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Applicability of Gaussian On-off Encoding for Quantum Annealing to Structural Analysis

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This study concerns an efficient random encoding method to structural analysis of two-dimensional truss problems based on quantum annealing. As the basic operation of a quantum annealing, real numbers are represented using binary variables and encoded into qubits, requiring an appropriate expression. In this study, the encoding method selects a certain number of digits within the range of real numbers, and then controls whether they work in the total summation of real number expression through the 0/1 quantum state. A Gaussian distribution are adopted in it to control the selection of digits to represent real numbers. Other three commonly used encoding methods are employed as comparison under different truss structures and load conditions. The results show that the Gaussian on-off encoding outperforms present methods in terms of accuracy, stability and qubit requirement.

Key Words : *Gaussian on-off encoding, QUBO, truss structure analysis, quantum annealing*

1. Introduction

Quantum computing is a rapidly advancing research field. Compared to classical algorithms, quantum algorithms can provide asymptotic acceleration in certain problems. Recently, there have been industrial efforts worldwide to construct commercial quantum computers. Among them, the D-Wave system [1] operates specifically for Quantum Annealing (QA) [2]. QA is a quantum algorithm specifically designed to solve combinatorial optimization problems. The underlying mathematical model of QA is the Quadratic Unconstrained Binary Optimization (QUBO) model. In essence, if a practical problem can be represented in the form of a QUBO model, its solution can be efficiently explored with QA.

To date, diverse applications of QA have been reported in biological science, machine learning, traffic control and structural engineering. Since solving a system of linear equations (hereafter simply referred to as "linear system") is one of the most fundamental problems in almost all sciences and engineering, there have been multiple previous studies by the application of QA[3,4]. However, these studies have not referred to a physical object. We wish to focus specifically on an arbitrary linear system that appears in matrix structural analysis (MSA) of two-dimensional (2D) trusses in this study.

Since the variables in the QUBO model are qubits, an encoding operation is inevitably required in MSA. The encoding can convert the objective function and relevant constraints of a target problem with real number variables into binary format to create the QUBO model, ensuring the compatibility with quantum annealing. Several currently available encoding methods, such as one-hot encoding and binary encoding, expand binary-variables to discrete real number variables with a customizable range, allowing the QA to execute this task with a certain accuracy. Unfortunately, for linear systems, the encoding methods that are generally used inevitably produce an undeniable error when the systems become even slightly larger.

To reduce the error introduced during the encoding stage in solving linear systems of equations, in this study we applies Gaussian on-off encoding[5], which encodes real numbers with a set of pre-selected candidate intervals (hereafter referred to as "digits"). The activation of n digits is then determined by controlling the 0/1 quantum state of n qubits. In the subsequent sections, a description of the setup of the 2D truss structures employed in this study is provided. Four encoding methods (one-hot encoding, binary encoding, on-off encoding, Gaussian on-off encoding) for various scales of truss structures are employed to demonstrate the superiority of proposed encoding method over the other three in the following aspects: accuracy, stability, qubit requirement.

2. Truss structure setup

In order to examine the performance of the QUBO model with different encoding methods, we consider three types of 2D truss structures with different numbers of members (rod elements) as shown in Fig. 1. All the members are assumed to have the same Young's modulus that is set to $2{\times}10^{11}\mathrm{N}/m^2$. A load of $F_1 = 1.0{\times}10^5$ N is applied to the lower right end of each truss structure. The analysis is also performed when the load is changed to $F_2 = 5.0 \times 10^5$ N in order to have more types of linear systems. Note that the self-weight of the structure is not considered in this study.

3. Gaussian on-off encoding

In this study, as a prerequisite for using QA, the truss analysis is characterized as a QUBO model as follows:

$$f(\boldsymbol{x}) = \boldsymbol{x}^T \boldsymbol{Q} \boldsymbol{x} = \sum_{i<j} Q_{ij} q_i q_j + \sum_{i=1}^{n} Q_{ii} q_i \quad (q_i \in 0, 1), \quad (1)$$

where Q is an upper diagonal coefficient matrix. q_i are the 0/1 binary variables, which can be simply transformed from Ising variables σ by $q = \frac{1}{2}(\sigma - 1)$. In truss analysis, each linear system is required to be characterized as a QUBO model. In this study, we define it by minimizing the total potential energy, defined as

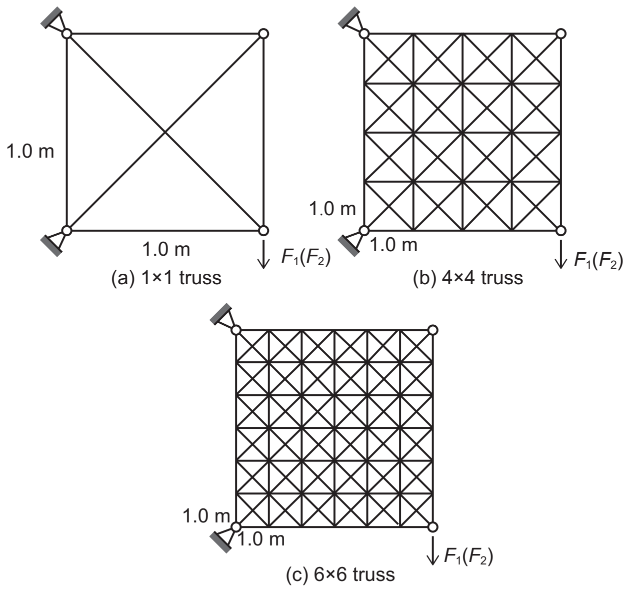

Fig. 1 2D truss structure models.

$$\Pi = \frac{1}{2} \boldsymbol{u}^T \boldsymbol{K} \boldsymbol{u} - \boldsymbol{u}^T \boldsymbol{F}. \quad (2)$$

Here, the $\boldsymbol{u}$ means the displacement (design variable) vector; $\boldsymbol{K}$ represents the stiffness matrix in the truss structure; $\boldsymbol{F}$ is the force vector defined by the load condition. The variables $\boldsymbol{u}$ in Eq. 2 take real numbers, each of which needs to be encoded with qubits. Since that the accuracy of an encoding method is undoubtedly affected by the number of qubits used, the number of qubits for each disign variable (displacement) corresponding to 1×1, 4×4, and 6×6 truss structures are set to 10, 20, and 30, respectively.

Gaussian on-off encoding express real value u_i as

$$u_i = \sum_{l=1}^{m} r_l q_{i,l}, \quad (3)$$

where $\boldsymbol{r}(r_1, r_2, ..., r_m) \sim N(\mu, \sigma)$, which defines the selection of digits within a certain range. The mean μ and standard deviation σ of the normal distribution are customized depending on the problem at hand. Since the first term in Eq. 2 is expressed as

$$\frac{1}{2} \sum_{i=1}^{n} \sum_{j=1}^{n} K_{i,j} u_i u_j = \frac{1}{2} \left(\sum_{i=1}^{n} K_{i,i} u_i^2 + 2 \sum_{i<j} K_{i,j} u_i u_j \right), \quad (4)$$

by the application of Gaussian on-off encoding, the first term yields

$$\frac{1}{2}\sum_{i=1}^{n}K_{i,i}u_i^2 = \frac{1}{2}\sum_{i=1}^{n}K_{i,i}\left(\sum_{l=1}^{m}r_l q_{i,l}\right)^2 \tag{5}$$

$$= \frac{1}{2}\sum_{i=1}^{n}\sum_{l=1}^{m}K_{i,i}r_l^2 q_{i,l} + \sum_{i=1}^{n}\sum_{l_1<l_2}K_{i,i}r_{l_1}r_{l_2}q_{i,l_1}q_{i,l_2}, \tag{6}$$

and the second term of Eq. 4 yields

$$\sum_{i<j}K_{i,j}u_i u_j = \sum_{i<j}\sum_{l_1=1}^{m}\sum_{l_2=1}^{m}K_{i,j}r_{l_1}r_{l_2}q_{i,l_1}q_{i,l_2}. \tag{7}$$

Additionally, the second term of Eq. 2 is

$$\sum_{i=1}^{n}F_i u_i = \sum_{i=1}^{n}\sum_{l=1}^{m}F_i r_l q_{i,l}. \tag{8}$$

Combining Eq. 2, Eq. 6, Eq. 7 and Eq. 8, the form of Gaussian on-off encoding can be finally expressed as

$$\begin{aligned}\frac{1}{2}\boldsymbol{u}^T\boldsymbol{K}\boldsymbol{u} - \boldsymbol{u}^T\boldsymbol{F} = &\frac{1}{2}\sum_{i=1}^{n}\sum_{l=1}^{m}K_{i,i}r_l^2 q_{i,l} \\ &+ \sum_{i=1}^{n}\sum_{l_1<l_2}K_{i,i}r_{l_1}r_{l_2}q_{i,l_1}q_{i,l_2} \\ &+ \sum_{i<j}\sum_{l_1=1}^{m}\sum_{l_2=1}^{m}K_{i,j}r_{l_1}r_{l_2}q_{i,l_1}q_{i,l_2} \\ &- \sum_{i=1}^{n}\sum_{l=1}^{m}F_i r_l q_{i,l}.\end{aligned} \tag{9}$$

4. Results of structural analysis by QA

In this section, the performances of the four encoding methods (one-hot encoding, binary encoding, on-off encoding, and Gaussian on-off encoding) are investigated comprehensively using the 2D truss structure models. A total of three aspects of performance examination (accuracy, stability and qubit requirement) are involved in this study, which are demonstrated sequentially. In addition, to avoid hardware errors in quantum annealers, all cases in this study are executed on a QA simulator.

(1) Accuracy and stability

The accuracy of QA in truss analysis with each encoding method is evaluated by the total potential energy Π and the maximum displacement u among the nodes in this study. Their quotients with the respective theoretical solutions were judged as the indices in the follow equations:

$$\eta_u = \frac{u_q}{u_c}, \qquad \eta_\Pi = \frac{\Pi_q}{\Pi_c}. \tag{10}$$

Here, u_q and Π_q denote the results of QA on u and Π respectively, while u_c and Π_c correspond to the theoretical solutions from a classical computer. For the sake of visualization, 2D scatter plots are provided in Fig. 2 to show the accuracy and stability of Gaussian on-off encoding with respect to other encoding methods. The coordinate (1.0, 1.0) in Fig. 2 represents the theoretical solution obtained by a classical computer. It indicates that as the coordinate approaches (1.0, 1.0), the level of accuracy increases. To examine the stability of the solutions, 10 independent runs were performed for each encoding method and the results are shown in the figure. It should be noted that to demonstrate the solutions with high accuracy among the results of the encoding methods, we have made a truncation of the results that deviate far from the theoretical solution so that they can be displayed at the edge of the figure. That is, the points at the edge are actually somewhere outside the figure.

Although all encoding methods show acceptable performance in 1×1 truss analysis, among which binary encoding, on-off encoding, Gaussian on-off encoding basically shows evident accuracy. In addition, as the scale of the truss structure increases, the results of binary encoding and one-hot encoding gradually deviate from the theoretical solution with increasing error. In the 6×6 truss structure, the on-off encoding and Gaussian on-off encoding yield the theoretical solution within 10 runs, while the Gaussian on-off encoding exhibits superior stability compared to on-off encoding. Approximately 75% and 50% of all the results of Gaussian on-off encoding reach the accuracy of more than 90% and 95%, respectively, which confirms its accuracy and stability.

The examples with the highest precision in 10 independent executions of the four encoding methods in 6×6 truss analysis with different load conditions are provided in Fig. 3, which visualizes the performance of the encoding methods.

(2) Qubit requirement

The number of qubits for each design variable (displacement component in each node) is fixed at 10, 20, and 30, respectively, where an increase in the number of qubits implies an increase in the number of real number digits in each encoding method. Theoretically, the more qubits are used, the accuracy and time cost boost accordingly. Therefore, for a certain scale of truss structure, it is crucial to

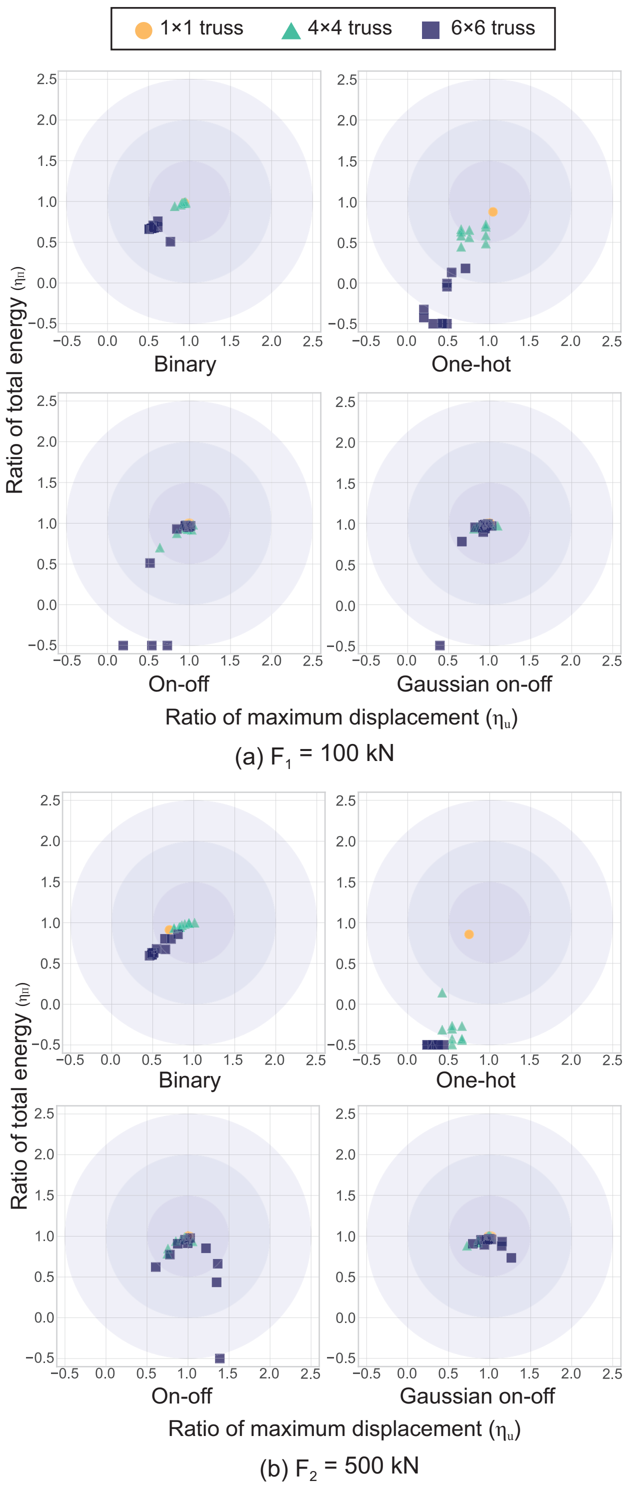

Fig. 2 Accuracy and stability of each encoding method.

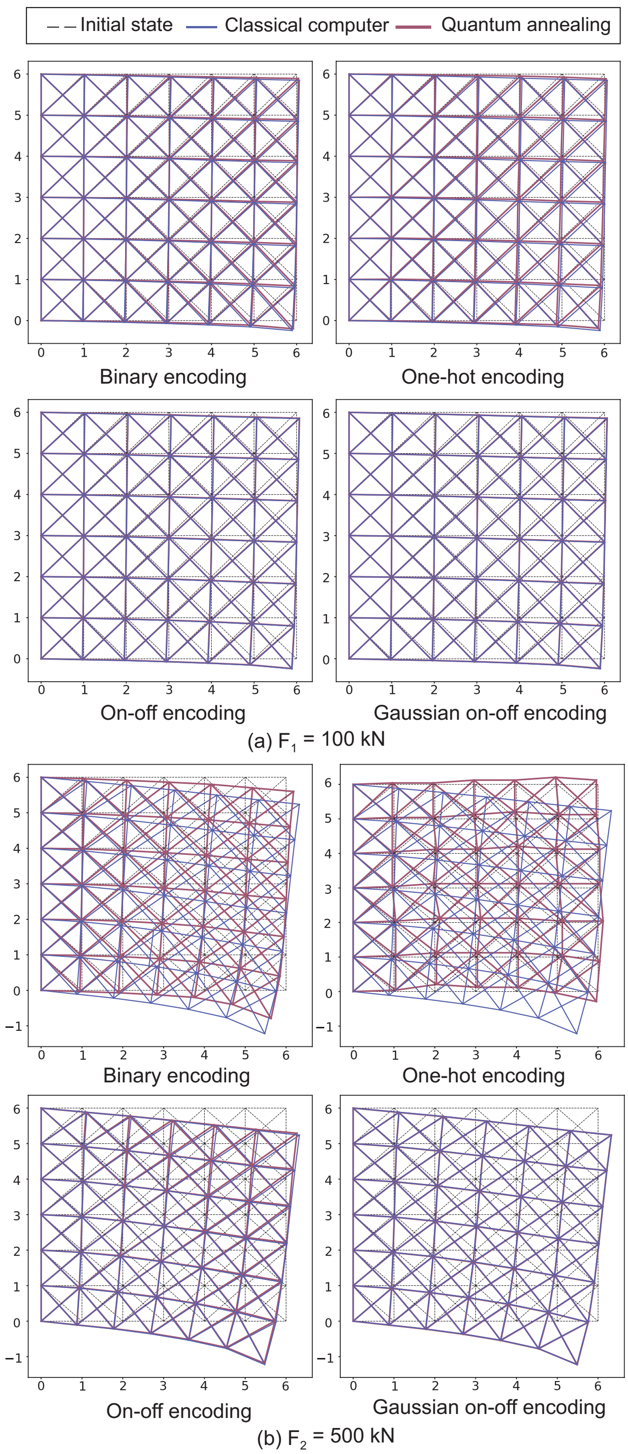

Fig. 3 6 × 6 truss analysis in different load conditions.

select the reasonable number of qubits.

Since only a few qubits are required for high accuracy in the 1 × 1 truss structure, it is different to fully discern the relationship between the accuracy and qubits. Therefore, the scenario of the 6 × 6 truss structure with the load condition F_2 is adopted to investigate the performance of each encoding method under different numbers of qubits, shown as Fig. 4. In the figure, the accuracy of the encoding methods in terms of total potential energy Π is defined as

$$\theta_\Pi = \left(1 - \left|\frac{\Pi_q - \Pi_c}{\Pi_c}\right|\right) \times 100. \qquad (11)$$

The definition of the symbols in Eq. 11 is consistent with Eq. 10. It should be note that in some executions, there may be results with extremely significant errors. In Fig. 4,

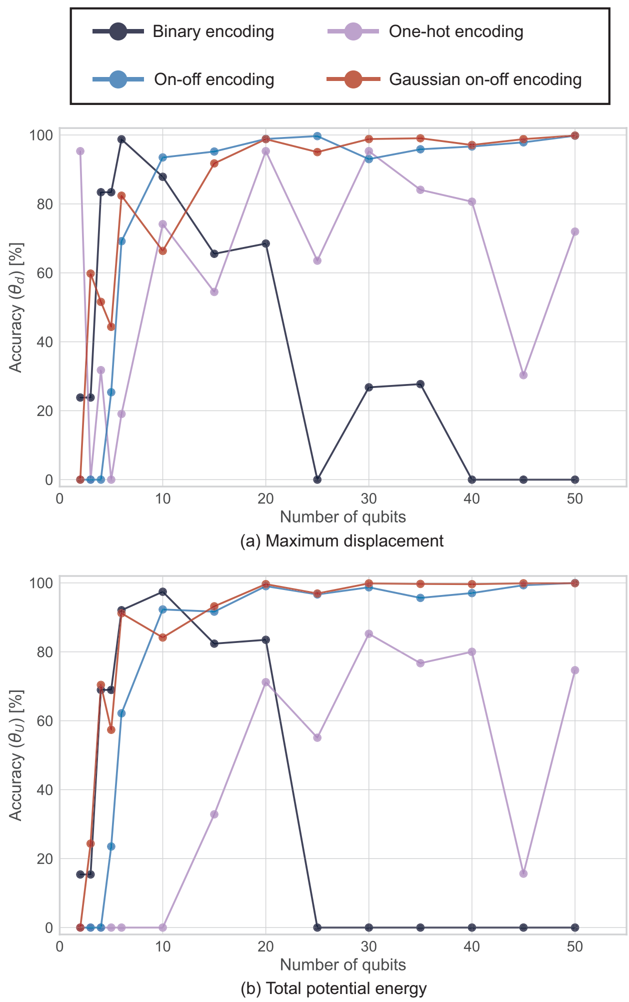

Fig. 4 Effect of the number of qubits on solution accuracy for different encoding methods.

the results with lower and upper limits may actually exceed the accuracy range. Therefore, in this study, we truncate them to values between 0 and 100.

According to Fig. 4, the accuracy of one-hot encoding is not ideal over the full range. It is difficult to identify the trend that its accuracy improves with the increase in the number of qubits. Furthermore, the accuracy of binary encoding is limited to a narrow range, an excessive or insufficient number of qubits can lead to its failure to obtain the theoretical solution. This can be attributed to the fact that if the number of qubits is excessive, there are digits that significantly deviate from the theoretical solution. If the digits with large deviations are selected by QA, the accuracy of binary encoding decreases significantly. While the accuracy and stability of Gaussian on-off encoding increase steadily with the number of qubits. Both in terms of accuracy and stability, Gaussian on-off encoding shows superior results to on-off encoding. According to this result, Gaussian on-off encoding is demonstrated to be efficient in utilizing qubits within a lenient applicability condition.

5. Conclusion

In this study, Gaussian on-off encoding in truss analysis are examined for accuracy, stability, and qubit requirement. Through these assessments, its applicability to such problems is also confirmed. It is anticipated to find application in large-scale truss analysis and engineering simulation, with the potential for significant enhancement in analysis efficiency should specialized hardware for quality assurance be developed in the future. Large-scale structure analysis is also expected to further examine the potential of the Gaussian on-off encoding.

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