論 文 の 内 容 の 要 旨

論文題目　　量子アニーリングを用いたブラックボックス最適化

(Black-Box Optimization with Quantum Annealing)

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In this thesis a new black-box optimization method, factorization machine for quantum annealing (FMQA), is proposed. The method targets at any combinatorial optimization problems. It is composed of a regression model called factorization machine (FM), and a heuristic minimization solver called quantum annealing (QA). A proof-of-principle demonstration of the FMQA's efficiency on a metamaterial designing problem is made, and it found better materials structure than the ones found with some classical algorithms. To improve the performance for further optimization problems, the FMQA is modified with a local modeling technique. It is tested on several benchmarking problems and on an application for feature selection problem. The method is revealed to be more robust than the original FMQA for the early steps of optimizations.

In science, industry, and engineering, there are often optimization problems where we have to get an objective value by experiments or simulations (e.g., maximizing energy conversion efficiency or minimizing resource consumption). We cannot always expect the objective function's analytical representation or 1st-degree gradient information in those cases. Such an optimization task is called black-box optimization (BBO).

In the recent development of BBO methods, optimization problems over discrete or binary variables are gathering more attention, for example, in materials informatics. In this thesis, our targets are limited for BBO problems with binary variables. The assumption in BBO is so common and there are several optimization algorithms for solving them. One of the naivest ways is greedy editing.　In the greedy editing, we apply single-variable flipping repeatedly as long as that improves the objective value. Simulated annealing and tabu search are variations of the greedy editing, where the variable flipping yielding the degraded objective value is sometimes allowed. They are suited for solving problems where the objective value is easily evaluated but not for all BBO problems. The most successful algorithms for BBO belong to surrogate-based methods. We construct a regression model (or surrogate model) using the data already obtained and select the most promising input configuration based on it. Afterward, we evaluate the objective function on the selected configuration and add the result to the dataset. The selections and evaluations are continued until some convergence criterion is met. Using the surrogate model makes the process aware of the objective function's landscape and it reduces the required evaluations of the objective function. That is what makes the surrogate-based methods appropriate for real-world BBO problems.

On the other hand, BBO algorithms may fail when the search space is too large because finding the most promising configuration can be difficult even on the surrogate model. To solve the increasingly larger problems, a new BBO algorithm that can deal with a huge search space is required.

Recent technological advancement for implementing multiple quantum bits (qubits) and manipulating their connections sparkled further exploration of quantum computing algorithms. Adiabatic quantum computing (AQC) is a special type of quantum computing, which utilizes the time development of an adiabatic quantum system for solving computational tasks. D-Wave Systems Inc. has developed D-Wave 2000Q™, a quantum annealing (QA) machine, for realizing an AQC process. The scope of AQC is more limited than the general quantum computing. However, the D-Wave 2000Q™, for example, is composed of 2000 qubits, which is an order of magnitude more than the ones implemented in general-purpose quantum computers so far. The machines are already used as the core of optimization systems for various commercial-scale problems.

QA is a heuristic similar to the simulated annealing algorithm, but its variables go through superposed states. QA's current implementation can solve combinatorial problems represented in the quadratic unconstrained binary optimization (QUBO) format, which includes NP-hard problems. QUBO is a minimization problem of the form:

$$\min_{\mathbf{x}\in\{0,1\}^d} \sum_{i\leq j} q_{ij} x_i x_j \qquad (1)$$

where d is the number of variables and $q_{ij} \in \mathbb{R}$ is a parameter for configuring the problem. Typically, we convert our optimization problems in this QUBO format and solve them with the QA machine.

QA's ability to deal with high-dimensional problems is desirable for BBO to overcome the limitation of searching in a large space. To fit the BBO problems to QA machines, we must use surrogate-based methods whose model is compatible with the QUBO format.

A quadratic regression function as a surrogate model is proposed for the BBO over continuous variables in [M. J. D. Powell, 2009]. Similarly, the objective function of QUBO in expression (1) can be used as a surrogate model for BBO over binary variables. However, a difficulty arises from that there are $d(d+1)/2+1 \sim \mathcal{O}(d^2)$ model parameters in (1), which requires the dataset of the size proportional to d^2. This is too demanding when d is large and when one evaluation cost is unignorable.

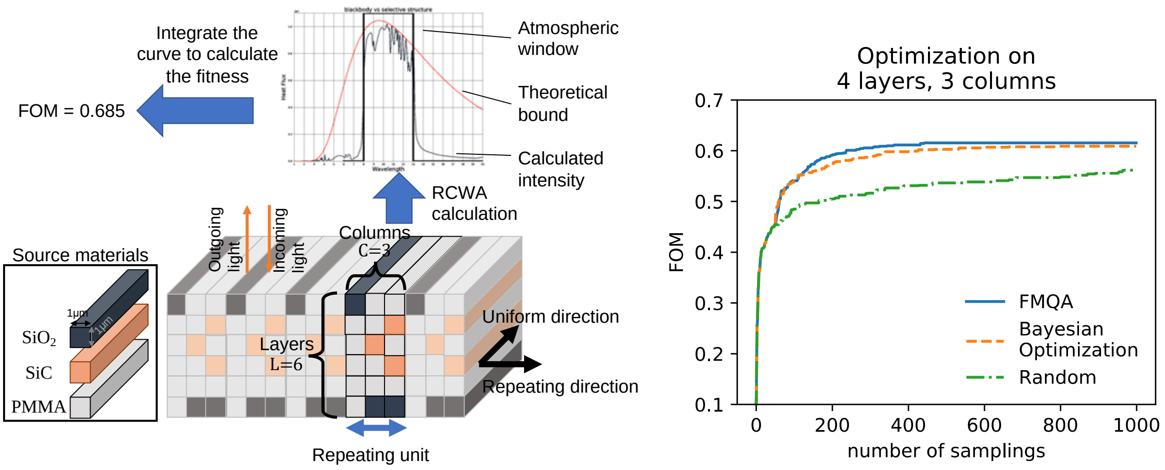

Figure 1: (Left) Materials structure and calculation of its FOM. (Right) Comparison of FMQA against Bayesian optimization and random search.

We instead use the factorization machine (FM) as a surrogate model. FM is the following quadratic function:

$$
\begin{aligned}
\hat{f}_\theta(\mathbf{x}) &= w_0 + \sum_{i=1}^{d} w_i x_i + \sum_{i=1}^{d} \sum_{j=i+1}^{d} \sum_{k=1}^{K} v_{ik} v_{jk} x_i x_j \\
&= \mathrm{w}_0 + \sum_{i=1}^{N} w_i x_i + \sum_{i=1}^{N} \sum_{j=i+1}^{N} (\mathbf{v}_i \cdot \mathbf{v}_j) x_i x_j, \qquad (2)
\end{aligned}
$$

where $w_i (i = 0, \cdots, d)$ is scalar and $\mathbf{v_i} (i = 1, \cdots, d)$ is a vector of size K (hyperparameter). Compared to QUBO's objective, the model parameters' size is reduced to $dK + d + 1$, leading to less size required for the training dataset. We can convert a trained FM model to QUBO's objective function easily by equations:

$$
\begin{aligned}
q_{ii} &= w_i \qquad\qquad (\, i \in \{1, \cdots, d\}) \\
q_{ij} &= \mathbf{v}_i \cdot \mathbf{v}_j \quad (i, j \in \{1, \cdots, d\}; i < j). \qquad (3)
\end{aligned}
$$

We then solve the resulting QUBO problem by the QA. Since the QA machine is specially designed hardware for the QUBO problem, a promising solution is obtained instantly. The combination of FM and QA is termed factorization machine for quantum annealing (FMQA).

A proof-of-principle experiment on a realistic application in materials science is made for validating the FMQA. A composition of different materials to show extraordinary properties than bulk materials is called metamaterial. Designing metamaterials became complex and difficult because of advancements in synthesizing technology. We tried to design metamaterials for selective radiative cooling as an example where such a designing task is represented in a BBO on binary variables.

Our target material was a stacking of fiber-shaped materials in a repeating pattern, with each fiber has a cross-section of a 1μm square (Fig.1 Left). The source materials (SiO_2, SiC, and PMMA) are stacked up to 9 layers. We can calculate spectral radiation by rigorous coupled-wave analysis (RCWA) simulation if a stacking pattern is specified.

What is to be optimized here is the radiation intensity's fitness to a wavelength band so-called atmospheric window (from 8 to 13μm). In other words, we have to keep the radiation intensity between the atmospheric window as close to a theoretical upper bound, while at outside keeping it as close to zero. The whole fitness is evaluated by a weighted integration over the entire wavelengths, resulting in a real value between -2.0 and 1.0 (higher is better), referred to as FOM (Figure of Merit).

By applying our method to the problem, we achieved faster optimization than Bayesian optimization, which is an algorithm known to works well for BBO on continuous variables, in designing structures with 4 layers and 3 columns (Fig.1 Right). We also tried to design many different sizes of the structures and found a configuration which shows an unprecedented performance of FOM=0.724.

We also developed the variation of the FMQA with localized FM models, local FMQA. The QA part needed to be replaced with SA due to the shortage of qubits, but the modification made the model faster and robust for a set of benchmarking problems especially in the beginning steps of the optimization. It is also applied for a feature selection task for efficiently modeling the androgen receptor (AR) activity of chemical compounds. The data is based on an open repository about quantitative structure-activity relationship (QSAR) analysis. As a result, the local FMQA was faster and better at choosing the relevant features to predict the output label of the compounds than other methods. The localization of surrogate models can be beneficial for a practical performance of BBO methods.

Throughout the thesis, effective applications of QA for black-box optimization are proposed with several use cases. The selection power of QA could help the optimization process, with the use of an FM as a surrogate model. The design and hyper-parameter tuning of the models could further accelerate it. The future work will be finding an effective strategy for achieving better optimization performance, along with other realistic applications other than the ones addressed here.