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

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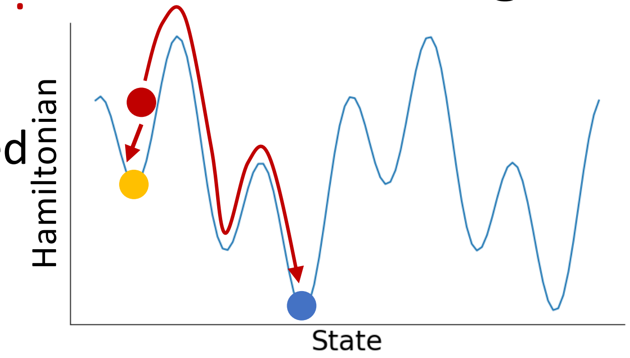
Background of FMQA

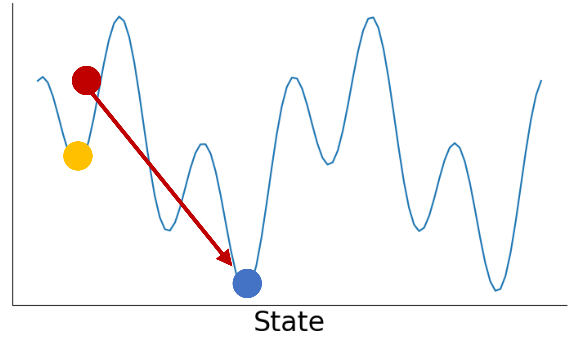
Quantum annealing(QA)[1]:

Combinatorial optimization with Quadratic Unconstrained Binary Optimization (QUBO) model attracted much attention.

Simulated annealing (SA)



Quantum annealing (QA)



Tunneling effect[2]

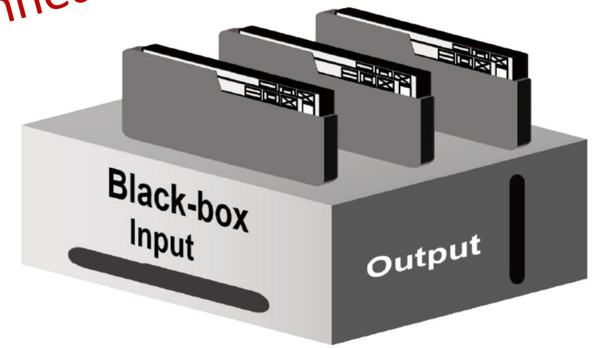
Black-box optimization:

Functions that are unknown or difficult to solve directly, search for the parameter sets corresponding to the minimum/maximum.

Factorization Machine with Quantum annealing(FMQA)[3]

Optimization issues as QUBO form.

FMQA has been applied in automated material search[3], but few examples in landslide risk assessment.

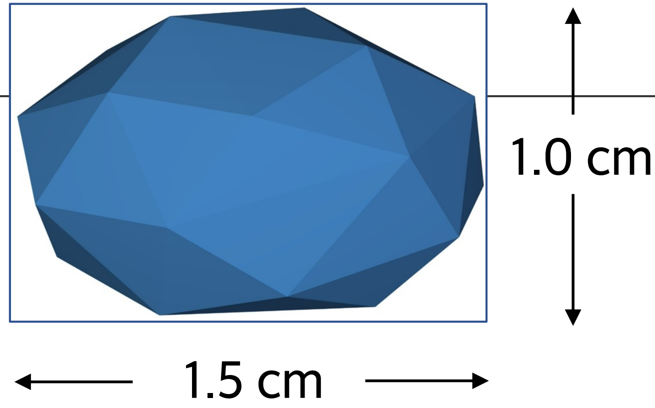


Black-box function

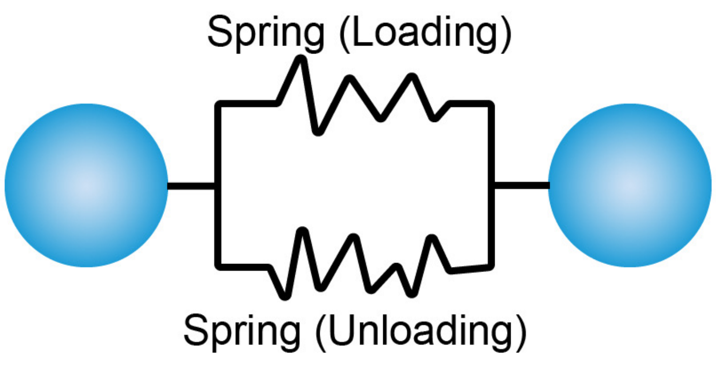
[1] Kadowaki T, Nishimori H. Quantum annealing in the transverse Ising model. Physical Review E. 1998;58(5):5355.
[2] Gunther, L. Quantum tunnelling of magnetisation. Phys. 1990;World 3, 28.
[3] Kitai K, Guo J, Ju S, et al. Designing metamaterials with quantum annealing and factorization machines. Physical Review Research.2020;2(1):013319.

DEM simulations (training data for metamodel)

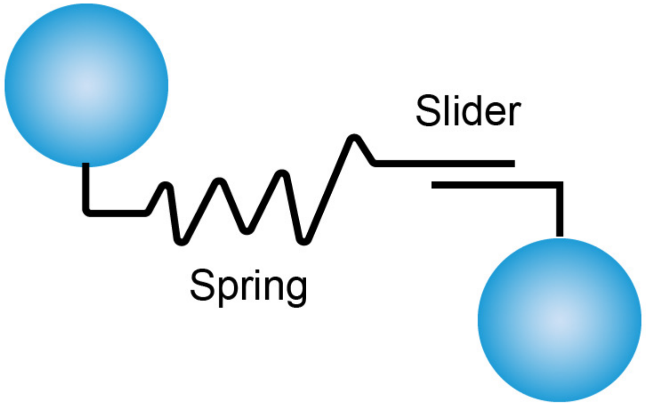
Particle model



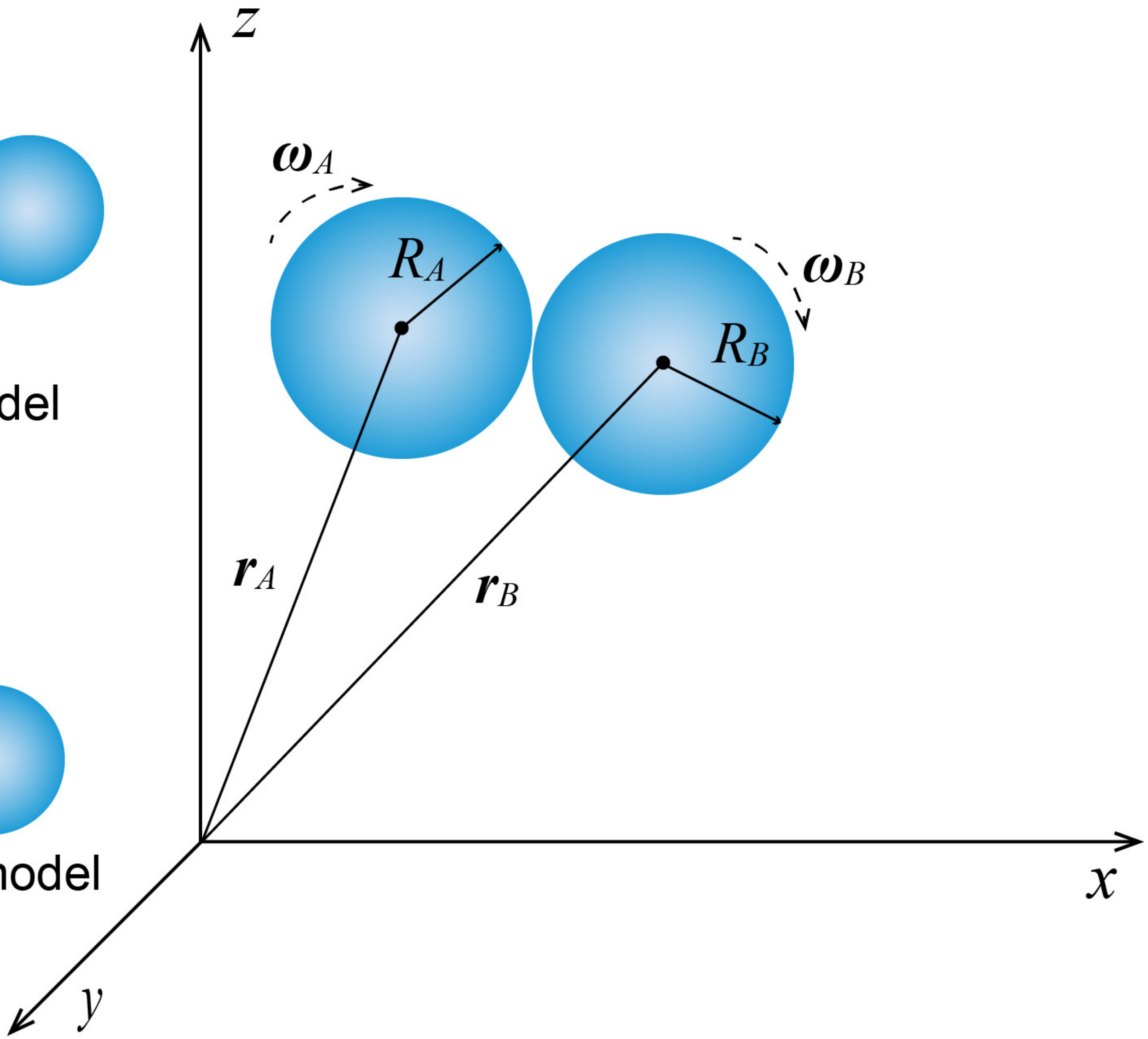
Contact force model



Normal contact force model



Tangential contact force model



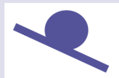
[4] Cundall, P. A.; Strack, O. D. L. (1979). "A discrete numerical model for granular assemblies". Geotechnique. 29 (1): 47–65.

Creation of metamodel (surrogate): input and output

Input $\boldsymbol{x}\,(FABE, FABS, COR, SC)$

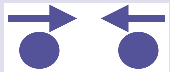
- x_1 : Friction angle between elements (FABE)

- x_2 : Friction angle with bottom surface (FABS)

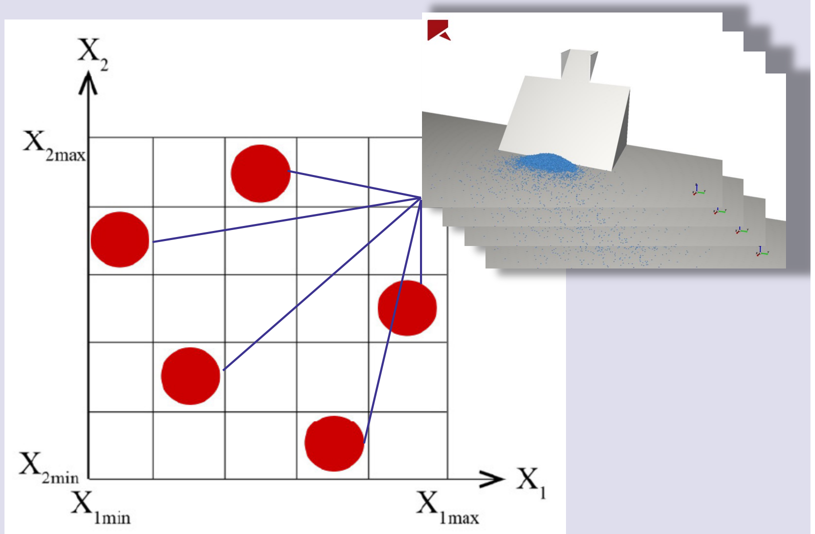


- x_3 : Coefficient of restitution (COR)

- x_4 : Spring coefficient (SC)



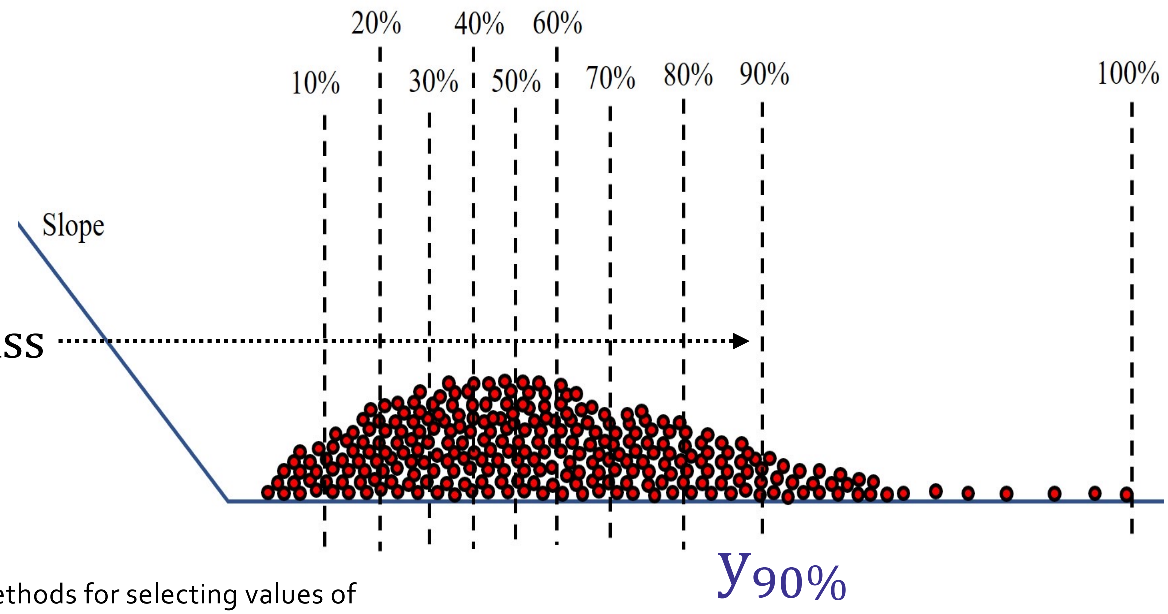
Latin hypercube sampling (LHS)[6]



Output y

Run-out distance (90%)

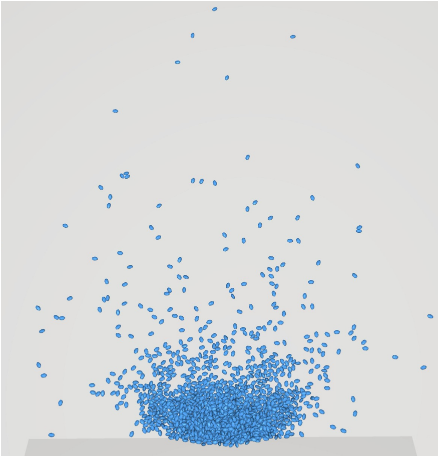
$y_{90\%}$ – Distance of 90% of total mass



[6] McKay, Beckman, Conover (2000). A comparison of three methods for selecting values of input variables in the analysis of output from a computer code. Technometrics 42, 55–61.

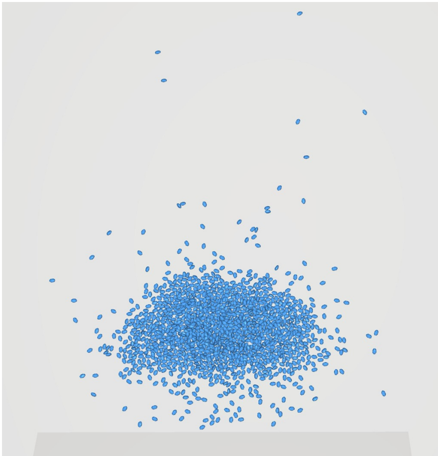
Creation of metamodel (surrogate): input and output

Examples



Setting of example 1

- Friction angle between elements 30.94°
- Friction angle with bottom surface 29.65°
- Coefficient of restitution 0.38
- Spring coefficient 8.46e+6 [N/m]



Setting of example 2

- Friction angle between elements 28.32°
- Friction angle with bottom surface 21.43°
- Coefficient of restitution 0.46
- Spring coefficient: 9.50e+6 [N/m]

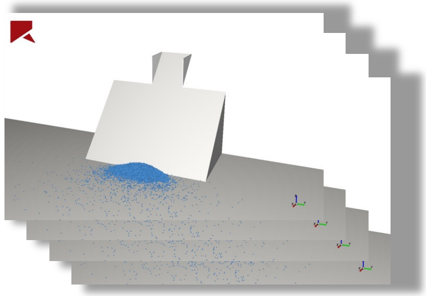
Problem 1: For various high-risk parameter set[5], excessive trials of DEM granular flow simulations are time consuming

[5] https://www.geospatial.jp/ckan/dataset/aas-disaster-201809/resource/7b043a45-59b4-408e-8046-eab11d1bb1a5

Optimization issues and objective

1. **Metamodel-based simulation optimization (MBSO)**

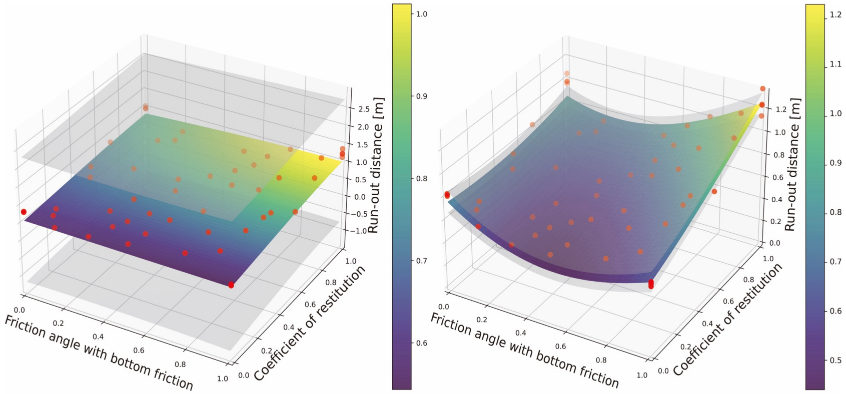
   Search for optimal parameter set using the created metamodel by the application of FMQA



Problem 2: Metamodel with/without HPO, traditional methods may be inefficient

2. **Hyper-parameter optimization (HPO) in metamodel**

   Determine optimal hyper-parameter set by the application of FMQA

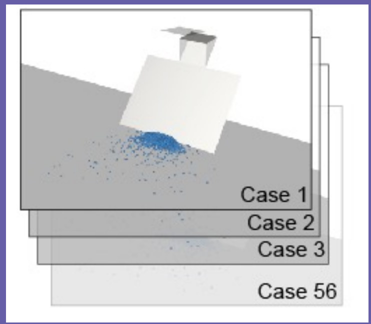


(a) Metamodel with default hyper-parameter value

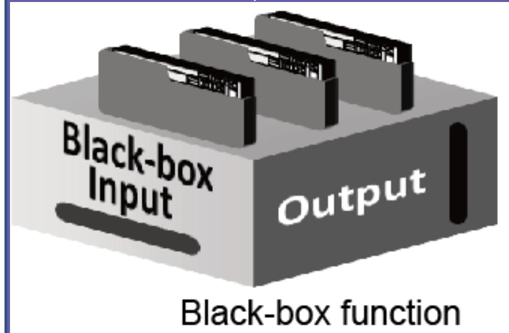
(b) Metamodel with hyper-parameter optimization (gradient-ascent method)

Objective : Examine the applicability of FMQA to HPO and MBSO in landslide risk assessment and compare its performance with existing optimization methods

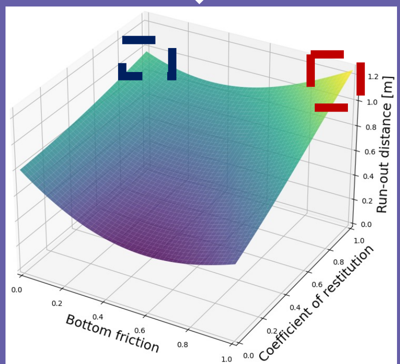
Methodology



DEM simulations y



Metamodel $\hat{y}$



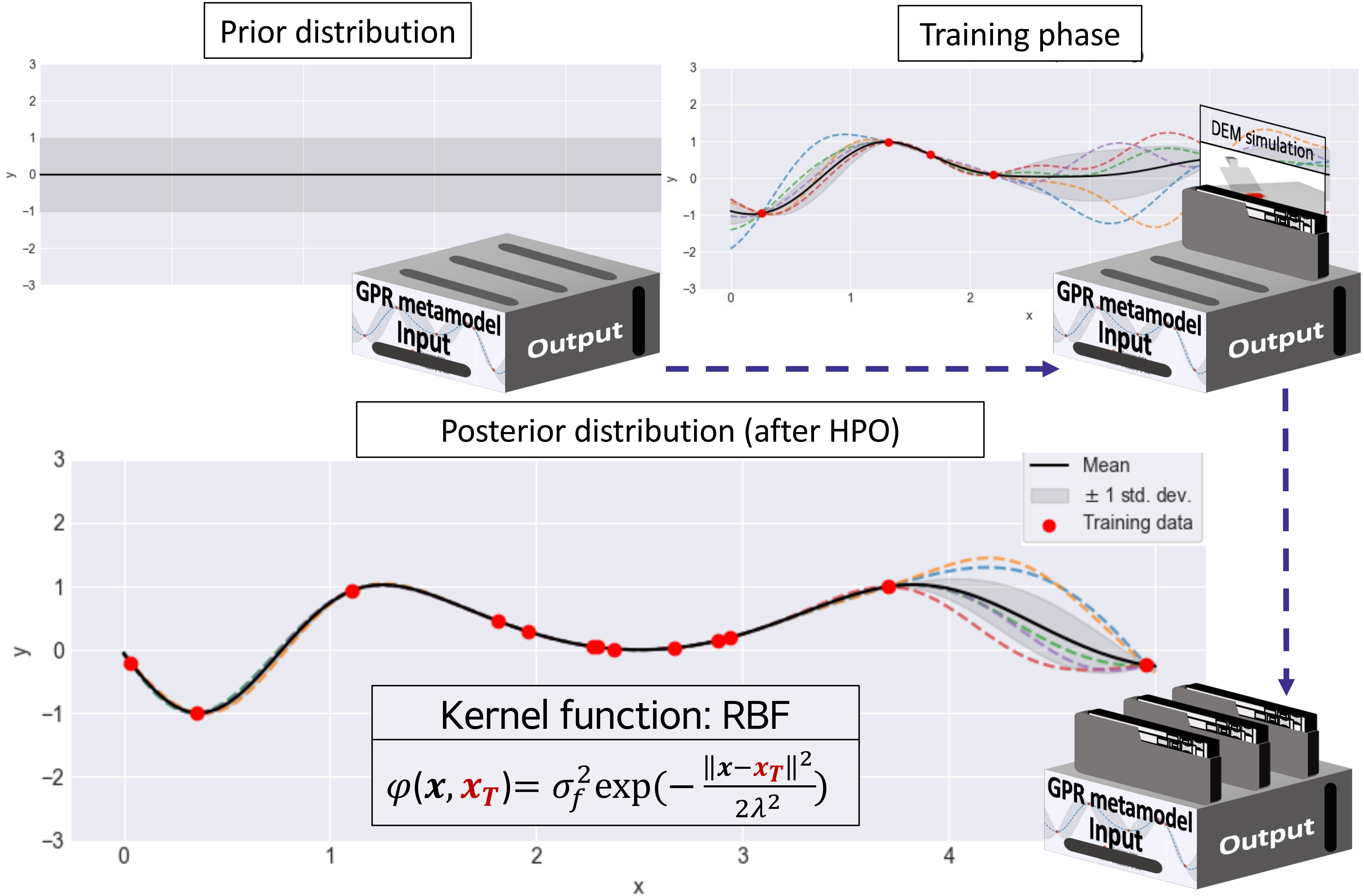
Optimal set

1. Prepare training data for metamodeling
   - DEM granular flow simulations
   - Latin hypercube sampling

2. Create metamodel
   - Gaussian process regression (GPR) metamodel
   - Hyper-parameter optimization with FMQA

3. Metamodel-based simulation optimization
   - FMQA

Gaussian process regression (GPR) metamodel[7]

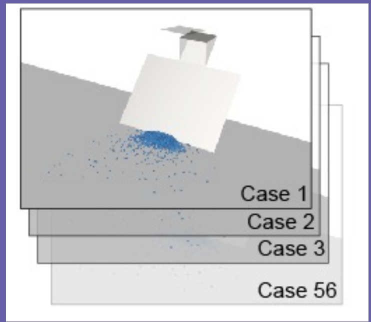


Kernel function: RBF

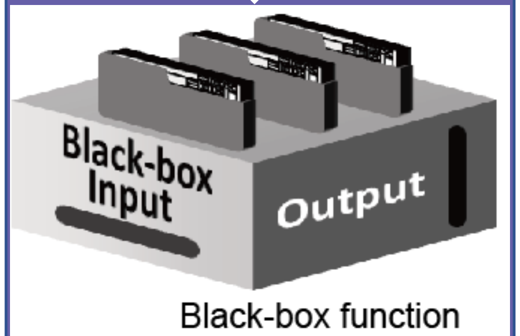
$$\varphi(\boldsymbol{x}, \boldsymbol{x_T}) = \sigma_f^2 \exp\left(-\frac{\|\boldsymbol{x}-\boldsymbol{x_T}\|^2}{2\lambda^2}\right)$$

[7] Williams, C. K. (1998). Prediction with Gaussian processes: From linear regression to linear prediction and beyond. In Learning in graphical models (pp. 599-621). Dordrecht: Springer Netherlands.

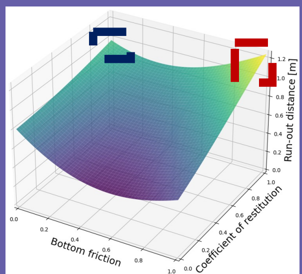
Hyper-parameter optimization



DEM simulations y



Metamodel $\hat{y}$



Optimal set

***Objective*: Search for the hyper-parameters that minimize loss of the metamodel**

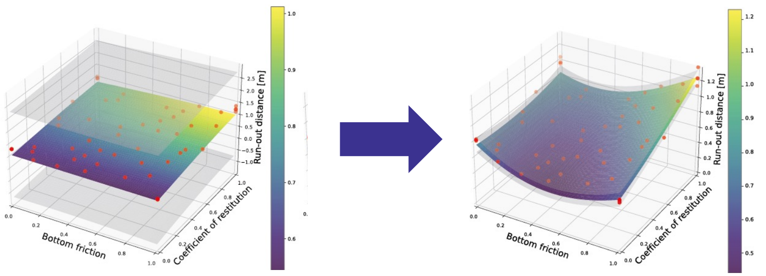
Input	**Output**
Hyper-parameter set	Loss
λ, σ_f^2	$L = L_{train} + \alpha L_{validation}$ ($\alpha = 10$)

- Training data: 56 DEM simulations sampled by LHS

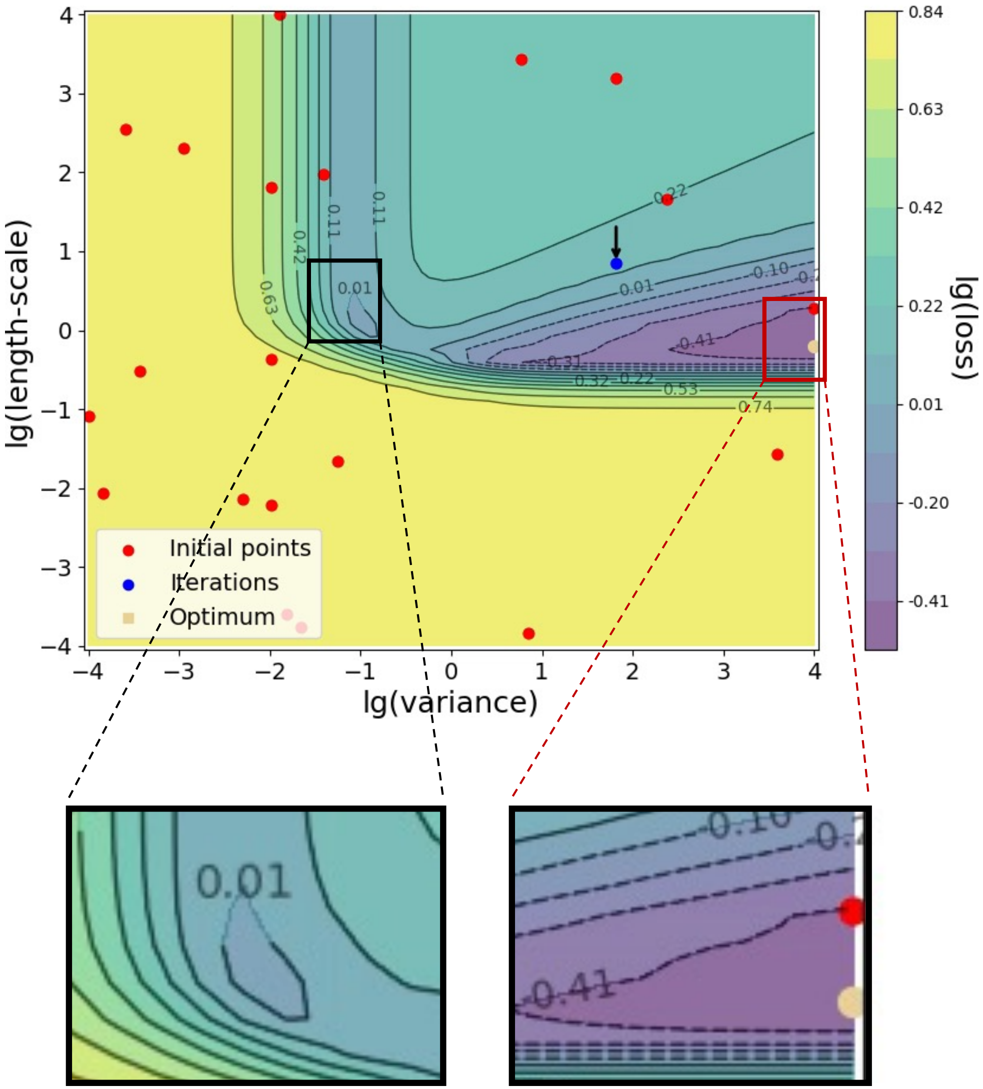
$$L_{train} = \sqrt{\frac{1}{56}\sum_{i=1}^{56}(\hat{y}_i - y_i^{(train)})^2}$$

- Validation data: 10 DEM simulations with random samples

$$L_{validation} = \sqrt{\frac{1}{10}\sum_{i=1}^{10}(\hat{y}_i - y_i^{(validation)})^2}$$

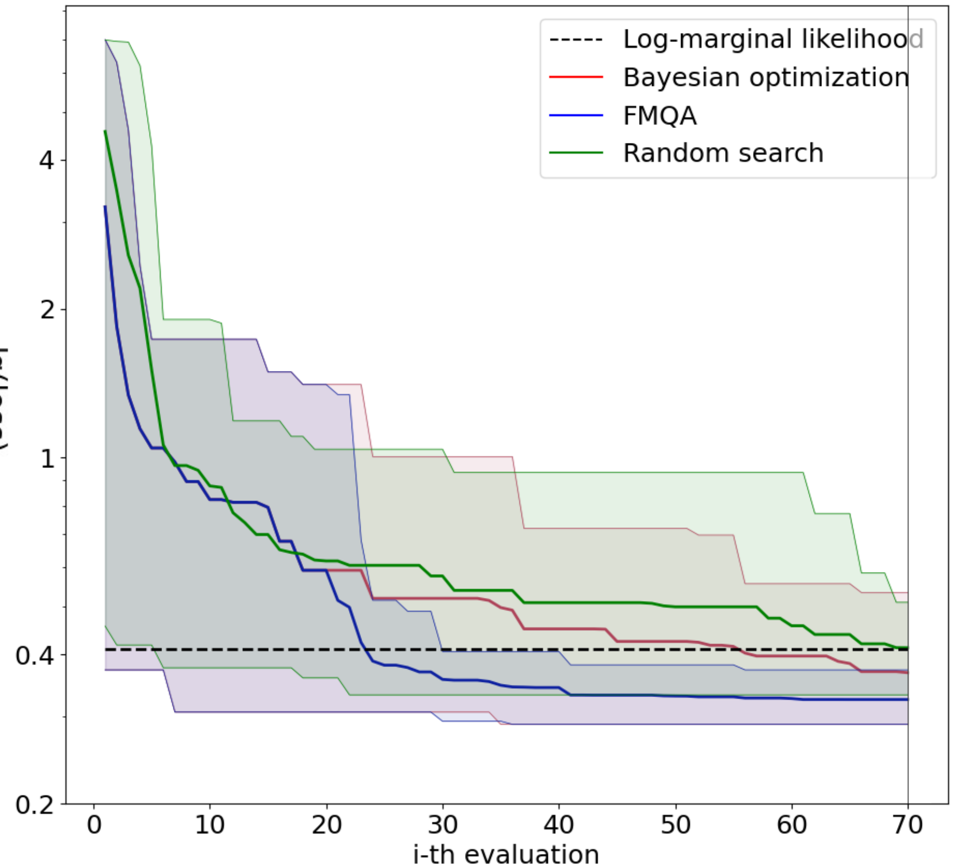


Hyper-parameter optimization (HPO)



Local optimum

Global optimum



Input hyper-parameters: σ_f^2, λ

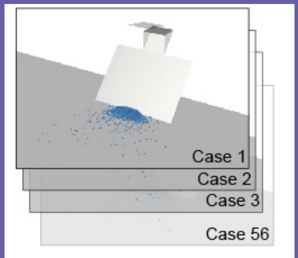
Range: (1e-4, 1e+4)

Initial points/Iterations: 20/50

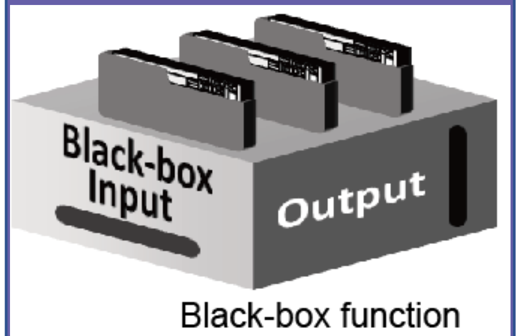
One-hot encoding digits: 100/axis

Total candidates for QA: 100^2

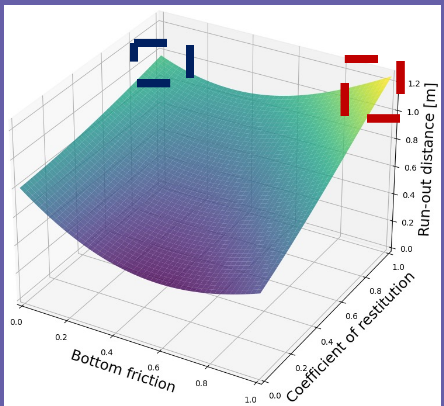
Metamodel-based simulation optimization (MBSO)



DEM simulations y



Metamodel $\hat{y}$



Optimal set

***Objective*: Search for a set of physical parameters set that gives the highest risk in landslide**

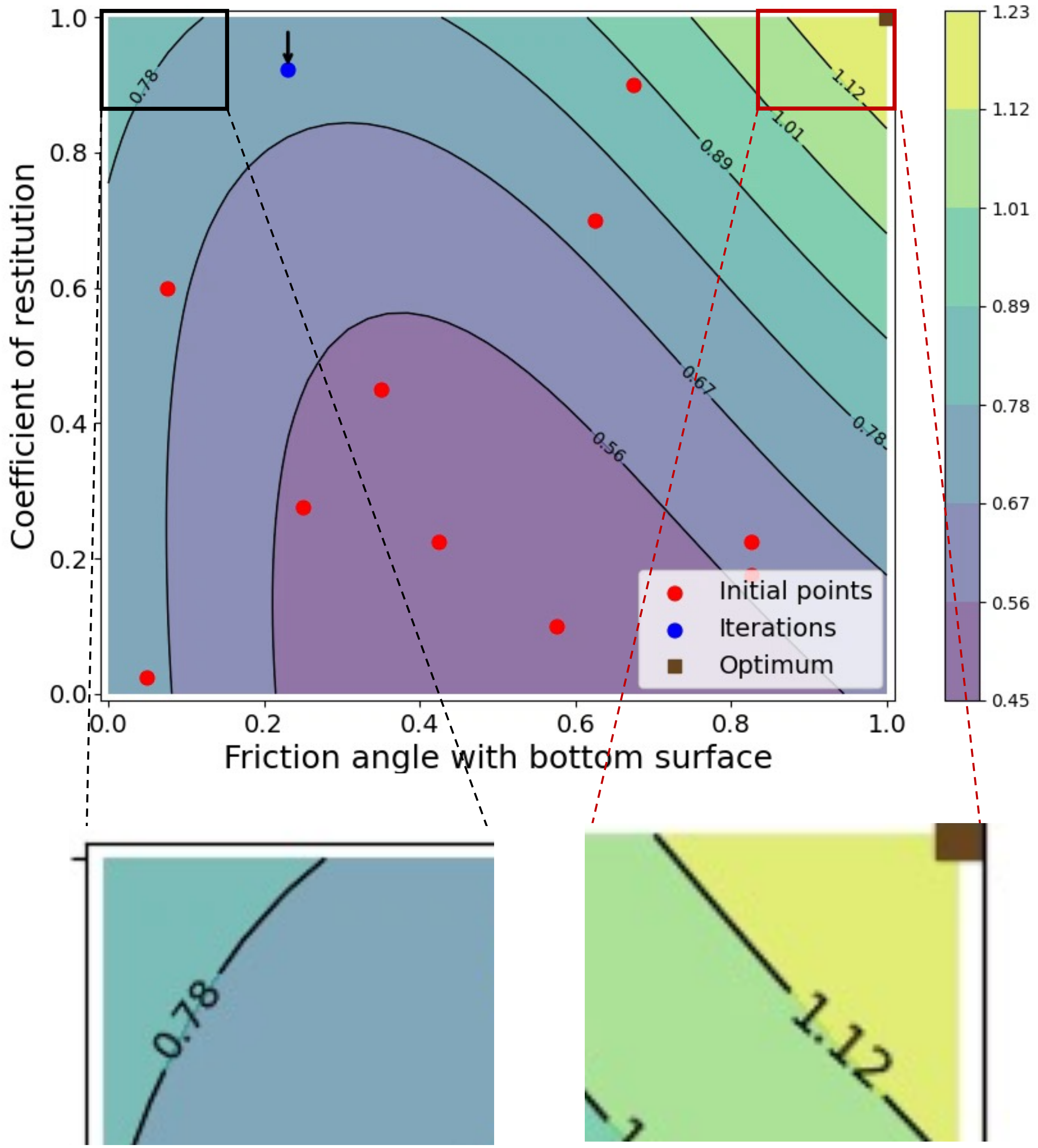
Input	**Output**
Physical parameters FABE, FABS, COR, SC	Runout distance

Parameters	Range	References
FABE [°]	20 – 40	Mao et al.[7], Guo et al.[8]
FABS [°]	20 – 40	Li & Zhao[9], Mao et al.[7]
COR	0.3 – 0.7	Girolami et al.[10]
SC [N/m]	1e+5 – 1e+7	Chen & Song[11]

[7] Mao, W., Wang, Y., Yang, P. et al. Dynamics of granular debris flows against slit dams based on the CFD–DEM method: effect of grain size distribution and ambient environments. (2023).
[8] Guo, J., Cui, Y., Xu, W. et al. Numerical investigation of the landslide-debris flow transformation process considering topographic and entrainment effects: a case study (2022).
[9] Li, X., & Zhao, J., A unified CFD-DEM approach for modeling of debris flow impacts on flexible barriers. (2018)
[10] Girolami, L., Hergault, V., Vinay, G. et al. A three-dimensional discrete-grain model for the simulation of dam-break rectangular collapses: comparison between numerical results and experiments. (2012).
[11] Chen, Z., Song, D. Numerical investigation of the recent Chenhecun landslide (Gansu, China) using the discrete element method. (2021).

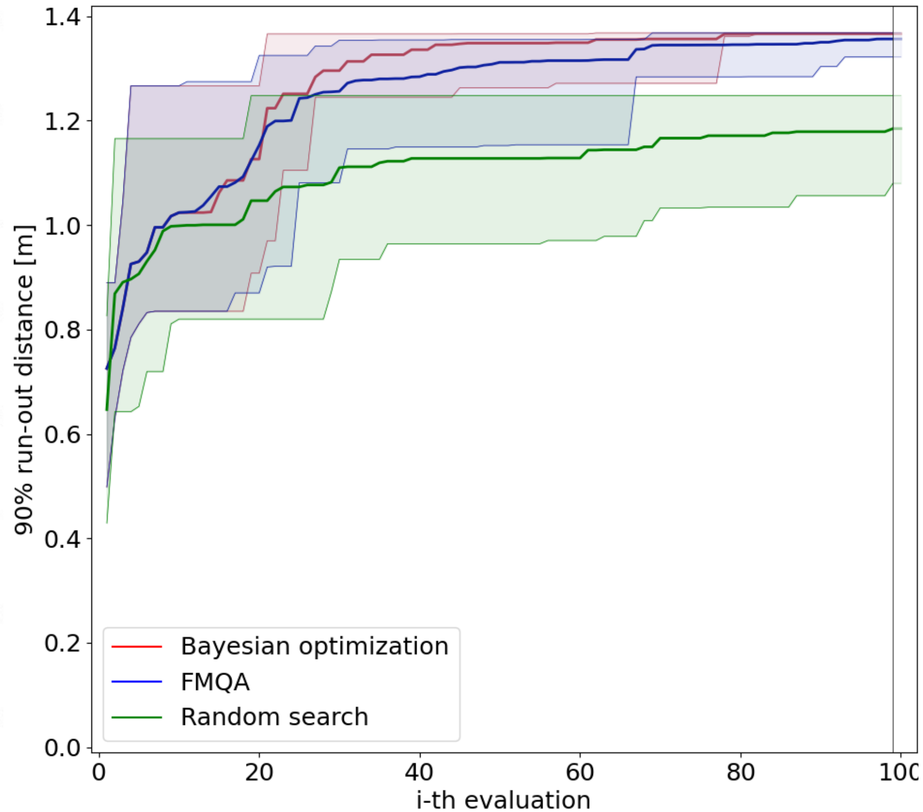
Metamodel-based simulation optimization

FMQA process in MBSO



Local optimum

Global optimum



Input parameters: $FABE, FABS, COR, SC$

Range: Normalized in (0, 1)

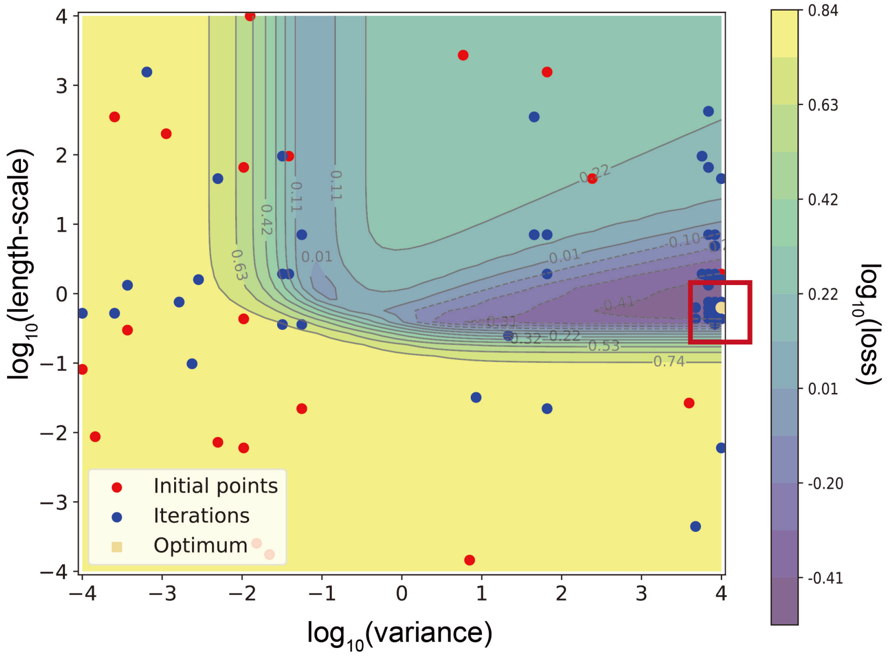
Initial points/Iterations: 10/90

One-hot encoding digits: 40/axis

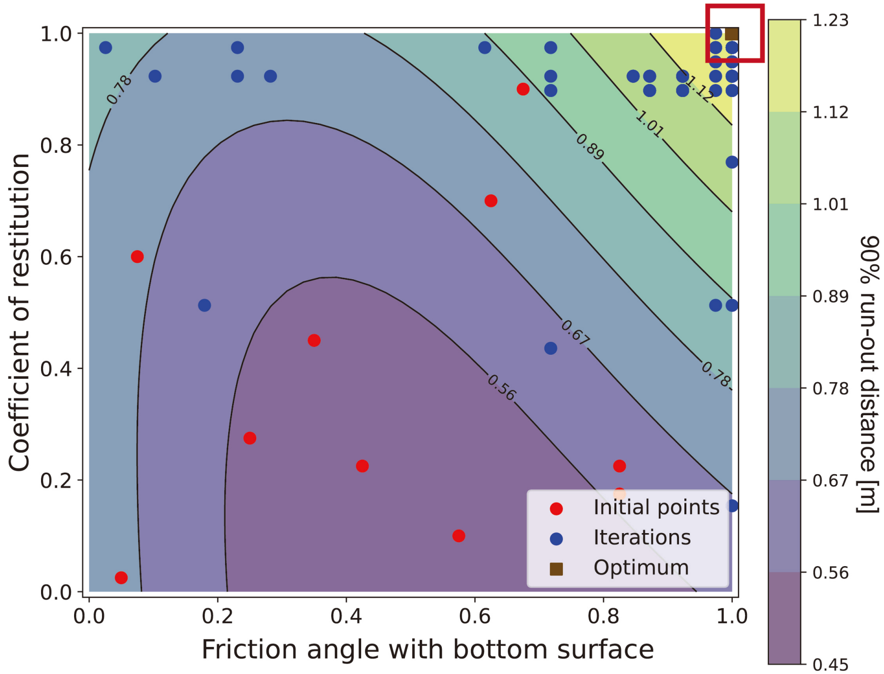
Total candidates for QA: 40^4

Conclusion

HPO for high-accuracy metamodeling



MBSO for high-risk physical parameter set



- Examined the applicability of QA for hyper-parameter optimization (HPO) and metamodel-based simulation optimization (MBSO) targeting granular flow simulation.
- FMQA is equivalent to Bayesian optimization and was applicable to the field of landslide risk assessment.

Future work

Further discuss the applicability of FMQA to more complex optimization problems.