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Application of FMQA in Hyper-parameter Optimization and Metamodel-based Optimization in DEM Granular Flow Simulations

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This study examined the applicability of factorization machines with quantum annealing (FMQA) to the field of landslide risk assessment for two specific black-box optimization problems, hyper-parameter optimization (HPO) for metamodeling and metamodel-based simulation optimization (MBSO) targeting granular flow simulation using discrete element method (DEM). These two optimization problems are solved successively: HPO is first performed to determine the hyperparameters of the Gaussian process regression (GPR) metamodel, which is then is used as a low-cost, fast approximate solver of granular flow simulations for MBSO. After conducting a series of granular flow simulations using DEM, a metamodel is created that outputs a risk index of interest, the run-out distance, from its input parameters by employing GPR with two hyperparameters, length-scale and signal variance. Subsequently, HPO is performed to obtain the optimal set of hyperparameters by applying FMQA. Finally, using the metamodel created by each optimization method as an approximate solver for DEM simulations, MBSO is performed to find the optimal target output, the maximum run-out distance, in the space of physical input parameters for risk assessment.

Key Words : *FMQA, metamodeling, Quantum annealing, granular flow simulation*

1. INTRODUCTION

Recent advances in computational mechanics have made high-precision numerical simulation an indispensable tool for hazard risk assessment. Among them, the discrete element method (DEM)[1], which models granular flow at the particle level, has been widely used in the field of landslide hazards. Regarding the use of DEM simulation in this field, it is expected that the exploration of parameter settings for high-risk target outputs (e.g., run-out distance[2], impact force, etc.) will provide comprehensive intelligence for risk assessment. However, the expensive computational cost of DEM simulations precludes such insight. Specifically, it is impossible to fully explore the entire parameter space, even when multiple simulation runs are conducted to ascertain the global optimum.

The advent of metamodeling, a kind of mathematical regression model for numerical simulation, has overcome the computational cost obstacles and made optimization more efficient. It identifies and estimates the relationship between the inputs and outputs of the simulation model, forming a mathematical function that is used to evaluate possible solutions in the optimization process. There are two typical black-box optimization problems that use metamodeling: hyperparameter optimization (HPO) and optimization that searches for effective factors for metamodel-based simulation, which is called metamodel-based simulation optimization (MBSO), respectively. The common used methods for performing black-box optimization are random search (RS) and Bayesian optimization (BO).

As a new streamline, D-Wave Systems has recently developed a device named D-Wave 2000Q[3] that physically implements quantum annealing (QA)[4]. The system is essentially an Ising machine that processes binary variables and can be utilized to search for low-energy solutions of quadratic unconstrained binary optimization (QUBO) models. Recently, factorization machines with Quantum annealing (FMQA) [5] provides a prospective approach for black-box optimization problems using quantum annealing. Previous studies have insufficiently discussed the suitability of FMQA in HPO and MBSO in the field of landslide risk assessment. Hence, the objective of this study is to examine the applicability of QA in HPO and MBSO to the field of landslide hazard/risk assessment.

2. Granular flow simulation and GPR-based metamodel

The run-out distance of particles in granular flow is typically an important index for landslide risk assessment, and it is taken as the target output of the MBSO problem in this study. In this context, Xiao et al.[2] performed 56 cases of DEM granular flow simulations to create a metamodel, which was referred to as the 'surrogate model' in the paper, and analyzed the effect of four parameters on the run-out distance of the granular flow. The settings of the DEM simulations and the sampling method for the input parameters involved in this study are basically consistent with theirs. After outlining the simulation conditions, we will explain how to use Gaussian process regression (GPR) to create a metamodel using these simulation cases as training data.

(1) DEM simulation conditions

The particle model employed in this study is a polygon particle model that is close to an ellipsoid as shown in Fig. 1. The shape and dimensions of this particle model are shown in the same figure. Here, the length of the minor axis d is 2 cm, and the aspect ratios of the length and width are 1.50 and 0.75, respectively. Fig. 2 shows the slope model for the DEM simulations, with an inclination angle of 45°. The dimensions of the collector are shown in Fig. 2.

In our previous study[2], a series of DEM simulations were performed for each of four different input parameters: friction angle between elements (FABE), friction angle with bottom surface (FABS), coefficient of restitution (COR), and spring coefficient (SC), and the target output was the runout distance. Each simulation case contained approximately 1300 polygon particles, and the average computation time was 45 minutes. Thus, it is efficient to create a metamodel with the runout distance as the target output for the four input parameters and to perform optimization based on this model, and it makes sense to investigate the applicability of FMQA in that optimization process.

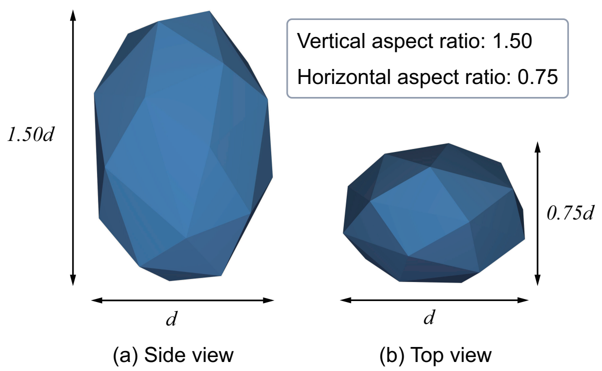

Fig. 1 Shape and dimensions of the particle model.

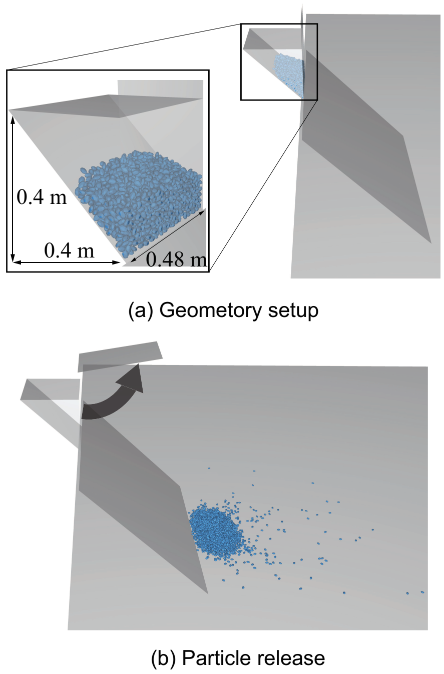

Fig. 2 Dimensions of the DEM slope model.

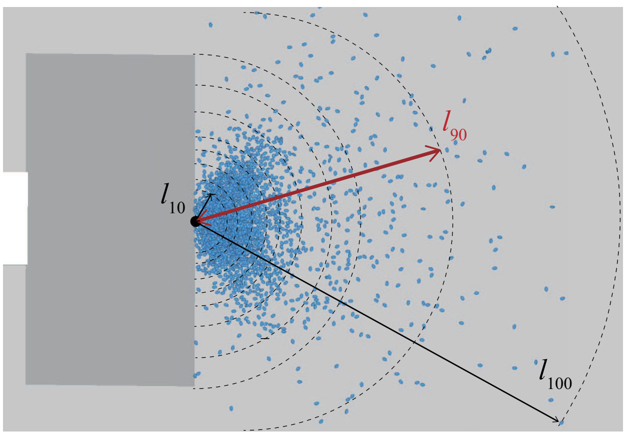

Fig. 3 Target output image for the MBSO problem (90% run-out distance).

(2) Sampling of input parameters

The ranges of the four input parameters are determined with reference to the authors' experience and values employed in related studies[2]. To minimize the sampling bias within each of these ranges, an appropriate sampling method must be employed to ensure that the DEM simulation case comprehensively covers the parameter space. To meet this requirement, Latin hypercube sampling (LHS) is adopted in this study. The number of simulation cases for training the metamodel in this study is 56.

In general, granular flows represented in DEM simulations have a high uncertainty in the run-out distance because individual particles move independently of each other at the front. In particular, DEM-based MBSO compares favorably with direct optimization by simulation in terms of efficiency, but its accuracy does not fully restore the numerical simulation itself. For this reason, a total of 10 metamodels with different target outputs were created, compared and examined in the study by Xiao et al. [2]. Here, one target output was defined for each 10th percentile from the 10th to the 100th percentile of the maximum run-out distance calculated for each mass ratio. The metamodel with 100% run-out distance (also called the maximum run-out distance of all particles) had an error of 12-13%, while this error was only approximately 6% in the 90% run-out distance scenario. Therefore, it would be difficult to predict the 100% run-out distance in a metamodel for risk assessment using DEM. Considering the efficiency, accuracy, and validity of the risk assessment, the target output of this study is defined as the 90% run-out distance and is denoted by l_{90}. As an example, Fig. 3 shows L_{90} in red.

In summary, four input parameters (FABE, FABS, COR, SC) and the target output (90% run-out distance) are used to create our metamodels for MBSO, each of which is intended to minimize the loss from the DEM simulation result.

(3) GPR-based metamodel

This study focuses on the physical processes of landslides, and the dependence of physical input parameters (friction, restitution and spring coefficient) on the target output. Gaussian process regression (GPR)[6] is known to provide a smooth regression for the target output, which accords well with the physical processes involved in this study. Therefore, GPR is employed to create the metamodel in this study.

GPR is a powerful Bayesian approach to regression problems with the reasonable assumption that the correlation between two points decreases with distance between the points increases. The most common kernel is the radial basis function (RBF) kernel, which is defined as

$$k(\boldsymbol{x}, \boldsymbol{x}') = \sigma_f^2 \exp\left(-\frac{|\boldsymbol{x}-\boldsymbol{x}'|^2}{2\lambda^2}\right), \tag{1}$$

where $k(\boldsymbol{x}, \boldsymbol{x}')$ is the covariance function that models the dependence between function values at different input points, $\boldsymbol{x}$ and $\boldsymbol{x}'$. The RBF is known for providing an expressive kernel for modeling smooth and stationary black-box functions. Here, by varying the two hyperparameters, λ (length-scale) and σ_f^2 (signal variance), the prior correlation between points can be increased or decreased, thereby controlling the accuracy and robustness of the metamodel.

The common method for optimizing these hyperparameters is to maximize the marginal (logarithmic) likelihood using the gradient-ascent method. In the HPO of this study, its performance was compared to that of FMQA.

3. FMQA for optimization problems

(1) Hyperparameter optimization in the metamodel

Similar to the optimization setup in the previous section, hyperparametric optimization (HPO) in this study is performed on the length scale λ and variance σ_f^2, with their initial ranges both set to $\left[10^{-4}, 10^{4}\right]$.

To evaluate the performance of machine learning models, two types of loss functions are usually used: training loss L_{train} and validation loss $L_{\text{validation}}$. In this study, L_{train} indicates the fitting degree of the created GPR metamodel with respect to the training data, and its value is calculated using the root mean square error (RMSE) as follows:

$$L_{\text{train}} = \sqrt{\frac{1}{M}\sum_{i=1}^{M}(\hat{y}_i - y_i^{(\text{train})})^2}, \tag{2}$$

where M denotes the number of DEM simulation cases for training[2] and is set to 56. Additionally, $y_i^{(\text{train})}$ and $\hat{y}_i$ are the simulation result and the prediction of the metamodel for the i-th training data, respectively. In contrast, $L_{\text{validation}}$ indicates the predictive performance of the metamodel, and is also used as an index to assess whether the metamodel is overfitting. In addition to the 56 sets of training data, 10 data points are randomly sampled in the parameter space and additional 10 DEM simulation cases are performed to generate 10 sets of validation data ($i = 1, \cdots, m = 10$). Then, the validation loss is calculated as

$$L_{\text{validation}} = \sqrt{\frac{1}{m}\sum_{i=1}^{m}(\hat{y}_i - y_i^{(\text{validation})})^2}, \tag{3}$$

where $y_i^{(\text{validation})}$ shows the simulation result on i-th validation data.

In this study, FMQA is applied to create a metamodel that adequately approximates the simulation results for an arbitrary set of four input parameters. To avoid overfitting to the training data, we designed the following multiobjective optimization metric:

$$L = L_{\text{train}} + \alpha L_{\text{validation}}, \tag{4}$$

where the parameter α is introduced to control the importance of $L_{\text{validation}}$. In general, the robustness of machine learning models is more important, so α is set to 10 in this study in order to create an optimal metamodel with generalizability. Fig. 4 shows the response surface of L with length-scale λ and variance σ_f^2 as independent variables. Here, the colors reflect the magnitude of L, and the horizontal and vertical axes and the magnitude of L are expressed on a logarithmic scale with a base of 10. It can be seen from this figure that the hyperparameter settings have a significant impact on the loss L. When the variance ranges from 10^3 to 10^4 and the length-scale is in $[0.1, 1]$, L appears to be at a minimum.

Under the above setup, FMQA is used to search for the minimum value of the loss L defined by Eq. (4) in the two-dimensional hyperparameter space. Fig. 5 illustrates the FMQA search process with a representative result of the FMQA performed in this study. Here, the red points are the initial training data and the blue points are the observed positions of FMQA during the process. It should be noted that here the training data are not the results of the

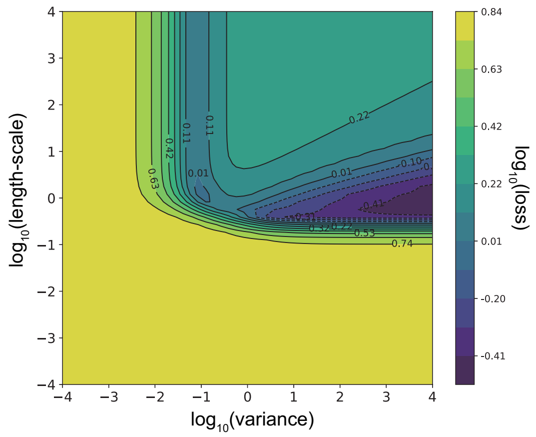

Fig. 4 Response surface of loss function with hyperparameters.

DEM simulations used to train the GPR metamodel but rather the initial samples in the hyperparameter space in Fig. 4. Since there is no general rule to define the number of iterations for FMQA, we define the number of initial data and evaluations in this study as 20 and 50, respectively. The final result of the FMQA search is 0.289, and the corresponding position in the parameter space is indicated by the white dot in the red box in the figure. Fig. 5 shows that FMQA converges to the global minimum at $(\sigma_f^2, \lambda) = (10^{4.0}, 10^{-0.2})$ rather than the local minimum at $(\sigma_f^2, \lambda) = (10^{-1.0}, 1.0)$ after 70 evaluations, exemplifying FMQA's high optimization ability.

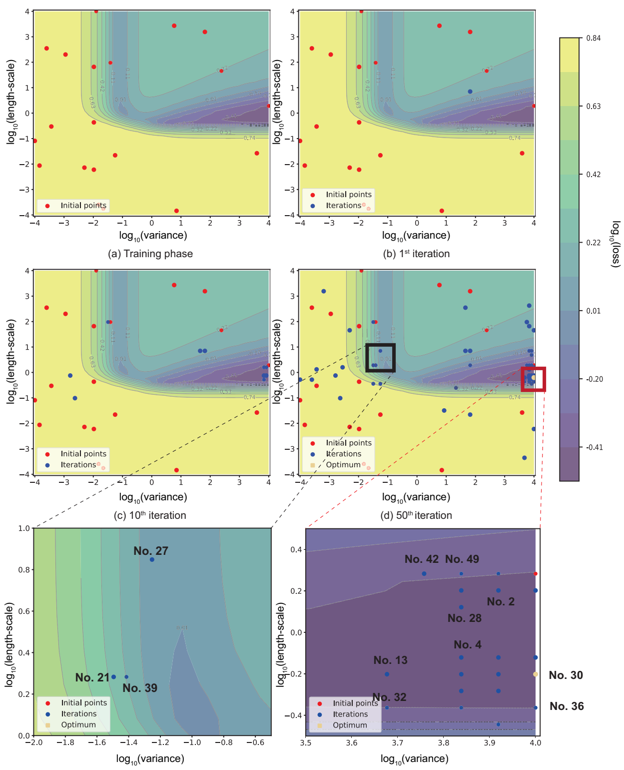

Fig. 5 FMQA search process in HPO.

Random search (RS) and Bayesian optimization (BO) are also performed for HPO as a comparison with the FMQA optimization performance. Note that the optimization performances of BO and FMQA vary depending on the initial points which are selected randomly, hence 10 independent optimization experiments for each method are conducted in this study to compare the optimization performances of these two methods and RS. Since the optimization performance of BO and FMQA depends on the randomly selected initial points, this study performs 10 independent optimization trials for each method in order to compare the optimization performance of these two methods and that of RS. Fig. 6 shows the evaluation histories of these optimization trials. Here, the vertical axis represents the minimum loss explored by each method, and the horizontal axis represents the total number of evaluations. The solid line in the figure represents the average performance of each method over 10 trials, and the width of each color band corresponds to the range between the best and worst performance of each method. The evaluation in BO and FMQA is divided into initial data and subsequent repeated observations. This is why FMQA and BO perform consistently in the first 20 evaluations in this figure. The dashed line in Fig. 6 is the optimization result of the gradient-ascent method, with a loss of 0.407.

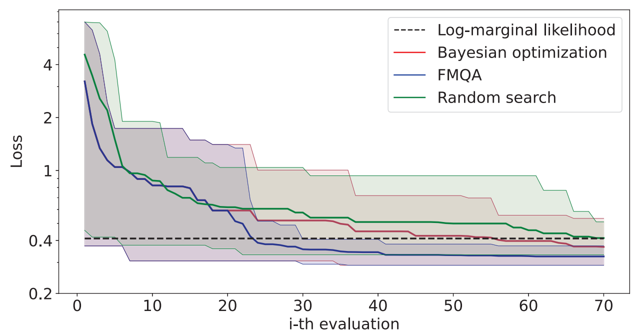

Fig. 6 Evaluation histories of FMQA.

The optimization results with RS shows that it achieves performance almost equal to that of the gradient-ascent method after 70 evaluations, but it has the widest color band of the three methods, indicating that it has the highest uncertainty. FMQA explores the loss below 0.407 around the 5th observation. Within a total of 70 evaluations, FMQA searches for a minimum loss value of 0.289, the best performance among the three methods. This section addressed the first problem in this study: hyperparameter optimization of the metamodel. In HPO, BO and FMQA exhibit insignificant strength compared to the exhaustive search method (RS), which can be attributed to the two-dimensional hyperparameter space. In the next subsection, the performances of FMQA, BO and RS are compared for a 4D MBSO problem using the created GPR metamodel with optimized hyperparameters.

(2) Metamodel-based simulation optimization

In this subsection, another FMQA is applied to the metamodel to search for the maximum 90% run-out distance in the space of physical input parameters (FABE, FABS, COR, SC) for optimal risk assessment.

As an example of MBSO here, we consider the problem of applying FMQA to the metamodel to find the physical input parameters (FABE, FABS, COR, SC) corresponding to the maximum 90% runout distance.

In accordance with Xiao et al. [2], the key parameters in determining run-out distance were FABS and COR. For visualization, Fig. 7 displays the GPR metamodel as a 3D response surface in contour format. Here, the horizontal and vertical axes are FABS and COR, respectively, and the color indicates the magnitude of the 90% run-out distance. As seen from the figure, the optimum solution for this MBSO example is intuitive to explore, but it is sufficient for verifying the performance of FMQA.

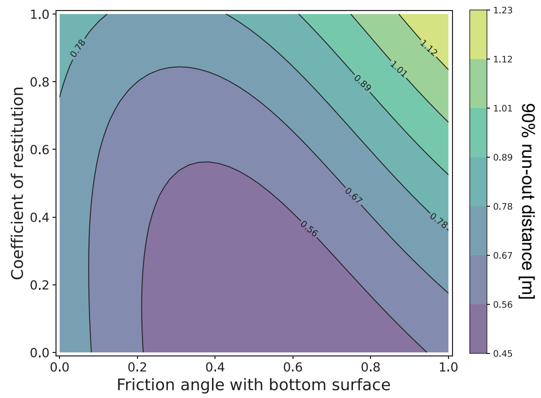

Fig. 7 Response surface of the 90% run-out distance with key physical input parameters (FABS, COR).

For MBSO using FMQA, BO and RS separately, 10 optimization trials are performed independently with different initial data arrangements. In a single FMQA optimization trial, 100 evaluations are performed with 10 initial data points and 90 subsequent iterative evaluations. Fig. 8 illustrates the FMQA search process for a representative result of the FMQA. The optimization results converge to the brown point in the red box. This point corresponds to (FABE, FABS, COR, SC) = (0, 1, 1, 0.872) in the physical parameter space, corresponding to a global maximum of 1.3681 m. As seen from Fig. 8, the local maximum (FABS, COR) = (0,1) was evaluated in the physical parameter space at a certain iterative step, but the global minimum was eventually selected. To further confirm the performance of FMQA, Fig. 9 compares the optimization history with those of BO and RS. On this particular MBSO problem, FMQA performed almost the same as BO. Indeed, these two performances are approximately 18% better than those of RS. FMQA's best performance over 10 independent runs was slightly better than BO's, but BO converged faster and more consistently.

(3) Discussion

To obtain a globally optimum solution to a black-box function, global optimization algorithms generally need

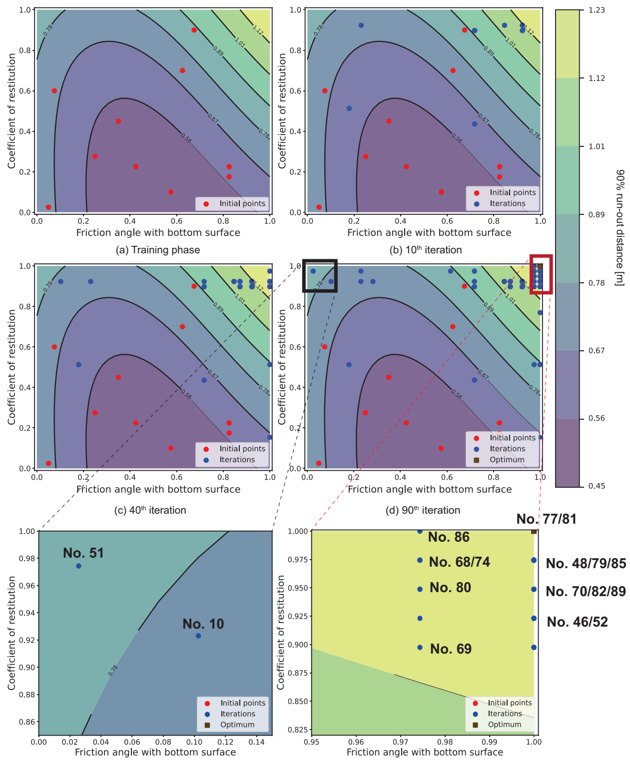

Fig. 8 FMQA search process in MBSO.

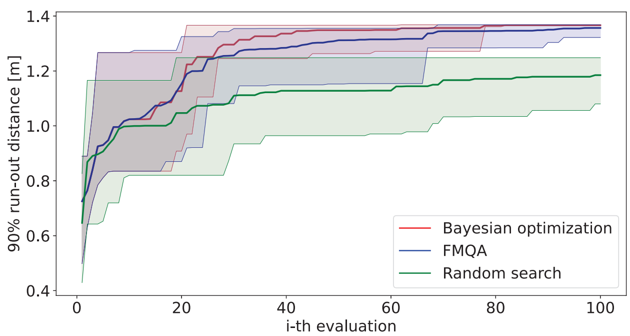

Fig. 9 Evaluation histories of FMQA for MBSO.

to balance exploration and exploitation, which is called the 'exploration-exploitation trade-off'. This trade-off is achieved through the two respective acquisition functions: the commonly used upper confidence bound (UCB) for BO and the FM model function, which is updated with each evaluation, for FMQA. In general, the focus on exploration helps the optimization method escape local optimum solutions and explore the entire parameter space in search of the global optimum solution.

In the HPO and MBSO problems in this study, the local optimum solutions were in the range $(\sigma_f^2, \lambda) = (10^{-1}, 1)$ and (FABS, COR) = (0, 1), respectively. As seen in Figs. 5 and 8, FMQA explores the locations of uncertainty throughout the optimization process and eventually converges to the global optimum. These results are a good illustration of the exploration-exploitation trade-off and the strength of FMQA. Although it is not the main objective to judge the superiority of methods, it is meaningful to explore the possibilities of FMQA by comparing it with other methods, and we will continue to study its applicability to the field of landslide risk assessment.

4. Conclusion

This study examined the applicability of FMQA for two optimization problems, hyperparameter optimization (HPO) for metamodeling and metamodel-based simulation optimization (MBSO) targeting granular flow simulation using DEM.

Daring to choose simple HPO and MBSO problems as examples for comparative studies, the results showed that FMQA using an Ising machine was equivalent to Bayesian optimization (BO), a state-of-the-art optimization algorithm, and was applicable to the field of landslide risk assessment. As quantum computers are expected to be exponentially faster than classical computers, the value of this study is that it provides a basis for direct application of QA to high-dimensional complex HPO and MBSO in the future as hardware is developed.

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