldsymbol{t}(\boldsymbol{x}_8)}$:

$$\begin{gathered}
\mathcal{F}_{\boldsymbol{t}(\boldsymbol{x}_8)} = X_{\gamma_1} \cup X_{\gamma_2} = G_{\boldsymbol{t}(\boldsymbol{x}_8)}(\boldsymbol{x}_8) \cup G_{\boldsymbol{t}(\boldsymbol{x}_8)}(\boldsymbol{x}_9) \cup G_{\boldsymbol{t}(\boldsymbol{x}_8)}(\boldsymbol{x}_{10}),\\
X_{\gamma_1} = \{\boldsymbol{x}_8, \boldsymbol{x}_{8,3}, \boldsymbol{x}_9, \boldsymbol{x}_{9,3}, \boldsymbol{x}_{10}, \boldsymbol{x}_{10,3}\},\\
X_{\gamma_2} = \{\boldsymbol{x}_{8,2}, \boldsymbol{x}_{8,4}, \boldsymbol{x}_{9,2}, \boldsymbol{x}_{9,4}, \boldsymbol{x}_{10,2}, \boldsymbol{x}_{10,4}\},\\
|\Gamma| = 2,\ |\Lambda| = 3,\\
|X_{\gamma_1} \cap G_{\boldsymbol{t}(\boldsymbol{x}_8)}(\boldsymbol{x}_8)| = |\{\boldsymbol{x}_8, \boldsymbol{x}_{8,3}\}| = 2,\\
\boldsymbol{x}_{10,2} = [(1122)(1211)(2111)(2222)],\\
\boldsymbol{x}_{10,3} = [(1112)(1221)(2121)(2212)],\\
\boldsymbol{x}_{10,4} = [(1121)(1212)(2112)(2221)].
\end{gathered}$$

minimal basis for $\mathcal{F}_{\boldsymbol{t}(\boldsymbol{x}_{17})}$: 16 kinds of 1 move.
minimal basis for $\mathcal{F}_{\boldsymbol{t}(\boldsymbol{x}_8)}$: 36 kinds of 1 move.
orbit graph for $\mathcal{F}_{\boldsymbol{t}(\boldsymbol{x}_{17})}$: unique indispensable orbit graph,

$$\{(X_{\gamma_1}, X_{\gamma_2})\}$$

which either of

$$\begin{gathered}
\mathcal{B}_1 = \{\boldsymbol{x}_{20,3} - \boldsymbol{x}_{20,4}, \boldsymbol{x}_{19,3} - \boldsymbol{x}_{19,4}, \boldsymbol{x}_{18} - \boldsymbol{x}_{18,2}, \boldsymbol{x}_{17} - \boldsymbol{x}_{17,2}\},\\
\mathcal{B}_2 = \{\boldsymbol{x}_{20,3} - \boldsymbol{x}_{18,2}, \boldsymbol{x}_{19,3} - \boldsymbol{x}_{17,2}, \boldsymbol{x}_{18} - \boldsymbol{x}_{20,4}, \boldsymbol{x}_{17} - \boldsymbol{x}_{19,4}\},\\
\mathcal{B}_3 = \{\boldsymbol{x}_{20,3} - \boldsymbol{x}_{19,4}, \boldsymbol{x}_{19,3} - \boldsymbol{x}_{20,4}, \boldsymbol{x}_{18} - \boldsymbol{x}_{17,2}, \boldsymbol{x}_{17} - \boldsymbol{x}_{18,2}\},\\
\mathcal{B}_4 = \{\boldsymbol{x}_{20,3} - \boldsymbol{x}_{17,2}, \boldsymbol{x}_{19,3} - \boldsymbol{x}_{18,2}, \boldsymbol{x}_{18} - \boldsymbol{x}_{19,4}, \boldsymbol{x}_{17} - \boldsymbol{x}_{20,4}\}
\end{gathered}$$

derives.
invariant minimal basis for $\mathcal{F}_{\boldsymbol{t}(\boldsymbol{x}_{17})}$: 4 kinds of 4 moves, $\mathcal{B}_1, \ldots, \mathcal{B}_4$.
orbit graph for $\mathcal{F}_{\boldsymbol{t}(\boldsymbol{x}_8)}$: unique indispensable orbit graph,

$$\{(X_{\gamma_1}, X_{\gamma_2})\}$$

which either of

$$\begin{gathered}
\mathcal{B}_1 = \{\boldsymbol{x}_8 - \boldsymbol{x}_{8,2}, \boldsymbol{x}_{8,3} - \boldsymbol{x}_{8,4}\},\ \mathcal{B}_2 = \{\boldsymbol{x}_8 - \boldsymbol{x}_{8,4}, \boldsymbol{x}_{8,3} - \boldsymbol{x}_{8,2}\},\\
\mathcal{B}_3 = \{\boldsymbol{x}_9 - \boldsymbol{x}_{9,2}, \boldsymbol{x}_{9,3} - \boldsymbol{x}_{9,4}\},\ \mathcal{B}_4 = \{\boldsymbol{x}_9 - \boldsymbol{x}_{9,4}, \boldsymbol{x}_{9,3} - \boldsymbol{x}_{9,2}\},\\
\mathcal{B}_5 = \{\boldsymbol{x}_{10} - \boldsymbol{x}_{10,2}, \boldsymbol{x}_{10,3} - \boldsymbol{x}_{10,4}\},\ \mathcal{B}_6 = \{\boldsymbol{x}_{10} - \boldsymbol{x}_{10,4}, \boldsymbol{x}_{10,3} - \boldsymbol{x}_{10,2}\},\\
\mathcal{B}_7 = \{\boldsymbol{x}_8 - \boldsymbol{x}_{9,2}, \boldsymbol{x}_8 - \boldsymbol{x}_{9,4}, \boldsymbol{x}_{8,3} - \boldsymbol{x}_{9,2}, \boldsymbol{x}_{8,3} - \boldsymbol{x}_{9,4},\\
\boldsymbol{x}_9 - \boldsymbol{x}_{8,2}, \boldsymbol{x}_9 - \boldsymbol{x}_{8,4}, \boldsymbol{x}_{9,3} - \boldsymbol{x}_{8,2}, \boldsymbol{x}_{9,3} - \boldsymbol{x}_{8,4}\},\\
\mathcal{B}_8 = \{\boldsymbol{x}_8 - \boldsymbol{x}_{10,2}, \boldsymbol{x}_8 - \boldsymbol{x}_{10,4}, \boldsymbol{x}_{8,3} - \boldsymbol{x}_{10,2}, \boldsymbol{x}_{8,3} - \boldsymbol{x}_{10,4},\\
\boldsymbol{x}_{10} - \boldsymbol{x}_{8,2}, \boldsymbol{x}_{10} - \boldsymbol{x}_{8,4}, \boldsymbol{x}_{10,3} - \boldsymbol{x}_{8,2}, \boldsymbol{x}_{10,3} - \boldsymbol{x}_{8,4}\},\\
\mathcal{B}_9 = \{\boldsymbol{x}_9 - \boldsymbol{x}_{10,2}, \boldsymbol{x}_9 - \boldsymbol{x}_{10,4}, \boldsymbol{x}_{9,3} - \boldsymbol{x}_{10,2}, \boldsymbol{x}_{9,3} - \boldsymbol{x}_{10,4},\\
\boldsymbol{x}_{10} - \boldsymbol{x}_{9,2}, \boldsymbol{x}_{10} - \boldsymbol{x}_{9,4}, \boldsymbol{x}_{10,3} - \boldsymbol{x}_{9,2}, \boldsymbol{x}_{10,3} - \boldsymbol{x}_{9,4}\}
\end{gathered}$$

derives.
invariant minimal basis for $\mathcal{F}_{\boldsymbol{t}(\boldsymbol{x}_8)}$: 9 kinds, i.e., 6 kinds of 2 moves, $\mathcal{B}_1, \ldots, \mathcal{B}_6$, or 3 kinds of 8 moves, $\mathcal{B}_7, \ldots, \mathcal{B}_9$.

Models with the independence graph (f)

- Model 123/4 (graphical, decomposable model)
  degree of freedom: 8
  indispensable moves: 20 moves of degree 2 with representative elements $\boldsymbol{y}_1, \boldsymbol{y}_2, \boldsymbol{y}_5, \boldsymbol{y}_6, \boldsymbol{y}_7$.
  uniqueness: unique minimal basis exists.

Models with the independence graph (g)

- Model 12/13/14 (graphical, decomposable model)
  degree of freedom: 8
  indispensable moves: 12 moves of degree 2 with representative elements $\boldsymbol{y}_2, \boldsymbol{y}_3, \boldsymbol{y}_5$.
  uniqueness: unique minimal basis does not exist.
  isomorphic structures of reference sets:

$$\mathcal{F}_{G(\boldsymbol{t}(\boldsymbol{y}_6))} = \mathcal{F}_{\boldsymbol{t}(\boldsymbol{y}_6)} \cup \mathcal{F}_{\boldsymbol{t}(\boldsymbol{y}'_6)} = G(\boldsymbol{y}_6),$$
$$|G(\boldsymbol{t}(\boldsymbol{y}_6))| = 2,\ |\mathcal{F}_{G(\boldsymbol{t}(\boldsymbol{y}_6))}/G| = 1,\ |\mathcal{F}_{\boldsymbol{t}(\boldsymbol{y}_6)}| = 4,$$
$$\boldsymbol{y}'_6 = [(2111)(2222)].$$

  direct product structure for $\mathcal{F}_{\boldsymbol{t}(\boldsymbol{y}_6)}$:

$$\mathcal{F}_{\boldsymbol{t}(\boldsymbol{y}_6)} = X_{\gamma_1} \cup X_{\gamma_2} \cup X_{\gamma_3} \cup X_{\gamma_4} = G_{\boldsymbol{t}(\boldsymbol{y}_6)}(\boldsymbol{y}_6),$$
$$X_{\gamma_1} = \{\boldsymbol{y}_6\},\ X_{\gamma_2} = \{\boldsymbol{y}_{6,2}\},\ X_{\gamma_3} = \{\boldsymbol{y}_{6,3}\},\ X_{\gamma_4} = \{\boldsymbol{y}_{6,4}\},$$
$$|\Gamma| = 4,\ |\Lambda| = 1,$$
$$|X_{\gamma_1} \cap G_{\boldsymbol{t}(\boldsymbol{y}_6)}(\boldsymbol{y}_6)| = |\{\boldsymbol{y}_6\}| = 1,$$
$$\boldsymbol{y}_{6,2} = [(1112)(1221)],$$
$$\boldsymbol{y}_{6,3} = [(1121)(1212)],$$
$$\boldsymbol{y}_{6,4} = [(1122)(1211)].$$

  minimal basis for $\mathcal{F}_{\boldsymbol{t}(\boldsymbol{y}_6)}$: 16 kinds of 3 moves.
  orbit graphs for $\mathcal{F}_{\boldsymbol{t}(\boldsymbol{y}_6)}$: 3 kinds of dispensable orbit graphs,

$$E_{\gamma_2} = \{(X_{\gamma_1}, X_{\gamma_2}), (X_{\gamma_3}, X_{\gamma_4})\},$$
$$E_{\gamma_3} = \{(X_{\gamma_1}, X_{\gamma_3}), (X_{\gamma_2}, X_{\gamma_4})\},$$
$$E_{\gamma_4} = \{(X_{\gamma_1}, X_{\gamma_4}), (X_{\gamma_2}, X_{\gamma_3})\},$$

  which correspond to

$$\mathcal{B}_{\gamma_2} = \{\boldsymbol{y}_6 - \boldsymbol{y}_{6,2}, \boldsymbol{y}_{6,3} - \boldsymbol{y}_{6,4}\},$$
$$\mathcal{B}_{\gamma_3} = \{\boldsymbol{y}_6 - \boldsymbol{y}_{6,3}, \boldsymbol{y}_{6,2} - \boldsymbol{y}_{6,4}\},$$
$$\mathcal{B}_{\gamma_4} = \{\boldsymbol{y}_6 - \boldsymbol{y}_{6,4}, \boldsymbol{y}_{6,2} - \boldsymbol{y}_{6,3}\},$$

  respectively.
  invariant minimal basis for $\mathcal{F}_{\boldsymbol{t}(\boldsymbol{y}_6)}$: 3 kinds of 4 moves,

$$\{\mathcal{B}_{\gamma_2}, \mathcal{B}_{\gamma_3}\},\ \{\mathcal{B}_{\gamma_2}, \mathcal{B}_{\gamma_4}\},\ \{\mathcal{B}_{\gamma_3}, \mathcal{B}_{\gamma_4}\}.$$

Models with the independence graph (h)

- Model 12/13/4 (graphical, decomposable model)
  degree of freedom: 9
  indispensable moves: 28 moves of degree 2 with representative elements

$$\boldsymbol{y}_1, \boldsymbol{y}_2, \boldsymbol{y}_3, \boldsymbol{y}_4, \boldsymbol{y}_5, \boldsymbol{y}_7, \boldsymbol{y}_8.$$

  uniqueness: unique minimal basis does not exist.
  isomorphic structures of reference sets:

$$\mathcal{F}_{G(\boldsymbol{t}(\boldsymbol{y}_6))} = \mathcal{F}_{\boldsymbol{t}(\boldsymbol{y}_6)} \cup \mathcal{F}_{\boldsymbol{t}(\boldsymbol{y}'_6)} = G(\boldsymbol{y}_6),$$
$$|G(\boldsymbol{t}(\boldsymbol{y}_6))| = 2,\ |\mathcal{F}_{G(\boldsymbol{t}(\boldsymbol{y}_6))}/G| = 1,\ |\mathcal{F}_{\boldsymbol{t}(\boldsymbol{y}_6)}| = 4.$$

direct product structure for $\mathcal{F}_{\boldsymbol{t}(\boldsymbol{y}_6)}$: same as model 12/13/14.
minimal basis for $\mathcal{F}_{\boldsymbol{t}(\boldsymbol{y}_6)}$: 16 kinds of 3 moves.
orbit graphs for $\mathcal{F}_{\boldsymbol{t}(\boldsymbol{y}_6)}$: 3 kinds of dispensable orbit graphs (same as model 12/13/14).
invariant minimal basis for $\mathcal{F}_{\boldsymbol{t}(\boldsymbol{y}_6)}$: 3 kinds of 4 moves (same as model 12/13/14).

Models with the independence graph (i)

- Model 12/34 (graphical, decomposable model)
  degree of freedom: 9
  indispensable moves: 36 moves of degree 2 with representative elements

$$\begin{gathered}\boldsymbol{y}_1,\ \boldsymbol{y}_2,\ \boldsymbol{y}_3,\ \boldsymbol{y}_4,\ \boldsymbol{y}_6,\ \boldsymbol{y}_7,\ \boldsymbol{y}_8,\\ \boldsymbol{y}_9 = [(1111)(2121)],\ \boldsymbol{y}_{10} = [(1111)(2221)].\end{gathered}$$

  uniqueness: unique minimal basis exists.

Models with the independence graph (j)

- Model 12/3/4 (graphical, decomposable model)
  degree of freedom: 10
  indispensable moves: 28 moves of degree 2 with representative elements

$$\boldsymbol{y}_1, \boldsymbol{y}_2, \boldsymbol{y}_3, \boldsymbol{y}_4, \boldsymbol{y}_5, \boldsymbol{y}_9, \boldsymbol{y}_{10}.$$

  uniqueness: unique minimal basis does not exist.
  isomorphic structures of reference sets:

$$\begin{gathered}\mathcal{F}_{G(\boldsymbol{t}(\boldsymbol{y}_6))} = \mathcal{F}_{\boldsymbol{t}(\boldsymbol{y}_6)} \cup \mathcal{F}_{\boldsymbol{t}(\boldsymbol{y}'_6)} = G(\boldsymbol{y}_6),\\ |G(\boldsymbol{t}(\boldsymbol{y}_6))| = 2,\ |\mathcal{F}_{G(\boldsymbol{t}(\boldsymbol{y}_6))}/G| = 1,\ |\mathcal{F}_{\boldsymbol{t}(\boldsymbol{y}_6)}| = 4,\\ \mathcal{F}_{G(\boldsymbol{t}(\boldsymbol{y}_7))} = \mathcal{F}_{\boldsymbol{t}(\boldsymbol{y}_7)} \cup \mathcal{F}_{\boldsymbol{t}(\boldsymbol{y}'_7)} = G(\boldsymbol{y}_7),\\ |G(\boldsymbol{t}(\boldsymbol{y}_7))| = 2,\ |\mathcal{F}_{G(\boldsymbol{t}(\boldsymbol{y}_7))}/G| = 1,\ |\mathcal{F}_{\boldsymbol{t}(\boldsymbol{y}_7)}| = 4,\\ \boldsymbol{y}'_7 = [(1211)(2222)],\\ \mathcal{F}_{G(\boldsymbol{t}(\boldsymbol{y}_8))} = \mathcal{F}_{\boldsymbol{t}(\boldsymbol{y}_8)} \cup \mathcal{F}_{\boldsymbol{t}(\boldsymbol{y}'_8)} = G(\boldsymbol{y}_8),\\ |G(\boldsymbol{t}(\boldsymbol{y}_8))| = 2,\ |\mathcal{F}_{G(\boldsymbol{t}(\boldsymbol{y}_8))}/G| = 1,\ |\mathcal{F}_{\boldsymbol{t}(\boldsymbol{y}_8)}| = 4,\\ \boldsymbol{y}'_8 = [(1211)(2122)].\end{gathered}$$

  direct product structure for $\mathcal{F}_{\boldsymbol{t}(\boldsymbol{y}_6)}$: same as model 12/13/14.
  direct product structure for $\mathcal{F}_{\boldsymbol{t}(\boldsymbol{y}_7)}$:

$$\begin{gathered}\mathcal{F}_{\boldsymbol{t}(\boldsymbol{y}_7)} = X_{\gamma_1} \cup X_{\gamma_2} \cup X_{\gamma_3} \cup X_{\gamma_4} = G_{\boldsymbol{t}(\boldsymbol{y}_7)}(\boldsymbol{y}_7),\\ X_{\gamma_1} = \{\boldsymbol{y}_7\},\ X_{\gamma_2} = \{\boldsymbol{y}_{7,2}\},\ X_{\gamma_3} = \{\boldsymbol{y}_{7,3}\},\ X_{\gamma_4} = \{\boldsymbol{y}_{7,4}\},\\ |\Gamma| = 4,\ |\Lambda| = 1,\\ |X_{\gamma_1} \cap G_{\boldsymbol{t}(\boldsymbol{y}_7)}(\boldsymbol{y}_7)| = |\{\boldsymbol{y}_7\}| = 1,\\ \boldsymbol{y}_{7,2} = [(1112)(2121)],\\ \boldsymbol{y}_{7,3} = [(1121)(2112)],\\ \boldsymbol{y}_{7,4} = [(1122)(2111)].\end{gathered}$$

direct product structure for $\mathcal{F}_{\boldsymbol{t}(\boldsymbol{y}_8)}$:

$$\begin{gathered}
\mathcal{F}_{\boldsymbol{t}(\boldsymbol{y}_8)} = X_{\gamma_1} \cup X_{\gamma_2} \cup X_{\gamma_3} \cup X_{\gamma_4} = G_{\boldsymbol{t}(\boldsymbol{y}_8)}(\boldsymbol{y}_8), \\
X_{\gamma_1} = \{\boldsymbol{y}_8\},\ X_{\gamma_2} = \{\boldsymbol{y}_{8,2}\},\ X_{\gamma_3} = \{\boldsymbol{y}_{8,3}\},\ X_{\gamma_4} = \{\boldsymbol{y}_{8,4}\}, \\
|\Gamma| = 4,\ |\Lambda| = 1, \\
|X_{\gamma_1} \cap G_{\boldsymbol{t}(\boldsymbol{y}_8)}(\boldsymbol{y}_8)| = |\{\boldsymbol{y}_8\}| = 1, \\
\boldsymbol{y}_{8,2} = [(1112)(2221)], \\
\boldsymbol{y}_{8,3} = [(1121)(2212)], \\
\boldsymbol{y}_{8,4} = [(1122)(2211)].
\end{gathered}$$

minimal basis for $\mathcal{F}_{\boldsymbol{t}(\boldsymbol{y}_6)}, \mathcal{F}_{\boldsymbol{t}(\boldsymbol{y}_7)}, \mathcal{F}_{\boldsymbol{t}(\boldsymbol{y}_8)}$: 16 kinds of 3 moves, respectively.
orbit graphs for $\mathcal{F}_{\boldsymbol{t}(\boldsymbol{y}_6)}, \mathcal{F}_{\boldsymbol{t}(\boldsymbol{y}_7)}, \mathcal{F}_{\boldsymbol{t}(\boldsymbol{y}_8)}$: 3 kinds of dispensable orbit graphs, respectively (same as model 12/13/14).
invariant minimal basis for $\mathcal{F}_{\boldsymbol{t}(\boldsymbol{y}_6)}, \mathcal{F}_{\boldsymbol{t}(\boldsymbol{y}_7)}, \mathcal{F}_{\boldsymbol{t}(\boldsymbol{y}_8)}$: 3 kinds of 4 moves, respectively (same as model 12/13/14).

Models with the independence graph (k)

- Model 12/3/4 (graphical, decomposable model)
  degree of freedom: 11
  indispensable moves: 24 moves of degree 2 with representative elements

$$\boldsymbol{y}_1,\ \boldsymbol{y}_2,\ \boldsymbol{y}_3,\ \boldsymbol{y}_5,\ \boldsymbol{y}_9,\ \boldsymbol{y}_{11} = [(1111)(2211)].$$

  uniqueness: unique minimal basis does not exist.
  isomorphic structures of reference sets:

$$\begin{gathered}
\mathcal{F}_{G(\boldsymbol{t}(\boldsymbol{y}_4))} = \mathcal{F}_{\boldsymbol{t}(\boldsymbol{y}_4)} \cup \mathcal{F}_{\boldsymbol{t}(\boldsymbol{y}'_4)} = G(\boldsymbol{y}_4), \\
|G(\boldsymbol{t}(\boldsymbol{y}_4))| = 2,\ |\mathcal{F}_{G(\boldsymbol{t}(\boldsymbol{y}_4))}/G| = 1,\ |\mathcal{F}_{\boldsymbol{t}(\boldsymbol{y}_4)}| = 4, \\
\boldsymbol{y}'_4 = [(1121)(2222)], \\
\mathcal{F}_{G(\boldsymbol{t}(\boldsymbol{y}_6))} = \mathcal{F}_{\boldsymbol{t}(\boldsymbol{y}_6)} \cup \mathcal{F}_{\boldsymbol{t}(\boldsymbol{y}'_6)} = G(\boldsymbol{y}_6), \\
|G(\boldsymbol{t}(\boldsymbol{y}_6))| = 2,\ |\mathcal{F}_{G(\boldsymbol{t}(\boldsymbol{y}_6))}/G| = 1,\ |\mathcal{F}_{\boldsymbol{t}(\boldsymbol{y}_6)}| = 4, \\
\mathcal{F}_{G(\boldsymbol{t}(\boldsymbol{y}_7))} = \mathcal{F}_{\boldsymbol{t}(\boldsymbol{y}_7)} \cup \mathcal{F}_{\boldsymbol{t}(\boldsymbol{y}'_7)} = G(\boldsymbol{y}_7), \\
|G(\boldsymbol{t}(\boldsymbol{y}_7))| = 2,\ |\mathcal{F}_{G(\boldsymbol{t}(\boldsymbol{y}_7))}/G| = 1,\ |\mathcal{F}_{\boldsymbol{t}(\boldsymbol{y}_7)}| = 4, \\
\mathcal{F}_{G(\boldsymbol{t}(\boldsymbol{y}_{10}))} = \mathcal{F}_{\boldsymbol{t}(\boldsymbol{y}_{10})} \cup \mathcal{F}_{\boldsymbol{t}(\boldsymbol{y}'_{10})} = G(\boldsymbol{y}_{10}), \\
|G(\boldsymbol{t}(\boldsymbol{y}_{10}))| = 2,\ |\mathcal{F}_{G(\boldsymbol{t}(\boldsymbol{y}_{10}))}/G| = 1,\ |\mathcal{F}_{\boldsymbol{t}(\boldsymbol{y}_{10})}| = 4, \\
\boldsymbol{y}'_{10} = [(1112)(2222)],
\end{gathered}$$

$$\begin{gathered}
\mathcal{F}_{\boldsymbol{t}(\boldsymbol{y}_8)} = G(\boldsymbol{y}_8), \\
|G(\boldsymbol{t}(\boldsymbol{y}_8))| = 1,\ |\mathcal{F}_{G(\boldsymbol{t}(\boldsymbol{y}_8))}/G| = 1,\ |\mathcal{F}_{\boldsymbol{t}(\boldsymbol{y}_8)}| = 8.
\end{gathered}$$

  direct product structure for $\mathcal{F}_{\boldsymbol{t}(\boldsymbol{y}_4)}$:

$$\begin{gathered}
\mathcal{F}_{\boldsymbol{t}(\boldsymbol{y}_4)} = X_{\gamma_1} \cup X_{\gamma_2} \cup X_{\gamma_3} \cup X_{\gamma_4} = G_{\boldsymbol{t}(\boldsymbol{y}_4)}(\boldsymbol{y}_4), \\
X_{\gamma_1} = \{\boldsymbol{y}_4\},\ X_{\gamma_2} = \{\boldsymbol{y}_{4,2}\},\ X_{\gamma_3} = \{\boldsymbol{y}_{4,3}\},\ X_{\gamma_4} = \{\boldsymbol{y}_{4,4}\}, \\
|\Gamma| = 4,\ |\Lambda| = 1, \\
|X_{\gamma_1} \cap G_{\boldsymbol{t}(\boldsymbol{y}_4)}(\boldsymbol{y}_4)| = |\{\boldsymbol{y}_4\}| = 1, \\
\boldsymbol{y}_{4,2} = [(1112)(2211)], \\
\boldsymbol{y}_{4,3} = [(1211)(2112)], \\
\boldsymbol{y}_{4,4} = [(1212)(2111)].
\end{gathered}$$

direct product structure for $\mathcal{F}_{\boldsymbol{t}(\boldsymbol{y}_6)}$: same as model 12/13/14.
direct product structure for $\mathcal{F}_{\boldsymbol{t}(\boldsymbol{y}_7)}$: same as model 12/3/4.
direct product structure for $\mathcal{F}_{\boldsymbol{t}(\boldsymbol{y}_{10})}$:

$$\begin{gathered}
\mathcal{F}_{\boldsymbol{t}(\boldsymbol{y}_{10})} = X_{\gamma_1} \cup X_{\gamma_2} \cup X_{\gamma_3} \cup X_{\gamma_4} = G_{\boldsymbol{t}(\boldsymbol{y}_{10})}(\boldsymbol{y}_{10}), \\
X_{\gamma_1} = \{\boldsymbol{y}_{10}\},\ X_{\gamma_2} = \{\boldsymbol{y}_{10,2}\},\ X_{\gamma_3} = \{\boldsymbol{y}_{10,3}\},\ X_{\gamma_4} = \{\boldsymbol{y}_{10,4}\}, \\
|\Gamma| = 4,\ |\Lambda| = 1, \\
|X_{\gamma_1} \cap G_{\boldsymbol{t}(\boldsymbol{y}_{10})}(\boldsymbol{y}_{10})| = |\{\boldsymbol{y}_{10}\}| = 1, \\
\boldsymbol{y}_{10,2} = [(1121)(2211)], \\
\boldsymbol{y}_{10,3} = [(1211)(2121)], \\
\boldsymbol{y}_{10,4} = [(1221)(2111)].
\end{gathered}$$

direct product structure for $\mathcal{F}_{\boldsymbol{t}(\boldsymbol{y}_8)}$:

$$\begin{gathered}
\mathcal{F}_{\boldsymbol{t}(\boldsymbol{y}_8)} = X_{\gamma_1} \cup X_{\gamma_2} \cup X_{\gamma_3} \cup X_{\gamma_4} \cup X_{\gamma_5} \cup X_{\gamma_6} \cup X_{\gamma_7} \cup X_{\gamma_8} = G_{\boldsymbol{t}(\boldsymbol{y}_8)}(\boldsymbol{y}_8), \\
X_{\gamma_1} = \{\boldsymbol{y}_8\},\ X_{\gamma_2} = \{\boldsymbol{y}_{8,2}\},\ X_{\gamma_3} = \{\boldsymbol{y}_{8,3}\},\ X_{\gamma_4} = \{\boldsymbol{y}_{8,4}\}, \\
X_{\gamma_5} = \{\boldsymbol{y}_{8,5}\},\ X_{\gamma_6} = \{\boldsymbol{y}_{8,6}\},\ X_{\gamma_7} = \{\boldsymbol{y}_{8,7}\},\ X_{\gamma_8} = \{\boldsymbol{y}_{8,8}\}, \\
|\Gamma| = 8,\ |\Lambda| = 1, \\
|X_{\gamma_1} \cap G_{\boldsymbol{t}(\boldsymbol{y}_8)}(\boldsymbol{y}_8)| = |\{\boldsymbol{y}_8\}| = 1, \\
\boldsymbol{y}_{8,2} = [(1112)(2221)], \\
\boldsymbol{y}_{8,3} = [(1121)(2212)], \\
\boldsymbol{y}_{8,4} = [(1122)(2211)], \\
\boldsymbol{y}_{8,5} = [(1211)(2122)], \\
\boldsymbol{y}_{8,6} = [(1212)(2121)], \\
\boldsymbol{y}_{8,7} = [(1221)(2112)], \\
\boldsymbol{y}_{8,8} = [(1222)(2111)].
\end{gathered}$$

minimal basis for $\mathcal{F}_{\boldsymbol{t}(\boldsymbol{y}_4)}, \mathcal{F}_{\boldsymbol{t}(\boldsymbol{y}_6)}, \mathcal{F}_{\boldsymbol{t}(\boldsymbol{y}_7)}, \mathcal{F}_{\boldsymbol{t}(\boldsymbol{y}_{10})}$: 16 kinds of 3 moves, respectively.
minimal basis for $\mathcal{F}_{\boldsymbol{t}(\boldsymbol{y}_8)}$: $8^{8-2} = 262144$ kinds of 7 moves.
orbit graphs for $\mathcal{F}_{\boldsymbol{t}(\boldsymbol{y}_4)}, \mathcal{F}_{\boldsymbol{t}(\boldsymbol{y}_6)}, \mathcal{F}_{\boldsymbol{t}(\boldsymbol{y}_7)}, \mathcal{F}_{\boldsymbol{t}(\boldsymbol{y}_{10})}$: 3 kinds of dispensable orbit graphs, respectively (same as model 12/13/14).
invariant minimal basis for $\mathcal{F}_{\boldsymbol{t}(\boldsymbol{y}_4)}, \mathcal{F}_{\boldsymbol{t}(\boldsymbol{y}_6)}, \mathcal{F}_{\boldsymbol{t}(\boldsymbol{y}_7)}, \mathcal{F}_{\boldsymbol{t}(\boldsymbol{y}_{10})}$: 3 kinds of 4 moves, respectively (same as model 12/13/14).
orbit graphs for $\mathcal{F}_{\boldsymbol{t}(\boldsymbol{y}_8)}$: 7 kinds of dispensable orbit graphs,

$$\begin{aligned}
E_{\gamma_2} &= \{(X_{\gamma_1}, X_{\gamma_2}), (X_{\gamma_3}, X_{\gamma_4}), (X_{\gamma_5}, X_{\gamma_6}), (X_{\gamma_7}, X_{\gamma_8})\}, \\
E_{\gamma_3} &= \{(X_{\gamma_1}, X_{\gamma_3}), (X_{\gamma_2}, X_{\gamma_4}), (X_{\gamma_5}, X_{\gamma_7}), (X_{\gamma_6}, X_{\gamma_8})\}, \\
E_{\gamma_4} &= \{(X_{\gamma_1}, X_{\gamma_4}), (X_{\gamma_2}, X_{\gamma_3}), (X_{\gamma_5}, X_{\gamma_8}), (X_{\gamma_6}, X_{\gamma_7})\}, \\
E_{\gamma_5} &= \{(X_{\gamma_1}, X_{\gamma_5}), (X_{\gamma_2}, X_{\gamma_6}), (X_{\gamma_3}, X_{\gamma_7}), (X_{\gamma_4}, X_{\gamma_8})\}, \\
E_{\gamma_6} &= \{(X_{\gamma_1}, X_{\gamma_6}), (X_{\gamma_2}, X_{\gamma_5}), (X_{\gamma_3}, X_{\gamma_8}), (X_{\gamma_4}, X_{\gamma_7})\}, \\
E_{\gamma_7} &= \{(X_{\gamma_1}, X_{\gamma_7}), (X_{\gamma_2}, X_{\gamma_8}), (X_{\gamma_3}, X_{\gamma_5}), (X_{\gamma_4}, X_{\gamma_6})\}, \\
E_{\gamma_8} &= \{(X_{\gamma_1}, X_{\gamma_8}), (X_{\gamma_2}, X_{\gamma_7}), (X_{\gamma_3}, X_{\gamma_6}), (X_{\gamma_4}, X_{\gamma_5})\},
\end{aligned}$$

which correspond to $\mathcal{B}_{\gamma_2}, \ldots, \mathcal{B}_{\gamma_8}$, respectively.
invariant minimal basis for $\mathcal{F}_{\boldsymbol{t}(\boldsymbol{y}_8)}$: 7 kinds of 12 moves,

$$\begin{gathered}
\{\mathcal{B}_{\gamma_2}, \mathcal{B}_{\gamma_3}, \mathcal{B}_{\gamma_4}\},\ \{\mathcal{B}_{\gamma_2}, \mathcal{B}_{\gamma_5}, \mathcal{B}_{\gamma_6}\},\ \{\mathcal{B}_{\gamma_2}, \mathcal{B}_{\gamma_7}, \mathcal{B}_{\gamma_8}\},\ \{\mathcal{B}_{\gamma_3}, \mathcal{B}_{\gamma_5}, \mathcal{B}_{\gamma_7}\}, \\
\{\mathcal{B}_{\gamma_3}, \mathcal{B}_{\gamma_6}, \mathcal{B}_{\gamma_8}\},\ \{\mathcal{B}_{\gamma_4}, \mathcal{B}_{\gamma_5}, \mathcal{B}_{\gamma_8}\},\ \{\mathcal{B}_{\gamma_4}, \mathcal{B}_{\gamma_6}, \mathcal{B}_{\gamma_7}\}.
\end{gathered}$$

3.6.4 Discussion

In this section we define an invariant minimal Markov basis and derive its basic characteristics. Of course, we can construct an invariant Markov basis from any Markov basis as the union of all orbits of the basis elements. However, even if we start with a minimal Markov basis, the union of all orbits of the basis elements is not necessarily an invariant minimal basis. For example, consider again the complete independence model of the three-way case of Example 3.6.11. A set of moves

$$\{\boldsymbol{x}_8 - \boldsymbol{x}_8',\ \boldsymbol{x}_8 - \boldsymbol{x}_8'',\ \boldsymbol{x}_8 - \boldsymbol{x}_8'''\}$$

connects the four elements $\boldsymbol{x}_8, \boldsymbol{x}_8', \boldsymbol{x}_8'', \boldsymbol{x}_8'''$ into a tree, and thus is a minimal basis elements for $\{\boldsymbol{x}_8, \boldsymbol{x}_8', \boldsymbol{x}_8'', \boldsymbol{x}_8'''\}$. However, it is seen that the union of the orbits of these three moves contains 6 moves, and hence not minimal invariant. From these considerations, structure of an invariant minimal Markov basis is important.

Theorem 3.6.1 states how to construct an invariant minimal Markov basis. This theorem is an extension of Theorem 3.5.1. To construct a minimal Markov basis, we can add basis elements step by step from low degree, by considering all reference sets as stated in Theorem 3.5.1. On the other hand, to construct an invariant minimal Markov basis, we have to add the orbit of moves step by step from low degree. Similar to the construction of a minimal Markov basis, it is difficult to construct an invariant minimal Markov basis by applying Theorem 3.6.1 directly. But if a minimal Markov basis is available, we can construct an invariant minimal Markov basis relatively easily, by considering all the reference sets one by one, which is covered by the dispensable moves in the minimal Markov basis. The results of Section 3.6.3 is obtained in such a way.

It seems also difficult to give a simple necessary and sufficient conditions on $D_1, \ldots, D_r$ such that an invariant minimal Markov basis is unique. It is of interest to derive conditions such that an invariant minimal Markov basis is unique even if a minimal Markov basis is not unique. As stated in Section 3.6.2, such an example we have found so far is the obvious one-way contingency table, except for the peculiar case of the Hardy-Weinberg model.

Chapter 4

Concluding remarks

This thesis focuses on the conditional inference for contingency tables. To compute the conditional expectation expressed as (1.3), two approaches, i.e., exact methods (Chapter 2) and Markov chain Monte Carlo methods (Chapter 3), are treated in this thesis. Each chapter includes several sections, which contain their own discussion parts, respectively. In this final chapter, we give some additional remarks.

In exact methods part, we have considered two topics of computing exact p values by the network algorithms. In both topics, the test statistic that we have treated is the Freeman-Halton exact test statistic, which are sometimes known as the generalized Fisher's exact test statistic. Of course, this is not the only statistic which the network algorithm can be adapted. For example, the likelihood ratio statistic and the Pearson χ^2 statistic, which we consider in Section 2.2.5, are also commonly used measures. To compute the exact p values for these test statistics, different optimization problems must be solved to evaluate bounds of LP and SP for each measure. If these bounds can be evaluated in efficient ways, the network algorithm also becomes a valuable tool for these test statistics. Note that the LP and SP can be calculated exactly by a dynamic programming in a single backward pass through the network, regardless of the test statistic. Whether this technique is feasible or not relies on the number of nodes in the network. In addition, some techniques of the discrete convex analysis can be used. See Section 10 of Murota (2003), for example.

Conversely, our idea of evaluating an approximate optimal solution of LP as the value at the maximum likelihood estimator can be applied to any Freeman-Halton type exact test statistic in calculating exact p value by the network algorithm, regardless of the model that we consider. Then for Freeman-Halton type exact test statistics, we only have to consider the evaluation of SP to adapt the network algorithm. The problem of Hardy-Weinberg exact test in Section 2.2 is an ideal problem to adapt the network algorithm since the closed form expression of the optimal solution of SP can be derived.

In the network representation of the reference set of all the two-way tables having the same row and column sums in Section 2.1, each arc expresses the fixed values of each column. Similarly, in the network representation of the reference set of all the genotype frequencies having the same allele counts in Section 2.2, each arc expresses the fixed value of each allele count. These correspondences, which completely characterize the structure of each network, are not the only ways. For example, if each cell count is fixed step by step, another network representation of the reference set can be derived. The choice of the network representations has to depend on several factors, such as, the number of nodes, whether the set of next nodes which are connected to the current node can be easily determined, and whether the efficient bounds for LP and SP of corresponding optimization problems can be evaluated. In the two problems that we have considered, the network representations described in this thesis seem to be optimal. However, in the problem of higher dimensional tables, e.g., three-way problem discussed in Section 2.1.5, the choice of the network representation is an important topic.

In Markov chain Monte Carlo part, we focus on the Markov basis defined by Diaconis and Sturmfels (1998). Of course, to construct a connected Markov chain for some given data set, all the elements of a minimal Markov basis are not necessarily needed. In fact, for many three-way data sets, we can construct a connected Markov chain over the reference set of fixed two-dimensional marginals only by basic moves. We also consider the similar basis reduction for two-way problem with structural zero cells in Section 3.4.7. However, it is difficult to determine whether a Markov chain constructed only by the basic moves is connected or not for given data set. This is one of the reasons and justifications that we consider a Markov basis. Other related problems to the connectivity by the basic moves are the problems concerning the extensions of the reference sets. In the three-way setting, for example, the following problem seems to be attractive and interesting.

> **Problem** If we permit one cell frequency to be -1 at each transition of the chain, does the set of basic moves connect all the elements in the reference set of $I \times J \times K$ contingency tables with any fixed two-dimensional marginals ?

In fact, this is another open problem at present, though we have found some indispensable moves contain ± 2. To see this, consider the following $3 \times 4 \times 6$ indispensable move of degree 14.

$$
\begin{aligned}
\boldsymbol{z} &= \begin{array}{|cccccc|}\hline +1 & -1 & 0 & 0 & 0 & 0 \\ 0 & +1 & -1 & 0 & 0 & 0 \\ 0 & 0 & +1 & 0 & 0 & -1 \\ -1 & 0 & 0 & 0 & 0 & +1 \\ \hline \end{array} \quad \begin{array}{|cccccc|}\hline 0 & +1 & 0 & -1 & 0 & 0 \\ 0 & -1 & 0 & 0 & +1 & 0 \\ 0 & 0 & 0 & +1 & 0 & -1 \\ 0 & 0 & 0 & 0 & -1 & +1 \\ \hline \end{array} \quad \begin{array}{|cccccc|}\hline -1 & 0 & 0 & +1 & 0 & 0 \\ 0 & 0 & +1 & 0 & -1 & 0 \\ 0 & 0 & -1 & -1 & 0 & +2 \\ +1 & 0 & 0 & 0 & +1 & -2 \\ \hline \end{array} \\
&= [(111, 122, 133, 146, 212, 225, 234, 246, 314, 323, 336, 336, 341, 345) \parallel \\
&\qquad (112, 123, 136, 141, 214, 222, 236, 245, 311, 325, 333, 334, 346, 346)] \\
&= \boldsymbol{z}^+ - \boldsymbol{z}^-
\end{aligned}
$$

This is indispensable in the sense that $\boldsymbol{z}^+$ and $\boldsymbol{z}^-$ are mutually accessible only by using $\boldsymbol{z}$. However, if we permit one cell frequency to be -1 at each transition of the chain, $\boldsymbol{z}^+$ and $\boldsymbol{z}^-$ are mutually accessible by basic moves as follows.

$$
\begin{aligned}
&\boldsymbol{z}^+ = [(111, 122, 133, 146, 212, 225, 234, 246, 314, 323, 336, 336, 341, 345)] \\
&\longrightarrow [(116, 122, 133, 141, 212, 225, 234, 246, 311, 314, 323, 336, 336, 345, 346) \parallel (316)] \\
&\longrightarrow [(114, 122, 133, 136, 141, 212, 225, 234, 246, 311, 323, 334, 336, 345, 346) \parallel (134)] \\
&\longrightarrow [(112, 122, 133, 136, 141, 214, 225, 232, 246, 311, 323, 334, 336, 345, 346) \parallel (132)] \\
&\longrightarrow [(112, 123, 136, 141, 214, 222, 225, 233, 246, 311, 323, 334, 336, 345, 346) \parallel (223)] \\
&\longrightarrow [(112, 123, 136, 141, 214, 222, 225, 236, 246, 311, 326, 333, 334, 345, 346) \parallel (226)] \\
&\longrightarrow [(112, 123, 136, 141, 214, 222, 236, 245, 311, 325, 333, 334, 346, 346)] = \boldsymbol{z}^-.
\end{aligned}
$$

If it is assured that the answer for the above problem is yes, we can easily construct a Markov chain Monte Carlo algorithm only by the basic moves.

Our contribution includes various topics and all these results are concerning a minimality and uniqueness of a Markov basis. Our study is motivated by the fact that the outputs of the algebraic algorithms are in general not minimal and not unique since they depend on the particular term order. Especially, we are interested in the no three-way interaction model for the three-way contingency tables since it is the simplest example of non-decomposable hierarchical models. As is shown in Section 3.2 and Section 3.3, we have found that a minimal Markov basis is uniquely determined for $3 \times 4 \times K$ and $4 \times 4 \times 4$ cases. This finding is very attractive, and the general problem we have given in Section 3.3.4 is one of the most interesting open problems.

As we have stated, the main contributions in the first half of Chapter 3 are for actually performing the Markov chain Monte Carlo method, rather than in new theoretical developments. In fact, to calculate the exact p value for given problem which the large-sample approximations are poor, we want to use exact methods if possible, and the Markov chain Monte Carlo methods become powerful tools only when exact calculations are infeasible. These days, algorithms such as the network algorithm can practically handle analyses for most $I \times J$ and $2 \times 2 \times K$ problems of moderate sizes (Agresti, 1992). However, it is believed at present that it is still difficult to calculate the p values efficiently by some exact computation algorithms for the no three-factor interaction problems. For these reasons, it is also important to consider the topics of the actual computation. However, our investigation for this area is not enough at present. As the first contribution, we exhibit the list of indispensable moves for three-way contingency tables obtained in this thesis in the author's web page:

`http://www.stat.t.u-tokyo.ac.jp/~aoki/list-of-indispensable-moves.html`

We hope that this database actually serves many statisticians who intend to use the Markov chain Monte Carlo methods to test the hypothesis of no three-factor interactions for three-way contingency tables.

On the other hand, the latter half of Chapter 3 gives some basic characterization of a minimal Markov basis. Though it is computationally difficult at present to actually construct a minimal and an invariant minimal Markov basis following our theorems, we believe that, with further refinement, it might be possible to implement an alternative efficient algorithm for constructing a minimal and an invariant minimal Markov basis. This is another attractive topic to be considered.

Appendix A

List of indispensable moves for larger tables produced by the separations and combinations of two-dimensional slices of $3 \times 4 \times K$ and $4 \times 4 \times 4$ indispensable moves

We list indispensable moves of larger sizes. All the indispensable moves listed below are produced by the separations and combinations of two-dimensional slices of $3 \times 4 \times K$ and $4 \times 4 \times 4$ indispensable moves (Section 3.3.1) and themselves. We specify each indispensable move by its size, degree and slice degree. We also give a simplified information as the form (3.9). All the informations in the list are available from the author's web page.

A.1 Indispensable moves of degree 11

- $3 \times 5 \times 5$ move of degree 11 with slice degree $\{3,4,4\} \times \{2,2,2,2,3\} \times \{2,2,2,2,3\}$
  $((3,5,5),(11),((3,4,4),(2,2,2,2,3),(2,2,2,2,3)),(fcs),\emptyset,$
  $((111,125,152,215,234,243,251,322,335,344,353),(115,122,151,211,235,244,253,325,334,343,352)))$

$$
\begin{array}{|ccccc|}\hline +1 & 0 & 0 & 0 & -1 \\ 0 & -1 & 0 & 0 & +1 \\ 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \\ -1 & +1 & 0 & 0 & 0 \\ \hline \end{array}
\quad
\begin{array}{|ccccc|}\hline -1 & 0 & 0 & 0 & +1 \\ 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & +1 & -1 \\ 0 & 0 & +1 & -1 & 0 \\ +1 & 0 & -1 & 0 & 0 \\ \hline \end{array}
\quad
\begin{array}{|ccccc|}\hline 0 & 0 & 0 & 0 & 0 \\ 0 & +1 & 0 & 0 & -1 \\ 0 & 0 & 0 & -1 & +1 \\ 0 & 0 & -1 & +1 & 0 \\ 0 & -1 & +1 & 0 & 0 \\ \hline \end{array}
$$

- $4 \times 4 \times 5$ move of degree 11 with slice degree $\{2,2,3,4\} \times \{2,3,3,3\} \times \{2,2,2,2,3\}$
  $((4,4,5),(11),((2,2,3,4),(2,3,3,3),(2,2,2,2,3)),(fcs),\emptyset,$
  $((121,135,225,242,314,333,345,413,422,431,444),(125,131,222,245,313,335,344,414,421,433,442)))$

$$
\begin{array}{|ccccc|}\hline 0 & 0 & 0 & 0 & 0 \\ +1 & 0 & 0 & 0 & -1 \\ -1 & 0 & 0 & 0 & +1 \\ 0 & 0 & 0 & 0 & 0 \\ \hline \end{array}
\quad
\begin{array}{|ccccc|}\hline 0 & 0 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 & +1 \\ 0 & 0 & 0 & 0 & 0 \\ 0 & +1 & 0 & 0 & -1 \\ \hline \end{array}
\quad
\begin{array}{|ccccc|}\hline 0 & 0 & -1 & +1 & 0 \\ 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & +1 & 0 & -1 \\ 0 & 0 & 0 & -1 & +1 \\ \hline \end{array}
\quad
\begin{array}{|ccccc|}\hline 0 & 0 & +1 & -1 & 0 \\ -1 & +1 & 0 & 0 & 0 \\ +1 & 0 & -1 & 0 & 0 \\ 0 & -1 & 0 & +1 & 0 \\ \hline \end{array}
$$

- $4 \times 4 \times 5$ move of degree 11 with slice degree $\{2,3,3,3\} \times \{2,3,3,3\} \times \{2,2,2,2,3\}$
$((4,4,5),(11),((2,3,3,3),(2,3,3,3),(2,2,2,2,3)),(fcs),\emptyset,$
$((121,145,222,233,241,314,325,332,415,434,443),(125,141,221,232,243,315,322,334,414,433,445)))$

$$\boxed{\begin{array}{ccccc} 0&0&0&0&0\\ +1&0&0&0&-1\\ 0&0&0&0&0\\ -1&0&0&0&+1 \end{array}}\ \boxed{\begin{array}{ccccc} 0&0&0&0&0\\ -1&+1&0&0&0\\ 0&-1&+1&0&0\\ +1&0&-1&0&0 \end{array}}\ \boxed{\begin{array}{ccccc} 0&0&0&+1&-1\\ 0&-1&0&0&+1\\ 0&+1&0&-1&0\\ 0&0&0&0&0 \end{array}}\ \boxed{\begin{array}{ccccc} 0&0&0&-1&+1\\ 0&0&0&0&0\\ 0&0&-1&+1&0\\ 0&0&+1&0&-1 \end{array}}$$

A.2 Indispensable moves of degree 12

- $3 \times 5 \times 6$ move of degree 12 with slice degree $\{3,4,5\} \times \{2,2,2,3,3\} \times \{2,2,2,2,2,2\}$
$((3,5,6),(12),((3,4,5),(2,2,2,3,3),(2,2,2,2,2,2)),(fcs),\emptyset,((121,143,152,$
$214,235,246,253,315,322,336,341,354),(122,141,153,215,236,243,254,314,321,335,346,352)))$

$$\boxed{\begin{array}{cccccc} 0&0&0&0&0&0\\ +1&-1&0&0&0&0\\ 0&0&0&0&0&0\\ -1&0&+1&0&0&0\\ 0&+1&-1&0&0&0 \end{array}}\ \boxed{\begin{array}{cccccc} 0&0&0&+1&-1&0\\ 0&0&0&0&0&0\\ 0&0&0&0&+1&-1\\ 0&0&-1&0&0&+1\\ 0&0&+1&-1&0&0 \end{array}}\ \boxed{\begin{array}{cccccc} 0&0&0&-1&+1&0\\ -1&+1&0&0&0&0\\ 0&0&0&0&-1&+1\\ +1&0&0&0&0&-1\\ 0&-1&0&+1&0&0 \end{array}}$$

- $3 \times 5 \times 6$ move of degree 12 with slice degree $\{4,4,4\} \times \{2,2,2,3,3\} \times \{2,2,2,2,2,2\}$
$((3,5,6),(12),((4,4,4),(2,2,2,3,3),(2,2,2,2,2,2)),(fcs),\emptyset,((111,123,144,$
$152,212,235,241,256,324,336,345,353),(112,124,141,153,211,236,245,252,323,335,344,356)))$

$$\boxed{\begin{array}{cccccc} +1&-1&0&0&0&0\\ 0&0&+1&-1&0&0\\ 0&0&0&0&0&0\\ -1&0&0&+1&0&0\\ 0&+1&-1&0&0&0 \end{array}}\ \boxed{\begin{array}{cccccc} -1&+1&0&0&0&0\\ 0&0&0&0&0&0\\ 0&0&0&0&+1&-1\\ +1&0&0&0&-1&0\\ 0&-1&0&0&0&+1 \end{array}}\ \boxed{\begin{array}{cccccc} 0&0&0&0&0&0\\ 0&0&-1&+1&0&0\\ 0&0&0&0&-1&+1\\ 0&0&0&-1&+1&0\\ 0&0&+1&0&0&-1 \end{array}}$$

- $4 \times 4 \times 5$ move(1) of degree 12 with slice degree $\{2,2,4,4\} \times \{3,3,3,3\} \times \{2,2,2,2,4\}$
$((4,4,5),(12),((2,2,4,4),(3,3,3,3),(2,2,2,2,4)),(fcs),\emptyset,((111,125,232,$
$245,313,321,334,342,415,424,435,443),(115,121,235,242,311,324,332,343,413,425,434,445)))$

$$\boxed{\begin{array}{ccccc} +1&0&0&0&-1\\ -1&0&0&0&+1\\ 0&0&0&0&0\\ 0&0&0&0&0 \end{array}}\ \boxed{\begin{array}{ccccc} 0&0&0&0&0\\ 0&0&0&0&0\\ 0&+1&0&0&-1\\ 0&-1&0&0&+1 \end{array}}\ \boxed{\begin{array}{ccccc} -1&0&+1&0&0\\ +1&0&0&-1&0\\ 0&-1&0&+1&0\\ 0&+1&-1&0&0 \end{array}}\ \boxed{\begin{array}{ccccc} 0&0&-1&0&+1\\ 0&0&0&+1&-1\\ 0&0&0&-1&+1\\ 0&0&+1&0&-1 \end{array}}$$

- $4 \times 4 \times 5$ move(2) of degree 12 with slice degree $\{2,2,4,4\} \times \{3,3,3,3\} \times \{2,2,2,2,4\}$
(not fundamental, circuit)
$((4,4,5),(12),((2,2,4,4),(3,3,3,3),(2,2,2,2,4)),(Fcs),(315,325,435,445),((111,125,232,245,313,321,335,$
$344,415,424,433,442),(115,121,235,242,311,324,333,345,413,425,432,444)))$

$$\boxed{\begin{array}{ccccc} +1&0&0&0&-1\\ -1&0&0&0&+1\\ 0&0&0&0&0\\ 0&0&0&0&0 \end{array}}\ \boxed{\begin{array}{ccccc} 0&0&0&0&0\\ 0&0&0&0&0\\ 0&+1&0&0&-1\\ 0&-1&0&0&+1 \end{array}}\ \boxed{\begin{array}{ccccc} -1&0&+1&0&(0)\\ +1&0&0&-1&(0)\\ 0&0&-1&0&+1\\ 0&0&0&+1&-1 \end{array}}\ \boxed{\begin{array}{ccccc} 0&0&-1&0&+1\\ 0&0&0&+1&-1\\ 0&-1&+1&0&(0)\\ 0&+1&0&-1&(0) \end{array}}$$

- $4 \times 4 \times 5$ move of degree 12 with slice degree $\{2,3,3,4\} \times \{2,3,3,4\} \times \{2,2,2,3,3\}$ (not fundamental, circuit)
$((4,4,5),(12),((2,3,3,4),(2,3,3,4),(2,2,2,3,3)),(Fcs),(244,445),((135,144,221,234,242,313,324,345,415,423,432,441),(134,145,224,232,241,315,323,344,413,421,435,442)))$

$$\boxed{\begin{array}{ccccc} 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & -1 & +1 \\ 0 & 0 & 0 & +1 & -1 \end{array}} \quad \boxed{\begin{array}{ccccc} 0 & 0 & 0 & 0 & 0 \\ +1 & 0 & 0 & -1 & 0 \\ 0 & -1 & 0 & +1 & 0 \\ -1 & +1 & 0 & (0) & 0 \end{array}} \quad \boxed{\begin{array}{ccccc} 0 & 0 & +1 & 0 & -1 \\ 0 & 0 & -1 & +1 & 0 \\ 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & -1 & +1 \end{array}} \quad \boxed{\begin{array}{ccccc} 0 & 0 & -1 & 0 & +1 \\ -1 & 0 & +1 & 0 & 0 \\ 0 & +1 & 0 & 0 & -1 \\ +1 & -1 & 0 & 0 & (0) \end{array}}$$

- $4 \times 4 \times 5$ move of degree 12 with slice degree $\{2,3,3,4\} \times \{3,3,3,3\} \times \{2,2,2,3,3\}$
$((4,4,5),(12),((2,3,3,4),(3,3,3,3),(2,2,2,3,3)),(fcs),(435),((111,124,214,235,242,325,333,344,415,421,432,443),(114,121,215,232,244,324,335,343,411,425,433,442)))$

$$\boxed{\begin{array}{ccccc} +1 & 0 & 0 & -1 & 0 \\ -1 & 0 & 0 & +1 & 0 \\ 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \end{array}} \quad \boxed{\begin{array}{ccccc} 0 & 0 & 0 & +1 & -1 \\ 0 & 0 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 & +1 \\ 0 & +1 & 0 & -1 & 0 \end{array}} \quad \boxed{\begin{array}{ccccc} 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & -1 & +1 \\ 0 & 0 & +1 & 0 & -1 \\ 0 & 0 & -1 & +1 & 0 \end{array}} \quad \boxed{\begin{array}{ccccc} -1 & 0 & 0 & 0 & +1 \\ +1 & 0 & 0 & 0 & -1 \\ 0 & +1 & -1 & 0 & (0) \\ 0 & -1 & +1 & 0 & 0 \end{array}}$$

- $4 \times 4 \times 6$ move of degree 12 with slice degree $\{2,2,4,4\} \times \{2,3,3,4\} \times \{2,2,2,2,2,2\}$
$((4,4,6),(12),((2,2,4,4),(2,3,3,4),(2,2,2,2,2,2)),(fcs),\emptyset,((122,141,233,244,315,321,336,343,416,425,434,442),(121,142,234,243,316,325,333,341,415,422,436,444)))$

$$\boxed{\begin{array}{cccccc} 0 & 0 & 0 & 0 & 0 & 0 \\ -1 & +1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ +1 & -1 & 0 & 0 & 0 & 0 \end{array}} \quad \boxed{\begin{array}{cccccc} 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & +1 & -1 & 0 & 0 \\ 0 & 0 & -1 & +1 & 0 & 0 \end{array}} \quad \boxed{\begin{array}{cccccc} 0 & 0 & 0 & 0 & +1 & -1 \\ +1 & 0 & 0 & 0 & -1 & 0 \\ 0 & 0 & -1 & 0 & 0 & +1 \\ -1 & 0 & +1 & 0 & 0 & 0 \end{array}} \quad \boxed{\begin{array}{cccccc} 0 & 0 & 0 & 0 & -1 & +1 \\ 0 & -1 & 0 & 0 & +1 & 0 \\ 0 & 0 & 0 & +1 & 0 & -1 \\ 0 & +1 & 0 & -1 & 0 & 0 \end{array}}$$

- $4 \times 4 \times 6$ move of degree 12 with slice degree $\{2,2,4,4\} \times \{3,3,3,3\} \times \{2,2,2,2,2,2\}$
$((4,4,6),(12),((2,2,4,4),(3,3,3,3),(2,2,2,2,2,2)),(fcs),\emptyset,((111,122,233,244,315,321,336,343,412,426,434,445),(112,121,234,243,311,326,333,345,415,422,436,444)))$

$$\boxed{\begin{array}{cccccc} +1 & -1 & 0 & 0 & 0 & 0 \\ -1 & +1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \end{array}} \quad \boxed{\begin{array}{cccccc} 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & +1 & -1 & 0 & 0 \\ 0 & 0 & -1 & +1 & 0 & 0 \end{array}} \quad \boxed{\begin{array}{cccccc} -1 & 0 & 0 & 0 & +1 & 0 \\ +1 & 0 & 0 & 0 & 0 & -1 \\ 0 & 0 & -1 & 0 & 0 & +1 \\ 0 & 0 & +1 & 0 & -1 & 0 \end{array}} \quad \boxed{\begin{array}{cccccc} 0 & +1 & 0 & 0 & -1 & 0 \\ 0 & -1 & 0 & 0 & 0 & +1 \\ 0 & 0 & 0 & +1 & 0 & -1 \\ 0 & 0 & 0 & -1 & +1 & 0 \end{array}}$$

- $4 \times 4 \times 6$ move of degree 12 with slice degree $\{2,3,3,4\} \times \{2,3,3,4\} \times \{2,2,2,2,2,2\}$
$((4,4,6),(12),((2,3,3,4),(2,3,3,4),(2,2,2,2,2,2)),(fcs),\emptyset,((121,142,223,234,241,316,335,344,415,422,433,456),(122,141,221,233,244,315,334,346,416,423,435,442)))$

$$\boxed{\begin{array}{cccccc} 0 & 0 & 0 & 0 & 0 & 0 \\ +1 & -1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ -1 & +1 & 0 & 0 & 0 & 0 \end{array}} \quad \boxed{\begin{array}{cccccc} 0 & 0 & 0 & 0 & 0 & 0 \\ -1 & 0 & +1 & 0 & 0 & 0 \\ 0 & 0 & -1 & +1 & 0 & 0 \\ +1 & 0 & 0 & -1 & 0 & 0 \end{array}} \quad \boxed{\begin{array}{cccccc} 0 & 0 & 0 & 0 & -1 & +1 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & -1 & +1 & 0 \\ 0 & 0 & 0 & +1 & 0 & -1 \end{array}} \quad \boxed{\begin{array}{cccccc} 0 & 0 & 0 & 0 & +1 & -1 \\ 0 & +1 & -1 & 0 & 0 & 0 \\ 0 & 0 & +1 & 0 & -1 & 0 \\ 0 & -1 & 0 & 0 & 0 & +1 \end{array}}$$

- $4 \times 5 \times 5$ move of degree 12 with slice degree $\{3,3,3,3\} \times \{2,2,2,2,4\} \times \{2,2,2,2,4\}$
$((4,5,5),(12),((3,3,3,3),(2,2,2,2,4),(2,2,2,2,4)),(fcs),\emptyset,((111,125,152,215,233,251,322,345,354,435,444,453),(115,122,151,211,235,253,325,344,352,433,445,454)))$

$$\boxed{\begin{array}{ccccc} +1 & 0 & 0 & 0 & -1 \\ 0 & -1 & 0 & 0 & +1 \\ 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \\ -1 & +1 & 0 & 0 & 0 \end{array}} \quad \boxed{\begin{array}{ccccc} -1 & 0 & 0 & 0 & +1 \\ 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & +1 & 0 & -1 \\ 0 & 0 & 0 & 0 & 0 \\ +1 & 0 & -1 & 0 & 0 \end{array}} \quad \boxed{\begin{array}{ccccc} 0 & 0 & 0 & 0 & 0 \\ 0 & +1 & 0 & 0 & -1 \\ 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & -1 & +1 \\ 0 & -1 & 0 & +1 & 0 \end{array}} \quad \boxed{\begin{array}{ccccc} 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & -1 & 0 & +1 \\ 0 & 0 & 0 & +1 & -1 \\ 0 & 0 & +1 & -1 & 0 \end{array}}$$

- $4 \times 5 \times 5$ move of degree 12 with slice degree $\{3,3,3,3\} \times \{2,2,2,3,3\} \times \{2,2,2,3,3\}$
$((4,5,5),(12),((3,3,3,3),(2,2,2,3,3),(2,2,2,3,3)),(fcs),\emptyset,((111,125,144,$
$214,221,255,333,342,354,432,445,453),(114,121,145,211,225,254,332,344,353,433,442,455)))$

$$\begin{array}{|ccccc|}\hline +1&0&0&-1&0\\ -1&0&0&0&+1\\ 0&0&0&0&0\\ 0&0&0&+1&-1\\ 0&0&0&0&0\\ \hline\end{array}\quad
\begin{array}{|ccccc|}\hline -1&0&0&+1&0\\ +1&0&0&0&-1\\ 0&0&0&0&0\\ 0&0&0&0&0\\ 0&0&0&-1&+1\\ \hline\end{array}\quad
\begin{array}{|ccccc|}\hline 0&0&0&0&0\\ 0&0&0&0&0\\ 0&-1&+1&0&0\\ 0&+1&0&-1&0\\ 0&0&-1&+1&0\\ \hline\end{array}\quad
\begin{array}{|ccccc|}\hline 0&0&0&0&0\\ 0&0&0&0&0\\ 0&+1&-1&0&0\\ 0&-1&0&0&+1\\ 0&0&+1&0&-1\\ \hline\end{array}$$

A.3 Indispensable moves of degree 13

- $3 \times 5 \times 6$ move of degree 13 with slice degree $\{4,4,5\} \times \{2,2,2,3,4\} \times \{2,2,2,2,2,3\}$
$((3,5,6),(13),((4,4,5),(2,2,2,3,4),(2,2,2,2,2,3)),(fcs),\emptyset,((111,126,143,152,216,234,241,255,322,336,345,$
$353,354),(116,122,141,153,211,236,245,254,326,334,343,352,355)))$

$$\begin{array}{|cccccc|}\hline +1&0&0&0&0&-1\\ 0&-1&0&0&0&+1\\ 0&0&0&0&0&0\\ -1&0&+1&0&0&0\\ 0&+1&-1&0&0&0\\ \hline\end{array}
\begin{array}{|cccccc|}\hline -1&0&0&0&0&+1\\ 0&0&0&0&0&0\\ 0&0&0&+1&0&-1\\ +1&0&0&0&-1&0\\ 0&0&0&-1&+1&0\\ \hline\end{array}
\begin{array}{|cccccc|}\hline 0&0&0&0&0&0\\ 0&+1&0&0&0&-1\\ 0&0&0&-1&0&+1\\ 0&0&-1&0&+1&0\\ 0&-1&+1&+1&-1&0\\ \hline\end{array}$$

- $3 \times 5 \times 6$ move of degree 13 with slice degree $\{4,4,5\} \times \{2,2,3,3,3\} \times \{2,2,2,2,2,3\}$
$((3,5,6),(13),((4,4,5),(2,2,3,3,3),(2,2,2,2,2,3)),(fcs),(356),((111,133,142,156,226,234,243,255,316,324,$
$331,345,352),(116,131,143,152,224,233,245,256,311,326,334,342,355)))$

$$\begin{array}{|cccccc|}\hline +1&0&0&0&0&-1\\ 0&0&0&0&0&0\\ -1&0&+1&0&0&0\\ 0&+1&-1&0&0&0\\ 0&-1&0&0&0&+1\\ \hline\end{array}
\begin{array}{|cccccc|}\hline 0&0&0&0&0&0\\ 0&0&0&-1&0&+1\\ 0&0&-1&+1&0&0\\ 0&0&+1&0&-1&0\\ 0&0&0&0&+1&-1\\ \hline\end{array}
\begin{array}{|cccccc|}\hline -1&0&0&0&0&+1\\ 0&0&0&+1&0&-1\\ +1&0&0&-1&0&0\\ 0&-1&0&0&+1&0\\ 0&+1&0&0&-1&(0)\\ \hline\end{array}$$

- $3 \times 6 \times 6$ move of degree 13 with slice degree $\{3,5,5\} \times \{2,2,2,2,2,3\} \times \{2,2,2,2,2,3\}$
$((3,6,6),(13),((3,5,5),(2,2,2,2,2,3),(2,2,2,2,2,3)),(fcs),\emptyset,((111,126,162,216,234,243,255,261,322,336,$
$345,354,363),(116,122,161,211,236,245,254,263,326,334,343,355,362)))$

$$\begin{array}{|cccccc|}\hline +1&0&0&0&0&-1\\ 0&-1&0&0&0&+1\\ 0&0&0&0&0&0\\ 0&0&0&0&0&0\\ 0&0&0&0&0&0\\ -1&+1&0&0&0&0\\ \hline\end{array}
\begin{array}{|cccccc|}\hline -1&0&0&0&0&+1\\ 0&0&0&0&0&0\\ 0&0&0&+1&0&-1\\ 0&0&+1&0&-1&0\\ 0&0&0&-1&+1&0\\ +1&0&-1&0&0&0\\ \hline\end{array}
\begin{array}{|cccccc|}\hline 0&0&0&0&0&0\\ 0&+1&0&0&0&-1\\ 0&0&0&-1&0&+1\\ 0&0&-1&0&+1&0\\ 0&0&0&+1&-1&0\\ 0&-1&+1&0&0&0\\ \hline\end{array}$$

- $3 \times 6 \times 6$ move of degree 13 with slice degree $\{4,4,5\} \times \{2,2,2,2,2,3\} \times \{2,2,2,2,2,3\}$
$((3,6,6),(13),((4,4,5),(2,2,2,2,2,3),(2,2,2,2,2,3)),(fcs),\emptyset,((111,126,133,162,216,245,254,261,323,332,$
$346,355,364),(116,123,132,161,211,246,255,264,326,333,345,354,362)))$

$$\begin{array}{|cccccc|}\hline +1&0&0&0&0&-1\\ 0&0&-1&0&0&+1\\ 0&-1&+1&0&0&0\\ 0&0&0&0&0&0\\ 0&0&0&0&0&0\\ -1&+1&0&0&0&0\\ \hline\end{array}
\begin{array}{|cccccc|}\hline -1&0&0&0&0&+1\\ 0&0&0&0&0&0\\ 0&0&0&0&0&0\\ 0&0&0&0&+1&-1\\ 0&0&0&+1&-1&0\\ +1&0&0&-1&0&0\\ \hline\end{array}
\begin{array}{|cccccc|}\hline 0&0&0&0&0&0\\ 0&0&+1&0&0&-1\\ 0&+1&-1&0&0&0\\ 0&0&0&0&-1&+1\\ 0&0&0&-1&+1&0\\ 0&-1&0&+1&0&0\\ \hline\end{array}$$

- $4 \times 4 \times 5$ move(1) of degree 13 with slice degree $\{3,3,3,4\} \times \{3,3,3,4\} \times \{2,2,3,3,3\}$
$((4,4,5),(13),((3,3,3,4),(3,3,3,4),(2,2,3,3,3)),(fcs),(443,444),((111,135,144,225,233,242,315,324,343,413,422,434,441),(115,134,141,222,235,243,313,325,344,411,424,433,442)))$

$$\begin{array}{|ccccc|}\hline +1&0&0&0&-1\\ 0&0&0&0&0\\ 0&0&0&-1&+1\\ -1&0&0&+1&0\\ \hline\end{array}\ \begin{array}{|ccccc|}\hline 0&0&0&0&0\\ 0&-1&0&0&+1\\ 0&0&+1&0&-1\\ 0&+1&-1&0&0\\ \hline\end{array}\ \begin{array}{|ccccc|}\hline 0&0&-1&0&+1\\ 0&0&0&+1&-1\\ 0&0&0&0&0\\ 0&0&+1&-1&0\\ \hline\end{array}\ \begin{array}{|ccccc|}\hline -1&0&+1&0&0\\ 0&+1&0&-1&0\\ 0&0&-1&+1&0\\ +1&-1&(0)&(0)&0\\ \hline\end{array}$$

- $4 \times 4 \times 5$ move(2) of degree 13 with slice degree $\{3,3,3,4\} \times \{3,3,3,4\} \times \{2,2,3,3,3\}$
(not fundamental, circuit)
$((4,4,5),(13),((3,3,3,4),(3,3,3,4),(2,2,3,3,3)),(Fcs),(244,323,415,443),((111,135,144,223,234,242,315,324,343,413,425,432,441),(115,134,141,224,232,243,313,325,344,411,423,435,442)))$

$$\begin{array}{|ccccc|}\hline +1&0&0&0&-1\\ 0&0&0&0&0\\ 0&0&0&-1&+1\\ -1&0&0&+1&0\\ \hline\end{array}\ \begin{array}{|ccccc|}\hline 0&0&0&0&0\\ 0&0&+1&-1&0\\ 0&-1&0&+1&0\\ 0&+1&-1&(0)&0\\ \hline\end{array}\ \begin{array}{|ccccc|}\hline 0&0&-1&0&+1\\ 0&0&(0)&+1&-1\\ 0&0&0&0&0\\ 0&0&+1&-1&0\\ \hline\end{array}\ \begin{array}{|ccccc|}\hline -1&0&+1&0&(0)\\ 0&0&-1&0&+1\\ 0&+1&0&0&-1\\ +1&-1&(0)&0&0\\ \hline\end{array}$$

- $4 \times 4 \times 6$ move of degree 13 with slice degree $\{2,3,3,5\} \times \{3,3,3,4\} \times \{2,2,2,2,2,3\}$
$((4,4,6),(13),((2,3,3,5),(3,3,3,4),(2,2,2,2,2,3)),(fcs),\emptyset,((111,126,216,233,242,325,336,344,412,421,434,443,445),(116,121,212,236,243,326,334,345,411,425,433,442,444)))$

$$\begin{array}{|cccccc|}\hline +1&0&0&0&0&-1\\ -1&0&0&0&0&+1\\ 0&0&0&0&0&0\\ 0&0&0&0&0&0\\ \hline\end{array}\ \begin{array}{|cccccc|}\hline 0&-1&0&0&0&+1\\ 0&0&0&0&0&0\\ 0&0&+1&0&0&-1\\ 0&+1&-1&0&0&0\\ \hline\end{array}\ \begin{array}{|cccccc|}\hline 0&0&0&0&0&0\\ 0&0&0&0&+1&-1\\ 0&0&0&-1&0&+1\\ 0&0&0&+1&-1&0\\ \hline\end{array}\ \begin{array}{|cccccc|}\hline -1&+1&0&0&0&0\\ +1&0&0&0&-1&0\\ 0&0&-1&+1&0&0\\ 0&-1&+1&-1&+1&0\\ \hline\end{array}$$

- $4 \times 4 \times 6$ move(1) of degree 13 with slice degree $\{2,3,4,4\} \times \{3,3,3,4\} \times \{2,2,2,2,2,3\}$
$((4,4,6),(13),((2,3,4,4),(3,3,3,4),(2,2,2,2,2,3)),(fcs),(446),((111,146,223,236,242,314,325,333,341,416,422,434,445),(116,141,222,233,246,311,323,334,345,414,425,436,442)))$

$$\begin{array}{|cccccc|}\hline +1&0&0&0&0&-1\\ 0&0&0&0&0&0\\ 0&0&0&0&0&0\\ -1&0&0&0&0&+1\\ \hline\end{array}\ \begin{array}{|cccccc|}\hline 0&0&0&0&0&0\\ 0&-1&+1&0&0&0\\ 0&0&-1&0&0&+1\\ 0&+1&0&0&0&-1\\ \hline\end{array}\ \begin{array}{|cccccc|}\hline -1&0&0&+1&0&0\\ 0&0&-1&0&+1&0\\ 0&0&+1&-1&0&0\\ +1&0&0&0&-1&0\\ \hline\end{array}\ \begin{array}{|cccccc|}\hline 0&0&0&-1&0&+1\\ 0&+1&0&0&-1&0\\ 0&0&0&+1&0&-1\\ 0&-1&0&0&+1&(0)\\ \hline\end{array}$$

- $4 \times 4 \times 6$ move(2) of degree 13 with slice degree $\{2,3,4,4\} \times \{3,3,3,4\} \times \{2,2,2,2,2,3\}$
$((4,4,6),(13),((2,3,4,4),(3,3,3,4),(2,2,2,2,2,3)),(fcs),\emptyset,((111,126,222,233,246,315,321,332,344,416,434,443,445),(116,121,226,232,243,311,322,334,345,415,433,444,446)))$

$$\begin{array}{|cccccc|}\hline +1&0&0&0&0&-1\\ -1&0&0&0&0&+1\\ 0&0&0&0&0&0\\ 0&0&0&0&0&0\\ \hline\end{array}\ \begin{array}{|cccccc|}\hline 0&0&0&0&0&0\\ 0&+1&0&0&0&-1\\ 0&-1&+1&0&0&0\\ 0&0&-1&0&0&+1\\ \hline\end{array}\ \begin{array}{|cccccc|}\hline -1&0&0&0&+1&0\\ +1&-1&0&0&0&0\\ 0&+1&0&-1&0&0\\ 0&0&0&+1&-1&0\\ \hline\end{array}\ \begin{array}{|cccccc|}\hline 0&0&0&0&-1&+1\\ 0&0&0&0&0&0\\ 0&0&-1&+1&0&0\\ 0&0&+1&-1&+1&-1\\ \hline\end{array}$$

- $4 \times 4 \times 6$ move of degree 13 with slice degree $\{3,3,3,4\} \times \{3,3,3,4\} \times \{2,2,2,2,2,3\}$
$((4,4,6),(13),((3,3,3,4),(3,3,3,4),(2,2,2,2,2,3)),(fcs),(416),((111,126,142,222,234,243,316,333,345,415,424,436,441),(116,122,141,224,233,242,315,336,343,411,426,434,445)))$

$$\begin{array}{|cccccc|}\hline +1&0&0&0&0&-1\\ 0&-1&0&0&0&+1\\ 0&0&0&0&0&0\\ -1&+1&0&0&0&0\\ \hline\end{array}\ \begin{array}{|cccccc|}\hline 0&0&0&0&0&0\\ 0&+1&0&-1&0&0\\ 0&0&-1&+1&0&0\\ 0&-1&+1&0&0&0\\ \hline\end{array}\ \begin{array}{|cccccc|}\hline 0&0&0&0&-1&+1\\ 0&0&0&0&0&0\\ 0&0&+1&0&0&-1\\ 0&0&-1&0&+1&0\\ \hline\end{array}\ \begin{array}{|cccccc|}\hline -1&0&0&0&+1&(0)\\ 0&0&0&+1&0&-1\\ 0&0&0&-1&0&+1\\ +1&0&0&0&-1&0\\ \hline\end{array}$$

- $4 \times 5 \times 5$ move of degree 13 with slice degree $\{2,3,3,5\} \times \{2,2,2,3,4\} \times \{2,2,3,3,3\}$
$((4,5,5),(13),((2,3,3,5),(2,2,2,3,4),(2,2,3,3,3)),(fcs),\emptyset,((113,144,221,245,254,335,343,352,414,425,432,451,453),(114,143,225,244,251,332,345,353,413,421,435,452,454)))$

0	0	+1	−1	0
0	0	0	0	0
0	0	0	0	0
0	0	−1	+1	0
0	0	0	0	0

0	0	0	0	0
+1	0	0	0	−1
0	0	0	0	0
0	0	0	−1	+1
−1	0	0	+1	0

0	0	0	0	0
0	0	0	0	0
0	−1	0	0	+1
0	0	+1	0	−1
0	+1	−1	0	0

0	0	−1	+1	0
−1	0	0	0	+1
0	+1	0	0	−1
0	0	0	0	0
+1	−1	+1	−1	0

- $4 \times 5 \times 5$ move of degree 13 with slice degree $\{2,3,4,4\} \times \{2,2,2,3,4\} \times \{2,2,3,3,3\}$
$((4,5,5),(13),((2,3,4,4),(2,2,2,3,4),(2,2,3,3,3)),(fcs),\emptyset,((113,154,235,241,252,314,325,331,343,424,442,453,455),(114,153,231,242,255,313,324,335,341,425,443,452,454)))$

0	0	+1	−1	0
0	0	0	0	0
0	0	0	0	0
0	0	0	0	0
0	0	−1	+1	0

0	0	0	0	0
0	0	0	0	0
−1	0	0	0	+1
+1	−1	0	0	0
0	+1	0	0	−1

0	0	−1	+1	0
0	0	0	−1	+1
+1	0	0	0	−1
−1	0	+1	0	0
0	0	0	0	0

0	0	0	0	0
0	0	0	+1	−1
0	0	0	0	0
0	+1	−1	0	0
0	−1	+1	−1	+1

- $4 \times 5 \times 5$ move of degree 13 with slice degree $\{3,3,3,4\} \times \{2,2,2,3,4\} \times \{2,2,2,3,4\}$
$((4,5,5),(13),((3,3,3,4),(2,2,2,3,4),(2,2,2,3,4)),(fcs),\emptyset,((114,135,152,225,241,253,334,343,355,412,421,444,455),(112,134,155,221,243,255,335,344,353,414,425,441,452)))$

0	−1	0	+1	0
0	0	0	0	0
0	0	0	−1	+1
0	0	0	0	0
0	+1	0	0	−1

0	0	0	0	0
−1	0	0	0	+1
0	0	0	0	0
+1	0	−1	0	0
0	0	+1	0	−1

0	0	0	0	0
0	0	0	0	0
0	0	0	+1	−1
0	0	+1	−1	0
0	0	−1	0	+1

0	+1	0	−1	0
+1	0	0	0	−1
0	0	0	0	0
−1	0	0	+1	0
0	−1	0	0	+1

- $4 \times 5 \times 5$ move of degree 13 with slice degree $\{3,3,3,4\} \times \{2,2,2,3,4\} \times \{2,2,3,3,3\}$
$((4,5,5),(13),((3,3,3,4),(2,2,2,3,4),(2,2,3,3,3)),(fcs),\emptyset,((113,125,134,214,243,251,323,342,355,435,441,452,454),(114,123,135,213,241,254,325,343,352,434,442,451,455)))$

0	0	+1	−1	0
0	0	−1	0	+1
0	0	0	+1	−1
0	0	0	0	0
0	0	0	0	0

0	0	−1	+1	0
0	0	0	0	0
0	0	0	0	0
−1	0	+1	0	0
+1	0	0	−1	0

0	0	0	0	0
0	0	+1	0	−1
0	0	0	0	0
0	+1	−1	0	0
0	−1	0	0	+1

0	0	0	0	0
0	0	0	0	0
0	0	0	−1	+1
+1	−1	0	0	0
−1	+1	0	+1	−1

- $4 \times 5 \times 6$ move of degree 13 with slice degree $\{2,3,3,5\} \times \{2,2,3,3,3\} \times \{2,2,2,2,2,3\}$
$((4,5,6),(13),((2,3,3,5),(2,2,3,3,3),(2,2,2,2,2,3)),(fcs),\emptyset,((131,146,212,236,253,324,345,356,413,425,432,441,454),(136,141,213,232,256,325,346,354,412,424,431,445,453)))$

0	0	0	0	0	0
0	0	0	0	0	0
+1	0	0	0	0	−1
−1	0	0	0	0	+1
0	0	0	0	0	0

0	+1	−1	0	0	0
0	0	0	0	0	0
0	−1	0	0	0	+1
0	0	0	0	0	0
0	0	+1	0	0	−1

0	0	0	0	0	0
0	0	0	+1	−1	0
0	0	0	0	0	0
0	0	0	0	+1	−1
0	0	0	−1	0	+1

0	−1	+1	0	0	0
0	0	0	−1	+1	0
−1	+1	0	0	0	0
+1	0	0	0	−1	0
0	0	−1	+1	0	0

- $4 \times 5 \times 6$ move(1) of degree 13 with slice degree $\{2,3,4,4\} \times \{2,2,2,3,4\} \times \{2,2,2,2,2,3\}$
$((4,5,6),(13),((2,3,4,4),(2,2,2,3,4),(2,2,2,2,2,3)),(fcs),\emptyset,((141,152,213,226,254,324,336,345,351,416,435,442,453),(142,151,216,224,253,326,335,341,354,413,436,445,452)))$

0	0	0	0	0	0
0	0	0	0	0	0
0	0	0	0	0	0
+1	−1	0	0	0	0
−1	+1	0	0	0	0

0	0	+1	0	0	−1
0	0	0	−1	0	+1
0	0	0	0	0	0
0	0	0	0	0	0
0	0	−1	+1	0	0

0	0	0	0	0	0
0	0	0	+1	0	−1
0	0	0	0	−1	+1
−1	0	0	0	+1	0
+1	0	0	−1	0	0

0	0	−1	0	0	+1
0	0	0	0	0	0
0	0	0	0	+1	−1
0	+1	0	0	−1	0
0	−1	+1	0	0	0

- $4 \times 5 \times 6$ move(2) of degree 13 with slice degree $\{2,3,4,4\} \times \{2,2,2,3,4\} \times \{2,2,2,2,2,3\}$
  $((4,5,6),(13),((2,3,4,4),(2,2,2,3,4),(2,2,2,2,2,3)),(fcs),\emptyset,((141,152,213,246,251,325,336,342,354,416,424,435,453),(142,151,216,241,253,324,335,346,352,413,425,436,454)))$

$$\begin{array}{|cccccc|}\hline 0&0&0&0&0&0\\0&0&0&0&0&0\\0&0&0&0&0&0\\+1&-1&0&0&0&0\\-1&+1&0&0&0&0\\\hline\end{array}\ \begin{array}{|cccccc|}\hline 0&0&+1&0&0&-1\\0&0&0&0&0&0\\0&0&0&0&0&0\\-1&0&0&0&0&+1\\+1&0&-1&0&0&0\\\hline\end{array}\ \begin{array}{|cccccc|}\hline 0&0&0&0&0&0\\0&0&0&-1&+1&0\\0&0&0&0&-1&+1\\0&+1&0&0&0&-1\\0&-1&0&+1&0&0\\\hline\end{array}\ \begin{array}{|cccccc|}\hline 0&0&-1&0&0&+1\\0&0&0&+1&-1&0\\0&0&0&0&+1&-1\\0&0&0&0&0&0\\0&0&+1&-1&0&0\\\hline\end{array}$$

- $4 \times 5 \times 6$ move(1) of degree 13 with slice degree $\{2,3,4,4\} \times \{2,2,3,3,3\} \times \{2,2,2,2,2,3\}$
  $((4,5,6),(13),((2,3,4,4),(2,2,3,3,3),(2,2,2,2,2,3)),(fcs),\emptyset,((136,141,216,234,253,322,331,345,354,413,425,446,452),(131,146,213,236,254,325,334,341,352,416,422,445,453)))$

$$\begin{array}{|cccccc|}\hline 0&0&0&0&0&0\\0&0&0&0&0&0\\-1&0&0&0&0&+1\\+1&0&0&0&0&-1\\0&0&0&0&0&0\\\hline\end{array}\ \begin{array}{|cccccc|}\hline 0&0&-1&0&0&+1\\0&0&0&0&0&0\\0&0&0&+1&0&-1\\0&0&0&0&0&0\\0&0&+1&-1&0&0\\\hline\end{array}\ \begin{array}{|cccccc|}\hline 0&0&0&0&0&0\\0&+1&0&0&-1&0\\+1&0&0&-1&0&0\\-1&0&0&0&+1&0\\0&-1&0&+1&0&0\\\hline\end{array}\ \begin{array}{|cccccc|}\hline 0&0&+1&0&0&-1\\0&-1&0&0&+1&0\\0&0&0&0&0&0\\0&0&0&0&-1&+1\\0&+1&-1&0&0&0\\\hline\end{array}$$

- $4 \times 5 \times 6$ move(2) of degree 13 with slice degree $\{2,3,4,4\} \times \{2,2,3,3,3\} \times \{2,2,2,2,2,3\}$
  $((4,5,6),(13),((2,3,4,4),(2,2,3,3,3),(2,2,2,2,2,3)),(fcs),\emptyset,((131,142,213,226,254,324,336,341,355,416,432,445,453),(132,141,216,224,253,326,331,345,354,413,436,442,455)))$

$$\begin{array}{|cccccc|}\hline 0&0&0&0&0&0\\0&0&0&0&0&0\\+1&-1&0&0&0&0\\-1&+1&0&0&0&0\\0&0&0&0&0&0\\\hline\end{array}\ \begin{array}{|cccccc|}\hline 0&0&+1&0&0&-1\\0&0&0&-1&0&+1\\0&0&0&0&0&0\\0&0&0&0&0&0\\0&0&-1&+1&0&0\\\hline\end{array}\ \begin{array}{|cccccc|}\hline 0&0&0&0&0&0\\0&0&0&+1&0&-1\\-1&0&0&0&0&+1\\+1&0&0&0&-1&0\\0&0&0&-1&+1&0\\\hline\end{array}\ \begin{array}{|cccccc|}\hline 0&0&-1&0&0&+1\\0&0&0&0&0&0\\0&+1&0&0&0&-1\\0&-1&0&0&+1&0\\0&0&+1&0&-1&0\\\hline\end{array}$$

- $4 \times 5 \times 6$ move of degree 13 with slice degree $\{3,3,3,4\} \times \{2,2,2,3,4\} \times \{2,2,2,2,2,3\}$
  $((4,5,6),(13),((3,3,3,4),(2,2,2,3,4),(2,2,2,2,2,3)),(fcs),\emptyset,((111,126,152,222,246,253,335,343,354,416,434,445,451),(116,122,151,226,243,252,334,345,353,411,435,446,454)))$

$$\begin{array}{|cccccc|}\hline +1&0&0&0&0&-1\\0&-1&0&0&0&+1\\0&0&0&0&0&0\\0&0&0&0&0&0\\-1&+1&0&0&0&0\\\hline\end{array}\ \begin{array}{|cccccc|}\hline 0&0&0&0&0&0\\0&+1&0&0&0&-1\\0&0&0&0&0&0\\0&0&-1&0&0&+1\\0&-1&+1&0&0&0\\\hline\end{array}\ \begin{array}{|cccccc|}\hline 0&0&0&0&0&0\\0&0&0&0&0&0\\0&0&0&-1&+1&0\\0&0&+1&0&-1&0\\0&0&-1&+1&0&0\\\hline\end{array}\ \begin{array}{|cccccc|}\hline -1&0&0&0&0&+1\\0&0&0&0&0&0\\0&0&0&+1&-1&0\\0&0&0&0&+1&-1\\+1&0&0&-1&0&0\\\hline\end{array}$$

- $4 \times 5 \times 6$ move(1) of degree 13 with slice degree $\{3,3,3,4\} \times \{2,2,3,3,3\} \times \{2,2,2,2,2,3\}$
  $((4,5,6),(13),((3,3,3,4),(2,2,3,3,3),(2,2,2,2,2,3)),(fcs),\emptyset,((131,143,152,216,234,241,325,346,353,414,426,432,455),(132,141,153,214,231,246,326,343,355,416,425,434,452)))$

$$\begin{array}{|cccccc|}\hline 0&0&0&0&0&0\\0&0&0&0&0&0\\+1&-1&0&0&0&0\\-1&0&+1&0&0&0\\0&+1&-1&0&0&0\\\hline\end{array}\ \begin{array}{|cccccc|}\hline 0&0&0&-1&0&+1\\0&0&0&0&0&0\\-1&0&0&+1&0&0\\+1&0&0&0&0&-1\\0&0&0&0&0&0\\\hline\end{array}\ \begin{array}{|cccccc|}\hline 0&0&0&0&0&0\\0&0&0&0&+1&-1\\0&0&0&0&0&0\\0&0&-1&0&0&+1\\0&0&+1&0&-1&0\\\hline\end{array}\ \begin{array}{|cccccc|}\hline 0&0&0&+1&0&-1\\0&0&0&0&-1&+1\\0&+1&0&-1&0&0\\0&0&0&0&0&0\\0&-1&0&0&+1&0\\\hline\end{array}$$

- $4 \times 5 \times 6$ move(2) of degree 13 with slice degree $\{3,3,3,4\} \times \{2,2,3,3,3\} \times \{2,2,2,2,2,3\}$
  $((4,5,6),(13),((3,3,3,4),(2,2,3,3,3),(2,2,2,2,2,3)),(fcs),\emptyset,((111,136,152,223,244,256,326,335,343,412,431,445,454),(112,131,156,226,243,254,323,336,345,411,435,444,452)))$

$$\begin{array}{|cccccc|}\hline +1&-1&0&0&0&0\\0&0&0&0&0&0\\-1&0&0&0&0&+1\\0&0&0&0&0&0\\0&+1&0&0&0&-1\\\hline\end{array}\ \begin{array}{|cccccc|}\hline 0&0&0&0&0&0\\0&0&+1&0&0&-1\\0&0&0&0&0&0\\0&0&-1&+1&0&0\\0&0&0&-1&0&+1\\\hline\end{array}\ \begin{array}{|cccccc|}\hline 0&0&0&0&0&0\\0&0&-1&0&0&+1\\0&0&0&0&+1&-1\\0&0&+1&0&-1&0\\0&0&0&0&0&0\\\hline\end{array}\ \begin{array}{|cccccc|}\hline -1&+1&0&0&0&0\\0&0&0&0&0&0\\+1&0&0&0&-1&0\\0&0&0&-1&+1&0\\0&-1&0&+1&0&0\\\hline\end{array}$$

- $5 \times 5 \times 5$ move of degree 13 with slice degree $\{2,2,2,3,4\} \times \{2,2,2,3,4\} \times \{2,2,3,3,3\}$
  $((5,5,5),(13),((2,2,2,3,4),(2,2,2,3,4),(2,2,3,3,3)),(fcs),\emptyset,((113,155,224,253,345,351,432,441,454,515,523,534,542),(115,153,223,254,341,355,434,442,451,513,524,532,545)))$

$$\begin{array}{|ccccc|}\hline 0&0&+1&0&-1\\ 0&0&0&0&0\\ 0&0&0&0&0\\ 0&0&0&0&0\\ 0&0&-1&0&+1\\ \hline\end{array}\quad \begin{array}{|ccccc|}\hline 0&0&0&0&0\\ 0&0&-1&+1&0\\ 0&0&0&0&0\\ 0&0&0&0&0\\ 0&0&+1&-1&0\\ \hline\end{array}\quad \begin{array}{|ccccc|}\hline 0&0&0&0&0\\ 0&0&0&0&0\\ 0&0&0&0&0\\ -1&0&0&0&+1\\ +1&0&0&0&-1\\ \hline\end{array}$$

$$\begin{array}{|ccccc|}\hline 0&0&0&0&0\\ 0&0&0&0&0\\ 0&+1&0&-1&0\\ +1&-1&0&0&0\\ -1&0&0&+1&0\\ \hline\end{array}\quad \begin{array}{|ccccc|}\hline 0&0&-1&0&+1\\ 0&0&+1&-1&0\\ 0&-1&0&+1&0\\ 0&+1&0&0&-1\\ 0&0&0&0&0\\ \hline\end{array}$$

- $5 \times 5 \times 5$ move(1) of degree 13 with slice degree $\{2,2,2,3,4\} \times \{2,2,3,3,3\} \times \{2,2,3,3,3\}$
  $((5,5,5),(13),((2,2,2,3,4),(2,2,3,3,3),(2,2,3,3,3)),(fcs),\emptyset,((135,153,231,245,313,354,424,442,455,514,522,533,541),(133,155,235,241,314,353,422,445,454,513,524,531,542)))$

$$\begin{array}{|ccccc|}\hline 0&0&0&0&0\\ 0&0&0&0&0\\ 0&0&-1&0&+1\\ 0&0&0&0&0\\ 0&0&+1&0&-1\\ \hline\end{array}\quad \begin{array}{|ccccc|}\hline 0&0&0&0&0\\ 0&0&0&0&0\\ +1&0&0&0&-1\\ -1&0&0&0&+1\\ 0&0&0&0&0\\ \hline\end{array}\quad \begin{array}{|ccccc|}\hline 0&0&+1&-1&0\\ 0&0&0&0&0\\ 0&0&0&0&0\\ 0&0&0&0&0\\ 0&0&-1&+1&0\\ \hline\end{array}$$

$$\begin{array}{|ccccc|}\hline 0&0&0&0&0\\ 0&-1&0&+1&0\\ 0&0&0&0&0\\ 0&+1&0&0&-1\\ 0&0&0&-1&+1\\ \hline\end{array}\quad \begin{array}{|ccccc|}\hline 0&0&-1&+1&0\\ 0&+1&0&-1&0\\ -1&0&+1&0&0\\ +1&-1&0&0&0\\ 0&0&0&0&0\\ \hline\end{array}$$

- $5 \times 5 \times 5$ move(2) of degree 13 with slice degree $\{2,2,2,3,4\} \times \{2,2,3,3,3\} \times \{2,2,3,3,3\}$
  $((5,5,5),(13),((2,2,2,3,4),(2,2,3,3,3),(2,2,3,3,3)),(fcs),\emptyset,((133,144,245,254,315,343,421,434,452,513,522,531,555),(134,143,244,255,313,345,422,431,454,515,521,533,552)))$

$$\begin{array}{|ccccc|}\hline 0&0&0&0&0\\ 0&0&0&0&0\\ 0&0&+1&-1&0\\ 0&0&-1&+1&0\\ 0&0&0&0&0\\ \hline\end{array}\quad \begin{array}{|ccccc|}\hline 0&0&0&0&0\\ 0&0&0&0&0\\ 0&0&0&0&0\\ 0&0&0&-1&+1\\ 0&0&0&+1&-1\\ \hline\end{array}\quad \begin{array}{|ccccc|}\hline 0&0&-1&0&+1\\ 0&0&0&0&0\\ 0&0&0&0&0\\ 0&0&+1&0&-1\\ 0&0&0&0&0\\ \hline\end{array}$$

$$\begin{array}{|ccccc|}\hline 0&0&0&0&0\\ +1&-1&0&0&0\\ -1&0&0&+1&0\\ 0&0&0&0&0\\ 0&+1&0&-1&0\\ \hline\end{array}\quad \begin{array}{|ccccc|}\hline 0&0&+1&0&-1\\ -1&+1&0&0&0\\ +1&0&-1&0&0\\ 0&0&0&0&0\\ 0&-1&0&0&+1\\ \hline\end{array}$$

- $5 \times 5 \times 5$ move(3) of degree 13 with slice degree $\{2,2,2,3,4\} \times \{2,2,3,3,3\} \times \{2,2,3,3,3\}$
$((5,5,5),(13),((2,2,2,3,4),(2,2,3,3,3),(2,2,3,3,3)),(fcs),\emptyset,((131,143,233,252,315,324,425,444,453,514,532,541,555),(133,141,232,253,314,325,424,443,455,515,531,544,552)))$

$$
\begin{array}{|ccccc|}\hline 0&0&0&0&0\\ 0&0&0&0&0\\ +1&0&-1&0&0\\ -1&0&+1&0&0\\ 0&0&0&0&0\\ \hline\end{array}
\quad
\begin{array}{|ccccc|}\hline 0&0&0&0&0\\ 0&0&0&0&0\\ 0&-1&+1&0&0\\ 0&0&0&0&0\\ 0&+1&-1&0&0\\ \hline\end{array}
\quad
\begin{array}{|ccccc|}\hline 0&0&0&-1&+1\\ 0&0&0&+1&-1\\ 0&0&0&0&0\\ 0&0&0&0&0\\ 0&0&0&0&0\\ \hline\end{array}
$$

$$
\begin{array}{|ccccc|}\hline 0&0&0&0&0\\ 0&0&0&-1&+1\\ 0&0&0&0&0\\ 0&0&-1&+1&0\\ 0&0&+1&0&-1\\ \hline\end{array}
\quad
\begin{array}{|ccccc|}\hline 0&0&0&+1&-1\\ 0&0&0&0&0\\ -1&+1&0&0&0\\ +1&0&0&-1&0\\ 0&-1&0&0&+1\\ \hline\end{array}
$$

A.4 Indispensable moves of degree 14

- $3 \times 5 \times 6$ move of degree 14 with slice degree $\{4,4,6\} \times \{2,2,3,3,4\} \times \{2,2,2,2,2,4\}$
$((3,5,6),(14),((4,4,6),(2,2,3,3,4),(2,2,2,2,2,4)),(fcS),\emptyset,((111,132,143,156,224,235,242,256,316,326,331,344,353,355),(116,131,142,153,226,232,244,255,311,324,335,343,356,356)))$

$$
\begin{array}{|cccccc|}\hline +1&0&0&0&0&-1\\ 0&0&0&0&0&0\\ -1&+1&0&0&0&0\\ 0&-1&+1&0&0&0\\ 0&0&-1&0&0&+1\\ \hline\end{array}
\quad
\begin{array}{|cccccc|}\hline 0&0&0&0&0&0\\ 0&0&0&+1&0&-1\\ 0&-1&0&0&+1&0\\ 0&+1&0&-1&0&0\\ 0&0&0&0&-1&+1\\ \hline\end{array}
\quad
\begin{array}{|cccccc|}\hline -1&0&0&0&0&+1\\ 0&0&0&-1&0&+1\\ +1&0&0&0&-1&0\\ 0&0&-1&+1&0&0\\ 0&0&+1&0&+1&-2\\ \hline\end{array}
$$

- $3 \times 5 \times 6$ move of degree 14 with slice degree $\{4,5,5\} \times \{2,3,3,3,3\} \times \{2,2,2,2,2,4\}$
$((3,5,6),(14),((4,5,5),(2,3,3,3,3),(2,2,2,2,2,4)),(fcs),\emptyset,((121,132,143,154,215,226,233,246,251,316,322,335,344,356),(122,133,144,151,216,221,235,243,256,315,326,332,346,354)))$

$$
\begin{array}{|cccccc|}\hline 0&0&0&0&0&0\\ +1&-1&0&0&0&0\\ 0&+1&-1&0&0&0\\ 0&0&+1&-1&0&0\\ -1&0&0&+1&0&0\\ \hline\end{array}
\quad
\begin{array}{|cccccc|}\hline 0&0&0&0&+1&-1\\ -1&0&0&0&0&+1\\ 0&0&+1&0&-1&0\\ 0&0&-1&0&0&+1\\ +1&0&0&0&0&-1\\ \hline\end{array}
\quad
\begin{array}{|cccccc|}\hline 0&0&0&0&-1&+1\\ 0&+1&0&0&0&-1\\ 0&-1&0&0&+1&0\\ 0&0&0&+1&0&-1\\ 0&0&0&-1&0&+1\\ \hline\end{array}
$$

- $3 \times 5 \times 7$ move(1) of degree 14 with slice degree $\{4,4,6\} \times \{2,2,3,3,4\} \times \{2,2,2,2,2,2,2\}$
$((3,5,7),(14),((4,4,6),(2,2,3,3,4),(2,2,2,2,2,2,2)),(fcs),\emptyset,((111,132,143,154,227,235,242,256,314,326,331,347,353,355),(114,131,142,153,226,232,247,255,311,327,335,343,354,356)))$

$$
\begin{array}{|ccccccc|}\hline +1&0&0&-1&0&0&0\\ 0&0&0&0&0&0&0\\ -1&+1&0&0&0&0&0\\ 0&-1&+1&0&0&0&0\\ 0&0&-1&+1&0&0&0\\ \hline\end{array}
\quad
\begin{array}{|ccccccc|}\hline 0&0&0&0&0&0&0\\ 0&0&0&0&0&-1&+1\\ 0&-1&0&0&+1&0&0\\ 0&+1&0&0&0&0&-1\\ 0&0&0&0&-1&+1&0\\ \hline\end{array}
\quad
\begin{array}{|ccccccc|}\hline -1&0&0&+1&0&0&0\\ 0&0&0&0&0&+1&-1\\ +1&0&0&0&-1&0&0\\ 0&0&-1&0&0&0&+1\\ 0&0&+1&-1&+1&-1&0\\ \hline\end{array}
$$

- $3 \times 5 \times 7$ move(2) of degree 14 with slice degree $\{4,4,6\} \times \{2,2,3,3,4\} \times \{2,2,2,2,2,2,2\}$
$((3,5,7),(14),((4,4,6),(2,2,3,3,4),(2,2,2,2,2,2,2)),(fcs),\emptyset,((111,132,143,154,226,235,242,257,314,325,331,347,353,356),(114,131,142,153,225,232,247,256,311,326,335,343,354,357)))$

$$
\begin{array}{|ccccccc|}\hline +1&0&0&-1&0&0&0\\ 0&0&0&0&0&0&0\\ -1&+1&0&0&0&0&0\\ 0&-1&+1&0&0&0&0\\ 0&0&-1&+1&0&0&0\\ \hline\end{array}
\quad
\begin{array}{|ccccccc|}\hline 0&0&0&0&0&0&0\\ 0&0&0&0&-1&+1&0\\ 0&-1&0&0&+1&0&0\\ 0&+1&0&0&0&0&-1\\ 0&0&0&0&0&-1&+1\\ \hline\end{array}
\quad
\begin{array}{|ccccccc|}\hline -1&0&0&+1&0&0&0\\ 0&0&0&0&+1&-1&0\\ +1&0&0&0&-1&0&0\\ 0&0&-1&0&0&0&+1\\ 0&0&+1&-1&0&+1&-1\\ \hline\end{array}
$$

- $3 \times 5 \times 7$ move(1) of degree 14 with slice degree $\{4,5,5\} \times \{2,2,3,3,4\} \times \{2,2,2,2,2,2,2\}$
$((3,5,7),(14),((4,5,5),(2,2,3,3,4),(2,2,2,2,2,2,2)),(fcs),\emptyset,((111,133,142,154,212,226,231,247,255,325,336,344,353,357),(112,131,144,153,211,225,236,242,257,326,333,347,354,355)))$

+1	−1	0	0	0	0	0
0	0	0	0	0	0	0
−1	0	+1	0	0	0	0
0	+1	0	−1	0	0	0
0	0	−1	+1	0	0	0

−1	+1	0	0	0	0	0
0	0	0	0	−1	+1	0
+1	0	0	0	0	−1	0
0	−1	0	0	0	0	+1
0	0	0	0	+1	0	−1

0	0	0	0	0	0	0
0	0	0	0	+1	−1	0
0	0	−1	0	0	+1	0
0	0	0	+1	0	0	−1
0	0	+1	−1	−1	0	+1

- $3 \times 5 \times 7$ move (2) of degree 14 with slice degree $\{4,5,5\} \times \{2,2,3,3,4\} \times \{2,2,2,2,2,2,2\}$
$((3,5,7),(14),((4,5,5),(2,2,3,3,4),(2,2,2,2,2,2,2)),(fcs),\emptyset,((131,144,152,153,215,226,237,243,251,316,327,332,345,354),(132,143,151,154,216,227,231,245,253,315,326,337,344,352)))$

0	0	0	0	0	0	0
0	0	0	0	0	0	0
+1	−1	0	0	0	0	0
0	0	−1	+1	0	0	0
−1	+1	+1	−1	0	0	0

0	0	0	0	+1	−1	0
0	0	0	0	0	+1	−1
−1	0	0	0	0	0	+1
0	0	+1	0	−1	0	0
+1	0	−1	0	0	0	0

0	0	0	0	−1	+1	0
0	0	0	0	0	−1	+1
0	+1	0	0	0	0	−1
0	0	0	−1	+1	0	0
0	−1	0	+1	0	0	0

- $3 \times 5 \times 7$ move of degree 14 with slice degree $\{4,5,5\} \times \{2,3,3,3,3\} \times \{2,2,2,2,2,2,2\}$
$((3,5,7),(14),((4,5,5),(2,3,3,3,3),(2,2,2,2,2,2,2)),(fcs),\emptyset,((121,133,142,154,216,222,237,245,253,315,326,331,344,357),(122,131,144,153,215,226,233,242,257,316,321,337,345,354)))$

0	0	0	0	0	0	0
+1	−1	0	0	0	0	0
−1	0	+1	0	0	0	0
0	+1	0	−1	0	0	0
0	0	−1	+1	0	0	0

0	0	0	0	−1	+1	0
0	+1	0	0	0	−1	0
0	0	−1	0	0	0	+1
0	−1	0	0	+1	0	0
0	0	+1	0	0	0	−1

0	0	0	0	+1	−1	0
−1	0	0	0	0	+1	0
+1	0	0	0	0	0	−1
0	0	0	+1	−1	0	0
0	0	0	−1	0	0	+1

- $3 \times 6 \times 6$ move(1) of degree 14 with slice degree $\{4,4,6\} \times \{2,2,2,2,3,3\} \times \{2,2,2,2,2,4\}$
$((3,6,6),(14),((4,4,6),(2,2,2,2,3,3),(2,2,2,2,2,4)),(fcs),\emptyset,((111,126,152,163,234,246,253,265,316,322,336,345,354,361),(116,122,153,161,236,245,254,263,311,326,334,346,352,365)))$

+1	0	0	0	0	−1
0	−1	0	0	0	+1
0	0	0	0	0	0
0	0	0	0	0	0
0	+1	−1	0	0	0
−1	0	+1	0	0	0

0	0	0	0	0	0
0	0	0	0	0	0
0	0	0	+1	0	−1
0	0	0	0	−1	+1
0	0	+1	−1	0	0
0	0	−1	0	+1	0

−1	0	0	0	0	+1
0	+1	0	0	0	−1
0	0	0	−1	0	+1
0	0	0	0	+1	−1
0	−1	0	+1	0	0
+1	0	0	0	−1	0

- $3 \times 6 \times 6$ move(2) of degree 14 with slice degree $\{4,4,6\} \times \{2,2,2,2,3,3\} \times \{2,2,2,2,2,4\}$
(not fundamental, circuit)
$((3,6,6),(14),((4,4,6),(2,2,2,2,3,3),(2,2,2,2,2,4)),(Fcs),(156),((111,126,152,163,234,246,253,265,316,322,335,344,356,361),(116,122,153,161,235,244,256,263,311,326,334,346,352,365)))$

+1	0	0	0	0	−1
0	−1	0	0	0	+1
0	0	0	0	0	0
0	0	0	0	0	0
0	+1	−1	0	0	(0)
−1	0	+1	0	0	0

0	0	0	0	0	0
0	0	0	0	0	0
0	0	0	+1	−1	0
0	0	0	−1	0	+1
0	0	+1	0	0	−1
0	0	−1	0	+1	0

−1	0	0	0	0	+1
0	+1	0	0	0	−1
0	0	0	−1	+1	0
0	0	0	+1	0	−1
0	−1	0	0	0	+1
+1	0	0	0	−1	0

- $3 \times 6 \times 7$ move of degree 14 with slice degree $\{4,4,6\} \times \{2,2,2,2,3,3\} \times \{2,2,2,2,2,2,2\}$
  $((3,6,7),(14),((4,4,6),(2,2,2,2,3,3),(2,2,2,2,2,2,2)),(fcs),\emptyset,((111,122,153,164,236,247,254,265,312,323,335,346,357,361),(112,123,154,161,235,246,257,264,311,322,336,347,353,365)))$

$$
\begin{array}{|ccccccc|}\hline
+1 & -1 & 0 & 0 & 0 & 0 & 0 \\
0 & +1 & -1 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & +1 & -1 & 0 & 0 & 0 \\
-1 & 0 & 0 & +1 & 0 & 0 & 0 \\ \hline
\end{array}
\begin{array}{|ccccccc|}\hline
0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & -1 & +1 & 0 \\
0 & 0 & 0 & 0 & 0 & -1 & +1 \\
0 & 0 & 0 & +1 & 0 & 0 & -1 \\
0 & 0 & 0 & -1 & +1 & 0 & 0 \\ \hline
\end{array}
\begin{array}{|ccccccc|}\hline
-1 & +1 & 0 & 0 & 0 & 0 & 0 \\
0 & -1 & +1 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & +1 & -1 & 0 \\
0 & 0 & 0 & 0 & 0 & +1 & -1 \\
0 & 0 & -1 & 0 & 0 & 0 & +1 \\
+1 & 0 & 0 & 0 & -1 & 0 & 0 \\ \hline
\end{array}
$$

- $3 \times 6 \times 7$ move of degree 14 with slice degree $\{4,5,5\} \times \{2,2,2,2,3,3\} \times \{2,2,2,2,2,2,2\}$
  $((3,6,7),(14),((4,5,5),(2,2,2,2,3,3),(2,2,2,2,2,2,2)),(fcs),\emptyset,((111,123,154,162,212,235,246,251,267,324,336,347,355,363),(112,124,151,163,211,236,247,255,262,323,335,346,354,367)))$

$$
\begin{array}{|ccccccc|}\hline
+1 & -1 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & +1 & -1 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 \\
-1 & 0 & 0 & +1 & 0 & 0 & 0 \\
0 & +1 & -1 & 0 & 0 & 0 & 0 \\ \hline
\end{array}
\begin{array}{|ccccccc|}\hline
-1 & +1 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & +1 & -1 & 0 \\
0 & 0 & 0 & 0 & 0 & +1 & -1 \\
+1 & 0 & 0 & 0 & -1 & 0 & 0 \\
0 & -1 & 0 & 0 & 0 & 0 & +1 \\ \hline
\end{array}
\begin{array}{|ccccccc|}\hline
0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & -1 & +1 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & -1 & +1 & 0 \\
0 & 0 & 0 & 0 & 0 & -1 & +1 \\
0 & 0 & 0 & -1 & +1 & 0 & 0 \\
0 & 0 & +1 & 0 & 0 & 0 & -1 \\ \hline
\end{array}
$$

- $4 \times 4 \times 5$ move(1) of degree 14 with slice degree $\{3,3,3,5\} \times \{3,3,3,5\} \times \{2,2,3,3,4\}$
  (not fundamental, circuit)
  $((4,4,5),(14),((3,3,3,5),(3,3,3,5),(2,2,3,3,4)),(FcS),(335,444),((111,123,144,222,233,245,313,334,345,415,424,435,441,442),(113,124,141,223,235,242,315,333,344,411,422,434,445,445)))$

$$
\begin{array}{|ccccc|}\hline
+1 & 0 & -1 & 0 & 0 \\
0 & 0 & +1 & -1 & 0 \\
0 & 0 & 0 & 0 & 0 \\
-1 & 0 & 0 & +1 & 0 \\ \hline
\end{array}
\begin{array}{|ccccc|}\hline
0 & 0 & 0 & 0 & 0 \\
0 & +1 & -1 & 0 & 0 \\
0 & 0 & +1 & 0 & -1 \\
0 & -1 & 0 & 0 & +1 \\ \hline
\end{array}
\begin{array}{|ccccc|}\hline
0 & 0 & +1 & 0 & -1 \\
0 & 0 & 0 & 0 & 0 \\
0 & 0 & -1 & +1 & (0) \\
0 & 0 & 0 & -1 & +1 \\ \hline
\end{array}
\begin{array}{|ccccc|}\hline
-1 & 0 & 0 & 0 & +1 \\
0 & -1 & 0 & +1 & 0 \\
0 & 0 & 0 & -1 & +1 \\
+1 & +1 & 0 & (0) & -2 \\ \hline
\end{array}
$$

- $4 \times 4 \times 5$ move(2) of degree 14 with slice degree $\{3,3,3,5\} \times \{3,3,3,5\} \times \{2,2,3,3,4\}$
  (not fundamental, circuit)
  $((4,4,5),(14),((3,3,3,5),(3,3,3,5),(2,2,3,3,4)),(FcS),(244,413),((111,133,144,222,234,245,313,324,345,415,423,435,441,442),(113,134,141,224,235,242,315,323,344,411,422,433,445,445)))$

$$
\begin{array}{|ccccc|}\hline
-1 & 0 & +1 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 \\
0 & 0 & -1 & +1 & 0 \\
+1 & 0 & 0 & -1 & 0 \\ \hline
\end{array}
\begin{array}{|ccccc|}\hline
0 & 0 & 0 & 0 & 0 \\
0 & -1 & 0 & +1 & 0 \\
0 & 0 & 0 & -1 & +1 \\
0 & +1 & 0 & (0) & -1 \\ \hline
\end{array}
\begin{array}{|ccccc|}\hline
0 & 0 & -1 & 0 & +1 \\
0 & 0 & +1 & -1 & 0 \\
0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & +1 & -1 \\ \hline
\end{array}
\begin{array}{|ccccc|}\hline
+1 & 0 & (0) & 0 & -1 \\
0 & +1 & -1 & 0 & 0 \\
0 & 0 & +1 & 0 & -1 \\
-1 & -1 & 0 & 0 & +2 \\ \hline
\end{array}
$$

- $4 \times 4 \times 5$ move(1) of degree 14 with slice degree $\{3,3,3,5\} \times \{3,3,4,4\} \times \{2,3,3,3,3\}$
  (not fundamental, circuit)
  $((4,4,5),(14),((3,3,3,5),(3,3,4,4),(2,3,3,3,3)),(Fcs),(132,245,424),((112,124,133,213,225,244,315,332,341,422,431,434,443,445),(113,122,134,215,224,243,312,331,345,425,432,433,441,444)))$

$$
\begin{array}{|ccccc|}\hline
0 & +1 & -1 & 0 & 0 \\
0 & -1 & 0 & +1 & 0 \\
0 & (0) & +1 & -1 & 0 \\
0 & 0 & 0 & 0 & 0 \\ \hline
\end{array}
\begin{array}{|ccccc|}\hline
0 & 0 & +1 & 0 & -1 \\
0 & 0 & 0 & -1 & +1 \\
0 & 0 & 0 & 0 & 0 \\
0 & 0 & -1 & +1 & (0) \\ \hline
\end{array}
\begin{array}{|ccccc|}\hline
0 & -1 & 0 & 0 & +1 \\
0 & 0 & 0 & 0 & 0 \\
-1 & +1 & 0 & 0 & 0 \\
+1 & 0 & 0 & 0 & -1 \\ \hline
\end{array}
\begin{array}{|ccccc|}\hline
0 & 0 & 0 & 0 & 0 \\
0 & +1 & 0 & (0) & -1 \\
+1 & -1 & -1 & +1 & 0 \\
-1 & 0 & +1 & -1 & +1 \\ \hline
\end{array}
$$

- $4 \times 4 \times 5$ move(2) of degree 14 with slice degree $\{3,3,3,5\} \times \{3,3,4,4\} \times \{2,3,3,3,3\}$
$((4,4,5),(14),((3,3,3,5),(3,3,4,4),(2,3,3,3,3)),(fcs),\emptyset,((112,124,133,213,225,244,315,331,342,$
$422,434,435,441,443),(113,122,134,215,224,243,312,335,341,425,431,433,442,444)))$

$$\begin{array}{|ccccc|}\hline 0 & +1 & -1 & 0 & 0 \\ 0 & -1 & 0 & +1 & 0 \\ 0 & 0 & +1 & -1 & 0 \\ 0 & 0 & 0 & 0 & 0 \\ \hline \end{array} \quad \begin{array}{|ccccc|}\hline 0 & 0 & +1 & 0 & -1 \\ 0 & 0 & 0 & -1 & +1 \\ 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & -1 & +1 & 0 \\ \hline \end{array} \quad \begin{array}{|ccccc|}\hline 0 & -1 & 0 & 0 & +1 \\ 0 & 0 & 0 & 0 & 0 \\ +1 & 0 & 0 & 0 & -1 \\ -1 & +1 & 0 & 0 & 0 \\ \hline \end{array} \quad \begin{array}{|ccccc|}\hline 0 & 0 & 0 & 0 & 0 \\ 0 & +1 & 0 & 0 & -1 \\ -1 & 0 & -1 & +1 & +1 \\ +1 & -1 & +1 & -1 & 0 \\ \hline \end{array}$$

- $4 \times 4 \times 6$ move of degree 14 with slice degree $\{2,3,4,5\} \times \{3,3,3,5\} \times \{2,2,2,2,2,4\}$
$((4,4,6),(14),((2,3,4,5),(3,3,3,5),(2,2,2,2,2,4)),(fcS),\emptyset,((111,146,225,233,246,312,323,334,341,$
$416,422,436,444,445),(116,141,223,236,245,311,322,333,344,412,425,434,446,446)))$

$$\begin{array}{|cccccc|}\hline +1 & 0 & 0 & 0 & 0 & -1 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ -1 & 0 & 0 & 0 & 0 & +1 \\ \hline \end{array} \quad \begin{array}{|cccccc|}\hline 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & -1 & 0 & +1 & 0 \\ 0 & 0 & +1 & 0 & 0 & -1 \\ 0 & 0 & 0 & 0 & -1 & +1 \\ \hline \end{array} \quad \begin{array}{|cccccc|}\hline -1 & +1 & 0 & 0 & 0 & 0 \\ 0 & -1 & +1 & 0 & 0 & 0 \\ 0 & 0 & -1 & +1 & 0 & 0 \\ +1 & 0 & 0 & -1 & 0 & 0 \\ \hline \end{array} \quad \begin{array}{|cccccc|}\hline 0 & -1 & 0 & 0 & 0 & +1 \\ 0 & +1 & 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & -1 & 0 & +1 \\ 0 & 0 & 0 & +1 & +1 & -2 \\ \hline \end{array}$$

- $4 \times 4 \times 6$ move of degree 14 with slice degree $\{2,4,4,4\} \times \{3,3,4,4\} \times \{2,2,2,2,2,4\}$
$((4,4,6),(14),((2,4,4,4),(3,3,4,4),(2,2,2,2,2,4)),(fcs),\emptyset,((131,142,213,226,236,241,314,323,332,$
$345,416,425,434,446),(132,141,216,223,231,246,313,325,334,342,414,426,436,445)))$

$$\begin{array}{|cccccc|}\hline 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ +1 & -1 & 0 & 0 & 0 & 0 \\ -1 & +1 & 0 & 0 & 0 & 0 \\ \hline \end{array} \quad \begin{array}{|cccccc|}\hline 0 & 0 & +1 & 0 & 0 & -1 \\ 0 & 0 & -1 & 0 & 0 & +1 \\ -1 & 0 & 0 & 0 & 0 & +1 \\ +1 & 0 & 0 & 0 & 0 & -1 \\ \hline \end{array} \quad \begin{array}{|cccccc|}\hline 0 & 0 & -1 & +1 & 0 & 0 \\ 0 & 0 & +1 & 0 & -1 & 0 \\ 0 & +1 & 0 & -1 & 0 & 0 \\ 0 & -1 & 0 & 0 & +1 & 0 \\ \hline \end{array} \quad \begin{array}{|cccccc|}\hline 0 & 0 & 0 & -1 & 0 & +1 \\ 0 & 0 & 0 & 0 & +1 & -1 \\ 0 & 0 & 0 & +1 & 0 & -1 \\ 0 & 0 & 0 & 0 & -1 & +1 \\ \hline \end{array}$$

- $4 \times 4 \times 6$ move(1) of degree 14 with slice degree $\{3,3,3,5\} \times \{3,3,3,5\} \times \{2,2,2,2,3,3\}$
$((4,4,6),(14),((3,3,3,5),(3,3,3,5),(2,2,2,2,3,3)),(fcs),(446),((111,125,142,215,233,246,326,335,$
$344,416,422,434,441,443),(115,122,141,216,235,243,325,334,346,411,426,433,442,444)))$

$$\begin{array}{|cccccc|}\hline +1 & 0 & 0 & 0 & -1 & 0 \\ 0 & -1 & 0 & 0 & +1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ -1 & +1 & 0 & 0 & 0 & 0 \\ \hline \end{array} \quad \begin{array}{|cccccc|}\hline 0 & 0 & 0 & 0 & +1 & -1 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & +1 & 0 & -1 & 0 \\ 0 & 0 & -1 & 0 & 0 & +1 \\ \hline \end{array} \quad \begin{array}{|cccccc|}\hline 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & -1 & +1 \\ 0 & 0 & 0 & -1 & +1 & 0 \\ 0 & 0 & 0 & +1 & 0 & -1 \\ \hline \end{array} \quad \begin{array}{|cccccc|}\hline -1 & 0 & 0 & 0 & 0 & +1 \\ 0 & +1 & 0 & 0 & 0 & -1 \\ 0 & 0 & -1 & +1 & 0 & 0 \\ +1 & -1 & +1 & -1 & 0 & (0) \\ \hline \end{array}$$

- $4 \times 4 \times 6$ move(2) of degree 14 with slice degree $\{3,3,3,5\} \times \{3,3,3,5\} \times \{2,2,2,2,3,3\}$
(not fundamental, circuit)
$((4,4,6),(14),((3,3,3,5),(3,3,3,5),(2,2,2,2,3,3)),(Fcs),(436),((111,125,142,215,236,243,326,334,$
$345,416,422,433,441,444),(115,122,141,216,233,245,325,336,344,411,426,434,442,443)))$

$$\begin{array}{|cccccc|}\hline +1 & 0 & 0 & 0 & -1 & 0 \\ 0 & -1 & 0 & 0 & +1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ -1 & +1 & 0 & 0 & 0 & 0 \\ \hline \end{array} \quad \begin{array}{|cccccc|}\hline 0 & 0 & 0 & 0 & +1 & -1 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & -1 & 0 & 0 & +1 \\ 0 & 0 & +1 & 0 & -1 & 0 \\ \hline \end{array} \quad \begin{array}{|cccccc|}\hline 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & -1 & +1 \\ 0 & 0 & 0 & +1 & 0 & -1 \\ 0 & 0 & 0 & -1 & +1 & 0 \\ \hline \end{array} \quad \begin{array}{|cccccc|}\hline -1 & 0 & 0 & 0 & 0 & +1 \\ 0 & +1 & 0 & 0 & 0 & -1 \\ 0 & 0 & +1 & -1 & 0 & (0) \\ +1 & -1 & -1 & +1 & 0 & 0 \\ \hline \end{array}$$

- $4 \times 4 \times 6$ move of degree 14 with slice degree $\{3,3,4,4\} \times \{3,3,4,4\} \times \{2,2,2,2,2,4\}$
$((4,4,6),(14),((3,3,4,4),(3,3,4,4),(2,2,2,2,2,4)),(fcs),\emptyset,((111,136,142,223,236,244,315,324,331,$
$346,412,425,433,446),(112,131,146,224,233,246,311,325,336,344,415,423,436,442)))$

$$\begin{array}{|cccccc|}\hline +1 & -1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ -1 & 0 & 0 & 0 & 0 & +1 \\ 0 & +1 & 0 & 0 & 0 & -1 \\ \hline \end{array} \quad \begin{array}{|cccccc|}\hline 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & +1 & -1 & 0 & 0 \\ 0 & 0 & -1 & 0 & 0 & +1 \\ 0 & 0 & 0 & +1 & 0 & -1 \\ \hline \end{array} \quad \begin{array}{|cccccc|}\hline -1 & 0 & 0 & 0 & +1 & 0 \\ 0 & 0 & 0 & +1 & -1 & 0 \\ +1 & 0 & 0 & 0 & 0 & -1 \\ 0 & 0 & 0 & -1 & 0 & +1 \\ \hline \end{array} \quad \begin{array}{|cccccc|}\hline 0 & +1 & 0 & 0 & -1 & 0 \\ 0 & 0 & -1 & 0 & +1 & 0 \\ 0 & 0 & +1 & 0 & 0 & -1 \\ 0 & -1 & 0 & 0 & 0 & +1 \\ \hline \end{array}$$

- $4 \times 4 \times 7$ move(1) of degree 14 with slice degree $\{2,3,4,5\} \times \{2,3,4,5\} \times \{2,2,2,2,2,2,2\}$
$((4,4,7),(14),((2,3,4,5),(2,3,4,5),(2,2,2,2,2,2,2)),(fcs),\emptyset,((133,145,222,231,243,314,321,337,346,$ $416,424,435,442,447),(135,143,221,233,242,316,324,331,347,414,422,437,445,446)))$

$$\begin{array}{|ccccccc|}\hline 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & +1 & 0 & -1 & 0 & 0 \\ 0 & 0 & -1 & 0 & +1 & 0 & 0 \\ \hline \end{array} \quad \begin{array}{|ccccccc|}\hline 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ -1 & +1 & 0 & 0 & 0 & 0 & 0 \\ +1 & 0 & -1 & 0 & 0 & 0 & 0 \\ 0 & -1 & +1 & 0 & 0 & 0 & 0 \\ \hline \end{array}$$

$$\begin{array}{|ccccccc|}\hline 0 & 0 & 0 & +1 & 0 & -1 & 0 \\ +1 & 0 & 0 & -1 & 0 & 0 & 0 \\ -1 & 0 & 0 & 0 & 0 & 0 & +1 \\ 0 & 0 & 0 & 0 & 0 & +1 & -1 \\ \hline \end{array} \quad \begin{array}{|ccccccc|}\hline 0 & 0 & 0 & -1 & 0 & +1 & 0 \\ 0 & -1 & 0 & +1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & +1 & 0 & -1 \\ 0 & +1 & 0 & 0 & -1 & -1 & +1 \\ \hline \end{array}$$

- $4 \times 4 \times 7$ move(2) of degree 14 with slice degree $\{2,3,4,5\} \times \{2,3,4,5\} \times \{2,2,2,2,2,2,2\}$
$((4,4,7),(14),((2,3,4,5),(2,3,4,5),(2,2,2,2,2,2,2)),(fcs),\emptyset,((131,142,223,234,245,316,324,332,347,$ $417,426,435,441,443),(132,141,224,235,243,317,326,334,342,416,423,431,445,447)))$

$$\begin{array}{|ccccccc|}\hline 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ +1 & -1 & 0 & 0 & 0 & 0 & 0 \\ -1 & +1 & 0 & 0 & 0 & 0 & 0 \\ \hline \end{array} \quad \begin{array}{|ccccccc|}\hline 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & +1 & -1 & 0 & 0 & 0 \\ 0 & 0 & 0 & +1 & -1 & 0 & 0 \\ 0 & 0 & -1 & 0 & +1 & 0 & 0 \\ \hline \end{array}$$

$$\begin{array}{|ccccccc|}\hline 0 & 0 & 0 & 0 & 0 & +1 & -1 \\ 0 & 0 & 0 & +1 & 0 & -1 & 0 \\ 0 & +1 & 0 & -1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 & 0 & 0 & +1 \\ \hline \end{array} \quad \begin{array}{|ccccccc|}\hline 0 & 0 & 0 & 0 & 0 & -1 & +1 \\ 0 & 0 & -1 & 0 & 0 & +1 & 0 \\ -1 & 0 & 0 & 0 & +1 & 0 & 0 \\ +1 & 0 & +1 & 0 & -1 & 0 & -1 \\ \hline \end{array}$$

- $4 \times 4 \times 7$ move of degree 14 with slice degree $\{2,3,4,5\} \times \{2,4,4,4\} \times \{2,2,2,2,2,2,2\}$
$((4,4,7),(14),((2,3,4,5),(2,4,4,4),(2,2,2,2,2,2,2)),(fcs),\emptyset,((121,132,223,231,244,315,322,337,346,$ $416,425,434,443,447),(122,131,221,234,243,316,325,332,347,415,423,437,444,446)))$

$$\begin{array}{|ccccccc|}\hline 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ +1 & -1 & 0 & 0 & 0 & 0 & 0 \\ -1 & +1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ \hline \end{array} \quad \begin{array}{|ccccccc|}\hline 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ -1 & 0 & +1 & 0 & 0 & 0 & 0 \\ +1 & 0 & 0 & -1 & 0 & 0 & 0 \\ 0 & 0 & -1 & +1 & 0 & 0 & 0 \\ \hline \end{array}$$

$$\begin{array}{|ccccccc|}\hline 0 & 0 & 0 & 0 & +1 & -1 & 0 \\ 0 & +1 & 0 & 0 & -1 & 0 & 0 \\ 0 & -1 & 0 & 0 & 0 & 0 & +1 \\ 0 & 0 & 0 & 0 & 0 & +1 & -1 \\ \hline \end{array} \quad \begin{array}{|ccccccc|}\hline 0 & 0 & 0 & 0 & -1 & +1 & 0 \\ 0 & 0 & -1 & 0 & +1 & 0 & 0 \\ 0 & 0 & 0 & +1 & 0 & 0 & -1 \\ 0 & 0 & +1 & -1 & 0 & -1 & +1 \\ \hline \end{array}$$

- $4 \times 4 \times 7$ move of degree 14 with slice degree $\{2,3,4,5\} \times \{3,3,3,5\} \times \{2,2,2,2,2,2,2\}$
$((4,4,7),(14),((2,3,4,5),(3,3,3,5),(2,2,2,2,2,2,2)),(fcs),\emptyset,((111,142,223,235,244,312,326,333,347,$ $416,424,437,441,445),(112,141,224,233,245,316,323,337,342,411,426,435,444,447)))$

$$\begin{array}{|ccccccc|}\hline +1 & -1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ -1 & +1 & 0 & 0 & 0 & 0 & 0 \\ \hline \end{array} \quad \begin{array}{|ccccccc|}\hline 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & +1 & -1 & 0 & 0 & 0 \\ 0 & 0 & -1 & 0 & +1 & 0 & 0 \\ 0 & 0 & 0 & +1 & -1 & 0 & 0 \\ \hline \end{array}$$

$$\begin{array}{|ccccccc|}\hline 0 & +1 & 0 & 0 & 0 & -1 & 0 \\ 0 & 0 & -1 & 0 & 0 & +1 & 0 \\ 0 & 0 & +1 & 0 & 0 & 0 & -1 \\ 0 & -1 & 0 & 0 & 0 & 0 & +1 \\ \hline \end{array} \quad \begin{array}{|ccccccc|}\hline -1 & 0 & 0 & 0 & 0 & +1 & 0 \\ 0 & 0 & 0 & +1 & 0 & -1 & 0 \\ 0 & 0 & 0 & 0 & -1 & 0 & +1 \\ +1 & 0 & 0 & -1 & +1 & 0 & -1 \\ \hline \end{array}$$

- $4 \times 4 \times 7$ move of degree 14 with slice degree $\{2,3,4,5\} \times \{3,3,4,4\} \times \{2,2,2,2,2,2,2\}$
$((4,4,7),(14),((2,3,4,5),(3,3,4,4),(2,2,2,2,2,2,2)),(fcs),\emptyset,((111,132,223,234,245,317,324,331,346,412,426,435,443,447),(112,131,224,235,243,311,326,334,347,417,423,432,445,446)))$

$$\begin{array}{|ccccccc|}\hline +1 & -1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ -1 & +1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ \hline \end{array} \quad \begin{array}{|ccccccc|}\hline 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & +1 & -1 & 0 & 0 & 0 \\ 0 & 0 & 0 & +1 & -1 & 0 & 0 \\ 0 & 0 & -1 & 0 & +1 & 0 & 0 \\ \hline \end{array}$$

$$\begin{array}{|ccccccc|}\hline -1 & 0 & 0 & 0 & 0 & 0 & +1 \\ 0 & 0 & 0 & +1 & 0 & -1 & 0 \\ +1 & 0 & 0 & -1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & +1 & -1 \\ \hline \end{array} \quad \begin{array}{|ccccccc|}\hline 0 & +1 & 0 & 0 & 0 & 0 & -1 \\ 0 & 0 & -1 & 0 & 0 & +1 & 0 \\ 0 & -1 & 0 & 0 & +1 & 0 & 0 \\ 0 & 0 & +1 & 0 & -1 & -1 & +1 \\ \hline \end{array}$$

- $4 \times 4 \times 7$ move(1) of degree 14 with slice degree $\{2,4,4,4\} \times \{3,3,4,4\} \times \{2,2,2,2,2,2,2\}$
$((4,4,7),(14),((2,4,4,4),(3,3,4,4),(2,2,2,2,2,2,2)),(fcs),\emptyset,((111,132,213,224,231,245,312,323,337,346,426,435,444,447),(112,131,211,223,235,244,313,326,332,347,424,437,445,446)))$

$$\begin{array}{|ccccccc|}\hline +1 & -1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ -1 & +1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ \hline \end{array} \quad \begin{array}{|ccccccc|}\hline -1 & 0 & +1 & 0 & 0 & 0 & 0 \\ 0 & 0 & -1 & +1 & 0 & 0 & 0 \\ +1 & 0 & 0 & 0 & -1 & 0 & 0 \\ 0 & 0 & 0 & -1 & +1 & 0 & 0 \\ \hline \end{array}$$

$$\begin{array}{|ccccccc|}\hline 0 & +1 & -1 & 0 & 0 & 0 & 0 \\ 0 & 0 & +1 & 0 & 0 & -1 & 0 \\ 0 & -1 & 0 & 0 & 0 & 0 & +1 \\ 0 & 0 & 0 & 0 & 0 & +1 & -1 \\ \hline \end{array} \quad \begin{array}{|ccccccc|}\hline 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & -1 & 0 & +1 & 0 \\ 0 & 0 & 0 & 0 & +1 & 0 & -1 \\ 0 & 0 & 0 & +1 & -1 & -1 & +1 \\ \hline \end{array}$$

- $4 \times 4 \times 7$ move(2) of degree 14 with slice degree $\{2,4,4,4\} \times \{3,3,4,4\} \times \{2,2,2,2,2,2,2\}$
$((4,4,7),(14),((2,4,4,4),(3,3,4,4),(2,2,2,2,2,2,2)),(fcs),\emptyset,((131,142,213,225,234,241,316,323,332,347,414,427,436,445),(132,141,214,223,231,245,313,327,336,342,416,425,434,447)))$

$$\begin{array}{|ccccccc|}\hline 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ +1 & -1 & 0 & 0 & 0 & 0 & 0 \\ -1 & +1 & 0 & 0 & 0 & 0 & 0 \\ \hline \end{array} \quad \begin{array}{|ccccccc|}\hline 0 & 0 & +1 & -1 & 0 & 0 & 0 \\ 0 & 0 & -1 & 0 & +1 & 0 & 0 \\ -1 & 0 & 0 & +1 & 0 & 0 & 0 \\ +1 & 0 & 0 & 0 & -1 & 0 & 0 \\ \hline \end{array}$$

$$\begin{array}{|ccccccc|}\hline 0 & 0 & -1 & 0 & 0 & +1 & 0 \\ 0 & 0 & +1 & 0 & 0 & 0 & -1 \\ 0 & +1 & 0 & 0 & 0 & -1 & 0 \\ 0 & -1 & 0 & 0 & 0 & 0 & +1 \\ \hline \end{array} \quad \begin{array}{|ccccccc|}\hline 0 & 0 & 0 & +1 & 0 & -1 & 0 \\ 0 & 0 & 0 & 0 & -1 & 0 & +1 \\ 0 & 0 & 0 & -1 & 0 & +1 & 0 \\ 0 & 0 & 0 & 0 & +1 & 0 & -1 \\ \hline \end{array}$$

- $4 \times 4 \times 7$ move of degree 14 with slice degree $\{3,3,3,5\} \times \{3,3,4,4\} \times \{2,2,2,2,2,2,2\}$
$((4,4,7),(14),((3,3,3,5),(3,3,4,4),(2,2,2,2,2,2,2)),(fcs),\emptyset,((111,123,132,212,235,244,326,333,347,414,421,437,445,446),(112,121,133,214,232,245,323,337,346,411,426,435,444,447)))$

$$\begin{array}{|ccccccc|}\hline +1 & -1 & 0 & 0 & 0 & 0 & 0 \\ -1 & 0 & +1 & 0 & 0 & 0 & 0 \\ 0 & +1 & -1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ \hline \end{array} \quad \begin{array}{|ccccccc|}\hline 0 & +1 & 0 & -1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 & +1 & 0 & 0 \\ 0 & 0 & 0 & +1 & -1 & 0 & 0 \\ \hline \end{array}$$

$$\begin{array}{|ccccccc|}\hline 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & -1 & 0 & 0 & +1 & 0 \\ 0 & 0 & +1 & 0 & 0 & 0 & -1 \\ 0 & 0 & 0 & 0 & 0 & -1 & +1 \\ \hline \end{array} \quad \begin{array}{|ccccccc|}\hline -1 & 0 & 0 & +1 & 0 & 0 & 0 \\ +1 & 0 & 0 & 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & 0 & -1 & 0 & +1 \\ 0 & 0 & 0 & -1 & +1 & +1 & -1 \\ \hline \end{array}$$

- $4 \times 4 \times 7$ move of degree 14 with slice degree $\{3,3,4,4\} \times \{3,3,4,4\} \times \{2,2,2,2,2,2,2\}$
  $((4,4,7),(14),((3,3,4,4),(3,3,4,4),(2,2,2,2,2,2,2)),(fcs),\emptyset,((111,133,142,224,236,245,317,325,331,343,412,427,434,446),(112,131,143,225,234,246,311,327,333,345,417,424,436,442)))$

$$\begin{array}{|ccccccc|}\hline +1 & -1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ -1 & 0 & +1 & 0 & 0 & 0 & 0 \\ 0 & +1 & -1 & 0 & 0 & 0 & 0 \\ \hline \end{array} \quad \begin{array}{|ccccccc|}\hline 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & +1 & -1 & 0 & 0 \\ 0 & 0 & 0 & -1 & 0 & +1 & 0 \\ 0 & 0 & 0 & 0 & +1 & -1 & 0 \\ \hline \end{array}$$

$$\begin{array}{|ccccccc|}\hline -1 & 0 & 0 & 0 & 0 & 0 & +1 \\ 0 & 0 & 0 & 0 & +1 & 0 & -1 \\ +1 & 0 & -1 & 0 & 0 & 0 & 0 \\ 0 & 0 & +1 & 0 & -1 & 0 & 0 \\ \hline \end{array} \quad \begin{array}{|ccccccc|}\hline 0 & +1 & 0 & 0 & 0 & 0 & -1 \\ 0 & 0 & 0 & -1 & 0 & 0 & +1 \\ 0 & 0 & 0 & +1 & 0 & -1 & 0 \\ 0 & -1 & 0 & 0 & 0 & +1 & 0 \\ \hline \end{array}$$

- $4 \times 5 \times 5$ move of degree 14 with slice degree $\{2,3,4,5\} \times \{2,2,2,4,4\} \times \{2,3,3,3,3\}$
  $((4,5,5),(14),((2,3,4,5),(2,2,2,4,4),(2,3,3,3,3)),(fcs),\emptyset,((142,153,214,245,251,322,335,343,344,411,424,433,452,455),(143,152,211,244,255,324,333,342,345,414,422,435,451,453)))$

$$\begin{array}{|ccccc|}\hline 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \\ 0 & +1 & -1 & 0 & 0 \\ 0 & -1 & +1 & 0 & 0 \\ \hline \end{array} \quad \begin{array}{|ccccc|}\hline -1 & 0 & 0 & +1 & 0 \\ 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & -1 & +1 \\ +1 & 0 & 0 & 0 & -1 \\ \hline \end{array} \quad \begin{array}{|ccccc|}\hline 0 & 0 & 0 & 0 & 0 \\ 0 & +1 & 0 & -1 & 0 \\ 0 & 0 & -1 & 0 & +1 \\ 0 & -1 & +1 & +1 & -1 \\ 0 & 0 & 0 & 0 & 0 \\ \hline \end{array} \quad \begin{array}{|ccccc|}\hline +1 & 0 & 0 & -1 & 0 \\ 0 & -1 & 0 & +1 & 0 \\ 0 & 0 & +1 & 0 & -1 \\ 0 & 0 & 0 & 0 & 0 \\ -1 & +1 & -1 & 0 & +1 \\ \hline \end{array}$$

- $4 \times 5 \times 5$ move(1) of degree 14 with slice degree $\{3,3,3,5\} \times \{2,2,3,3,4\} \times \{2,3,3,3,3\}$
  (not fundamental, circuit)
  $((4,5,5),(14),((3,3,3,5),(2,2,3,3,4),(2,3,3,3,3)),(Fcs),(353,445),((111,132,153,225,234,242,333,345,354,412,424,443,451,455),(112,133,151,224,232,245,334,343,355,411,425,442,453,454)))$

$$\begin{array}{|ccccc|}\hline +1 & -1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \\ 0 & +1 & -1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \\ -1 & 0 & +1 & 0 & 0 \\ \hline \end{array} \quad \begin{array}{|ccccc|}\hline 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & -1 & +1 \\ 0 & -1 & 0 & +1 & 0 \\ 0 & +1 & 0 & 0 & -1 \\ 0 & 0 & 0 & 0 & 0 \\ \hline \end{array} \quad \begin{array}{|ccccc|}\hline 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & +1 & -1 & 0 \\ 0 & 0 & -1 & 0 & +1 \\ 0 & 0 & (0) & +1 & -1 \\ \hline \end{array} \quad \begin{array}{|ccccc|}\hline -1 & +1 & 0 & 0 & 0 \\ 0 & 0 & 0 & +1 & -1 \\ 0 & 0 & 0 & 0 & 0 \\ 0 & -1 & +1 & 0 & (0) \\ +1 & 0 & -1 & -1 & +1 \\ \hline \end{array}$$

- $4 \times 5 \times 5$ move(2) of degree 14 with slice degree $\{3,3,3,5\} \times \{2,2,3,3,4\} \times \{2,3,3,3,3\}$
  $((4,5,5),(14),((3,3,3,5),(2,2,3,3,4),(2,3,3,3,3)),(fcs),(445),((111,132,153,224,233,245,334,342,355,412,425,443,451,454),(112,133,151,225,234,243,332,345,354,411,424,442,453,455)))$

$$\begin{array}{|ccccc|}\hline +1 & -1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \\ 0 & +1 & -1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \\ -1 & 0 & +1 & 0 & 0 \\ \hline \end{array} \quad \begin{array}{|ccccc|}\hline 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & +1 & -1 \\ 0 & 0 & +1 & -1 & 0 \\ 0 & 0 & -1 & 0 & +1 \\ 0 & 0 & 0 & 0 & 0 \\ \hline \end{array} \quad \begin{array}{|ccccc|}\hline 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \\ 0 & -1 & 0 & +1 & 0 \\ 0 & +1 & 0 & 0 & -1 \\ 0 & 0 & 0 & -1 & +1 \\ \hline \end{array} \quad \begin{array}{|ccccc|}\hline -1 & +1 & 0 & 0 & 0 \\ 0 & 0 & 0 & -1 & +1 \\ 0 & 0 & 0 & 0 & 0 \\ 0 & -1 & +1 & 0 & (0) \\ +1 & 0 & -1 & +1 & -1 \\ \hline \end{array}$$

- $4 \times 5 \times 5$ move(1) of degree 14 with slice degree $\{3,3,4,4\} \times \{2,3,3,3,3\} \times \{2,3,3,3,3\}$
  $((4,5,5),(14),((3,3,4,4),(2,3,3,3,3),(2,3,3,3,3)),(fcs),(322,455),((122,135,153,224,242,255,314,323,332,341,413,431,445,454),(123,132,155,222,245,254,313,324,331,342,414,435,441,453)))$

$$\begin{array}{|ccccc|}\hline 0 & 0 & 0 & 0 & 0 \\ 0 & +1 & -1 & 0 & 0 \\ 0 & -1 & 0 & 0 & +1 \\ 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & +1 & 0 & -1 \\ \hline \end{array} \quad \begin{array}{|ccccc|}\hline 0 & 0 & 0 & 0 & 0 \\ 0 & -1 & 0 & +1 & 0 \\ 0 & 0 & 0 & 0 & 0 \\ 0 & +1 & 0 & 0 & -1 \\ 0 & 0 & 0 & -1 & +1 \\ \hline \end{array} \quad \begin{array}{|ccccc|}\hline 0 & 0 & -1 & +1 & 0 \\ 0 & (0) & +1 & -1 & 0 \\ -1 & +1 & 0 & 0 & 0 \\ +1 & -1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \\ \hline \end{array} \quad \begin{array}{|ccccc|}\hline 0 & 0 & +1 & -1 & 0 \\ 0 & 0 & 0 & 0 & 0 \\ +1 & 0 & 0 & 0 & -1 \\ -1 & 0 & 0 & 0 & +1 \\ 0 & 0 & -1 & +1 & (0) \\ \hline \end{array}$$

- $4 \times 5 \times 5$ move(2) of degree 14 with slice degree $\{3,3,4,4\} \times \{2,3,3,3,3\} \times \{2,3,3,3,3\}$
  $((4,5,5),(14),((3,3,4,4),(2,3,3,3,3),(2,3,3,3,3)),(fcs),\emptyset,((122,135,153,224,242,255,314,323,331,345,413,432,441,454),(123,132,155,222,245,254,313,324,335,341,414,431,442,453)))$

$$
\boxed{\begin{array}{ccccc} 0 & 0 & 0 & 0 & 0 \\ 0 & +1 & -1 & 0 & 0 \\ 0 & -1 & 0 & 0 & +1 \\ 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & +1 & 0 & -1 \end{array}}
\boxed{\begin{array}{ccccc} 0 & 0 & 0 & 0 & 0 \\ 0 & -1 & 0 & +1 & 0 \\ 0 & 0 & 0 & 0 & 0 \\ 0 & +1 & 0 & 0 & -1 \\ 0 & 0 & 0 & -1 & +1 \end{array}}
\boxed{\begin{array}{ccccc} 0 & 0 & -1 & +1 & 0 \\ 0 & 0 & +1 & -1 & 0 \\ +1 & 0 & 0 & 0 & -1 \\ -1 & 0 & 0 & 0 & +1 \\ 0 & 0 & 0 & 0 & 0 \end{array}}
\boxed{\begin{array}{ccccc} 0 & 0 & +1 & -1 & 0 \\ 0 & 0 & 0 & 0 & 0 \\ -1 & +1 & 0 & 0 & 0 \\ +1 & -1 & 0 & 0 & 0 \\ 0 & 0 & -1 & +1 & 0 \end{array}}
$$

- $4 \times 5 \times 6$ move(1) of degree 14 with slice degree $\{2,3,4,5\} \times \{2,3,3,3,3\} \times \{2,2,2,2,2,4\}$
  $((4,5,6),(14),((2,3,4,5),(2,3,3,3,3),(2,2,2,2,2,4)),(fcs),\emptyset,((121,136,216,242,253,324,331,343,355,412,426,435,444,456),(126,131,212,243,256,321,335,344,353,416,424,436,442,455)))$

$$
\boxed{\begin{array}{cccccc} 0 & 0 & 0 & 0 & 0 & 0 \\ +1 & 0 & 0 & 0 & 0 & -1 \\ -1 & 0 & 0 & 0 & 0 & +1 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \end{array}}
\boxed{\begin{array}{cccccc} 0 & -1 & 0 & 0 & 0 & +1 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & +1 & -1 & 0 & 0 & 0 \\ 0 & 0 & +1 & 0 & 0 & -1 \end{array}}
\boxed{\begin{array}{cccccc} 0 & 0 & 0 & 0 & 0 & 0 \\ -1 & 0 & 0 & +1 & 0 & 0 \\ +1 & 0 & 0 & 0 & -1 & 0 \\ 0 & 0 & +1 & -1 & 0 & 0 \\ 0 & 0 & -1 & 0 & +1 & 0 \end{array}}
\boxed{\begin{array}{cccccc} 0 & +1 & 0 & 0 & 0 & -1 \\ 0 & 0 & 0 & -1 & 0 & +1 \\ 0 & 0 & 0 & 0 & +1 & -1 \\ 0 & -1 & 0 & +1 & 0 & 0 \\ 0 & 0 & 0 & 0 & -1 & +1 \end{array}}
$$

- $4 \times 5 \times 6$ move(2) of degree 14 with slice degree $\{2,3,4,5\} \times \{2,3,3,3,3\} \times \{2,2,2,2,2,4\}$
  $((4,5,6),(14),((2,3,4,5),(2,3,3,3,3),(2,2,2,2,2,4)),(fcs),\emptyset,((121,136,212,246,253,326,335,344,356,413,424,431,442,455),(126,131,213,242,256,324,336,346,355,412,421,435,444,453)))$

$$
\boxed{\begin{array}{cccccc} 0 & 0 & 0 & 0 & 0 & 0 \\ +1 & 0 & 0 & 0 & 0 & -1 \\ -1 & 0 & 0 & 0 & 0 & +1 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \end{array}}
\boxed{\begin{array}{cccccc} 0 & +1 & -1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 & 0 & +1 \\ 0 & 0 & +1 & 0 & 0 & -1 \end{array}}
\boxed{\begin{array}{cccccc} 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & -1 & 0 & +1 \\ 0 & 0 & 0 & 0 & +1 & -1 \\ 0 & 0 & 0 & +1 & 0 & -1 \\ 0 & 0 & 0 & 0 & -1 & +1 \end{array}}
\boxed{\begin{array}{cccccc} 0 & -1 & +1 & 0 & 0 & 0 \\ -1 & 0 & 0 & +1 & 0 & 0 \\ +1 & 0 & 0 & 0 & -1 & 0 \\ 0 & +1 & 0 & -1 & 0 & 0 \\ 0 & 0 & -1 & 0 & +1 & 0 \end{array}}
$$

- $4 \times 5 \times 6$ move(3) of degree 14 with slice degree $\{2,3,4,5\} \times \{2,3,3,3,3\} \times \{2,2,2,2,2,4\}$
  (not fundamental, circuit)
  $((4,5,6),(14),((2,3,4,5),(2,3,3,3,3),(2,2,2,2,2,4)),(Fcs),(326,336,446,456),((121,136,212,246,253,324,331,345,356,413,426,435,442,454),(126,131,213,242,256,321,335,346,354,412,424,436,445,453)))$

$$
\boxed{\begin{array}{cccccc} 0 & 0 & 0 & 0 & 0 & 0 \\ +1 & 0 & 0 & 0 & 0 & -1 \\ -1 & 0 & 0 & 0 & 0 & +1 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \end{array}}
\boxed{\begin{array}{cccccc} 0 & +1 & -1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 & 0 & +1 \\ 0 & 0 & +1 & 0 & 0 & -1 \end{array}}
\boxed{\begin{array}{cccccc} 0 & 0 & 0 & 0 & 0 & 0 \\ -1 & 0 & 0 & +1 & 0 & (0) \\ +1 & 0 & 0 & 0 & -1 & (0) \\ 0 & 0 & 0 & 0 & +1 & -1 \\ 0 & 0 & 0 & -1 & 0 & +1 \end{array}}
\boxed{\begin{array}{cccccc} 0 & -1 & +1 & 0 & 0 & 0 \\ 0 & 0 & 0 & -1 & 0 & +1 \\ 0 & 0 & 0 & 0 & +1 & -1 \\ 0 & +1 & 0 & 0 & -1 & (0) \\ 0 & 0 & -1 & +1 & 0 & (0) \end{array}}
$$

- $4 \times 5 \times 6$ move of degree 14 with slice degree $\{3,3,3,5\} \times \{2,2,3,3,4\} \times \{2,2,2,2,2,4\}$
  $((4,5,6),(14),((3,3,3,5),(2,2,3,3,4),(2,2,2,2,2,4)),(fcs),\emptyset,((111,136,152,232,243,254,326,344,355,416,425,433,446,451),(116,132,151,233,244,252,325,346,354,411,426,436,443,455)))$

$$
\boxed{\begin{array}{cccccc} +1 & 0 & 0 & 0 & 0 & -1 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 & 0 & +1 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ -1 & +1 & 0 & 0 & 0 & 0 \end{array}}
\boxed{\begin{array}{cccccc} 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & +1 & -1 & 0 & 0 & 0 \\ 0 & 0 & +1 & -1 & 0 & 0 \\ 0 & -1 & 0 & +1 & 0 & 0 \end{array}}
\boxed{\begin{array}{cccccc} 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & -1 & +1 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & +1 & 0 & -1 \\ 0 & 0 & 0 & -1 & +1 & 0 \end{array}}
\boxed{\begin{array}{cccccc} -1 & 0 & 0 & 0 & 0 & +1 \\ 0 & 0 & 0 & 0 & +1 & -1 \\ 0 & 0 & +1 & 0 & 0 & -1 \\ 0 & 0 & -1 & 0 & 0 & +1 \\ +1 & 0 & 0 & 0 & -1 & 0 \end{array}}
$$

- $4 \times 5 \times 6$ move of degree 14 with slice degree $\{3,3,3,5\} \times \{2,3,3,3,3\} \times \{2,2,2,2,3,3\}$
  $((4,5,6),(14),((3,3,3,5),(2,3,3,3,3),(2,2,2,2,3,3)),(fcs),(456),((111,125,132,226,245,253,335,344,$ $356,412,421,436,443,454),(112,121,135,225,243,256,336,345,354,411,426,432,444,453)))$

$$
\begin{array}{|cccccc|}\hline +1 & -1 & 0 & 0 & 0 & 0 \\ -1 & 0 & 0 & 0 & +1 & 0 \\ 0 & +1 & 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ \hline \end{array}
\begin{array}{|cccccc|}\hline 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & -1 & +1 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & -1 & 0 & +1 & 0 \\ 0 & 0 & +1 & 0 & 0 & -1 \\ \hline \end{array}
\begin{array}{|cccccc|}\hline 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & +1 & -1 \\ 0 & 0 & 0 & +1 & -1 & 0 \\ 0 & 0 & 0 & -1 & 0 & +1 \\ \hline \end{array}
\begin{array}{|cccccc|}\hline -1 & +1 & 0 & 0 & 0 & 0 \\ +1 & 0 & 0 & 0 & 0 & -1 \\ 0 & -1 & 0 & 0 & 0 & +1 \\ 0 & 0 & +1 & -1 & 0 & 0 \\ 0 & 0 & -1 & +1 & 0 & (0) \\ \hline \end{array}
$$

- $4 \times 5 \times 6$ move of degree 14 with slice degree $\{3,3,4,4\} \times \{2,2,2,4,4\} \times \{2,2,2,2,2,4\}$
  $((4,5,6),(14),((3,3,4,4),(2,2,2,4,4),(2,2,2,2,2,4)),(fcs),\emptyset,((111,146,153,226,243,252,316,335,344,$ $351,422,434,446,455),(116,143,151,222,246,253,311,334,346,355,426,435,444,452)))$

$$
\begin{array}{|cccccc|}\hline +1 & 0 & 0 & 0 & 0 & -1 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & -1 & 0 & 0 & +1 \\ -1 & 0 & +1 & 0 & 0 & 0 \\ \hline \end{array}
\begin{array}{|cccccc|}\hline 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 & 0 & +1 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & +1 & 0 & 0 & -1 \\ 0 & +1 & -1 & 0 & 0 & 0 \\ \hline \end{array}
\begin{array}{|cccccc|}\hline -1 & 0 & 0 & 0 & 0 & +1 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & -1 & +1 & 0 \\ 0 & 0 & 0 & +1 & 0 & -1 \\ +1 & 0 & 0 & 0 & -1 & 0 \\ \hline \end{array}
\begin{array}{|cccccc|}\hline 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & +1 & 0 & 0 & 0 & -1 \\ 0 & 0 & 0 & +1 & -1 & 0 \\ 0 & 0 & 0 & -1 & 0 & +1 \\ 0 & -1 & 0 & 0 & +1 & 0 \\ \hline \end{array}
$$

- $4 \times 5 \times 6$ move of degree 14 with slice degree $\{3,3,4,4\} \times \{2,2,2,4,4\} \times \{2,2,2,2,3,3\}$
  $((4,5,6),(14),((3,3,4,4),(2,2,2,4,4),(2,2,2,2,3,3)),(fcs),\emptyset,((111,142,155,226,243,254,315,323,336,$ $341,435,444,452,456),(115,141,152,223,244,256,311,326,335,343,436,442,454,455)))$

$$
\begin{array}{|cccccc|}\hline +1 & 0 & 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ -1 & +1 & 0 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 & +1 & 0 \\ \hline \end{array}
\begin{array}{|cccccc|}\hline 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & -1 & 0 & 0 & +1 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & +1 & -1 & 0 & 0 \\ 0 & 0 & 0 & +1 & 0 & -1 \\ \hline \end{array}
\begin{array}{|cccccc|}\hline -1 & 0 & 0 & 0 & +1 & 0 \\ 0 & 0 & +1 & 0 & 0 & -1 \\ 0 & 0 & 0 & 0 & -1 & +1 \\ +1 & 0 & -1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ \hline \end{array}
\begin{array}{|cccccc|}\hline 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & +1 & -1 \\ 0 & -1 & 0 & +1 & 0 & 0 \\ 0 & +1 & 0 & -1 & -1 & +1 \\ \hline \end{array}
$$

- $4 \times 5 \times 6$ move of degree 14 with slice degree $\{3,3,4,4\} \times \{2,2,3,3,4\} \times \{2,2,2,2,2,4\}$
  $((4,5,6),(14),((3,3,4,4),(2,2,3,3,4),(2,2,2,2,2,4)),(fcs),\emptyset,((111,132,156,223,244,256,316,331,345,$ $354,426,435,443,452),(116,131,152,226,243,254,311,335,344,356,423,432,445,456)))$

$$
\begin{array}{|cccccc|}\hline -1 & 0 & 0 & 0 & 0 & +1 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ +1 & -1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & +1 & 0 & 0 & 0 & -1 \\ \hline \end{array}
\begin{array}{|cccccc|}\hline 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & -1 & 0 & 0 & +1 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & +1 & -1 & 0 & 0 \\ 0 & 0 & 0 & +1 & 0 & -1 \\ \hline \end{array}
\begin{array}{|cccccc|}\hline +1 & 0 & 0 & 0 & 0 & -1 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ -1 & 0 & 0 & 0 & +1 & 0 \\ 0 & 0 & 0 & +1 & -1 & 0 \\ 0 & 0 & 0 & -1 & 0 & +1 \\ \hline \end{array}
\begin{array}{|cccccc|}\hline 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & +1 & 0 & 0 & -1 \\ 0 & +1 & 0 & 0 & -1 & 0 \\ 0 & 0 & -1 & 0 & +1 & 0 \\ 0 & -1 & 0 & 0 & 0 & +1 \\ \hline \end{array}
$$

- $4 \times 5 \times 7$ move(1) of degree 14 with slice degree $\{2,3,4,5\} \times \{2,2,3,3,4\} \times \{2,2,2,2,2,2,2\}$
  $((4,5,7),(14),((2,3,4,5),(2,2,3,3,4),(2,2,2,2,2,2,2)),(fcs),\emptyset,((131,152,213,244,255,327,336,345,351,$ $414,426,432,447,453),(132,151,214,245,253,326,331,347,355,413,427,436,444,452)))$

$$
\begin{array}{|ccccccc|}\hline 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ +1 & -1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ -1 & +1 & 0 & 0 & 0 & 0 & 0 \\ \hline \end{array}
\quad
\begin{array}{|ccccccc|}\hline 0 & 0 & +1 & -1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & +1 & -1 & 0 & 0 \\ 0 & 0 & -1 & 0 & +1 & 0 & 0 \\ \hline \end{array}
$$

$$
\begin{array}{|ccccccc|}\hline 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & -1 & +1 \\ -1 & 0 & 0 & 0 & 0 & +1 & 0 \\ 0 & 0 & 0 & 0 & +1 & 0 & -1 \\ +1 & 0 & 0 & 0 & -1 & 0 & 0 \\ \hline \end{array}
\quad
\begin{array}{|ccccccc|}\hline 0 & 0 & -1 & +1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & +1 & -1 \\ 0 & +1 & 0 & 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & -1 & 0 & 0 & +1 \\ 0 & -1 & +1 & 0 & 0 & 0 & 0 \\ \hline \end{array}
$$

- $4 \times 5 \times 7$ move(2) of degree 14 with slice degree $\{2,3,4,5\} \times \{2,2,3,3,4\} \times \{2,2,2,2,2,2,2\}$
$((4,5,7),(14),((2,3,4,5),(2,2,3,3,4),(2,2,2,2,2,2,2)),(fcs),\emptyset,((132,151,231,243,254,316,327,344,355,415,426,433,447,452),(131,152,233,244,251,315,326,347,354,416,427,432,443,455)))$

$$\begin{array}{|ccccccc|}\hline 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ -1 & +1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ +1 & -1 & 0 & 0 & 0 & 0 & 0 \\ \hline \end{array} \qquad \begin{array}{|ccccccc|}\hline 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ +1 & 0 & -1 & 0 & 0 & 0 & 0 \\ 0 & 0 & +1 & -1 & 0 & 0 & 0 \\ -1 & 0 & 0 & +1 & 0 & 0 & 0 \\ \hline \end{array}$$

$$\begin{array}{|ccccccc|}\hline 0 & 0 & 0 & 0 & -1 & +1 & 0 \\ 0 & 0 & 0 & 0 & 0 & -1 & +1 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & +1 & 0 & 0 & -1 \\ 0 & 0 & 0 & -1 & +1 & 0 & 0 \\ \hline \end{array} \qquad \begin{array}{|ccccccc|}\hline 0 & 0 & 0 & 0 & +1 & -1 & 0 \\ 0 & 0 & 0 & 0 & 0 & +1 & -1 \\ 0 & -1 & +1 & 0 & 0 & 0 & 0 \\ 0 & 0 & -1 & 0 & 0 & 0 & +1 \\ 0 & +1 & 0 & 0 & -1 & 0 & 0 \\ \hline \end{array}$$

- $4 \times 5 \times 7$ move of degree 14 with slice degree $\{2,3,4,5\} \times \{2,3,3,3,3\} \times \{2,2,2,2,2,2,2\}$
$((4,5,7),(14),((2,3,4,5),(2,3,3,3,3),(2,2,2,2,2,2,2)),(fcs),\emptyset,((121,132,214,243,255,326,331,345,357,413,422,437,446,454),(122,131,213,245,254,321,337,346,355,414,426,432,443,457)))$

$$\begin{array}{|ccccccc|}\hline 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ +1 & -1 & 0 & 0 & 0 & 0 & 0 \\ -1 & +1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ \hline \end{array} \qquad \begin{array}{|ccccccc|}\hline 0 & 0 & -1 & +1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & +1 & 0 & -1 & 0 & 0 \\ 0 & 0 & 0 & -1 & +1 & 0 & 0 \\ \hline \end{array}$$

$$\begin{array}{|ccccccc|}\hline 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ -1 & 0 & 0 & 0 & 0 & +1 & 0 \\ +1 & 0 & 0 & 0 & 0 & 0 & -1 \\ 0 & 0 & 0 & 0 & +1 & -1 & 0 \\ 0 & 0 & 0 & 0 & -1 & 0 & +1 \\ \hline \end{array} \qquad \begin{array}{|ccccccc|}\hline 0 & 0 & +1 & -1 & 0 & 0 & 0 \\ 0 & +1 & 0 & 0 & 0 & -1 & 0 \\ 0 & -1 & 0 & 0 & 0 & 0 & +1 \\ 0 & 0 & -1 & 0 & 0 & +1 & 0 \\ 0 & 0 & 0 & +1 & 0 & 0 & -1 \\ \hline \end{array}$$

- $4 \times 5 \times 7$ move of degree 14 with slice degree $\{2,4,4,4\} \times \{2,2,3,3,4\} \times \{2,2,2,2,2,2,2\}$
$((4,5,7),(14),((2,4,4,4),(2,2,3,3,4),(2,2,2,2,2,2,2)),(fcs),\emptyset,((131,152,213,235,244,251,326,332,345,357,414,427,446,453),(132,151,214,231,245,253,327,335,346,352,413,426,444,457)))$

$$\begin{array}{|ccccccc|}\hline 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ +1 & -1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ -1 & +1 & 0 & 0 & 0 & 0 & 0 \\ \hline \end{array} \qquad \begin{array}{|ccccccc|}\hline 0 & 0 & +1 & -1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ -1 & 0 & 0 & 0 & +1 & 0 & 0 \\ 0 & 0 & 0 & +1 & -1 & 0 & 0 \\ +1 & 0 & -1 & 0 & 0 & 0 & 0 \\ \hline \end{array}$$

$$\begin{array}{|ccccccc|}\hline 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & +1 & -1 \\ 0 & +1 & 0 & 0 & -1 & 0 & 0 \\ 0 & 0 & 0 & 0 & +1 & -1 & 0 \\ 0 & -1 & 0 & 0 & 0 & 0 & +1 \\ \hline \end{array} \qquad \begin{array}{|ccccccc|}\hline 0 & 0 & -1 & +1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & -1 & +1 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & -1 & 0 & +1 & 0 \\ 0 & 0 & +1 & 0 & 0 & 0 & -1 \\ \hline \end{array}$$

- $4 \times 5 \times 7$ move of degree 14 with slice degree $\{3,3,3,5\} \times \{2,2,3,3,4\} \times \{2,2,2,2,2,2,2\}$
$((4,5,7),(14),((3,3,3,5),(2,2,3,3,4),(2,2,2,2,2,2,2)),(fcs),\emptyset,((111,133,152,232,245,254,327,344,356,413,426,435,447,451),(113,132,151,235,244,252,326,347,354,411,427,433,445,456)))$

$$\begin{array}{|ccccccc|}\hline +1 & 0 & -1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & -1 & +1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ -1 & +1 & 0 & 0 & 0 & 0 & 0 \\ \hline \end{array} \qquad \begin{array}{|ccccccc|}\hline 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & +1 & 0 & 0 & -1 & 0 & 0 \\ 0 & 0 & 0 & -1 & +1 & 0 & 0 \\ 0 & -1 & 0 & +1 & 0 & 0 & 0 \\ \hline \end{array}$$

$$\begin{array}{|ccccccc|}\hline 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & -1 & +1 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & +1 & 0 & 0 & -1 \\ 0 & 0 & 0 & -1 & 0 & +1 & 0 \\ \hline \end{array} \qquad \begin{array}{|ccccccc|}\hline -1 & 0 & +1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & +1 & -1 \\ 0 & 0 & -1 & 0 & +1 & 0 & 0 \\ 0 & 0 & 0 & 0 & -1 & 0 & +1 \\ +1 & 0 & 0 & 0 & 0 & -1 & 0 \\ \hline \end{array}$$

- $4 \times 5 \times 7$ move of degree 14 with slice degree $\{3,3,4,4\} \times \{2,2,2,4,4\} \times \{2,2,2,2,2,2,2\}$
$((4,5,7),(14),((3,3,4,4),(2,2,2,4,4),(2,2,2,2,2,2,2)),(fcs),\emptyset,((111,143,152,225,244,253,312,336,341,357,424,437,446,455),(112,141,153,224,243,255,311,337,346,352,425,436,444,457)))$

$$\begin{array}{|ccccccc|}\hline +1 & -1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ -1 & 0 & +1 & 0 & 0 & 0 & 0 \\ 0 & +1 & -1 & 0 & 0 & 0 & 0 \\ \hline \end{array} \qquad \begin{array}{|ccccccc|}\hline 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & -1 & +1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & -1 & +1 & 0 & 0 & 0 \\ 0 & 0 & +1 & 0 & -1 & 0 & 0 \\ \hline \end{array}$$

$$\begin{array}{|ccccccc|}\hline -1 & +1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & +1 & -1 \\ +1 & 0 & 0 & 0 & 0 & -1 & 0 \\ 0 & -1 & 0 & 0 & 0 & 0 & +1 \\ \hline \end{array} \qquad \begin{array}{|ccccccc|}\hline 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & +1 & -1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & -1 & +1 \\ 0 & 0 & 0 & -1 & 0 & +1 & 0 \\ 0 & 0 & 0 & 0 & +1 & 0 & -1 \\ \hline \end{array}$$

- $4 \times 5 \times 7$ move of degree 14 with slice degree $\{3,3,4,4\} \times \{2,2,3,3,4\} \times \{2,2,2,2,2,2,2\}$
$((4,5,7),(14),((3,3,4,4),(2,2,3,3,4),(2,2,2,2,2,2,2)),(fcs),\emptyset,((111,132,153,224,245,256,312,337,346,351,425,433,447,454),(112,133,151,225,246,254,311,332,347,356,424,437,445,453)))$

$$\begin{array}{|ccccccc|}\hline +1 & -1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & +1 & -1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ -1 & 0 & +1 & 0 & 0 & 0 & 0 \\ \hline \end{array} \qquad \begin{array}{|ccccccc|}\hline 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & +1 & -1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & +1 & -1 & 0 \\ 0 & 0 & 0 & -1 & 0 & +1 & 0 \\ \hline \end{array}$$

$$\begin{array}{|ccccccc|}\hline -1 & +1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 & 0 & 0 & +1 \\ 0 & 0 & 0 & 0 & 0 & +1 & -1 \\ +1 & 0 & 0 & 0 & 0 & -1 & 0 \\ \hline \end{array} \qquad \begin{array}{|ccccccc|}\hline 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & -1 & +1 & 0 & 0 \\ 0 & 0 & +1 & 0 & 0 & 0 & -1 \\ 0 & 0 & 0 & 0 & -1 & 0 & +1 \\ 0 & 0 & -1 & +1 & 0 & 0 & 0 \\ \hline \end{array}$$

- $4 \times 6 \times 6$ move of degree 14 with slice degree $\{3, 3, 4, 4\} \times \{2, 2, 2, 2, 3, 3\} \times \{2, 2, 2, 2, 2, 4\}$
  $((4, 6, 6), (14), ((3, 3, 4, 4), (2, 2, 2, 2, 3, 3), (2, 2, 2, 2, 2, 4)), (fcs), \emptyset, ((111, 126, 152, 233, 246, 264, 322, 336, 355, 363, 416, 444, 451, 465), (116, 122, 151, 236, 244, 263, 326, 333, 352, 365, 411, 446, 455, 464)))$

+1	0	0	0	0	−1
0	−1	0	0	0	+1
0	0	0	0	0	0
0	0	0	0	0	0
−1	+1	0	0	0	0
0	0	0	0	0	0

0	0	0	0	0	0
0	0	0	0	0	0
0	0	+1	0	0	−1
0	0	0	−1	0	+1
0	0	0	0	0	0
0	0	−1	+1	0	0

0	0	0	0	0	0
0	+1	0	0	0	−1
0	0	−1	0	0	+1
0	0	0	0	0	0
0	−1	0	0	+1	0
0	0	+1	0	−1	0

−1	0	0	0	0	+1
0	0	0	0	0	0
0	0	0	0	0	0
0	0	0	+1	0	−1
+1	0	0	0	−1	0
0	0	0	−1	+1	0

- $5 \times 5 \times 5$ move of degree 14 with slice degree $\{2, 2, 2, 4, 4\} \times \{2, 2, 3, 3, 4\} \times \{2, 3, 3, 3, 3\}$
  $((5, 5, 5), (14), ((2, 2, 2, 4, 4), (2, 2, 3, 3, 4), (2, 3, 3, 3, 3)), (fcs), \emptyset, ((131, 145, 242, 255, 313, 354, 424, 435, 452, 453, 514, 522, 533, 541), (135, 141, 245, 252, 314, 353, 422, 433, 454, 455, 513, 524, 531, 542)))$

0	0	0	0	0
0	0	0	0	0
+1	0	0	0	−1
−1	0	0	0	+1
0	0	0	0	0

0	0	0	0	0
0	0	0	0	0
0	0	0	0	0
0	+1	0	0	−1
0	−1	0	0	+1

0	0	+1	−1	0
0	0	0	0	0
0	0	0	0	0
0	0	0	0	0
0	0	−1	+1	0

0	0	0	0	0
0	−1	0	+1	0
0	0	−1	0	+1
0	0	0	0	0
0	+1	+1	−1	−1

0	0	−1	+1	0
0	+1	0	−1	0
−1	0	+1	0	0
+1	−1	0	0	0
0	0	0	0	0

- $5 \times 5 \times 5$ move(1) of degree 14 with slice degree $\{2, 2, 3, 3, 4\} \times \{2, 3, 3, 3, 3\} \times \{2, 3, 3, 3, 3\}$
  $((5, 5, 5), (14), ((2, 2, 3, 3, 4), (2, 3, 3, 3, 3), (2, 3, 3, 3, 3)), (fcs), (555), ((112, 123, 231, 244, 322, 334, 355, 424, 445, 453, 513, 535, 541, 552), (113, 122, 234, 241, 324, 335, 352, 423, 444, 455, 512, 531, 545, 553)))$

0	+1	−1	0	0
0	−1	+1	0	0
0	0	0	0	0
0	0	0	0	0
0	0	0	0	0

0	0	0	0	0
0	0	0	0	0
+1	0	0	−1	0
−1	0	0	+1	0
0	0	0	0	0

0	0	0	0	0
0	+1	0	−1	0
0	0	0	+1	−1
0	0	0	0	0
0	−1	0	0	+1

0	0	0	0	0
0	0	−1	+1	0
0	0	0	0	0
0	0	0	−1	+1
0	0	+1	0	−1

0	−1	+1	0	0
0	0	0	0	0
−1	0	0	0	+1
+1	0	0	0	−1
0	+1	−1	0	(0)

- $5 \times 5 \times 5$ move(2) of degree 14 with slice degree $\{2,2,3,3,4\} \times \{2,3,3,3,3\} \times \{2,3,3,3,3\}$
  $((5,5,5),(14),((2,2,3,3,4),(2,3,3,3,3),(2,3,3,3,3)),(fcs),\emptyset,((112,123,231,244,322,345,354,425,434,453,513,535,541,552),(113,122,234,241,325,344,352,423,435,454,512,531,545,553)))$

$$\begin{array}{|ccccc|}\hline 0 & +1 & -1 & 0 & 0 \\ 0 & -1 & +1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \\ \hline\end{array} \quad \begin{array}{|ccccc|}\hline 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \\ +1 & 0 & 0 & -1 & 0 \\ -1 & 0 & 0 & +1 & 0 \\ 0 & 0 & 0 & 0 & 0 \\ \hline\end{array} \quad \begin{array}{|ccccc|}\hline 0 & 0 & 0 & 0 & 0 \\ 0 & +1 & 0 & 0 & -1 \\ 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & -1 & +1 \\ 0 & -1 & 0 & +1 & 0 \\ \hline\end{array}$$

$$\begin{array}{|ccccc|}\hline 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & -1 & 0 & +1 \\ 0 & 0 & 0 & +1 & -1 \\ 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & +1 & -1 & 0 \\ \hline\end{array} \quad \begin{array}{|ccccc|}\hline 0 & -1 & +1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \\ -1 & 0 & 0 & 0 & +1 \\ +1 & 0 & 0 & 0 & -1 \\ 0 & +1 & -1 & 0 & 0 \\ \hline\end{array}$$

- $5 \times 5 \times 5$ move(3) of degree 14 with slice degree $\{2,2,3,3,4\} \times \{2,3,3,3,3\} \times \{2,3,3,3,3\}$
  $((5,5,5),(14),((2,2,3,3,4),(2,3,3,3,3),(2,3,3,3,3)),(fcs),\emptyset,((121,135,213,252,334,345,353,425,442,454,512,524,531,543),(125,131,212,253,335,343,354,424,445,452,513,521,534,542)))$

$$\begin{array}{|ccccc|}\hline 0 & 0 & 0 & 0 & 0 \\ +1 & 0 & 0 & 0 & -1 \\ -1 & 0 & 0 & 0 & +1 \\ 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \\ \hline\end{array} \quad \begin{array}{|ccccc|}\hline 0 & -1 & +1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \\ 0 & +1 & -1 & 0 & 0 \\ \hline\end{array} \quad \begin{array}{|ccccc|}\hline 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & +1 & -1 \\ 0 & 0 & -1 & 0 & +1 \\ 0 & 0 & +1 & -1 & 0 \\ \hline\end{array}$$

$$\begin{array}{|ccccc|}\hline 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & -1 & +1 \\ 0 & 0 & 0 & 0 & 0 \\ 0 & +1 & 0 & 0 & -1 \\ 0 & -1 & 0 & +1 & 0 \\ \hline\end{array} \quad \begin{array}{|ccccc|}\hline 0 & +1 & -1 & 0 & 0 \\ -1 & 0 & 0 & +1 & 0 \\ +1 & 0 & 0 & -1 & 0 \\ 0 & -1 & +1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \\ \hline\end{array}$$

- $5 \times 5 \times 6$ move of degree 14 with slice degree $\{2,2,3,3,4\} \times \{2,3,3,3,3\} \times \{2,2,2,2,2,4\}$
  $((5,5,6),(14),((2,2,3,3,4),(2,3,3,3,3),(2,2,2,2,2,4)),(fcs),\emptyset,((121,136,232,246,316,344,353,413,426,455,525,531,542,554),(126,131,236,242,313,346,354,416,425,453,521,532,544,555)))$

$$\begin{array}{|cccccc|}\hline 0 & 0 & 0 & 0 & 0 & 0 \\ -1 & 0 & 0 & 0 & 0 & +1 \\ +1 & 0 & 0 & 0 & 0 & -1 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ \hline\end{array} \quad \begin{array}{|cccccc|}\hline 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 & 0 & +1 \\ 0 & +1 & 0 & 0 & 0 & -1 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ \hline\end{array} \quad \begin{array}{|cccccc|}\hline 0 & 0 & +1 & 0 & 0 & -1 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & -1 & 0 & +1 \\ 0 & 0 & -1 & +1 & 0 & 0 \\ \hline\end{array}$$

$$\begin{array}{|cccccc|}\hline 0 & 0 & -1 & 0 & 0 & +1 \\ 0 & 0 & 0 & 0 & +1 & -1 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & +1 & 0 & -1 & 0 \\ \hline\end{array} \quad \begin{array}{|cccccc|}\hline 0 & 0 & 0 & 0 & 0 & 0 \\ +1 & 0 & 0 & 0 & -1 & 0 \\ -1 & +1 & 0 & 0 & 0 & 0 \\ 0 & -1 & 0 & +1 & 0 & 0 \\ 0 & 0 & 0 & -1 & +1 & 0 \\ \hline\end{array}$$

- $5 \times 5 \times 6$ move of degree 14 with slice degree $\{2,3,3,3,3\} \times \{2,3,3,3,3\} \times \{2,2,2,2,3,3\}$
  $((5,5,6),(14),((2,3,3,3,3),(2,3,3,3,3),(2,2,2,2,3,3)),(fcs),\emptyset,((121,132,213,245,254,314,343,356,425,431,446,522,536,555),(122,131,214,243,255,313,346,354,421,436,445,525,532,556)))$

0	0	0	0	0	0
+1	−1	0	0	0	0
−1	+1	0	0	0	0
0	0	0	0	0	0
0	0	0	0	0	0

0	0	+1	−1	0	0
0	0	0	0	0	0
0	0	0	0	0	0
0	0	−1	0	+1	0
0	0	0	+1	−1	0

0	0	−1	+1	0	0
0	0	0	0	0	0
0	0	0	0	0	0
0	0	+1	0	0	−1
0	0	0	−1	0	+1

0	0	0	0	0	0
−1	0	0	0	+1	0
+1	0	0	0	0	−1
0	0	0	0	−1	+1
0	0	0	0	0	0

0	0	0	0	0	0
0	+1	0	0	−1	0
0	−1	0	0	0	+1
0	0	0	0	0	0
0	0	0	0	+1	−1

A.5 Indispensable moves of degree 15

- $3 \times 5 \times 7$ move of degree 15 with slice degree $\{4,5,6\} \times \{2,3,3,3,4\} \times \{2,2,2,2,2,2,3\}$
  (not fundamental, circuit)
  $((3,5,7),(15),((4,5,6),(2,3,3,3,4),(2,2,2,2,2,2,3)),(Fcs),(257,337),((121,137,142,153,217,222,236,244,255,314,325,331,343,356,357),(122,131,143,157,214,225,237,242,256,317,321,336,344,353,355)))$

0	0	0	0	0	0	0
+1	−1	0	0	0	0	0
−1	0	0	0	0	0	+1
0	+1	−1	0	0	0	0
0	0	+1	0	0	0	−1

0	0	0	−1	0	0	+1
0	+1	0	0	−1	0	0
0	0	0	0	0	+1	−1
0	−1	0	+1	0	0	0
0	0	0	0	+1	−1	(0)

0	0	0	+1	0	0	−1
−1	0	0	0	+1	0	0
+1	0	0	0	0	−1	(0)
0	0	+1	−1	0	0	0
0	0	−1	0	−1	+1	+1

- $4 \times 4 \times 7$ move of degree 15 with slice degree $\{2,4,4,5\} \times \{3,3,4,5\} \times \{2,2,2,2,2,2,3\}$
  (not fundamental, circuit)
  $((4,4,7),(15),((2,4,4,5),(3,3,4,5),(2,2,2,2,2,2,3)),(Fcs),(347,437),((131,147,213,222,234,241,312,326,337,345,417,424,435,443,446),(137,141,212,224,231,243,317,322,335,346,413,426,434,445,447)))$

0	0	0	0	0	0	0
0	0	0	0	0	0	0
−1	0	0	0	0	0	+1
+1	0	0	0	0	0	−1

0	+1	−1	0	0	0	0
0	−1	0	+1	0	0	0
+1	0	0	−1	0	0	0
−1	0	+1	0	0	0	0

0	−1	0	0	0	0	+1
0	+1	0	0	0	−1	0
0	0	0	0	+1	0	−1
0	0	0	0	−1	+1	(0)

0	0	+1	0	0	0	−1
0	0	0	−1	0	+1	0
0	0	0	+1	−1	0	(0)
0	0	−1	0	+1	−1	+1

- $4 \times 4 \times 7$ move(1) of degree 15 with slice degree $\{3,3,4,5\} \times \{3,3,4,5\} \times \{2,2,2,2,2,2,3\}$
(not fundamental, circuit)
$((4,4,7),(15),((3,3,4,5),(3,3,4,5),(2,2,2,2,2,2,3)),(Fcs),(147,437),((111,137,142,223,234,247,315,$
$324,336,341,417,425,432,443,446),(117,132,141,224,237,243,311,325,334,346,415,423,436,442,447)))$

$$
\begin{array}{|ccccccc|}\hline
+1 & 0 & 0 & 0 & 0 & 0 & -1 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & -1 & 0 & 0 & 0 & 0 & +1 \\
-1 & +1 & 0 & 0 & 0 & 0 & (0) \\ \hline
\end{array}
\quad
\begin{array}{|ccccccc|}\hline
0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & +1 & -1 & 0 & 0 & 0 \\
0 & 0 & 0 & +1 & 0 & 0 & -1 \\
0 & 0 & -1 & 0 & 0 & 0 & +1 \\ \hline
\end{array}
$$

$$
\begin{array}{|ccccccc|}\hline
-1 & 0 & 0 & 0 & +1 & 0 & 0 \\
0 & 0 & 0 & +1 & -1 & 0 & 0 \\
0 & 0 & 0 & -1 & 0 & +1 & 0 \\
+1 & 0 & 0 & 0 & 0 & -1 & 0 \\ \hline
\end{array}
\quad
\begin{array}{|ccccccc|}\hline
0 & 0 & 0 & 0 & -1 & 0 & +1 \\
0 & 0 & -1 & 0 & +1 & 0 & 0 \\
0 & +1 & 0 & 0 & 0 & -1 & (0) \\
0 & -1 & +1 & 0 & 0 & +1 & -1 \\ \hline
\end{array}
$$

- $4 \times 4 \times 7$ move(2) of degree 15 with slice degree $\{3,3,4,5\} \times \{3,3,4,5\} \times \{2,2,2,2,2,2,3\}$
(not fundamental, circuit)
$((4,4,7),(15),((3,3,4,5),(3,3,4,5),(2,2,2,2,2,2,3)),(Fcs),(247,437),((111,137,142,227,234,243,315,$
$323,331,346,412,425,436,444,447),(112,131,147,223,237,244,311,325,336,343,415,427,434,442,446)))$

$$
\begin{array}{|ccccccc|}\hline
+1 & -1 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 \\
-1 & 0 & 0 & 0 & 0 & 0 & +1 \\
0 & +1 & 0 & 0 & 0 & 0 & -1 \\ \hline
\end{array}
\quad
\begin{array}{|ccccccc|}\hline
0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & -1 & 0 & 0 & 0 & +1 \\
0 & 0 & 0 & +1 & 0 & 0 & -1 \\
0 & 0 & +1 & -1 & 0 & 0 & (0) \\ \hline
\end{array}
$$

$$
\begin{array}{|ccccccc|}\hline
-1 & 0 & 0 & 0 & +1 & 0 & 0 \\
0 & 0 & +1 & 0 & -1 & 0 & 0 \\
+1 & 0 & 0 & 0 & 0 & -1 & 0 \\
0 & 0 & -1 & 0 & 0 & +1 & 0 \\ \hline
\end{array}
\quad
\begin{array}{|ccccccc|}\hline
0 & +1 & 0 & 0 & -1 & 0 & 0 \\
0 & 0 & 0 & 0 & +1 & 0 & -1 \\
0 & 0 & 0 & -1 & 0 & +1 & (0) \\
0 & -1 & 0 & +1 & 0 & -1 & +1 \\ \hline
\end{array}
$$

- $4 \times 5 \times 6$ move of degree 15 with slice degree $\{3,3,4,5\} \times \{2,2,3,3,5\} \times \{2,2,2,2,3,4\}$
$((4,5,6),(15),((3,3,4,5),(2,2,3,3,5),(2,2,2,2,3,4)),(fcS),\emptyset,((111,125,156,234,243,256,315,333,342,$
$351,426,435,446,452,454),(115,126,151,233,246,254,311,335,343,352,425,434,442,456,456)))$

$$
\begin{array}{|cccccc|}\hline
+1 & 0 & 0 & 0 & -1 & 0 \\
0 & 0 & 0 & 0 & +1 & -1 \\
0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 \\
-1 & 0 & 0 & 0 & 0 & +1 \\ \hline
\end{array}
\quad
\begin{array}{|cccccc|}\hline
0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & -1 & +1 & 0 & 0 \\
0 & 0 & +1 & 0 & 0 & -1 \\
0 & 0 & 0 & -1 & 0 & +1 \\ \hline
\end{array}
\quad
\begin{array}{|cccccc|}\hline
-1 & 0 & 0 & 0 & +1 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & +1 & 0 & -1 & 0 \\
0 & +1 & -1 & 0 & 0 & 0 \\
+1 & -1 & 0 & 0 & 0 & 0 \\ \hline
\end{array}
\quad
\begin{array}{|cccccc|}\hline
0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & -1 & +1 \\
0 & 0 & 0 & -1 & +1 & 0 \\
0 & -1 & 0 & 0 & 0 & +1 \\
0 & +1 & 0 & +1 & 0 & -2 \\ \hline
\end{array}
$$

- $4 \times 5 \times 7$ move(1) of degree 15 with slice degree $\{2,4,4,5\} \times \{2,3,3,3,4\} \times \{2,2,2,2,2,2,3\}$
$((4,5,7),(15),((2,4,4,5),(2,3,3,3,4),(2,2,2,2,2,2,3)),(fcs),(457),((121,157,222,234,243,251,316,337,$
$344,355,415,427,432,446,453),(127,151,221,232,244,253,315,334,346,357,416,422,437,443,455)))$

$$
\begin{array}{|ccccccc|}\hline
0 & 0 & 0 & 0 & 0 & 0 & 0 \\
+1 & 0 & 0 & 0 & 0 & 0 & -1 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 \\
-1 & 0 & 0 & 0 & 0 & 0 & +1 \\ \hline
\end{array}
\quad
\begin{array}{|ccccccc|}\hline
0 & 0 & 0 & 0 & 0 & 0 & 0 \\
-1 & +1 & 0 & 0 & 0 & 0 & 0 \\
0 & -1 & 0 & +1 & 0 & 0 & 0 \\
0 & 0 & +1 & -1 & 0 & 0 & 0 \\
+1 & 0 & -1 & 0 & 0 & 0 & 0 \\ \hline
\end{array}
$$

$$
\begin{array}{|ccccccc|}\hline
0 & 0 & 0 & 0 & -1 & +1 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & -1 & 0 & 0 & +1 \\
0 & 0 & 0 & +1 & 0 & -1 & 0 \\
0 & 0 & 0 & 0 & +1 & 0 & -1 \\ \hline
\end{array}
\quad
\begin{array}{|ccccccc|}\hline
0 & 0 & 0 & 0 & +1 & -1 & 0 \\
0 & -1 & 0 & 0 & 0 & 0 & +1 \\
0 & +1 & 0 & 0 & 0 & 0 & -1 \\
0 & 0 & -1 & 0 & 0 & +1 & 0 \\
0 & 0 & +1 & 0 & -1 & 0 & (0) \\ \hline
\end{array}
$$

- $4 \times 5 \times 7$ move(2) of degree 15 with slice degree $\{2,4,4,5\} \times \{2,3,3,3,4\} \times \{2,2,2,2,2,2,3\}$
  $((4,5,7),(15),((2,4,4,5),(2,3,3,3,4),(2,2,2,2,2,2,3)),(fcs),(457),((121,157,222,234,243,251,317,335,344,356,415,427,432,446,453),(127,151,221,232,244,253,315,334,346,357,417,422,435,443,456)))$

$$\begin{array}{|ccccccc|}\hline 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ +1 & 0 & 0 & 0 & 0 & 0 & -1 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ -1 & 0 & 0 & 0 & 0 & 0 & +1 \\ \hline\end{array} \quad \begin{array}{|ccccccc|}\hline 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ -1 & +1 & 0 & 0 & 0 & 0 & 0 \\ 0 & -1 & 0 & +1 & 0 & 0 & 0 \\ 0 & 0 & +1 & -1 & 0 & 0 & 0 \\ +1 & 0 & -1 & 0 & 0 & 0 & 0 \\ \hline\end{array}$$

$$\begin{array}{|ccccccc|}\hline 0 & 0 & 0 & 0 & -1 & 0 & +1 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & -1 & +1 & 0 & 0 \\ 0 & 0 & 0 & +1 & 0 & -1 & 0 \\ 0 & 0 & 0 & 0 & 0 & +1 & -1 \\ \hline\end{array} \quad \begin{array}{|ccccccc|}\hline 0 & 0 & 0 & 0 & +1 & 0 & -1 \\ 0 & -1 & 0 & 0 & 0 & 0 & +1 \\ 0 & +1 & 0 & 0 & -1 & 0 & 0 \\ 0 & 0 & -1 & 0 & 0 & +1 & 0 \\ 0 & 0 & +1 & 0 & 0 & -1 & (0) \\ \hline\end{array}$$

- $4 \times 5 \times 7$ move of degree 15 with slice degree $\{3,3,4,5\} \times \{2,2,3,3,5\} \times \{2,2,2,2,2,2,3\}$
  $((4,5,7),(15),((3,3,4,5),(2,2,3,3,5),(2,2,2,2,2,2,3)),(fcs),\emptyset,((111,127,152,233,245,254,317,336,343,351,422,434,447,455,456),(117,122,151,234,243,255,311,333,347,356,427,436,445,452,454)))$

$$\begin{array}{|ccccccc|}\hline +1 & 0 & 0 & 0 & 0 & 0 & -1 \\ 0 & -1 & 0 & 0 & 0 & 0 & +1 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ -1 & +1 & 0 & 0 & 0 & 0 & 0 \\ \hline\end{array} \quad \begin{array}{|ccccccc|}\hline 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & +1 & -1 & 0 & 0 & 0 \\ 0 & 0 & -1 & 0 & +1 & 0 & 0 \\ 0 & 0 & 0 & +1 & -1 & 0 & 0 \\ \hline\end{array}$$

$$\begin{array}{|ccccccc|}\hline -1 & 0 & 0 & 0 & 0 & 0 & +1 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & -1 & 0 & 0 & +1 & 0 \\ 0 & 0 & +1 & 0 & 0 & 0 & -1 \\ +1 & 0 & 0 & 0 & 0 & -1 & 0 \\ \hline\end{array} \quad \begin{array}{|ccccccc|}\hline 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & +1 & 0 & 0 & 0 & 0 & -1 \\ 0 & 0 & 0 & +1 & 0 & -1 & 0 \\ 0 & 0 & 0 & 0 & -1 & 0 & +1 \\ 0 & -1 & 0 & -1 & +1 & +1 & 0 \\ \hline\end{array}$$

- $4 \times 5 \times 7$ move(1) of degree 15 with slice degree $\{3,3,4,5\} \times \{2,3,3,3,4\} \times \{2,2,2,2,2,2,3\}$
  $((4,5,7),(15),((3,3,4,5),(2,3,3,3,4),(2,2,2,2,2,2,3)),(fcs),(457),((111,122,157,233,247,254,326,335,343,352,417,421,434,456,455),(117,121,152,234,243,257,322,333,346,355,411,426,435,447,454)))$

$$\begin{array}{|ccccccc|}\hline +1 & 0 & 0 & 0 & 0 & 0 & -1 \\ -1 & +1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 & 0 & 0 & +1 \\ \hline\end{array} \quad \begin{array}{|ccccccc|}\hline 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & +1 & -1 & 0 & 0 & 0 \\ 0 & 0 & -1 & 0 & 0 & 0 & +1 \\ 0 & 0 & 0 & +1 & 0 & 0 & -1 \\ \hline\end{array}$$

$$\begin{array}{|ccccccc|}\hline 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 & 0 & +1 & 0 \\ 0 & 0 & -1 & 0 & +1 & 0 & 0 \\ 0 & 0 & +1 & 0 & 0 & -1 & 0 \\ 0 & +1 & 0 & 0 & -1 & 0 & 0 \\ \hline\end{array} \quad \begin{array}{|ccccccc|}\hline -1 & 0 & 0 & 0 & 0 & 0 & +1 \\ +1 & 0 & 0 & 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & +1 & -1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & +1 & -1 \\ 0 & 0 & 0 & -1 & +1 & 0 & (0) \\ \hline\end{array}$$

- $4 \times 5 \times 7$ move(2) of degree 15 with slice degree $\{3,3,4,5\} \times \{2,3,3,3,4\} \times \{2,2,2,2,2,2,3\}$
$((4,5,7),(15),((3,3,4,5),(2,3,3,3,4),(2,2,2,2,2,2,3)),(fcs),(457),((111,122,157,233,245,254,326,337,$ $343,352,417,421,434,446,455),(117,121,152,234,243,255,322,333,346,357,411,426,437,445,454)))$

$$\begin{array}{|ccccccc|}\hline +1 & 0 & 0 & 0 & 0 & 0 & -1 \\ -1 & +1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 & 0 & 0 & +1 \\ \hline \end{array} \quad \begin{array}{|ccccccc|}\hline 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & +1 & -1 & 0 & 0 & 0 \\ 0 & 0 & -1 & 0 & +1 & 0 & 0 \\ 0 & 0 & 0 & +1 & -1 & 0 & 0 \\ \hline \end{array}$$

$$\begin{array}{|ccccccc|}\hline 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 & 0 & +1 & 0 \\ 0 & 0 & -1 & 0 & 0 & 0 & +1 \\ 0 & 0 & +1 & 0 & 0 & -1 & 0 \\ 0 & +1 & 0 & 0 & 0 & 0 & -1 \\ \hline \end{array} \quad \begin{array}{|ccccccc|}\hline -1 & 0 & 0 & 0 & 0 & 0 & +1 \\ +1 & 0 & 0 & 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & +1 & 0 & 0 & -1 \\ 0 & 0 & 0 & 0 & -1 & +1 & 0 \\ 0 & 0 & 0 & -1 & +1 & 0 & (0) \\ \hline \end{array}$$

- $4 \times 5 \times 7$ move of degree 15 with slice degree $\{3,3,4,5\} \times \{3,3,3,3,3\} \times \{2,2,2,2,2,2,3\}$
$((4,5,7),(15),((3,3,4,5),(3,3,3,3,3),(2,2,2,2,2,2,3)),(fcs),(437),((111,127,132,237,243,254,315,321,$ $346,353,412,426,434,447,455),(112,121,137,234,247,253,311,326,343,355,415,427,432,446,454)))$

$$\begin{array}{|ccccccc|}\hline +1 & -1 & 0 & 0 & 0 & 0 & 0 \\ -1 & 0 & 0 & 0 & 0 & 0 & +1 \\ 0 & +1 & 0 & 0 & 0 & 0 & -1 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ \hline \end{array} \quad \begin{array}{|ccccccc|}\hline 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & -1 & 0 & 0 & +1 \\ 0 & 0 & +1 & 0 & 0 & 0 & -1 \\ 0 & 0 & -1 & +1 & 0 & 0 & 0 \\ \hline \end{array}$$

$$\begin{array}{|ccccccc|}\hline -1 & 0 & 0 & 0 & +1 & 0 & 0 \\ +1 & 0 & 0 & 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & -1 & 0 & 0 & +1 & 0 \\ 0 & 0 & +1 & 0 & -1 & 0 & 0 \\ \hline \end{array} \quad \begin{array}{|ccccccc|}\hline 0 & +1 & 0 & 0 & -1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & +1 & -1 \\ 0 & -1 & 0 & +1 & 0 & 0 & (0) \\ 0 & 0 & 0 & 0 & 0 & -1 & +1 \\ 0 & 0 & 0 & -1 & +1 & 0 & 0 \\ \hline \end{array}$$

- $4 \times 5 \times 7$ move of degree 15 with slice degree $\{3,4,4,4\} \times \{2,3,3,3,4\} \times \{2,2,2,2,2,2,3\}$
$((4,5,7),(15),((3,4,4,4),(2,3,3,3,4),(2,2,2,2,2,2,3)),(fcs),(457),((122,131,157,221,234,243,255,317,$ $323,346,352,416,437,445,454),(121,137,152,223,231,245,254,316,322,343,357,417,434,446,455)))$

$$\begin{array}{|ccccccc|}\hline 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ -1 & +1 & 0 & 0 & 0 & 0 & 0 \\ +1 & 0 & 0 & 0 & 0 & 0 & -1 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 & 0 & 0 & +1 \\ \hline \end{array} \quad \begin{array}{|ccccccc|}\hline 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ +1 & 0 & -1 & 0 & 0 & 0 & 0 \\ -1 & 0 & 0 & +1 & 0 & 0 & 0 \\ 0 & 0 & +1 & 0 & -1 & 0 & 0 \\ 0 & 0 & 0 & -1 & +1 & 0 & 0 \\ \hline \end{array}$$

$$\begin{array}{|ccccccc|}\hline 0 & 0 & 0 & 0 & 0 & -1 & +1 \\ 0 & -1 & +1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & -1 & 0 & 0 & +1 & 0 \\ 0 & +1 & 0 & 0 & 0 & 0 & -1 \\ \hline \end{array} \quad \begin{array}{|ccccccc|}\hline 0 & 0 & 0 & 0 & 0 & +1 & -1 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & -1 & 0 & 0 & +1 \\ 0 & 0 & 0 & 0 & +1 & -1 & 0 \\ 0 & 0 & 0 & +1 & -1 & 0 & (0) \\ \hline \end{array}$$

- $4 \times 6 \times 6$ move of degree 15 with slice degree $\{2,4,4,5\} \times \{2,2,2,3,3,3\} \times \{2,2,2,2,3,4\}$
$((4,6,6),(15),((2,4,4,5),(2,2,2,3,3,3),(2,2,2,2,3,4)),(fcs),\emptyset,((141,156,215,243,251,262,312,325,336,$
$364,426,434,446,455,463),(146,151,212,241,255,263,315,326,334,362,425,436,443,456,464)))$

$$\begin{array}{|cccccc|}\hline 0&0&0&0&0&0\\ 0&0&0&0&0&0\\ 0&0&0&0&0&0\\ +1&0&0&0&0&-1\\ -1&0&0&0&0&+1\\ 0&0&0&0&0&0\\ \hline\end{array}\quad \begin{array}{|cccccc|}\hline 0&-1&0&0&+1&0\\ 0&0&0&0&0&0\\ 0&0&0&0&0&0\\ -1&0&+1&0&0&0\\ +1&0&0&0&-1&0\\ 0&+1&-1&0&0&0\\ \hline\end{array}\quad \begin{array}{|cccccc|}\hline 0&+1&0&0&-1&0\\ 0&0&0&0&+1&-1\\ 0&0&0&-1&0&+1\\ 0&0&0&0&0&0\\ 0&0&0&0&0&0\\ 0&-1&0&+1&0&0\\ \hline\end{array}\quad \begin{array}{|cccccc|}\hline 0&0&0&0&0&0\\ 0&0&0&0&-1&+1\\ 0&0&0&+1&0&-1\\ 0&0&-1&0&0&+1\\ 0&0&0&0&+1&-1\\ 0&0&+1&-1&0&0\\ \hline\end{array}$$

- $4 \times 6 \times 6$ move of degree 15 with slice degree $\{3,3,3,6\} \times \{2,2,2,2,3,4\} \times \{2,2,2,3,3,3\}$
(not fundamental, circuit)
$((4,6,6),(15),((3,3,3,6),(2,2,2,2,3,4),(2,2,2,3,3,3)),(Fcs),(456),((111,125,164,236,253,262,324,345,$
$356,415,432,446,454,461,463),(115,124,161,232,256,263,325,346,354,411,436,445,453,462,464)))$

$$\begin{array}{|cccccc|}\hline +1&0&0&0&-1&0\\ 0&0&0&-1&+1&0\\ 0&0&0&0&0&0\\ 0&0&0&0&0&0\\ 0&0&0&0&0&0\\ -1&0&0&+1&0&0\\ \hline\end{array}\quad \begin{array}{|cccccc|}\hline 0&0&0&0&0&0\\ 0&0&0&0&0&0\\ 0&-1&0&0&0&+1\\ 0&0&0&0&0&0\\ 0&0&+1&0&0&-1\\ 0&+1&-1&0&0&0\\ \hline\end{array}\quad \begin{array}{|cccccc|}\hline 0&0&0&0&0&0\\ 0&0&0&+1&-1&0\\ 0&0&0&0&0&0\\ 0&0&0&0&+1&-1\\ 0&0&0&-1&0&+1\\ 0&0&0&0&0&0\\ \hline\end{array}\quad \begin{array}{|cccccc|}\hline -1&0&0&0&+1&0\\ 0&0&0&0&0&0\\ 0&+1&0&0&0&-1\\ 0&0&0&0&-1&+1\\ 0&0&-1&+1&0&(0)\\ +1&-1&+1&-1&0&0\\ \hline\end{array}$$

- $4 \times 6 \times 6$ move of degree 15 with slice degree $\{3,3,4,5\} \times \{2,2,2,2,3,4\} \times \{2,2,2,3,3,3\}$
$((4,6,6),(15),((3,3,4,5),(2,2,2,2,3,4),(2,2,2,3,3,3)),(fcs),\emptyset,((142,151,164,216,225,263,315,336,344,$
$352,423,434,455,461,466),(144,152,161,215,223,266,316,334,342,355,425,436,451,463,464)))$

$$\begin{array}{|cccccc|}\hline 0&0&0&0&0&0\\ 0&0&0&0&0&0\\ 0&0&0&0&0&0\\ 0&+1&0&-1&0&0\\ +1&-1&0&0&0&0\\ -1&0&0&+1&0&0\\ \hline\end{array}\quad \begin{array}{|cccccc|}\hline 0&0&0&0&-1&+1\\ 0&0&-1&0&+1&0\\ 0&0&0&0&0&0\\ 0&0&0&0&0&0\\ 0&0&0&0&0&0\\ 0&0&+1&0&0&-1\\ \hline\end{array}\quad \begin{array}{|cccccc|}\hline 0&0&0&0&+1&-1\\ 0&0&0&0&0&0\\ 0&0&0&-1&0&+1\\ 0&-1&0&+1&0&0\\ 0&+1&0&0&-1&0\\ 0&0&0&0&0&0\\ \hline\end{array}\quad \begin{array}{|cccccc|}\hline 0&0&0&0&0&0\\ 0&0&+1&0&-1&0\\ 0&0&0&+1&0&-1\\ 0&0&0&0&0&0\\ -1&0&0&0&+1&0\\ +1&0&-1&-1&0&+1\\ \hline\end{array}$$

- $4 \times 6 \times 7$ move of degree 15 with slice degree $\{2,4,4,5\} \times \{2,2,2,3,3,3\} \times \{2,2,2,2,2,2,3\}$
$((4,6,7),(15),((2,4,4,5),(2,2,2,3,3,3),(2,2,2,2,2,2,3)),(fcs),\emptyset,((151,162,213,224,237,245,335,346,357,$
$361,417,423,444,452,466),(152,161,217,223,235,244,337,345,351,366,413,424,446,457,462)))$

$$\begin{array}{|ccccccc|}\hline 0&0&0&0&0&0&0\\ 0&0&0&0&0&0&0\\ 0&0&0&0&0&0&0\\ 0&0&0&0&0&0&0\\ +1&-1&0&0&0&0&0\\ -1&+1&0&0&0&0&0\\ \hline\end{array}\quad \begin{array}{|ccccccc|}\hline 0&0&+1&0&0&0&-1\\ 0&0&-1&+1&0&0&0\\ 0&0&0&0&-1&0&+1\\ 0&0&0&-1&+1&0&0\\ 0&0&0&0&0&0&0\\ 0&0&0&0&0&0&0\\ \hline\end{array}$$

$$\begin{array}{|ccccccc|}\hline 0&0&0&0&0&0&0\\ 0&0&0&0&0&0&0\\ 0&0&0&0&+1&0&-1\\ 0&0&0&0&-1&+1&0\\ -1&0&0&0&0&0&+1\\ +1&0&0&0&0&-1&0\\ \hline\end{array}\quad \begin{array}{|ccccccc|}\hline 0&0&-1&0&0&0&+1\\ 0&0&+1&-1&0&0&0\\ 0&0&0&0&0&0&0\\ 0&0&0&+1&0&-1&0\\ 0&+1&0&0&0&0&-1\\ 0&-1&0&0&0&+1&0\\ \hline\end{array}$$

- $4 \times 6 \times 7$ move of degree 15 with slice degree $\{3,3,4,5\} \times \{2,2,2,3,3,3\} \times \{2,2,2,2,2,2,3\}$
  $((4,6,7),(15),((3,3,4,5),(2,2,2,3,3,3),(2,2,2,2,2,2,3)),(fcs),\emptyset,((111,127,142,233,255,264,317,341,356,365,422,434,446,453,467),(117,122,141,234,253,265,311,346,355,367,427,433,442,456,464)))$

$$\begin{array}{|ccccccc|}\hline +1&0&0&0&0&0&-1\\ 0&-1&0&0&0&0&+1\\ 0&0&0&0&0&0&0\\ -1&+1&0&0&0&0&0\\ 0&0&0&0&0&0&0\\ 0&0&0&0&0&0&0\\ \hline\end{array} \quad \begin{array}{|ccccccc|}\hline 0&0&0&0&0&0&0\\ 0&0&0&0&0&0&0\\ 0&0&+1&-1&0&0&0\\ 0&0&0&0&0&0&0\\ 0&0&-1&0&+1&0&0\\ 0&0&0&+1&-1&0&0\\ \hline\end{array}$$

$$\begin{array}{|ccccccc|}\hline -1&0&0&0&0&0&+1\\ 0&0&0&0&0&0&0\\ 0&0&0&0&0&0&0\\ +1&0&0&0&0&-1&0\\ 0&0&0&0&-1&+1&0\\ 0&0&0&0&+1&0&-1\\ \hline\end{array} \quad \begin{array}{|ccccccc|}\hline 0&0&0&0&0&0&0\\ 0&+1&0&0&0&0&-1\\ 0&0&-1&+1&0&0&0\\ 0&-1&0&0&0&+1&0\\ 0&0&+1&0&0&-1&0\\ 0&0&0&-1&0&0&+1\\ \hline\end{array}$$

- $4 \times 6 \times 7$ move of degree 15 with slice degree $\{3,4,4,4\} \times \{2,2,2,3,3,3\} \times \{2,2,2,2,2,2,3\}$
  $((4,6,7),(15),((3,4,4,4),(2,2,2,3,3,3),(2,2,2,2,2,2,3)),(fcs),\emptyset,((111,147,152,217,223,251,264,336,342,354,365,427,435,446,463),(117,142,151,211,227,254,263,335,346,352,364,423,436,447,465)))$

$$\begin{array}{|ccccccc|}\hline -1&0&0&0&0&0&+1\\ 0&0&0&0&0&0&0\\ 0&0&0&0&0&0&0\\ 0&+1&0&0&0&0&-1\\ +1&-1&0&0&0&0&0\\ 0&0&0&0&0&0&0\\ \hline\end{array} \quad \begin{array}{|ccccccc|}\hline +1&0&0&0&0&0&-1\\ 0&0&-1&0&0&0&+1\\ 0&0&0&0&0&0&0\\ 0&0&0&0&0&0&0\\ -1&0&0&+1&0&0&0\\ 0&0&+1&-1&0&0&0\\ \hline\end{array}$$

$$\begin{array}{|ccccccc|}\hline 0&0&0&0&0&0&0\\ 0&0&0&0&0&0&0\\ 0&0&0&0&+1&-1&0\\ 0&-1&0&0&0&+1&0\\ 0&+1&0&-1&0&0&0\\ 0&0&0&+1&-1&0&0\\ \hline\end{array} \quad \begin{array}{|ccccccc|}\hline 0&0&0&0&0&0&0\\ 0&0&+1&0&0&0&-1\\ 0&0&0&0&-1&+1&0\\ 0&0&0&0&0&-1&+1\\ 0&0&0&0&0&0&0\\ 0&0&-1&0&+1&0&0\\ \hline\end{array}$$

- $5 \times 5 \times 6$ move(1) of degree 15 with slice degree $\{2,2,3,3,5\} \times \{2,3,3,3,4\} \times \{2,2,2,2,3,4\}$
  $((5,5,6),(15),((2,2,3,3,5),(2,3,3,3,4),(2,2,2,2,3,4)),(fcs),\emptyset,((121,155,225,246,316,333,352,434,445,453,512,526,536,544,551),(125,151,226,245,312,336,353,433,444,455,516,521,534,546,552)))$

$$\begin{array}{|cccccc|}\hline 0&0&0&0&0&0\\ +1&0&0&0&-1&0\\ 0&0&0&0&0&0\\ 0&0&0&0&0&0\\ -1&0&0&0&+1&0\\ \hline\end{array} \quad \begin{array}{|cccccc|}\hline 0&0&0&0&0&0\\ 0&0&0&0&+1&-1\\ 0&0&0&0&0&0\\ 0&0&0&0&-1&+1\\ 0&0&0&0&0&0\\ \hline\end{array} \quad \begin{array}{|cccccc|}\hline 0&-1&0&0&0&+1\\ 0&0&0&0&0&0\\ 0&0&+1&0&0&-1\\ 0&0&0&0&0&0\\ 0&+1&-1&0&0&0\\ \hline\end{array}$$

$$\begin{array}{|cccccc|}\hline 0&0&0&0&0&0\\ 0&0&0&0&0&0\\ 0&0&-1&+1&0&0\\ 0&0&0&-1&+1&0\\ 0&0&+1&0&-1&0\\ \hline\end{array} \quad \begin{array}{|cccccc|}\hline 0&+1&0&0&0&-1\\ -1&0&0&0&0&+1\\ 0&0&0&-1&0&+1\\ 0&0&0&+1&0&-1\\ +1&-1&0&0&0&0\\ \hline\end{array}$$

- $5 \times 5 \times 6$ move(2) of degree 15 with slice degree $\{2,2,3,3,5\} \times \{2,3,3,3,4\} \times \{2,2,2,2,3,4\}$
$((5,5,6),(15),((2,2,3,3,5),(2,3,3,3,4),(2,2,2,2,3,4)),(fcs),\emptyset,((121,156,232,255,323,345,351,416,435,444,514,526,536,543,552),(126,151,235,252,321,343,355,414,436,445,516,523,532,544,556)))$

$$\boxed{\begin{array}{cccccc} 0&0&0&0&0&0\\ +1&0&0&0&0&-1\\ 0&0&0&0&0&0\\ 0&0&0&0&0&0\\ -1&0&0&0&0&+1 \end{array}} \quad \boxed{\begin{array}{cccccc} 0&0&0&0&0&0\\ 0&0&0&0&0&0\\ 0&+1&0&0&-1&0\\ 0&0&0&0&0&0\\ 0&-1&0&0&+1&0 \end{array}} \quad \boxed{\begin{array}{cccccc} 0&0&0&0&0&0\\ -1&0&+1&0&0&0\\ 0&0&0&0&0&0\\ 0&0&-1&0&+1&0\\ +1&0&0&0&-1&0 \end{array}}$$

$$\boxed{\begin{array}{cccccc} 0&0&0&-1&0&+1\\ 0&0&0&0&0&0\\ 0&0&0&0&+1&-1\\ 0&0&0&+1&-1&0\\ 0&0&0&0&0&0 \end{array}} \quad \boxed{\begin{array}{cccccc} 0&0&0&+1&0&-1\\ 0&0&-1&0&0&+1\\ 0&-1&0&0&0&+1\\ 0&0&+1&-1&0&0\\ 0&+1&0&0&0&-1 \end{array}}$$

- $5 \times 5 \times 6$ move of degree 15 with slice degree $\{2,3,3,3,4\} \times \{2,3,3,3,4\} \times \{2,2,2,2,3,4\}$
$((5,5,6),(15),((2,3,3,3,4),(2,3,3,3,4),(2,2,2,2,3,4)),(fcs),\emptyset,((141,156,222,245,251,324,333,352,416,425,434,515,536,546,553),(146,151,225,241,252,322,334,353,415,424,436,516,533,545,556)))$

$$\boxed{\begin{array}{cccccc} 0&0&0&0&0&0\\ 0&0&0&0&0&0\\ 0&0&0&0&0&0\\ +1&0&0&0&0&-1\\ -1&0&0&0&0&+1 \end{array}} \quad \boxed{\begin{array}{cccccc} 0&0&0&0&0&0\\ 0&+1&0&0&-1&0\\ 0&0&0&0&0&0\\ -1&0&0&0&+1&0\\ +1&-1&0&0&0&0 \end{array}} \quad \boxed{\begin{array}{cccccc} 0&0&0&0&0&0\\ 0&-1&0&+1&0&0\\ 0&0&+1&-1&0&0\\ 0&0&0&0&0&0\\ 0&+1&-1&0&0&0 \end{array}}$$

$$\boxed{\begin{array}{cccccc} 0&0&0&0&-1&+1\\ 0&0&0&-1&+1&0\\ 0&0&0&+1&0&-1\\ 0&0&0&0&0&0\\ 0&0&0&0&0&0 \end{array}} \quad \boxed{\begin{array}{cccccc} 0&0&0&0&+1&-1\\ 0&0&0&0&0&0\\ 0&0&-1&0&0&+1\\ 0&0&0&0&-1&+1\\ 0&0&+1&0&0&-1 \end{array}}$$

- $5 \times 5 \times 7$ move(1) of degree 15 with slice degree $\{2,2,3,3,5\} \times \{2,3,3,3,4\} \times \{2,2,2,2,2,2,3\}$
$((5,5,7),(15),((2,2,3,3,5),(2,3,3,3,4),(2,2,2,2,2,2,3)),(fcs),\emptyset,((127,131,222,257,337,343,354,416,444,455,515,521,533,546,552),(121,137,227,252,333,344,357,415,446,454,516,522,531,543,555)))$

$$\boxed{\begin{array}{ccccccc} 0&0&0&0&0&0&0\\ -1&0&0&0&0&0&+1\\ +1&0&0&0&0&0&-1\\ 0&0&0&0&0&0&0\\ 0&0&0&0&0&0&0 \end{array}} \quad \boxed{\begin{array}{ccccccc} 0&0&0&0&0&0&0\\ 0&+1&0&0&0&0&-1\\ 0&0&0&0&0&0&0\\ 0&0&0&0&0&0&0\\ 0&-1&0&0&0&0&+1 \end{array}} \quad \boxed{\begin{array}{ccccccc} 0&0&0&0&0&0&0\\ 0&0&0&0&0&0&0\\ 0&0&-1&0&0&0&+1\\ 0&0&+1&-1&0&0&0\\ 0&0&0&+1&0&0&-1 \end{array}}$$

$$\boxed{\begin{array}{ccccccc} 0&0&0&0&-1&+1&0\\ 0&0&0&0&0&0&0\\ 0&0&0&0&0&0&0\\ 0&0&0&+1&0&-1&0\\ 0&0&0&-1&+1&0&0 \end{array}} \quad \boxed{\begin{array}{ccccccc} 0&0&0&0&+1&-1&0\\ +1&-1&0&0&0&0&0\\ -1&0&+1&0&0&0&0\\ 0&0&-1&0&0&+1&0\\ 0&+1&0&0&-1&0&0 \end{array}}$$

- $5 \times 5 \times 7$ move(2) of degree 15 with slice degree $\{2,2,3,3,5\} \times \{2,3,3,3,4\} \times \{2,2,2,2,2,2,3\}$
$((5,5,7),(15),((2,2,3,3,5),(2,3,3,3,4),(2,2,2,2,2,2,3)),(fcs),\emptyset,((121,152,233,257,324,347,351,415,437,446,516,522,535,544,553),(122,151,237,253,321,344,357,416,435,447,515,524,533,546,552)))$

$$\begin{array}{|ccccccc|}\hline 0&0&0&0&0&0&0\\ +1&-1&0&0&0&0&0\\ 0&0&0&0&0&0&0\\ 0&0&0&0&0&0&0\\ -1&+1&0&0&0&0&0\\ \hline\end{array} \quad \begin{array}{|ccccccc|}\hline 0&0&0&0&0&0&0\\ 0&0&0&0&0&0&0\\ 0&0&+1&0&0&0&-1\\ 0&0&0&0&0&0&0\\ 0&0&-1&0&0&0&+1\\ \hline\end{array} \quad \begin{array}{|ccccccc|}\hline 0&0&0&0&0&0&0\\ -1&0&0&+1&0&0&0\\ 0&0&0&0&0&0&0\\ 0&0&0&-1&0&0&+1\\ +1&0&0&0&0&0&-1\\ \hline\end{array}$$

$$\begin{array}{|ccccccc|}\hline 0&0&0&0&+1&-1&0\\ 0&0&0&0&0&0&0\\ 0&0&0&0&-1&0&+1\\ 0&0&0&0&0&+1&-1\\ 0&0&0&0&0&0&0\\ \hline\end{array} \quad \begin{array}{|ccccccc|}\hline 0&0&0&0&-1&+1&0\\ 0&+1&0&-1&0&0&0\\ 0&0&-1&0&+1&0&0\\ 0&0&0&+1&0&-1&0\\ 0&-1&+1&0&0&0&0\\ \hline\end{array}$$

- $5 \times 5 \times 7$ move(1) of degree 15 with slice degree $\{2,2,3,4,4\} \times \{2,3,3,3,4\} \times \{2,2,2,2,2,2,3\}$
$((5,5,7),(15),((2,2,3,4,4),(2,3,3,3,4),(2,2,2,2,2,2,3)),(fcs),\emptyset,((141,157,232,247,316,325,354,424,433,442,451,515,523,537,556),(147,151,237,242,315,324,356,423,432,441,454,516,525,533,557)))$

$$\begin{array}{|ccccccc|}\hline 0&0&0&0&0&0&0\\ 0&0&0&0&0&0&0\\ 0&0&0&0&0&0&0\\ -1&0&0&0&0&0&+1\\ +1&0&0&0&0&0&-1\\ \hline\end{array} \quad \begin{array}{|ccccccc|}\hline 0&0&0&0&0&0&0\\ 0&0&0&0&0&0&0\\ 0&-1&0&0&0&0&+1\\ 0&+1&0&0&0&0&-1\\ 0&0&0&0&0&0&0\\ \hline\end{array} \quad \begin{array}{|ccccccc|}\hline 0&0&0&0&+1&-1&0\\ 0&0&0&+1&-1&0&0\\ 0&0&0&0&0&0&0\\ 0&0&0&0&0&0&0\\ 0&0&0&-1&0&+1&0\\ \hline\end{array}$$

$$\begin{array}{|ccccccc|}\hline 0&0&0&0&0&0&0\\ 0&0&+1&-1&0&0&0\\ 0&+1&-1&0&0&0&0\\ +1&-1&0&0&0&0&0\\ -1&0&0&+1&0&0&0\\ \hline\end{array} \quad \begin{array}{|ccccccc|}\hline 0&0&0&0&-1&+1&0\\ 0&0&-1&0&+1&0&0\\ 0&0&+1&0&0&0&-1\\ 0&0&0&0&0&0&0\\ 0&0&0&0&0&-1&+1\\ \hline\end{array}$$

- $5 \times 5 \times 7$ move(2) of degree 15 with slice degree $\{2,2,3,4,4\} \times \{2,3,3,3,4\} \times \{2,2,2,2,2,2,3\}$
$((5,5,7),(15),((2,2,3,4,4),(2,3,3,3,4),(2,2,2,2,2,2,3)),(fcs),\emptyset,((121,157,232,253,314,327,345,425,433,446,451,517,536,544,552),(127,151,233,252,317,325,344,421,436,445,453,514,532,546,557)))$

$$\begin{array}{|ccccccc|}\hline 0&0&0&0&0&0&0\\ -1&0&0&0&0&0&+1\\ 0&0&0&0&0&0&0\\ 0&0&0&0&0&0&0\\ +1&0&0&0&0&0&-1\\ \hline\end{array} \quad \begin{array}{|ccccccc|}\hline 0&0&0&0&0&0&0\\ 0&0&0&0&0&0&0\\ 0&-1&+1&0&0&0&0\\ 0&0&0&0&0&0&0\\ 0&+1&-1&0&0&0&0\\ \hline\end{array} \quad \begin{array}{|ccccccc|}\hline 0&0&0&-1&0&0&+1\\ 0&0&0&0&+1&0&-1\\ 0&0&0&0&0&0&0\\ 0&0&0&+1&-1&0&0\\ 0&0&0&0&0&0&0\\ \hline\end{array}$$

$$\begin{array}{|ccccccc|}\hline 0&0&0&0&0&0&0\\ +1&0&0&0&-1&0&0\\ 0&0&-1&0&0&+1&0\\ 0&0&0&0&+1&-1&0\\ -1&0&+1&0&0&0&0\\ \hline\end{array} \quad \begin{array}{|ccccccc|}\hline 0&0&0&+1&0&0&-1\\ 0&0&0&0&0&0&0\\ 0&+1&0&0&0&-1&0\\ 0&0&0&-1&0&+1&0\\ 0&-1&0&0&0&0&+1\\ \hline\end{array}$$

- $5 \times 5 \times 7$ move(1) of degree 15 with slice degree $\{2,3,3,3,4\} \times \{2,3,3,3,4\} \times \{2,2,2,2,2,2,3\}$
$((5,5,7),(15),((2,3,3,3,4),(2,3,3,3,4),(2,2,2,2,2,2,3)),(fcs),\emptyset,((121,152,223,237,251,316,345,357,417,434,446,522,533,544,555),(122,151,221,233,257,317,346,355,416,437,444,523,534,545,552)))$

$$\begin{array}{|ccccccc|}\hline 0&0&0&0&0&0&0\\ +1&-1&0&0&0&0&0\\ 0&0&0&0&0&0&0\\ 0&0&0&0&0&0&0\\ -1&+1&0&0&0&0&0\\ \hline\end{array} \quad \begin{array}{|ccccccc|}\hline 0&0&0&0&0&0&0\\ -1&0&+1&0&0&0&0\\ 0&0&-1&0&0&0&+1\\ 0&0&0&0&0&0&0\\ +1&0&0&0&0&0&-1\\ \hline\end{array} \quad \begin{array}{|ccccccc|}\hline 0&0&0&0&0&+1&-1\\ 0&0&0&0&0&0&0\\ 0&0&0&0&0&0&0\\ 0&0&0&0&+1&-1&0\\ 0&0&0&0&-1&0&+1\\ \hline\end{array}$$

$$\begin{array}{|ccccccc|}\hline 0&0&0&0&0&-1&+1\\ 0&0&0&0&0&0&0\\ 0&0&0&+1&0&0&-1\\ 0&0&0&-1&0&+1&0\\ 0&0&0&0&0&0&0\\ \hline\end{array} \quad \begin{array}{|ccccccc|}\hline 0&0&0&0&0&0&0\\ 0&+1&-1&0&0&0&0\\ 0&0&+1&-1&0&0&0\\ 0&0&0&+1&-1&0&0\\ 0&-1&0&0&+1&0&0\\ \hline\end{array}$$

- $5 \times 5 \times 7$ move(2) of degree 15 with slice degree $\{2,3,3,3,4\} \times \{2,3,3,3,4\} \times \{2,2,2,2,2,2,3\}$
$((5,5,7),(15),((2,3,3,3,4),(2,3,3,3,4),(2,2,2,2,2,2,3)),(fcs),\emptyset,((121,152,234,245,253,327,343,351,416,435,447,517,522,536,554),(122,151,235,243,254,321,347,353,417,436,445,516,527,534,552)))$

$$\begin{array}{|ccccccc|}\hline 0&0&0&0&0&0&0\\ +1&-1&0&0&0&0&0\\ 0&0&0&0&0&0&0\\ 0&0&0&0&0&0&0\\ -1&+1&0&0&0&0&0\\ \hline\end{array} \quad \begin{array}{|ccccccc|}\hline 0&0&0&0&0&0&0\\ 0&0&0&0&0&0&0\\ 0&0&0&+1&-1&0&0\\ 0&0&-1&0&+1&0&0\\ 0&0&+1&-1&0&0&0\\ \hline\end{array} \quad \begin{array}{|ccccccc|}\hline 0&0&0&0&0&0&0\\ -1&0&0&0&0&0&+1\\ 0&0&0&0&0&0&0\\ 0&0&+1&0&0&0&-1\\ +1&0&-1&0&0&0&0\\ \hline\end{array}$$

$$\begin{array}{|ccccccc|}\hline 0&0&0&0&0&+1&-1\\ 0&0&0&0&0&0&0\\ 0&0&0&0&+1&-1&0\\ 0&0&0&0&-1&0&+1\\ 0&0&0&0&0&0&0\\ \hline\end{array} \quad \begin{array}{|ccccccc|}\hline 0&0&0&0&0&-1&+1\\ 0&+1&0&0&0&0&-1\\ 0&0&0&-1&0&+1&0\\ 0&0&0&0&0&0&0\\ 0&-1&0&+1&0&0&0\\ \hline\end{array}$$

- $5 \times 5 \times 7$ move of degree 15 with slice degree $\{2,3,3,3,4\} \times \{3,3,3,3,3\} \times \{2,2,2,2,2,2,3\}$
$((5,5,7),(15),((2,3,3,3,4),(3,3,3,3,3),(2,2,2,2,2,2,3)),(fcs),\emptyset,((111,127,217,233,242,326,337,355,435,443,454,512,521,544,556),(117,121,212,237,243,327,335,356,433,444,455,511,526,542,554)))$

$$\begin{array}{|ccccccc|}\hline +1&0&0&0&0&0&-1\\ -1&0&0&0&0&0&+1\\ 0&0&0&0&0&0&0\\ 0&0&0&0&0&0&0\\ 0&0&0&0&0&0&0\\ \hline\end{array} \quad \begin{array}{|ccccccc|}\hline 0&-1&0&0&0&0&+1\\ 0&0&0&0&0&0&0\\ 0&0&+1&0&0&0&-1\\ 0&+1&-1&0&0&0&0\\ 0&0&0&0&0&0&0\\ \hline\end{array} \quad \begin{array}{|ccccccc|}\hline 0&0&0&0&0&0&0\\ 0&0&0&0&0&+1&-1\\ 0&0&0&0&-1&0&+1\\ 0&0&0&0&0&0&0\\ 0&0&0&0&+1&-1&0\\ \hline\end{array}$$

$$\begin{array}{|ccccccc|}\hline 0&0&0&0&0&0&0\\ 0&0&0&0&0&0&0\\ 0&0&-1&0&+1&0&0\\ 0&0&+1&-1&0&0&0\\ 0&0&0&+1&-1&0&0\\ \hline\end{array} \quad \begin{array}{|ccccccc|}\hline -1&+1&0&0&0&0&0\\ +1&0&0&0&0&-1&0\\ 0&0&0&0&0&0&0\\ 0&-1&0&+1&0&0&0\\ 0&0&0&-1&0&+1&0\\ \hline\end{array}$$

- $5 \times 6 \times 6$ move of degree 15 with slice degree $\{2,2,3,4,4\} \times \{2,2,2,2,3,4\} \times \{2,2,2,3,3,3\}$
  $((5,6,6),(15),((2,2,3,4,4),(2,2,2,2,3,4),(2,2,2,3,3,3)),(fcs),\emptyset,((151,164,214,265,326,345,362,415,433,$ $446,454,522,536,553,561),(154,161,215,264,322,346,365,414,436,445,453,526,533,551,562)))$

$$\boxed{\begin{array}{cccccc} 0&0&0&0&0&0\\ 0&0&0&0&0&0\\ 0&0&0&0&0&0\\ 0&0&0&0&0&0\\ +1&0&0&-1&0&0\\ -1&0&0&+1&0&0 \end{array}} \quad \boxed{\begin{array}{cccccc} 0&0&0&+1&-1&0\\ 0&0&0&0&0&0\\ 0&0&0&0&0&0\\ 0&0&0&0&0&0\\ 0&0&0&0&0&0\\ 0&0&0&-1&+1&0 \end{array}} \quad \boxed{\begin{array}{cccccc} 0&0&0&0&0&0\\ 0&-1&0&0&0&+1\\ 0&0&0&0&0&0\\ 0&0&0&0&+1&-1\\ 0&0&0&0&0&0\\ 0&+1&0&0&-1&0 \end{array}}$$

$$\boxed{\begin{array}{cccccc} 0&0&0&-1&+1&0\\ 0&0&0&0&0&0\\ 0&0&+1&0&0&-1\\ 0&0&0&0&-1&+1\\ 0&0&-1&+1&0&0\\ 0&0&0&0&0&0 \end{array}} \quad \boxed{\begin{array}{cccccc} 0&0&0&0&0&0\\ 0&+1&0&0&0&-1\\ 0&0&-1&0&0&+1\\ 0&0&0&0&0&0\\ -1&0&+1&0&0&0\\ +1&-1&0&0&0&0 \end{array}}$$

- $5 \times 6 \times 6$ move(1) of degree 15 with slice degree $\{2,3,3,3,4\} \times \{2,2,2,2,3,4\} \times \{2,2,2,3,3,3\}$
  $((5,6,6),(15),((2,3,3,3,4),(2,2,2,2,3,4),(2,2,2,3,3,3)),(fcs),\emptyset,((151,164,212,255,261,326,344,363,435,$ $446,454,515,523,536,562),(154,161,215,251,262,323,346,364,436,444,455,512,526,535,563)))$

$$\boxed{\begin{array}{cccccc} 0&0&0&0&0&0\\ 0&0&0&0&0&0\\ 0&0&0&0&0&0\\ 0&0&0&0&0&0\\ +1&0&0&-1&0&0\\ -1&0&0&+1&0&0 \end{array}} \quad \boxed{\begin{array}{cccccc} 0&+1&0&0&-1&0\\ 0&0&0&0&0&0\\ 0&0&0&0&0&0\\ 0&0&0&0&0&0\\ -1&0&0&0&+1&0\\ +1&-1&0&0&0&0 \end{array}} \quad \boxed{\begin{array}{cccccc} 0&0&0&0&0&0\\ 0&0&-1&0&0&+1\\ 0&0&0&0&0&0\\ 0&0&0&+1&0&-1\\ 0&0&0&0&0&0\\ 0&0&+1&-1&0&0 \end{array}}$$

$$\boxed{\begin{array}{cccccc} 0&0&0&0&0&0\\ 0&0&0&0&0&0\\ 0&0&0&0&+1&-1\\ 0&0&0&-1&0&+1\\ 0&0&0&+1&-1&0\\ 0&0&0&0&0&0 \end{array}} \quad \boxed{\begin{array}{cccccc} 0&-1&0&0&+1&0\\ 0&0&+1&0&0&-1\\ 0&0&0&0&-1&+1\\ 0&0&0&0&0&0\\ 0&0&0&0&0&0\\ 0&+1&-1&0&0&0 \end{array}}$$

- $5 \times 6 \times 6$ move(2) of degree 15 with slice degree $\{2,3,3,3,4\} \times \{2,2,2,2,3,4\} \times \{2,2,2,3,3,3\}$
  $((5,6,6),(15),((2,3,3,3,4),(2,2,2,2,3,4),(2,2,2,3,3,3)),(fcs),\emptyset,((114,165,221,252,264,335,346,363,443,$ $456,462,515,524,536,551),(115,164,224,251,262,336,343,365,446,452,463,514,521,535,556)))$

$$\boxed{\begin{array}{cccccc} 0&0&0&+1&-1&0\\ 0&0&0&0&0&0\\ 0&0&0&0&0&0\\ 0&0&0&0&0&0\\ 0&0&0&0&0&0\\ 0&0&0&-1&+1&0 \end{array}} \quad \boxed{\begin{array}{cccccc} 0&0&0&0&0&0\\ +1&0&0&-1&0&0\\ 0&0&0&0&0&0\\ 0&0&0&0&0&0\\ -1&+1&0&0&0&0\\ 0&-1&0&+1&0&0 \end{array}} \quad \boxed{\begin{array}{cccccc} 0&0&0&0&0&0\\ 0&0&0&0&0&0\\ 0&0&0&0&+1&-1\\ 0&0&-1&0&0&+1\\ 0&0&0&0&0&0\\ 0&0&+1&0&-1&0 \end{array}}$$

$$\boxed{\begin{array}{cccccc} 0&0&0&0&0&0\\ 0&0&0&0&0&0\\ 0&0&0&0&0&0\\ 0&0&+1&0&0&-1\\ 0&-1&0&0&0&+1\\ 0&+1&-1&0&0&0 \end{array}} \quad \boxed{\begin{array}{cccccc} 0&0&0&-1&+1&0\\ -1&0&0&+1&0&0\\ 0&0&0&0&-1&+1\\ 0&0&0&0&0&0\\ +1&0&0&0&0&-1\\ 0&0&0&0&0&0 \end{array}}$$

- $5 \times 6 \times 6$ move(3) of degree 15 with slice degree $\{2,3,3,3,4\} \times \{2,2,2,2,3,4\} \times \{2,2,2,3,3,3\}$
  $((5,6,6),(15),((2,3,3,3,4),(2,2,2,2,3,4),(2,2,2,3,3,3)),(fcs),\emptyset,((114,165,222,251,264,335,346,363,415,$ $436,454,521,543,556,562),(115,164,221,254,262,336,343,365,414,435,456,522,546,551,563)))$

$$
\begin{array}{|cccccc|}\hline 0&0&0&+1&-1&0\\ 0&0&0&0&0&0\\ 0&0&0&0&0&0\\ 0&0&0&0&0&0\\ 0&0&0&0&0&0\\ 0&0&0&-1&+1&0\\ \hline\end{array}
\quad
\begin{array}{|cccccc|}\hline 0&0&0&0&0&0\\ -1&+1&0&0&0&0\\ 0&0&0&0&0&0\\ 0&0&0&0&0&0\\ +1&0&0&-1&0&0\\ 0&-1&0&+1&0&0\\ \hline\end{array}
\quad
\begin{array}{|cccccc|}\hline 0&0&0&0&0&0\\ 0&0&0&0&0&0\\ 0&0&0&0&+1&-1\\ 0&0&-1&0&0&+1\\ 0&0&0&0&0&0\\ 0&0&+1&0&-1&0\\ \hline\end{array}
$$

$$
\begin{array}{|cccccc|}\hline 0&0&0&-1&+1&0\\ 0&0&0&0&0&0\\ 0&0&0&0&-1&+1\\ 0&0&0&0&0&0\\ 0&0&0&+1&0&-1\\ 0&0&0&0&0&0\\ \hline\end{array}
\quad
\begin{array}{|cccccc|}\hline 0&0&0&0&0&0\\ +1&-1&0&0&0&0\\ 0&0&0&0&0&0\\ 0&0&+1&0&0&-1\\ -1&0&0&0&0&+1\\ 0&+1&-1&0&0&0\\ \hline\end{array}
$$

A.6 Indispensable moves of degree 16

- $3 \times 5 \times 7$ move(1) of degree 16 with slice degree $\{4,6,6\} \times \{2,3,3,3,5\} \times \{2,2,2,2,2,2,4\}$
  $((3,5,7),(16),((4,6,6),(2,3,3,3,5),(2,2,2,2,2,2,4)),(fcS),\emptyset,((121,133,142,154,217,222,237,245,253,$ $256,315,326,331,344,357,357),(122,131,144,153,215,226,233,242,257,257,317,321,337,345,354,356)))$

$$
\begin{array}{|ccccccc|}\hline 0&0&0&0&0&0&0\\ +1&-1&0&0&0&0&0\\ -1&0&+1&0&0&0&0\\ 0&+1&0&-1&0&0&0\\ 0&0&-1&+1&0&0&0\\ \hline\end{array}
\begin{array}{|ccccccc|}\hline 0&0&0&0&-1&0&+1\\ 0&+1&0&0&0&-1&0\\ 0&0&-1&0&0&0&+1\\ 0&-1&0&0&+1&0&0\\ 0&0&+1&0&0&+1&-2\\ \hline\end{array}
\begin{array}{|ccccccc|}\hline 0&0&0&0&+1&0&-1\\ -1&0&0&0&0&+1&0\\ +1&0&0&0&0&0&-1\\ 0&0&0&+1&-1&0&0\\ 0&0&0&-1&0&-1&+2\\ \hline\end{array}
$$

- $3 \times 5 \times 7$ move(2) of degree 16 with slice degree $\{4,6,6\} \times \{2,3,3,3,5\} \times \{2,2,2,2,2,2,4\}$
  (not fundamental, not circuit)
  $((3,5,7),(16),((4,6,6),(2,3,3,3,5),(2,2,2,2,2,2,4)),(FCs),\emptyset,((121,133,142,154,216,222,237,247,253,$ $255,317,325,331,344,356,357),(122,131,144,153,217,225,233,242,256,257,316,321,337,347,354,355)))$

$$
\begin{array}{|ccccccc|}\hline 0&0&0&0&0&0&0\\ +1&-1&0&0&0&0&0\\ -1&0&+1&0&0&0&0\\ 0&+1&0&-1&0&0&0\\ 0&0&-1&+1&0&0&0\\ \hline\end{array}
\begin{array}{|ccccccc|}\hline 0&0&0&0&0&+1&-1\\ 0&+1&0&0&-1&0&0\\ 0&0&-1&0&0&0&+1\\ 0&-1&0&0&0&0&+1\\ 0&0&+1&0&+1&-1&-1\\ \hline\end{array}
\begin{array}{|ccccccc|}\hline 0&0&0&0&0&-1&+1\\ -1&0&0&0&+1&0&0\\ +1&0&0&0&0&0&-1\\ 0&0&0&+1&0&0&-1\\ 0&0&0&-1&-1&+1&+1\\ \hline\end{array}
$$

- $3 \times 5 \times 8$ move of degree 16 with slice degree $\{4,6,6\} \times \{2,3,3,3,5\} \times \{2,2,2,2,2,2,2,2\}$
  $((3,5,8),(16),((4,6,6),(2,3,3,3,5),(2,2,2,2,2,2,2,2)),(fcs),\emptyset,((121,133,142,154,216,222,238,245,253,$ $257,315,327,331,344,356,358),(122,131,144,153,215,227,233,242,256,258,316,321,338,345,354,357)))$

$$
\begin{array}{|cccccccc|}\hline 0&0&0&0&0&0&0&0\\ +1&-1&0&0&0&0&0&0\\ -1&0&+1&0&0&0&0&0\\ 0&+1&0&-1&0&0&0&0\\ 0&0&-1&+1&0&0&0&0\\ \hline\end{array}
\begin{array}{|cccccccc|}\hline 0&0&0&0&-1&+1&0&0\\ 0&+1&0&0&0&0&-1&0\\ 0&0&-1&0&0&0&0&+1\\ 0&-1&0&0&+1&0&0&0\\ 0&0&+1&0&0&-1&+1&-1\\ \hline\end{array}
\begin{array}{|cccccccc|}\hline 0&0&0&0&+1&-1&0&0\\ -1&0&0&0&0&0&+1&0\\ +1&0&0&0&0&0&0&-1\\ 0&0&0&+1&-1&0&0&0\\ 0&0&0&-1&0&+1&-1&+1\\ \hline\end{array}
$$

- $3 \times 6 \times 7$ move of degree 16 with slice degree $\{4,6,6\} \times \{2,2,3,3,3,3\} \times \{2,2,2,2,2,2,4\}$
  $((3,6,7),(16),((4,6,6),(2,2,3,3,3,3),(2,2,2,2,2,2,4)),(fcs),\emptyset,((131,143,152,164,217,226,232,245,257,263,315,327,337,341,354,366),(132,141,154,163,215,227,237,243,252,266,317,326,331,345,357,364)))$

$$\boxed{\begin{array}{ccccccc} 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ +1 & -1 & 0 & 0 & 0 & 0 & 0 \\ -1 & 0 & +1 & 0 & 0 & 0 & 0 \\ 0 & +1 & 0 & -1 & 0 & 0 & 0 \\ 0 & 0 & -1 & +1 & 0 & 0 & 0 \end{array}} \; \boxed{\begin{array}{ccccccc} 0 & 0 & 0 & 0 & -1 & 0 & +1 \\ 0 & 0 & 0 & 0 & 0 & +1 & -1 \\ 0 & +1 & 0 & 0 & 0 & 0 & -1 \\ 0 & 0 & -1 & 0 & +1 & 0 & 0 \\ 0 & -1 & 0 & 0 & 0 & 0 & +1 \\ 0 & 0 & +1 & 0 & 0 & -1 & 0 \end{array}} \; \boxed{\begin{array}{ccccccc} 0 & 0 & 0 & 0 & +1 & 0 & -1 \\ 0 & 0 & 0 & 0 & 0 & -1 & +1 \\ -1 & 0 & 0 & 0 & 0 & 0 & +1 \\ +1 & 0 & 0 & 0 & -1 & 0 & 0 \\ 0 & 0 & 0 & +1 & 0 & 0 & -1 \\ 0 & 0 & 0 & -1 & 0 & +1 & 0 \end{array}}$$

- $4 \times 4 \times 7$ move of degree 16 with slice degree $\{2,4,4,6\} \times \{3,3,5,5\} \times \{2,2,2,2,2,2,4\}$
  $((4,4,7),(16),((2,4,4,6),(3,3,5,5),(2,2,2,2,2,2,4)),(fcS),\emptyset,((131,147,212,224,233,241,315,322,336,347,413,426,437,437,444,445),(137,141,213,222,231,244,312,326,337,345,415,424,433,436,447,447)))$

$$\boxed{\begin{array}{ccccccc} 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ +1 & 0 & 0 & 0 & 0 & 0 & -1 \\ -1 & 0 & 0 & 0 & 0 & 0 & +1 \end{array}} \quad \boxed{\begin{array}{ccccccc} 0 & +1 & -1 & 0 & 0 & 0 & 0 \\ 0 & -1 & 0 & +1 & 0 & 0 & 0 \\ -1 & 0 & +1 & 0 & 0 & 0 & 0 \\ +1 & 0 & 0 & -1 & 0 & 0 & 0 \end{array}}$$

$$\boxed{\begin{array}{ccccccc} 0 & -1 & 0 & 0 & +1 & 0 & 0 \\ 0 & +1 & 0 & 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & 0 & 0 & +1 & -1 \\ 0 & 0 & 0 & 0 & -1 & 0 & +1 \end{array}} \quad \boxed{\begin{array}{ccccccc} 0 & 0 & +1 & 0 & -1 & 0 & 0 \\ 0 & 0 & 0 & -1 & 0 & +1 & 0 \\ 0 & 0 & -1 & 0 & 0 & -1 & +2 \\ 0 & 0 & 0 & +1 & +1 & 0 & -2 \end{array}}$$

- $4 \times 4 \times 7$ move of degree 16 with slice degree $\{3,3,4,6\} \times \{3,3,5,5\} \times \{2,2,2,2,2,2,4\}$
  $((4,4,7),(16),((3,3,4,6),(3,3,5,5),(2,2,2,2,2,2,4)),(fcS),\emptyset,((111,137,142,223,237,244,315,324,331,346,412,425,433,436,447,447),(112,131,147,224,233,247,311,325,336,344,415,423,437,437,442,446)))$

$$\boxed{\begin{array}{ccccccc} +1 & -1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ -1 & 0 & 0 & 0 & 0 & 0 & +1 \\ 0 & +1 & 0 & 0 & 0 & 0 & -1 \end{array}} \quad \boxed{\begin{array}{ccccccc} 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & +1 & -1 & 0 & 0 & 0 \\ 0 & 0 & -1 & 0 & 0 & 0 & +1 \\ 0 & 0 & 0 & +1 & 0 & 0 & -1 \end{array}}$$

$$\boxed{\begin{array}{ccccccc} -1 & 0 & 0 & 0 & +1 & 0 & 0 \\ 0 & 0 & 0 & +1 & -1 & 0 & 0 \\ +1 & 0 & 0 & 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & -1 & 0 & +1 & 0 \end{array}} \quad \boxed{\begin{array}{ccccccc} 0 & +1 & 0 & 0 & -1 & 0 & 0 \\ 0 & 0 & -1 & 0 & +1 & 0 & 0 \\ 0 & 0 & +1 & 0 & 0 & +1 & -2 \\ 0 & -1 & 0 & 0 & 0 & -1 & +2 \end{array}}$$

- $4 \times 4 \times 8$ move of degree 16 with slice degree $\{2,4,4,6\} \times \{3,3,5,5\} \times \{2,2,2,2,2,2,2,2\}$
  $((4,4,8),(16),((2,4,4,6),(3,3,5,5),(2,2,2,2,2,2,2,2)),(fcs),\emptyset,((131,142,213,225,234,241,316,323,337,348,414,427,432,438,445,446),(132,141,214,223,231,245,313,327,338,346,416,425,434,437,442,448)))$

$$\boxed{\begin{array}{cccccccc} 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ +1 & -1 & 0 & 0 & 0 & 0 & 0 & 0 \\ -1 & +1 & 0 & 0 & 0 & 0 & 0 & 0 \end{array}} \quad \boxed{\begin{array}{cccccccc} 0 & 0 & +1 & -1 & 0 & 0 & 0 & 0 \\ 0 & 0 & -1 & 0 & +1 & 0 & 0 & 0 \\ -1 & 0 & 0 & +1 & 0 & 0 & 0 & 0 \\ +1 & 0 & 0 & 0 & -1 & 0 & 0 & 0 \end{array}}$$

$$\boxed{\begin{array}{cccccccc} 0 & 0 & -1 & 0 & 0 & +1 & 0 & 0 \\ 0 & 0 & +1 & 0 & 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & +1 & -1 \\ 0 & 0 & 0 & 0 & 0 & -1 & 0 & +1 \end{array}} \quad \boxed{\begin{array}{cccccccc} 0 & 0 & 0 & +1 & 0 & -1 & 0 & 0 \\ 0 & 0 & 0 & 0 & -1 & 0 & +1 & 0 \\ 0 & +1 & 0 & -1 & 0 & 0 & -1 & +1 \\ 0 & -1 & 0 & 0 & +1 & +1 & 0 & -1 \end{array}}$$

- $4 \times 4 \times 8$ move of degree 16 with slice degree $\{3,3,4,6\} \times \{3,3,5,5\} \times \{2,2,2,2,2,2,2,2\}$
$((4,4,8),(16),((3,3,4,6),(3,3,5,5),(2,2,2,2,2,2,2,2)),(fcs),\emptyset,((111,133,142,224,236,245,317,325,331,348,412,427,434,438,443,446),(112,131,143,225,234,246,311,327,338,345,417,424,433,436,442,448)))$

$$\begin{array}{|cccccccc|}\hline +1 & -1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ -1 & 0 & +1 & 0 & 0 & 0 & 0 & 0 \\ 0 & +1 & -1 & 0 & 0 & 0 & 0 & 0 \\ \hline \end{array} \qquad \begin{array}{|cccccccc|}\hline 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & +1 & -1 & 0 & 0 & 0 \\ 0 & 0 & 0 & -1 & 0 & +1 & 0 & 0 \\ 0 & 0 & 0 & 0 & +1 & -1 & 0 & 0 \\ \hline \end{array}$$

$$\begin{array}{|cccccccc|}\hline -1 & 0 & 0 & 0 & 0 & 0 & +1 & 0 \\ 0 & 0 & 0 & 0 & +1 & 0 & -1 & 0 \\ +1 & 0 & 0 & 0 & 0 & 0 & 0 & -1 \\ 0 & 0 & 0 & 0 & -1 & 0 & 0 & +1 \\ \hline \end{array} \qquad \begin{array}{|cccccccc|}\hline 0 & +1 & 0 & 0 & 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & -1 & 0 & 0 & +1 & 0 \\ 0 & 0 & -1 & +1 & 0 & -1 & 0 & +1 \\ 0 & -1 & +1 & 0 & 0 & +1 & 0 & -1 \\ \hline \end{array}$$

- $4 \times 5 \times 7$ move of degree 16 with slice degree $\{2,4,4,6\} \times \{2,3,3,3,5\} \times \{2,2,2,2,2,2,4\}$
$((4,5,7),(16),((2,4,4,6),(2,3,3,3,5),(2,2,2,2,2,2,4)),(fcS),\emptyset,((121,157,222,233,244,251,316,335,343,357,417,427,432,446,454,455),(127,151,221,232,243,254,317,333,346,355,416,422,435,444,457,457)))$

$$\begin{array}{|ccccccc|}\hline 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ +1 & 0 & 0 & 0 & 0 & 0 & -1 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ -1 & 0 & 0 & 0 & 0 & 0 & +1 \\ \hline \end{array} \qquad \begin{array}{|ccccccc|}\hline 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ -1 & +1 & 0 & 0 & 0 & 0 & 0 \\ 0 & -1 & +1 & 0 & 0 & 0 & 0 \\ 0 & 0 & -1 & +1 & 0 & 0 & 0 \\ +1 & 0 & 0 & -1 & 0 & 0 & 0 \\ \hline \end{array}$$

$$\begin{array}{|ccccccc|}\hline 0 & 0 & 0 & 0 & 0 & +1 & -1 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & -1 & 0 & +1 & 0 & 0 \\ 0 & 0 & +1 & 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & 0 & -1 & 0 & +1 \\ \hline \end{array} \qquad \begin{array}{|ccccccc|}\hline 0 & 0 & 0 & 0 & 0 & -1 & +1 \\ 0 & -1 & 0 & 0 & 0 & 0 & +1 \\ 0 & +1 & 0 & 0 & -1 & 0 & 0 \\ 0 & 0 & 0 & -1 & 0 & +1 & 0 \\ 0 & 0 & 0 & +1 & +1 & 0 & -2 \\ \hline \end{array}$$

- $4 \times 5 \times 7$ move of degree 16 with slice degree $\{3,3,4,6\} \times \{2,3,3,3,5\} \times \{2,2,2,2,2,2,4\}$
$((4,5,7),(16),((3,3,4,6),(2,3,3,3,5),(2,2,2,2,2,2,4)),(fcS),\emptyset,((111,122,157,233,244,257,325,336,343,352,417,421,437,445,454,456),(117,121,152,237,243,254,322,333,345,356,411,425,436,444,457,457)))$

$$\begin{array}{|ccccccc|}\hline +1 & 0 & 0 & 0 & 0 & 0 & -1 \\ -1 & +1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 & 0 & 0 & +1 \\ \hline \end{array} \qquad \begin{array}{|ccccccc|}\hline 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & +1 & 0 & 0 & 0 & -1 \\ 0 & 0 & -1 & +1 & 0 & 0 & 0 \\ 0 & 0 & 0 & -1 & 0 & 0 & +1 \\ \hline \end{array}$$

$$\begin{array}{|ccccccc|}\hline 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 & +1 & 0 & 0 \\ 0 & 0 & -1 & 0 & 0 & +1 & 0 \\ 0 & 0 & +1 & 0 & -1 & 0 & 0 \\ 0 & +1 & 0 & 0 & 0 & -1 & 0 \\ \hline \end{array} \qquad \begin{array}{|ccccccc|}\hline -1 & 0 & 0 & 0 & 0 & 0 & +1 \\ +1 & 0 & 0 & 0 & -1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & -1 & +1 \\ 0 & 0 & 0 & -1 & +1 & 0 & 0 \\ 0 & 0 & 0 & +1 & 0 & +1 & -2 \\ \hline \end{array}$$

- $4 \times 5 \times 7$ move of degree 16 with slice degree $\{3,3,5,5\} \times \{2,3,3,4,4\} \times \{2,2,2,2,2,2,4\}$
$((4,5,7),(16),((3,3,5,5),(2,3,3,4,4),(2,2,2,2,2,2,4)),(fcs),\emptyset,((121,143,152,234,245,253,316,327,337,$
$341,354,417,422,435,446,457),(122,141,153,235,243,254,317,321,334,346,357,416,427,437,445,452)))$

$$\begin{array}{|ccccccc|}\hline 0&0&0&0&0&0&0\\ +1&-1&0&0&0&0&0\\ 0&0&0&0&0&0&0\\ -1&0&+1&0&0&0&0\\ 0&+1&-1&0&0&0&0\\ \hline\end{array}\qquad\begin{array}{|ccccccc|}\hline 0&0&0&0&0&0&0\\ 0&0&0&0&0&0&0\\ 0&0&0&+1&-1&0&0\\ 0&0&-1&0&+1&0&0\\ 0&0&+1&-1&0&0&0\\ \hline\end{array}$$

$$\begin{array}{|ccccccc|}\hline 0&0&0&0&0&+1&-1\\ -1&0&0&0&0&0&+1\\ 0&0&0&-1&0&0&+1\\ +1&0&0&0&0&-1&0\\ 0&0&0&+1&0&0&-1\\ \hline\end{array}\qquad\begin{array}{|ccccccc|}\hline 0&0&0&0&0&-1&+1\\ 0&+1&0&0&0&0&-1\\ 0&0&0&0&+1&0&-1\\ 0&0&0&0&-1&+1&0\\ 0&-1&0&0&0&0&+1\\ \hline\end{array}$$

- $4 \times 5 \times 8$ move of degree 16 with slice degree $\{2,3,5,6\} \times \{2,3,3,4,4\} \times \{2,2,2,2,2,2,2,2\}$
$((4,5,8),(16),((2,3,5,6),(2,3,3,4,4),(2,2,2,2,2,2,2,2)),(fcs),\emptyset,((121,142,234,245,253,317,322,338,344,$
$356,418,426,433,441,455,457),(122,141,233,244,255,318,326,334,342,357,417,421,438,445,453,456)))$

$$\begin{array}{|cccccccc|}\hline 0&0&0&0&0&0&0&0\\ +1&-1&0&0&0&0&0&0\\ 0&0&0&0&0&0&0&0\\ -1&+1&0&0&0&0&0&0\\ 0&0&0&0&0&0&0&0\\ \hline\end{array}\qquad\begin{array}{|cccccccc|}\hline 0&0&0&0&0&0&0&0\\ 0&0&0&0&0&0&0&0\\ 0&0&-1&+1&0&0&0&0\\ 0&0&0&-1&+1&0&0&0\\ 0&0&+1&0&-1&0&0&0\\ \hline\end{array}$$

$$\begin{array}{|cccccccc|}\hline 0&0&0&0&0&0&+1&-1\\ 0&+1&0&0&0&-1&0&0\\ 0&0&0&-1&0&0&0&+1\\ 0&-1&0&+1&0&0&0&0\\ 0&0&0&0&0&+1&-1&0\\ \hline\end{array}\qquad\begin{array}{|cccccccc|}\hline 0&0&0&0&0&0&-1&+1\\ -1&0&0&0&0&+1&0&0\\ 0&0&+1&0&0&0&0&-1\\ +1&0&0&0&-1&0&0&0\\ 0&0&-1&0&+1&-1&+1&0\\ \hline\end{array}$$

- $4 \times 5 \times 8$ move(1) of degree 16 with slice degree $\{2,4,4,6\} \times \{2,3,3,3,5\} \times \{2,2,2,2,2,2,2,2\}$
$((4,5,8),(16),((2,4,4,6),(2,3,3,3,5),(2,2,2,2,2,2,2,2)),(fcs),\emptyset,((121,152,223,234,245,251,316,338,344,$
$357,417,422,433,446,455,458),(122,151,221,233,244,255,317,334,346,358,416,423,438,445,452,457)))$

$$\begin{array}{|cccccccc|}\hline 0&0&0&0&0&0&0&0\\ +1&-1&0&0&0&0&0&0\\ 0&0&0&0&0&0&0&0\\ 0&0&0&0&0&0&0&0\\ -1&+1&0&0&0&0&0&0\\ \hline\end{array}\qquad\begin{array}{|cccccccc|}\hline 0&0&0&0&0&0&0&0\\ -1&0&+1&0&0&0&0&0\\ 0&0&-1&+1&0&0&0&0\\ 0&0&0&-1&+1&0&0&0\\ +1&0&0&0&-1&0&0&0\\ \hline\end{array}$$

$$\begin{array}{|cccccccc|}\hline 0&0&0&0&0&+1&-1&0\\ 0&0&0&0&0&0&0&0\\ 0&0&0&-1&0&0&0&+1\\ 0&0&0&+1&0&-1&0&0\\ 0&0&0&0&0&0&+1&-1\\ \hline\end{array}\qquad\begin{array}{|cccccccc|}\hline 0&0&0&0&0&-1&+1&0\\ 0&+1&-1&0&0&0&0&0\\ 0&0&+1&0&0&0&0&-1\\ 0&0&0&0&-1&+1&0&0\\ 0&-1&0&0&+1&0&-1&+1\\ \hline\end{array}$$

- $4 \times 5 \times 8$ move(2) of degree 16 with slice degree $\{2,4,4,6\} \times \{2,3,3,3,5\} \times \{2,2,2,2,2,2,2,2\}$
$((4,5,8),(16),((2,4,4,6),(2,3,3,3,5),(2,2,2,2,2,2,2,2)),(fcs),\emptyset,((121,152,223,234,245,251,316,338,344,357,418,422,433,447,455,456),(122,151,221,233,244,255,318,334,347,356,416,423,438,445,452,457)))$

$$\begin{array}{|cccccccc|}\hline 0&0&0&0&0&0&0&0\\ -1&+1&0&0&0&0&0&0\\ 0&0&0&0&0&0&0&0\\ 0&0&0&0&0&0&0&0\\ +1&-1&0&0&0&0&0&0\\ \hline\end{array} \quad \begin{array}{|cccccccc|}\hline 0&0&0&0&0&0&0&0\\ +1&0&-1&0&0&0&0&0\\ 0&0&+1&-1&0&0&0&0\\ 0&0&0&+1&-1&0&0&0\\ -1&0&0&0&+1&0&0&0\\ \hline\end{array}$$

$$\begin{array}{|cccccccc|}\hline 0&0&0&0&0&-1&0&+1\\ 0&0&0&0&0&0&0&0\\ 0&0&0&+1&0&0&0&-1\\ 0&0&0&-1&0&0&+1&0\\ 0&0&0&0&0&+1&-1&0\\ \hline\end{array} \quad \begin{array}{|cccccccc|}\hline 0&0&0&0&0&+1&0&-1\\ 0&-1&+1&0&0&0&0&0\\ 0&0&-1&0&0&0&0&+1\\ 0&0&0&0&+1&0&-1&0\\ 0&+1&0&0&-1&-1&+1&0\\ \hline\end{array}$$

- $4 \times 5 \times 8$ move of degree 16 with slice degree $\{3,3,4,6\} \times \{2,3,3,3,5\} \times \{2,2,2,2,2,2,2,2\}$
$((4,5,8),(16),((3,3,4,6),(2,3,3,3,5),(2,2,2,2,2,2,2,2)),(fcs),\emptyset,((111,123,152,234,246,255,327,338,344,353,412,421,435,447,456,458),(112,121,153,235,244,256,323,334,347,358,411,427,438,446,452,455)))$

$$\begin{array}{|cccccccc|}\hline +1&-1&0&0&0&0&0&0\\ -1&0&+1&0&0&0&0&0\\ 0&0&0&0&0&0&0&0\\ 0&0&0&0&0&0&0&0\\ 0&+1&-1&0&0&0&0&0\\ \hline\end{array} \quad \begin{array}{|cccccccc|}\hline 0&0&0&0&0&0&0&0\\ 0&0&0&0&0&0&0&0\\ 0&0&0&+1&-1&0&0&0\\ 0&0&0&-1&0&+1&0&0\\ 0&0&0&0&+1&-1&0&0\\ \hline\end{array}$$

$$\begin{array}{|cccccccc|}\hline 0&0&0&0&0&0&0&0\\ 0&0&-1&0&0&0&+1&0\\ 0&0&0&-1&0&0&0&+1\\ 0&0&0&+1&0&0&-1&0\\ 0&0&+1&0&0&0&0&-1\\ \hline\end{array} \quad \begin{array}{|cccccccc|}\hline -1&+1&0&0&0&0&0&0\\ +1&0&0&0&0&0&-1&0\\ 0&0&0&0&+1&0&0&-1\\ 0&0&0&0&0&-1&+1&0\\ 0&-1&0&0&-1&+1&0&+1\\ \hline\end{array}$$

- $4 \times 5 \times 8$ move of degree 16 with slice degree $\{3,3,4,6\} \times \{3,3,3,3,4\} \times \{2,2,2,2,2,2,2,2\}$
$((4,5,8),(16),((3,3,4,6),(3,3,3,3,4),(2,2,2,2,2,2,2,2)),(fcs),\emptyset,((111,123,152,234,246,255,313,327,336,348,418,422,437,445,451,454),(113,122,151,236,245,254,318,323,337,346,411,427,434,448,452,455)))$

$$\begin{array}{|cccccccc|}\hline +1&0&-1&0&0&0&0&0\\ 0&-1&+1&0&0&0&0&0\\ 0&0&0&0&0&0&0&0\\ 0&0&0&0&0&0&0&0\\ -1&+1&0&0&0&0&0&0\\ \hline\end{array} \quad \begin{array}{|cccccccc|}\hline 0&0&0&0&0&0&0&0\\ 0&0&0&0&0&0&0&0\\ 0&0&0&+1&0&-1&0&0\\ 0&0&0&0&-1&+1&0&0\\ 0&0&0&-1&+1&0&0&0\\ \hline\end{array}$$

$$\begin{array}{|cccccccc|}\hline 0&0&+1&0&0&0&0&-1\\ 0&0&-1&0&0&0&+1&0\\ 0&0&0&0&0&+1&-1&0\\ 0&0&0&0&0&-1&0&+1\\ 0&0&0&0&0&0&0&0\\ \hline\end{array} \quad \begin{array}{|cccccccc|}\hline -1&0&0&0&0&0&0&+1\\ 0&+1&0&0&0&0&-1&0\\ 0&0&0&-1&0&0&+1&0\\ 0&0&0&0&+1&0&0&-1\\ +1&-1&0&+1&-1&0&0&0\\ \hline\end{array}$$

- $4 \times 5 \times 8$ move(1) of degree 16 with slice degree $\{3, 3, 5, 5\} \times \{2, 3, 3, 4, 4\} \times \{2, 2, 2, 2, 2, 2, 2, 2\}$
$((4, 5, 8), (16), ((3, 3, 5, 5), (2, 3, 3, 4, 4), (2, 2, 2, 2, 2, 2, 2, 2)), (fcs), \emptyset, ((111, 133, 152, 224, 246, 255, 312, 327, 331, 348, 354, 426, 438, 445, 447, 453), (112, 131, 153, 226, 245, 254, 311, 324, 338, 347, 352, 427, 433, 446, 448, 455)))$

$$\begin{array}{|cccccccc|}\hline +1 & -1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ -1 & 0 & +1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & +1 & -1 & 0 & 0 & 0 & 0 & 0 \\ \hline \end{array} \quad \begin{array}{|cccccccc|}\hline 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & +1 & 0 & -1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & -1 & +1 & 0 & 0 \\ 0 & 0 & 0 & -1 & +1 & 0 & 0 & 0 \\ \hline \end{array}$$

$$\begin{array}{|cccccccc|}\hline -1 & +1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & -1 & 0 & 0 & +1 & 0 \\ +1 & 0 & 0 & 0 & 0 & 0 & 0 & -1 \\ 0 & 0 & 0 & 0 & 0 & 0 & -1 & +1 \\ 0 & -1 & 0 & +1 & 0 & 0 & 0 & 0 \\ \hline \end{array} \quad \begin{array}{|cccccccc|}\hline 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & +1 & -1 & 0 \\ 0 & 0 & -1 & 0 & 0 & 0 & 0 & +1 \\ 0 & 0 & 0 & 0 & +1 & -1 & +1 & -1 \\ 0 & 0 & +1 & 0 & -1 & 0 & 0 & 0 \\ \hline \end{array}$$

- $4 \times 5 \times 8$ move(2) of degree 16 with slice degree $\{3, 3, 5, 5\} \times \{2, 3, 3, 4, 4\} \times \{2, 2, 2, 2, 2, 2, 2, 2\}$
$((4, 5, 8), (16), ((3, 3, 5, 5), (2, 3, 3, 4, 4), (2, 2, 2, 2, 2, 2, 2, 2)), (fcs), \emptyset, ((121, 143, 152, 234, 245, 253, 317, 326, 338, 341, 354, 418, 422, 435, 447, 456), (122, 141, 153, 235, 243, 254, 318, 321, 334, 347, 356, 417, 426, 438, 445, 452)))$

$$\begin{array}{|cccccccc|}\hline 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ +1 & -1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ -1 & 0 & +1 & 0 & 0 & 0 & 0 & 0 \\ 0 & +1 & -1 & 0 & 0 & 0 & 0 & 0 \\ \hline \end{array} \quad \begin{array}{|cccccccc|}\hline 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & +1 & -1 & 0 & 0 & 0 \\ 0 & 0 & -1 & 0 & +1 & 0 & 0 & 0 \\ 0 & 0 & +1 & -1 & 0 & 0 & 0 & 0 \\ \hline \end{array}$$

$$\begin{array}{|cccccccc|}\hline 0 & 0 & 0 & 0 & 0 & 0 & +1 & -1 \\ -1 & 0 & 0 & 0 & 0 & +1 & 0 & 0 \\ 0 & 0 & 0 & -1 & 0 & 0 & 0 & +1 \\ +1 & 0 & 0 & 0 & 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & +1 & 0 & -1 & 0 & 0 \\ \hline \end{array} \quad \begin{array}{|cccccccc|}\hline 0 & 0 & 0 & 0 & 0 & 0 & -1 & +1 \\ 0 & +1 & 0 & 0 & 0 & -1 & 0 & 0 \\ 0 & 0 & 0 & 0 & +1 & 0 & 0 & -1 \\ 0 & 0 & 0 & 0 & -1 & 0 & +1 & 0 \\ 0 & -1 & 0 & 0 & 0 & +1 & 0 & 0 \\ \hline \end{array}$$

- $4 \times 5 \times 8$ move of degree 16 with slice degree $\{3, 4, 4, 5\} \times \{2, 3, 3, 3, 5\} \times \{2, 2, 2, 2, 2, 2, 2, 2\}$
$((4, 5, 8), (16), ((3, 4, 4, 5), (2, 3, 3, 3, 5), (2, 2, 2, 2, 2, 2, 2, 2)), (fcs), \emptyset, ((131, 143, 152, 224, 236, 241, 255, 318, 327, 344, 353, 417, 425, 432, 456, 458), (132, 141, 153, 225, 231, 244, 256, 317, 324, 343, 358, 418, 427, 436, 452, 455)))$

$$\begin{array}{|cccccccc|}\hline 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ +1 & -1 & 0 & 0 & 0 & 0 & 0 & 0 \\ -1 & 0 & +1 & 0 & 0 & 0 & 0 & 0 \\ 0 & +1 & -1 & 0 & 0 & 0 & 0 & 0 \\ \hline \end{array} \quad \begin{array}{|cccccccc|}\hline 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & +1 & -1 & 0 & 0 & 0 \\ -1 & 0 & 0 & 0 & 0 & +1 & 0 & 0 \\ +1 & 0 & 0 & -1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & +1 & -1 & 0 & 0 \\ \hline \end{array}$$

$$\begin{array}{|cccccccc|}\hline 0 & 0 & 0 & 0 & 0 & 0 & -1 & +1 \\ 0 & 0 & 0 & -1 & 0 & 0 & +1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & -1 & +1 & 0 & 0 & 0 & 0 \\ 0 & 0 & +1 & 0 & 0 & 0 & 0 & -1 \\ \hline \end{array} \quad \begin{array}{|cccccccc|}\hline 0 & 0 & 0 & 0 & 0 & 0 & +1 & -1 \\ 0 & 0 & 0 & 0 & +1 & 0 & -1 & 0 \\ 0 & +1 & 0 & 0 & 0 & -1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 & -1 & +1 & 0 & +1 \\ \hline \end{array}$$

- $4 \times 6 \times 6$ move of degree 16 with slice degree $\{2,4,4,6\} \times \{2,2,3,3,3,3\} \times \{2,2,2,2,4,4\}$
$((4,6,6),(16),((2,4,4,6),(2,2,3,3,3,3),(2,2,2,2,4,4)),(fcs),\emptyset,((135,146,231,245,255,262,313,326,354,$ $365,416,424,436,442,451,463),(136,145,235,242,251,265,316,324,355,363,413,426,431,446,454,462)))$

$$\begin{array}{|cccccc|}\hline 0&0&0&0&0&0\\ 0&0&0&0&0&0\\ 0&0&0&0&+1&-1\\ 0&0&0&0&-1&+1\\ 0&0&0&0&0&0\\ 0&0&0&0&0&0\\ \hline\end{array} \quad \begin{array}{|cccccc|}\hline 0&0&0&0&0&0\\ 0&0&0&0&0&0\\ +1&0&0&0&-1&0\\ 0&-1&0&0&+1&0\\ -1&0&0&0&+1&0\\ 0&+1&0&0&-1&0\\ \hline\end{array} \quad \begin{array}{|cccccc|}\hline 0&0&+1&0&0&-1\\ 0&0&0&-1&0&+1\\ 0&0&0&0&0&0\\ 0&0&0&0&0&0\\ 0&0&0&+1&-1&0\\ 0&0&-1&0&+1&0\\ \hline\end{array} \quad \begin{array}{|cccccc|}\hline 0&0&-1&0&0&+1\\ 0&0&0&+1&0&-1\\ -1&0&0&0&0&+1\\ 0&+1&0&0&0&-1\\ +1&0&0&-1&0&0\\ 0&-1&+1&0&0&0\\ \hline\end{array}$$

- $4 \times 6 \times 6$ move(1) of degree 16 with slice degree $\{3,3,4,6\} \times \{2,2,3,3,3,3\} \times \{2,2,2,2,4,4\}$
$((4,6,6),(16),((3,3,4,6),(2,2,3,3,3,3),(2,2,2,2,4,4)),(fcs),\emptyset,((115,131,146,226,255,262,334,341,352,$ $363,416,425,435,443,454,466),(116,135,141,225,252,266,331,343,354,362,415,426,434,446,455,463)))$

$$\begin{array}{|cccccc|}\hline 0&0&0&0&+1&-1\\ 0&0&0&0&0&0\\ +1&0&0&0&-1&0\\ -1&0&0&0&0&+1\\ 0&0&0&0&0&0\\ 0&0&0&0&0&0\\ \hline\end{array} \quad \begin{array}{|cccccc|}\hline 0&0&0&0&0&0\\ 0&0&0&0&-1&+1\\ 0&0&0&0&0&0\\ 0&0&0&0&0&0\\ 0&-1&0&0&+1&0\\ 0&+1&0&0&0&-1\\ \hline\end{array} \quad \begin{array}{|cccccc|}\hline 0&0&0&0&0&0\\ 0&0&0&0&0&0\\ -1&0&0&+1&0&0\\ +1&0&-1&0&0&0\\ 0&+1&0&-1&0&0\\ 0&-1&+1&0&0&0\\ \hline\end{array} \quad \begin{array}{|cccccc|}\hline 0&0&0&0&-1&+1\\ 0&0&0&0&+1&-1\\ 0&0&0&-1&+1&0\\ 0&0&+1&0&0&-1\\ 0&0&0&+1&-1&0\\ 0&0&-1&0&0&+1\\ \hline\end{array}$$

- $4 \times 6 \times 6$ move(2) of degree 16 with slice degree $\{3,3,4,6\} \times \{2,2,3,3,3,3\} \times \{2,2,2,2,4,4\}$
$((4,6,6),(16),((3,3,4,6),(2,2,3,3,3,3),(2,2,2,2,4,4)),(fcs),\emptyset,((111,135,146,226,252,265,334,345,355,$ $363,416,422,431,443,454,466),(116,131,145,222,255,266,335,343,354,365,411,426,434,446,452,463)))$

$$\begin{array}{|cccccc|}\hline +1&0&0&0&0&-1\\ 0&0&0&0&0&0\\ -1&0&0&0&+1&0\\ 0&0&0&0&-1&+1\\ 0&0&0&0&0&0\\ 0&0&0&0&0&0\\ \hline\end{array} \quad \begin{array}{|cccccc|}\hline 0&0&0&0&0&0\\ 0&-1&0&0&0&+1\\ 0&0&0&0&0&0\\ 0&0&0&0&0&0\\ 0&+1&0&0&-1&0\\ 0&0&0&0&+1&-1\\ \hline\end{array} \quad \begin{array}{|cccccc|}\hline 0&0&0&0&0&0\\ 0&0&0&0&0&0\\ 0&0&0&+1&-1&0\\ 0&0&-1&0&+1&0\\ 0&0&0&-1&+1&0\\ 0&0&+1&0&-1&0\\ \hline\end{array} \quad \begin{array}{|cccccc|}\hline -1&0&0&0&0&+1\\ 0&+1&0&0&0&-1\\ +1&0&0&-1&0&0\\ 0&0&+1&0&0&-1\\ 0&-1&0&+1&0&0\\ 0&0&-1&0&0&+1\\ \hline\end{array}$$

- $4 \times 6 \times 7$ move(1) of degree 16 with slice degree $\{2,4,4,6\} \times \{2,2,3,3,3,3\} \times \{2,2,2,2,2,2,4\}$
$((4,6,7),(16),((2,4,4,6),(2,2,3,3,3,3),(2,2,2,2,2,2,4)),(fcs),\emptyset,((131,147,232,241,254,263,315,327,356,$ $364,417,426,437,443,452,465),(137,141,231,243,252,264,317,326,354,365,415,427,432,447,456,463)))$

$$\begin{array}{|ccccccc|}\hline 0&0&0&0&0&0&0\\ 0&0&0&0&0&0&0\\ +1&0&0&0&0&0&-1\\ -1&0&0&0&0&0&+1\\ 0&0&0&0&0&0&0\\ 0&0&0&0&0&0&0\\ \hline\end{array} \quad \begin{array}{|ccccccc|}\hline 0&0&0&0&0&0&0\\ 0&0&0&0&0&0&0\\ -1&+1&0&0&0&0&0\\ +1&0&-1&0&0&0&0\\ 0&-1&0&+1&0&0&0\\ 0&0&+1&-1&0&0&0\\ \hline\end{array}$$

$$\begin{array}{|ccccccc|}\hline 0&0&0&0&+1&0&-1\\ 0&0&0&0&0&-1&+1\\ 0&0&0&0&0&0&0\\ 0&0&0&0&0&0&0\\ 0&0&0&-1&0&+1&0\\ 0&0&0&+1&-1&0&0\\ \hline\end{array} \quad \begin{array}{|ccccccc|}\hline 0&0&0&0&-1&0&+1\\ 0&0&0&0&0&+1&-1\\ 0&-1&0&0&0&0&+1\\ 0&0&+1&0&0&0&-1\\ 0&+1&0&0&0&-1&0\\ 0&0&-1&0&+1&0&0\\ \hline\end{array}$$

- $4 \times 6 \times 7$ move(2) of degree 16 with slice degree $\{2, 4, 4, 6\} \times \{2, 2, 3, 3, 3, 3\} \times \{2, 2, 2, 2, 2, 2, 4\}$
  $((4, 6, 7), (16), ((2, 4, 4, 6), (2, 2, 3, 3, 3, 3), (2, 2, 2, 2, 2, 2, 4)), (fcs), \emptyset, ((131, 147, 237, 243, 252, 267, 316, 325, 357, 364, 415, 424, 432, 441, 456, 463), (137, 141, 232, 247, 257, 263, 315, 324, 356, 367, 416, 425, 431, 443, 452, 464)))$

0	0	0	0	0	0	0
0	0	0	0	0	0	0
−1	0	0	0	0	0	+1
+1	0	0	0	0	0	−1
0	0	0	0	0	0	0
0	0	0	0	0	0	0

0	0	0	0	0	0	0
0	0	0	0	0	0	0
0	+1	0	0	0	0	−1
0	0	−1	0	0	0	+1
0	−1	0	0	0	0	+1
0	0	+1	0	0	0	−1

0	0	0	0	+1	−1	0
0	0	0	+1	−1	0	0
0	0	0	0	0	0	0
0	0	0	0	0	0	0
0	0	0	0	0	+1	−1
0	0	0	−1	0	0	+1

0	0	0	0	−1	+1	0
0	0	0	−1	+1	0	0
+1	−1	0	0	0	0	0
−1	0	+1	0	0	0	0
0	+1	0	0	0	−1	0
0	0	−1	+1	0	0	0

- $4 \times 6 \times 7$ move(3) of degree 16 with slice degree $\{2, 4, 4, 6\} \times \{2, 2, 3, 3, 3, 3\} \times \{2, 2, 2, 2, 2, 2, 4\}$
  (not fundamental, circuit)
  $((4, 6, 7), (16), ((2, 4, 4, 6), (2, 2, 3, 3, 3, 3), (2, 2, 2, 2, 2, 2, 4)), (Fcs), (437, 447), ((131, 147, 237, 243, 252, 264, 316, 327, 354, 365, 417, 425, 432, 441, 456, 463), (137, 141, 232, 247, 254, 263, 317, 325, 356, 364, 416, 427, 431, 443, 452, 465)))$

0	0	0	0	0	0	0
0	0	0	0	0	0	0
−1	0	0	0	0	0	+1
+1	0	0	0	0	0	−1
0	0	0	0	0	0	0
0	0	0	0	0	0	0

0	0	0	0	0	0	0
0	0	0	0	0	0	0
0	+1	0	0	0	0	−1
0	0	−1	0	0	0	+1
0	−1	0	+1	0	0	0
0	0	+1	−1	0	0	0

0	0	0	0	0	−1	+1
0	0	0	0	+1	0	−1
0	0	0	0	0	0	0
0	0	0	0	0	0	0
0	0	0	−1	0	+1	0
0	0	0	+1	−1	0	0

0	0	0	0	0	+1	−1
0	0	0	0	−1	0	+1
+1	−1	0	0	0	0	(0)
−1	0	+1	0	0	0	(0)
0	+1	0	0	0	−1	0
0	0	−1	0	+1	0	0

- $4 \times 6 \times 7$ move(1) of degree 16 with slice degree $\{3, 3, 4, 6\} \times \{2, 2, 3, 3, 3, 3\} \times \{2, 2, 2, 2, 2, 2, 4\}$
  $((4, 6, 7), (16), ((3, 3, 4, 6), (2, 2, 3, 3, 3, 3), (2, 2, 2, 2, 2, 2, 4)), (fcs), \emptyset, ((111, 132, 147, 227, 253, 264, 335, 342, 354, 366, 417, 423, 431, 446, 455, 467), (117, 131, 142, 223, 254, 267, 332, 346, 355, 364, 411, 427, 435, 447, 453, 466)))$

+1	0	0	0	0	0	−1
0	0	0	0	0	0	0
−1	+1	0	0	0	0	0
0	−1	0	0	0	0	+1
0	0	0	0	0	0	0
0	0	0	0	0	0	0

0	0	0	0	0	0	0
0	0	−1	0	0	0	+1
0	0	0	0	0	0	0
0	0	0	0	0	0	0
0	0	+1	−1	0	0	0
0	0	0	+1	0	0	−1

0	0	0	0	0	0	0
0	0	0	0	0	0	0
0	−1	0	0	+1	0	0
0	+1	0	0	0	−1	0
0	0	0	+1	−1	0	0
0	0	0	−1	0	+1	0

−1	0	0	0	0	0	+1
0	0	+1	0	0	0	−1
+1	0	0	0	−1	0	0
0	0	0	0	0	+1	−1
0	0	−1	0	+1	0	0
0	0	0	0	0	−1	+1

- $4 \times 6 \times 7$ move(2) of degree 16 with slice degree $\{3,3,4,6\} \times \{2,2,3,3,3,3\} \times \{2,2,2,2,2,2,4\}$
  $((4,6,7),(16),((3,3,4,6),(2,2,3,3,3,3),(2,2,2,2,2,2,4)),(fcs),\emptyset,((111,132,147,223,254,267,335,342,356,$ $364,417,427,431,446,453,465),(117,131,142,227,253,264,332,346,354,365,411,423,435,447,456,467)))$

$$\begin{array}{|ccccccc|}\hline -1 & 0 & 0 & 0 & 0 & 0 & +1 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ +1 & -1 & 0 & 0 & 0 & 0 & 0 \\ 0 & +1 & 0 & 0 & 0 & 0 & -1 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ \hline \end{array} \quad \begin{array}{|ccccccc|}\hline 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & -1 & 0 & 0 & 0 & +1 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & +1 & -1 & 0 & 0 & 0 \\ 0 & 0 & 0 & +1 & 0 & 0 & -1 \\ \hline \end{array}$$

$$\begin{array}{|ccccccc|}\hline 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & +1 & 0 & 0 & -1 & 0 & 0 \\ 0 & -1 & 0 & 0 & 0 & +1 & 0 \\ 0 & 0 & 0 & +1 & 0 & -1 & 0 \\ 0 & 0 & 0 & -1 & +1 & 0 & 0 \\ \hline \end{array} \quad \begin{array}{|ccccccc|}\hline +1 & 0 & 0 & 0 & 0 & 0 & -1 \\ 0 & 0 & +1 & 0 & 0 & 0 & -1 \\ -1 & 0 & 0 & 0 & +1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & -1 & +1 \\ 0 & 0 & -1 & 0 & 0 & +1 & 0 \\ 0 & 0 & 0 & 0 & -1 & 0 & +1 \\ \hline \end{array}$$

- $4 \times 6 \times 7$ move(3) of degree 16 with slice degree $\{3,3,4,6\} \times \{2,2,3,3,3,3\} \times \{2,2,2,2,2,2,4\}$
  $((4,6,7),(16),((3,3,4,6),(2,2,3,3,3,3),(2,2,2,2,2,2,4)),(fcs),\emptyset,((111,137,142,223,257,264,336,347,355,$ $367,412,424,431,445,453,466),(112,131,147,224,253,267,337,345,357,366,411,423,436,442,455,464)))$

$$\begin{array}{|ccccccc|}\hline +1 & -1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ -1 & 0 & 0 & 0 & 0 & 0 & +1 \\ 0 & +1 & 0 & 0 & 0 & 0 & -1 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ \hline \end{array} \quad \begin{array}{|ccccccc|}\hline 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & +1 & -1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & -1 & 0 & 0 & 0 & +1 \\ 0 & 0 & 0 & +1 & 0 & 0 & -1 \\ \hline \end{array}$$

$$\begin{array}{|ccccccc|}\hline 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & +1 & -1 \\ 0 & 0 & 0 & 0 & -1 & 0 & +1 \\ 0 & 0 & 0 & 0 & +1 & 0 & -1 \\ 0 & 0 & 0 & 0 & 0 & -1 & +1 \\ \hline \end{array} \quad \begin{array}{|ccccccc|}\hline -1 & +1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & -1 & +1 & 0 & 0 & 0 \\ +1 & 0 & 0 & 0 & 0 & -1 & 0 \\ 0 & -1 & 0 & 0 & +1 & 0 & 0 \\ 0 & 0 & +1 & 0 & -1 & 0 & 0 \\ 0 & 0 & 0 & -1 & 0 & +1 & 0 \\ \hline \end{array}$$

- $4 \times 6 \times 8$ move of degree 16 with slice degree $\{2,4,4,6\} \times \{2,2,3,3,3,3\} \times \{2,2,2,2,2,2,2,2\}$
  $((4,6,8),(16),((2,4,4,6),(2,2,3,3,3,3),(2,2,2,2,2,2,2,2)),(fcs),\emptyset,((131,142,233,241,255,264,316,328,357,$ $365,417,426,432,444,453,468),(132,141,231,244,253,265,317,326,355,368,416,428,433,442,457,464)))$

$$\begin{array}{|cccccccc|}\hline 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ +1 & -1 & 0 & 0 & 0 & 0 & 0 & 0 \\ -1 & +1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ \hline \end{array} \quad \begin{array}{|cccccccc|}\hline 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ -1 & 0 & +1 & 0 & 0 & 0 & 0 & 0 \\ +1 & 0 & 0 & -1 & 0 & 0 & 0 & 0 \\ 0 & 0 & -1 & 0 & +1 & 0 & 0 & 0 \\ 0 & 0 & 0 & +1 & -1 & 0 & 0 & 0 \\ \hline \end{array}$$

$$\begin{array}{|cccccccc|}\hline 0 & 0 & 0 & 0 & 0 & +1 & -1 & 0 \\ 0 & 0 & 0 & 0 & 0 & -1 & 0 & +1 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & -1 & 0 & +1 & 0 \\ 0 & 0 & 0 & 0 & +1 & 0 & 0 & -1 \\ \hline \end{array} \quad \begin{array}{|cccccccc|}\hline 0 & 0 & 0 & 0 & 0 & -1 & +1 & 0 \\ 0 & 0 & 0 & 0 & 0 & +1 & 0 & -1 \\ 0 & +1 & -1 & 0 & 0 & 0 & 0 & 0 \\ 0 & -1 & 0 & +1 & 0 & 0 & 0 & 0 \\ 0 & 0 & +1 & 0 & 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & -1 & 0 & 0 & 0 & +1 \\ \hline \end{array}$$

- $4 \times 6 \times 8$ move of degree 16 with slice degree $\{3,3,4,6\} \times \{2,2,3,3,3,3\} \times \{2,2,2,2,2,2,2,2\}$
  $((4,6,8),(16),((3,3,4,6),(2,2,3,3,3,3),(2,2,2,2,2,2,2,2)),(fcs),\emptyset,((111,133,142,224,256,265,337,343,358,366,412,425,431,448,454,467),(112,131,143,225,254,266,333,348,356,367,411,424,437,442,458,465)))$

$$\begin{array}{|cccccccc|}\hline +1 & -1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ -1 & 0 & +1 & 0 & 0 & 0 & 0 & 0 \\ 0 & +1 & -1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ \hline \end{array} \qquad \begin{array}{|cccccccc|}\hline 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & +1 & -1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & -1 & 0 & +1 & 0 & 0 \\ 0 & 0 & 0 & 0 & +1 & -1 & 0 & 0 \\ \hline \end{array}$$

$$\begin{array}{|cccccccc|}\hline 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & -1 & 0 & 0 & 0 & +1 & 0 \\ 0 & 0 & +1 & 0 & 0 & 0 & 0 & -1 \\ 0 & 0 & 0 & 0 & 0 & -1 & 0 & +1 \\ 0 & 0 & 0 & 0 & 0 & +1 & -1 & 0 \\ \hline \end{array} \qquad \begin{array}{|cccccccc|}\hline -1 & +1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & -1 & +1 & 0 & 0 & 0 \\ +1 & 0 & 0 & 0 & 0 & 0 & -1 & 0 \\ 0 & -1 & 0 & 0 & 0 & 0 & 0 & +1 \\ 0 & 0 & 0 & +1 & 0 & 0 & 0 & -1 \\ 0 & 0 & 0 & 0 & -1 & 0 & +1 & 0 \\ \hline \end{array}$$

- $5 \times 5 \times 7$ move(1) of degree 16 with slice degree $\{2,3,3,3,5\} \times \{2,3,3,4,4\} \times \{2,2,2,2,2,2,4\}$
  $((5,5,7),(16),((2,3,3,3,5),(2,3,3,4,4),(2,2,2,2,2,2,4)),(fcs),\emptyset,((121,147,222,241,253,334,343,355,417,435,456,516,527,537,544,552),(127,141,221,243,252,335,344,353,416,437,455,517,522,534,547,556)))$

$$\begin{array}{|ccccccc|}\hline 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ +1 & 0 & 0 & 0 & 0 & 0 & -1 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ -1 & 0 & 0 & 0 & 0 & 0 & +1 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ \hline \end{array} \qquad \begin{array}{|ccccccc|}\hline 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ -1 & +1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ +1 & 0 & -1 & 0 & 0 & 0 & 0 \\ 0 & -1 & +1 & 0 & 0 & 0 & 0 \\ \hline \end{array} \qquad \begin{array}{|ccccccc|}\hline 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & +1 & -1 & 0 & 0 \\ 0 & 0 & +1 & -1 & 0 & 0 & 0 \\ 0 & 0 & -1 & 0 & +1 & 0 & 0 \\ \hline \end{array}$$

$$\begin{array}{|ccccccc|}\hline 0 & 0 & 0 & 0 & 0 & -1 & +1 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & +1 & 0 & -1 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & -1 & +1 & 0 \\ \hline \end{array} \qquad \begin{array}{|ccccccc|}\hline 0 & 0 & 0 & 0 & 0 & +1 & -1 \\ 0 & -1 & 0 & 0 & 0 & 0 & +1 \\ 0 & 0 & 0 & -1 & 0 & 0 & +1 \\ 0 & 0 & 0 & +1 & 0 & 0 & -1 \\ 0 & +1 & 0 & 0 & 0 & -1 & 0 \\ \hline \end{array}$$

- $5 \times 5 \times 7$ move(2) of degree 16 with slice degree $\{2,3,3,3,5\} \times \{2,3,3,4,4\} \times \{2,2,2,2,2,2,4\}$
  (not fundamental, circuit)
  $((5,5,7),(16),((2,3,3,3,5),(2,3,3,4,4),(2,2,2,2,2,2,4)),(Fcs),(527,547),((121,147,233,244,252,327,342,355,416,437,453,517,525,534,541,556),(127,141,234,242,253,325,347,352,417,433,456,516,521,537,544,555)))$

$$\begin{array}{|ccccccc|}\hline 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ -1 & 0 & 0 & 0 & 0 & 0 & +1 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ +1 & 0 & 0 & 0 & 0 & 0 & -1 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ \hline \end{array} \qquad \begin{array}{|ccccccc|}\hline 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & -1 & +1 & 0 & 0 & 0 \\ 0 & +1 & 0 & -1 & 0 & 0 & 0 \\ 0 & -1 & +1 & 0 & 0 & 0 & 0 \\ \hline \end{array} \qquad \begin{array}{|ccccccc|}\hline 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & +1 & 0 & -1 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 & 0 & 0 & +1 \\ 0 & +1 & 0 & 0 & -1 & 0 & 0 \\ \hline \end{array}$$

$$\begin{array}{|ccccccc|}\hline 0 & 0 & 0 & 0 & 0 & -1 & +1 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & +1 & 0 & 0 & 0 & -1 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & -1 & 0 & 0 & +1 & 0 \\ \hline \end{array} \qquad \begin{array}{|ccccccc|}\hline 0 & 0 & 0 & 0 & 0 & +1 & -1 \\ +1 & 0 & 0 & 0 & -1 & 0 & (0) \\ 0 & 0 & 0 & -1 & 0 & 0 & +1 \\ -1 & 0 & 0 & +1 & 0 & 0 & (0) \\ 0 & 0 & 0 & 0 & +1 & -1 & 0 \\ \hline \end{array}$$

- $5 \times 5 \times 8$ move of degree 16 with slice degree $\{2,3,3,3,5\} \times \{2,3,3,4,4\} \times \{2,2,2,2,2,2,2,2\}$
  $((5,5,8),(16),((2,3,3,3,5),(2,3,3,4,4),(2,2,2,2,2,2,2,2)),(fcs),\emptyset,((121,142,223,241,254,335,344,356,418,436,457,517,522,538,545,553),(122,141,221,244,253,336,345,354,417,438,456,518,523,535,542,557)))$

$$\begin{array}{|cccccccc|}\hline 0&0&0&0&0&0&0&0\\ +1&-1&0&0&0&0&0&0\\ 0&0&0&0&0&0&0&0\\ -1&+1&0&0&0&0&0&0\\ 0&0&0&0&0&0&0&0\\ \hline\end{array} \quad \begin{array}{|cccccccc|}\hline 0&0&0&0&0&0&0&0\\ -1&0&+1&0&0&0&0&0\\ 0&0&0&0&0&0&0&0\\ +1&0&0&-1&0&0&0&0\\ 0&0&-1&+1&0&0&0&0\\ \hline\end{array} \quad \begin{array}{|cccccccc|}\hline 0&0&0&0&0&0&0&0\\ 0&0&0&0&0&0&0&0\\ 0&0&0&0&+1&-1&0&0\\ 0&0&0&+1&-1&0&0&0\\ 0&0&0&-1&0&+1&0&0\\ \hline\end{array}$$

$$\begin{array}{|cccccccc|}\hline 0&0&0&0&0&0&-1&+1\\ 0&0&0&0&0&0&0&0\\ 0&0&0&0&0&+1&0&-1\\ 0&0&0&0&0&0&0&0\\ 0&0&0&0&0&-1&+1&0\\ \hline\end{array} \quad \begin{array}{|cccccccc|}\hline 0&0&0&0&0&0&+1&-1\\ 0&+1&-1&0&0&0&0&0\\ 0&0&0&0&-1&0&0&+1\\ 0&-1&0&0&+1&0&0&0\\ 0&0&+1&0&0&0&-1&0\\ \hline\end{array}$$

- $5 \times 6 \times 6$ move(1) of degree 16 with slice degree $\{2,3,3,4,4\} \times \{2,2,2,2,4,4\} \times \{2,2,3,3,3,3\}$
  $((5,6,6),(16),((2,3,3,4,4),(2,2,2,2,4,4),(2,2,3,3,3,3)),(fcs),\emptyset,((153,164,211,225,263,334,346,362,415,442,456,461,523,536,554,555),(154,163,215,223,261,336,342,364,411,446,455,462,525,534,553,556)))$

$$\begin{array}{|cccccc|}\hline 0&0&0&0&0&0\\ 0&0&0&0&0&0\\ 0&0&0&0&0&0\\ 0&0&0&0&0&0\\ 0&0&+1&-1&0&0\\ 0&0&-1&+1&0&0\\ \hline\end{array} \quad \begin{array}{|cccccc|}\hline +1&0&0&0&-1&0\\ 0&0&-1&0&+1&0\\ 0&0&0&0&0&0\\ 0&0&0&0&0&0\\ 0&0&0&0&0&0\\ -1&0&+1&0&0&0\\ \hline\end{array} \quad \begin{array}{|cccccc|}\hline 0&0&0&0&0&0\\ 0&0&0&0&0&0\\ 0&0&0&+1&0&-1\\ 0&-1&0&0&0&+1\\ 0&0&0&0&0&0\\ 0&+1&0&-1&0&0\\ \hline\end{array}$$

$$\begin{array}{|cccccc|}\hline -1&0&0&0&+1&0\\ 0&0&0&0&0&0\\ 0&0&0&0&0&0\\ 0&+1&0&0&0&-1\\ 0&0&0&0&-1&+1\\ +1&-1&0&0&0&0\\ \hline\end{array} \quad \begin{array}{|cccccc|}\hline 0&0&0&0&0&0\\ 0&0&+1&0&-1&0\\ 0&0&0&-1&0&+1\\ 0&0&0&0&0&0\\ 0&0&-1&+1&+1&-1\\ 0&0&0&0&0&0\\ \hline\end{array}$$

- $5 \times 6 \times 6$ move(2) of degree 16 with slice degree $\{2,3,3,4,4\} \times \{2,2,2,2,4,4\} \times \{2,2,3,3,3,3\}$
  $((5,6,6),(16),((2,3,3,4,4),(2,2,2,2,4,4),(2,2,3,3,3,3)),(fcs),\emptyset,((113,164,225,251,263,344,356,362,414,423,435,446,536,552,555,561),(114,163,223,255,261,346,352,364,413,425,436,444,535,551,556,562)))$

$$\begin{array}{|cccccc|}\hline 0&0&+1&-1&0&0\\ 0&0&0&0&0&0\\ 0&0&0&0&0&0\\ 0&0&0&0&0&0\\ 0&0&0&0&0&0\\ 0&0&-1&+1&0&0\\ \hline\end{array} \quad \begin{array}{|cccccc|}\hline 0&0&0&0&0&0\\ 0&0&-1&0&+1&0\\ 0&0&0&0&0&0\\ 0&0&0&0&0&0\\ +1&0&0&0&-1&0\\ -1&0&+1&0&0&0\\ \hline\end{array} \quad \begin{array}{|cccccc|}\hline 0&0&0&0&0&0\\ 0&0&0&0&0&0\\ 0&0&0&0&0&0\\ 0&0&0&+1&0&-1\\ 0&-1&0&0&0&+1\\ 0&+1&0&-1&0&0\\ \hline\end{array}$$

$$\begin{array}{|cccccc|}\hline 0&0&-1&+1&0&0\\ 0&0&+1&0&-1&0\\ 0&0&0&0&+1&-1\\ 0&0&0&-1&0&+1\\ 0&0&0&0&0&0\\ 0&0&0&0&0&0\\ \hline\end{array} \quad \begin{array}{|cccccc|}\hline 0&0&0&0&0&0\\ 0&0&0&0&0&0\\ 0&0&0&0&-1&+1\\ 0&0&0&0&0&0\\ -1&+1&0&0&+1&-1\\ +1&-1&0&0&0&0\\ \hline\end{array}$$

- $5 \times 6 \times 6$ move(3) of degree 16 with slice degree $\{2,3,3,4,4\} \times \{2,2,2,2,4,4\} \times \{2,2,3,3,3,3\}$
$((5,6,6),(16),((2,3,3,4,4),(2,2,2,2,4,4),(2,2,3,3,3,3)),(fcs),\emptyset,((113,164,221,255,263,346,354,362,414,435,453,456,525,536,542,561),(114,163,225,253,261,342,356,364,413,436,454,455,521,535,546,562)))$

$$\begin{array}{|cccccc|}\hline 0&0&+1&-1&0&0\\ 0&0&0&0&0&0\\ 0&0&0&0&0&0\\ 0&0&0&0&0&0\\ 0&0&0&0&0&0\\ 0&0&-1&+1&0&0\\ \hline\end{array} \quad \begin{array}{|cccccc|}\hline 0&0&0&0&0&0\\ +1&0&0&0&-1&0\\ 0&0&0&0&0&0\\ 0&0&0&0&0&0\\ 0&0&-1&0&+1&0\\ -1&0&+1&0&0&0\\ \hline\end{array} \quad \begin{array}{|cccccc|}\hline 0&0&0&0&0&0\\ 0&0&0&0&0&0\\ 0&0&0&0&0&0\\ 0&-1&0&0&0&+1\\ 0&0&0&+1&0&-1\\ 0&+1&0&-1&0&0\\ \hline\end{array}$$

$$\begin{array}{|cccccc|}\hline 0&0&-1&+1&0&0\\ 0&0&0&0&0&0\\ 0&0&0&0&+1&-1\\ 0&0&0&0&0&0\\ 0&0&+1&-1&-1&+1\\ 0&0&0&0&0&0\\ \hline\end{array} \quad \begin{array}{|cccccc|}\hline 0&0&0&0&0&0\\ -1&0&0&0&+1&0\\ 0&0&0&0&-1&+1\\ 0&+1&0&0&0&-1\\ 0&0&0&0&0&0\\ +1&-1&0&0&0&0\\ \hline\end{array}$$

- $5 \times 6 \times 7$ move of degree 16 with slice degree $\{2,3,3,4,4\} \times \{2,2,3,3,3,3\} \times \{2,2,2,2,2,2,4\}$
$((5,6,7),(16),((2,3,3,4,4),(2,2,3,3,3,3),(2,2,2,2,2,2,4)),(fcs),\emptyset,((131,147,212,237,253,327,345,364,433,441,456,465,517,524,552,566),(137,141,217,233,252,324,347,365,431,445,453,466,512,527,556,564)))$

$$\begin{array}{|ccccccc|}\hline 0&0&0&0&0&0&0\\ 0&0&0&0&0&0&0\\ +1&0&0&0&0&0&-1\\ -1&0&0&0&0&0&+1\\ 0&0&0&0&0&0&0\\ 0&0&0&0&0&0&0\\ \hline\end{array} \quad \begin{array}{|ccccccc|}\hline 0&+1&0&0&0&0&-1\\ 0&0&0&0&0&0&0\\ 0&0&-1&0&0&0&+1\\ 0&0&0&0&0&0&0\\ 0&-1&+1&0&0&0&0\\ 0&0&0&0&0&0&0\\ \hline\end{array} \quad \begin{array}{|ccccccc|}\hline 0&0&0&0&0&0&0\\ 0&0&0&-1&0&0&+1\\ 0&0&0&0&0&0&0\\ 0&0&0&0&+1&0&-1\\ 0&0&0&0&0&0&0\\ 0&0&0&+1&-1&0&0\\ \hline\end{array}$$

$$\begin{array}{|ccccccc|}\hline 0&0&0&0&0&0&0\\ 0&0&0&0&0&0&0\\ -1&0&+1&0&0&0&0\\ +1&0&0&0&-1&0&0\\ 0&0&-1&0&0&+1&0\\ 0&0&0&0&+1&-1&0\\ \hline\end{array} \quad \begin{array}{|ccccccc|}\hline 0&-1&0&0&0&0&+1\\ 0&0&0&+1&0&0&-1\\ 0&0&0&0&0&0&0\\ 0&0&0&0&0&0&0\\ 0&+1&0&0&0&-1&0\\ 0&0&0&-1&0&+1&0\\ \hline\end{array}$$

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