A Bayesian approach for designing experiments based on information criteria to reduce prediction uncertainty of fuel fracture during LOCA

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Abstract: To ensure reactor safety during a loss-of-coolant accident (LOCA), it is necessary to accurately estimate the fracture limit of fuel cladding tubes during LOCA. However, the scarcity of test materials for certain types of the tubes, such as high-burnup fuel cladding tubes, poses a significant challenge to conduct comprehensive experiments. Therefore, the development of method to effectively reduce prediction uncertainty of fuel fracture from a limited experimental data is important. In this study, we propose a Bayesian approach for designing experimental conditions based on a widely applicable information criterion (WAIC) in order to effectively reduce the uncertainty of fuel cladding fracture prediction with limited data. Numerical experiments are conducted to evaluate the effectiveness of the proposed method. As a result, the use of WAIC has the potential to reduce uncertainty compared to conventional methods using functional variance and empirical loss in realistic situations where the true model is unknown.

Keywords: LOCA, fuel cladding tube, fracture limit, information criteria, Bayesian update

1. INTRODUCTION

To maintain the reactor core's coolable geometry during a loss-of-coolant accident (LOCA) in light-water reactors, it is important to accurately estimate the fracture limit of fuel cladding tubes. For this purpose, a Bayesian model has been developed using LOCA-simulated experiment results concerning the fracture and non-fracture of the tubes. However, the scarcity of test materials for certain types of the tubes, such as high-burnup fuel cladding tubes, poses a significant challenge to conduct comprehensive experiments. This necessitates the development of methodologies to effectively reduce the fracture limit uncertainty derived from a limited experimental dataset. Therefore, this study proposes a Bayesian approach for designing experimental conditions based on an information criterion to effectively reduce prediction uncertainty of fuel cladding tube fracture even with limited data.

A previous study developed a method for designing experimental condition to effectively reduce the uncertainty of Bayesian models by minimizing information entropy [1]. This method minimizes the Kullback-Leibler (KL) divergence between the true model and a predictive model by conducting experiments in a way that minimizes entropy. However, when using limited data, minimizing information entropy does not necessarily represent minimizing the KL divergence between the true model and the model [2]. Therefore, in order to effectively reduce the prediction uncertainty of fuel cladding tube fracture even with limited data, we propose a method to design experimental conditions based on the widely applicable information criterion (WAIC) [3]. WAIC is an information criterion that asymptotically approaches the KL divergence between the true model and a predictive model. Also, to evaluate the effectiveness of the proposed method, we conduct numerical experiments by applying it to the fracture probability estimation model [4].

2. REDUCTION OF PREDICTION UNCERTANITY

WAIC has been developed as a measure of the prediction accuracy of Bayesian models [3]. WAIC calculated for each experimental condition represents the prediction accuracy of the model for each condition, and this information can be used to determine the value of a new experiment. In this study, we propose a method to reduce the prediction uncertainty of the model by preferentially conducting experiments under experimental conditions where WAIC is large (where the model's prediction accuracy is low) and using the obtained data for Bayesian update of the model.

WAIC is defined as follows:

$$WAIC = T + \frac{V}{n} \tag{1}$$

$$V = \sum_{i=1}^{n} \mathrm{E}_{\omega}[(\log p(y_i \mid \boldsymbol{\omega}))^2] - \mathrm{E}_{\omega}[(\log p(y_i \mid \boldsymbol{\omega}))]^2 \tag{2}$$

$$T = -\frac{1}{n}\sum_{i=1}^{n} \log p^*(y_i) \tag{3}$$

$$p^*(y_i) = \mathrm{E}_{\omega}[p(y_i \mid \boldsymbol{\omega})] \tag{4}$$

where T is the empirical loss, V is the functional variance, y_i is a random variable, $\boldsymbol{\omega}$ is the vector of parameters, $p(y_i \mid \boldsymbol{\omega})$ is a Bayesian model, $\mathrm{E}_{\omega}[]$ is the expectation value over the posterior distribution of $\boldsymbol{\omega}$, $p^*(y_i)$ is the posterior predictive distribution, and n is the number of samples.

As shown in equation (5) below, the average of WAIC asymptotically approaches the average of the Bayes generalization loss G [3], which represents the prediction accuracy of the model. Therefore, WAIC can be used as a measure of the prediction accuracy of Bayesian models.

$$\mathrm{E}[G] = \mathrm{E}[WAIC] + O(\frac{1}{n^2}) \tag{5}$$

$$S = -\int q(y) \log q(y) \tag{6}$$

$$KL = \int q(y) \log \frac{q(y)}{p^*(y)} dy \tag{7}$$

$$G = S + KL = -\int q(y) \log p^*(y) dy \tag{8}$$

where $q(y)$ is the true model, E[] is the expected value, S is the entropy, and KL is the KL divergence between $q(y)$ and $p^*(y)$.

In this study, we propose a method to reduce prediction uncertainty of the model by preferentially conducting experiments under experimental conditions where the WAIC is large (where the prediction accuracy of the model is low). The proposed method consists of the following three steps as shown in Figure 1.

[Step1] Bayesian update 1
The first Bayesian update is performed using the experimental data and prior distribution to obtain the posterior distribution.

[Step2] Design of data sampling points
WAIC at each point on the design space of the data sampling points is calculated from the posterior distribution of parameters, and the experiment is conducted at the data sampling point with a large WAIC value to obtain new data.

[Step3] Bayesian update 2
Then, the second Bayesian update is performed including the newly added experimental data, and the posterior distribution of parameters is updated. In this way, a new posterior distribution with reduced parameter uncertainty is obtained.

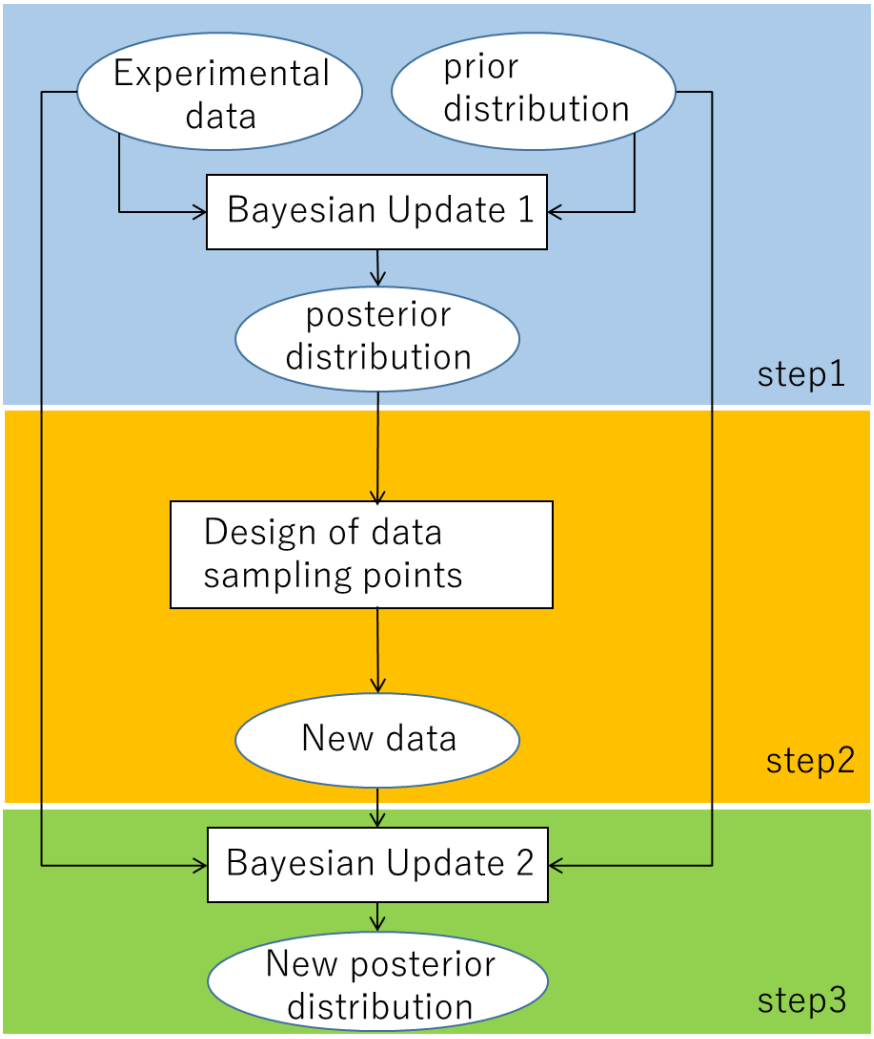

Figure 1. Flow of Reduction of Prediction Uncertainty

3. NUMERICAL EXPERIMENTS

To evaluate the effectiveness of the proposed prediction uncertainty reduction method, numerical experiments were conducted by applying the proposed method to a fracture probability estimation model [4]. The fracture probability estimation model provides an estimate of the fracture probability of a non-irradiated Zircaloy-4 cladding tube under LOCA conditions. In these numerical experiments, we assume a true model that generate data concerning fracture/non-fracture of the fuel cladding tube. In the real world, it is impossible to construct a model identical to the true model. Therefore, in this study, we conducted numerical experiments on two cases: one where the true model and the predictive model share the same mathematical structure (Case 1) and one where they have different mathematical structures (Case 2). We evaluated the effectiveness of the proposed method in both cases.

3.1. Case 1: True and Predictive Models Have the Same Mathematical Structure

3.1.1. Model Definition

The true model is defined as follows, as in the previous study [5]:

$$Y \sim Bernoulli(P_{true}(Y=1 \mid \boldsymbol{X})) \tag{9}$$

$$P_{true} = \Phi(10 + 7\log(\frac{X_1}{100}) + 20\log(1+\frac{X_2}{10000})) \tag{10}$$

where Y is LOCA-simulated test data binarized to 1 for fracture and 0 for non-fracture, $Bernoulli()$ is Bernoulli distribution, P_{true} is the fracture probability estimated by the true model, X_1 is an explanatory variable for equivalent cladding reacted (ECR, %), X_2 is an explanatory variable for the initial hydrogen concentration (wtppm), and Φ is the cumulative distribution function of the standard normal distribution.

The predictive model is defined as follows:

$$Y \sim Bernoulli(P(Y=1 \mid \boldsymbol{X})) \tag{11}$$

$$P = \Phi(\omega_0 + \omega_1 \log(\frac{X_1}{100}) + \omega_2 \log(1+\frac{X_2}{10000})) \tag{12}$$

where P is the fracture probability estimated by the predictive model and $(\omega_0, \omega_1, \omega_2)$ are parameters to be estimated.

Marginal prior distributions of these parameters are assumed to follow the following noninformative prior distribution:

$$\omega_k \sim Normal(0, 100) \quad (k = 0,1,2) \tag{13}$$

3.1.2. Calculation Flow

Numerical experiments were conducted in the following steps a) to f).

a) The design space of data sampling points was defined as a two-dimensional space consisting of ECR and initial hydrogen concentration. The design space consists of 403 sampling points in which ECR ranges from 10% to 40% in 1% increments and the initial hydrogen concentration ranges from 0 wtppm to 1200 wtppm in 100 wtppm increments.
b) Initial data were set as in the previous study [5], as shown in Figure 2.
c) Bayesian inference was performed to obtain the joint posterior distribution of parameters using the Markov chain Monte Carlo (MCMC) method with the initial data generated in step b) and the prior distributions. The MCMC sampling was performed using Stan via the rstan package version 2.21.7 for R language version 4.1.3. For the MCMC sampling, 27,000 iterations were run for each of the four chains (with the first 2,000 iterations excluded as a warm-up), resulting in a total of 100,000 iterations.
d) WAIC was calculated for each sampling point of the design space using the joint posterior distribution of parameters, and the data sampling points were determined so that the sampling points having large WAIC would be preferably selected. The number of data sampling points was gradually increased to 1, 3, 5, 7, 10, 15, and 20. For comparison, data sampling points were also designed for conventional methods [1,5] using functional variance and empirical loss in addition to WAIC.
e) New data were generated from the true model at the sampling points designed in step d), and Bayesian update of the predictive model was performed using the new data, the initial data, and the marginal prior distributions. For this Bayesian update, 2,700 iterations of MCMC sampling were performed in each of the four chains (with the first 200 iterations excluded as a warm-up), and a total of 10,000 iterations were run. To account for the effect of randomness of the new data, the above Bayesian update was performed 100 times with different random number seeds when generating new data from the true model.
f) Bayes generalization loss, a measure of the model's prediction accuracy in the design space, was calculated using the joint posterior distribution of parameters obtained in step e) to evaluate the predictive accuracy of the fracture probability estimation model.

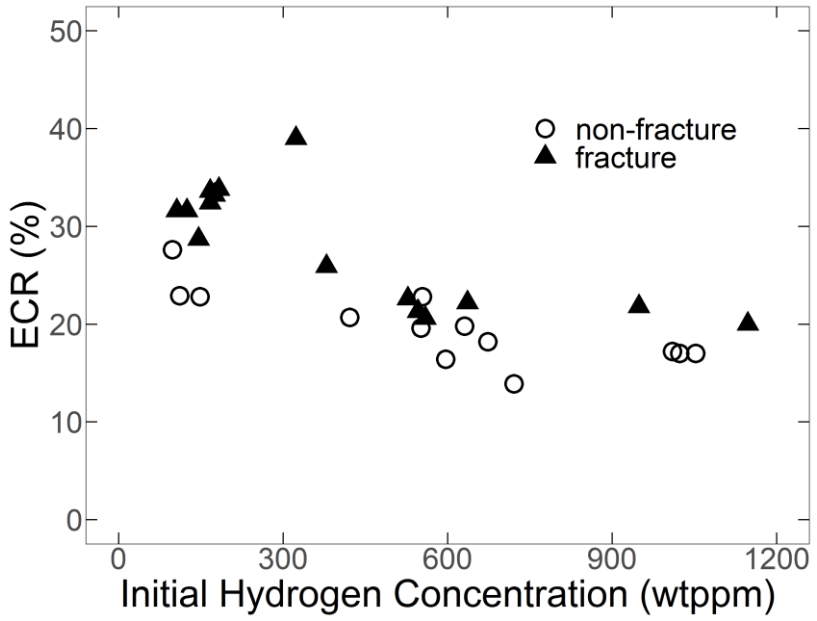

Figure 2. Initial Data generated from the true model

3.1.3. Results and Discussion

The relationship between the Bayes generalization loss and the number of data points added is shown in Figure 3. The results of 100 independent experiments with different random number seeds are shown in this figure as box plots. For comparison, the results of conventional methods [1,5] using the functional variance and the empirical loss (information entropy) are also shown in this figure.

As shown in this figure, the Bayes generalization loss was lowest on average when the empirical loss was used, which demonstrates effective reduction of predictive uncertainty of fracture when using the emprical loss. Our proposed method showed a minimal reduction in generalization loss when the amount of additional data was small (fewer than ~10). However, as the number of additional data points increased, it tended to achieve a generalization loss comparable to that obtained using the empirical loss.

These results can be attributed to the consistent mathematical structure between the true model and the predictive model. Since the mathematical structures of the true model and the predictive model are identical, it is clear from their mathematical definitions that minimizing the empirical loss, which is the expected value of the negative log-likelihood of the predictive model, will also minimize the Bayesian generalization loss, which is the KL divergence between the true model and the predictive model.

Moreover, the relationship between the estimated parameters and the number of data points added is shown in Figure 4. As shown in this figure, the method using empirical loss is more capable of bringing the parameters closer to the true value than the proposed method when the amount of additional data is small (less than ~10 data). However, as the number of additional data points increased, our proposed method approached the true value as well as the method using empirical loss. This shows that the proposed method accurately predicts the true values of the parameters.

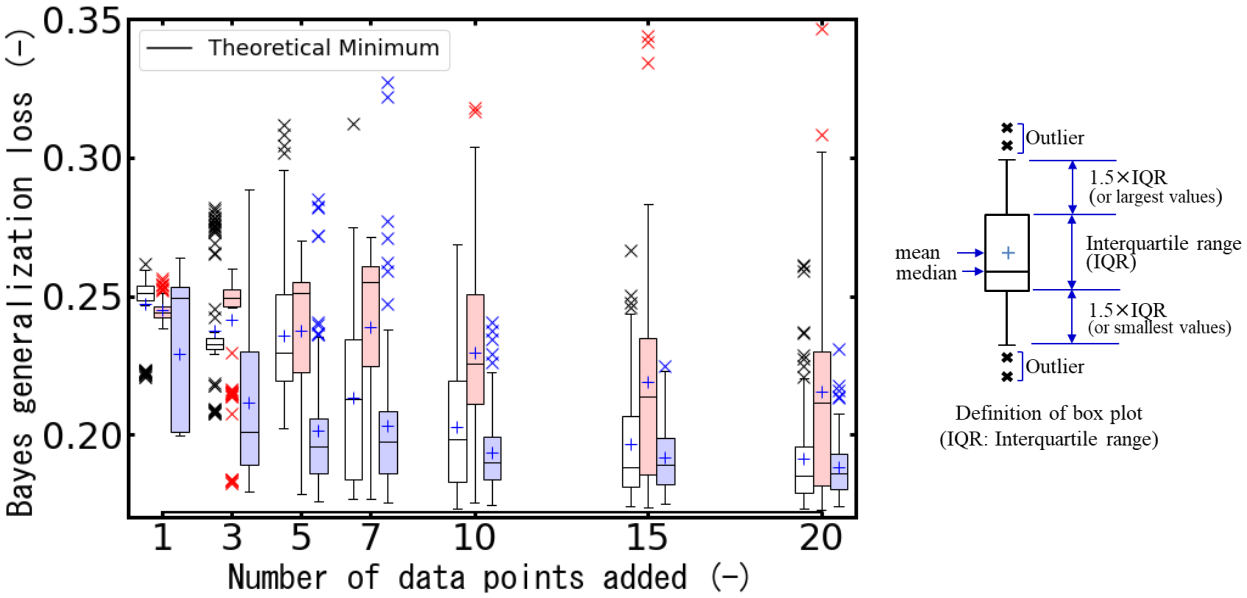

Figure 3. Relationship between the Number of Data Added and Bayes Generalization Loss
(White: WAIC; Red: Functional Variance; Blue: Empirical loss)

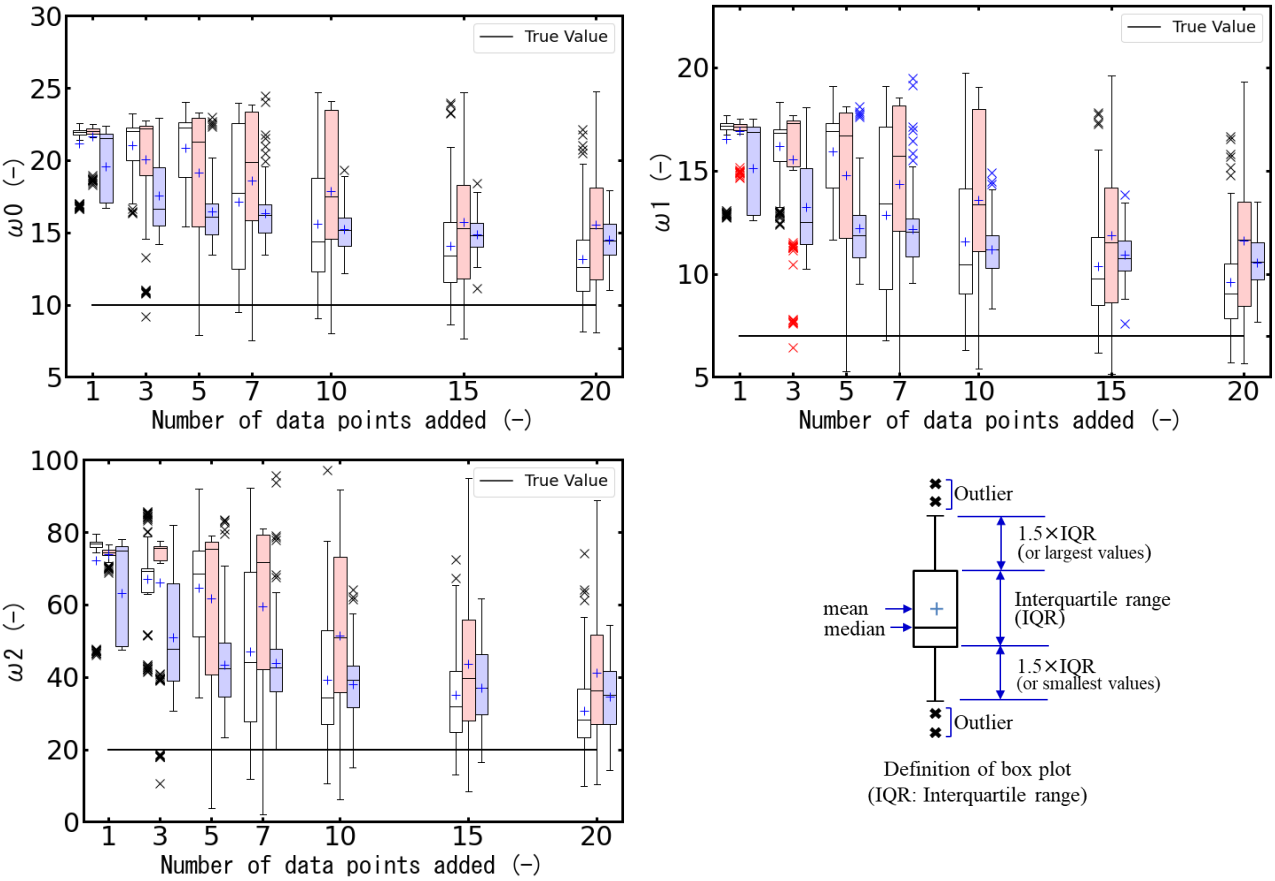

Figure 4. Relationship between the Number of Data Added and each parameters' values
(White: WAIC; Red: Functional Variance; Blue: Empirical loss)

3.2. Case 2: True and Predictive Models Have Different Mathematical Structures

3.2.1. Model Definition

The true model is defined as same as Section 3.1.1.

In the real world, the true model cannot be known, and thus the true model and the predictive model will not match. Therefore, in this Case 2, a predictive model is defined as a model with a mathematical structure different from that of the true model. The following changes to the true model were applied to the predictive model:

- The standard normal cumulative distribution function Φ was changed to the logistic function.
- No logarithm was taken for explanatory variables.
- A cross term was added for the explanatory variables (X_1, X_2).

Finally, the predictive model is defined as follows:

$$Y \sim Bernoulli(P(Y=1 \mid X)) \tag{14}$$

$$P(Y=1 \mid \mathbf{X}) = Logistic(\omega_0 + \omega_1 X_1 + \frac{\omega_2 X_2}{10000} + \frac{\omega_3 X_1 X_2}{10000}) = \frac{1}{1+\exp(-(\omega_0 + \omega_1 X_1 + \frac{\omega_2 X_2}{10000} + \frac{\omega_3 X_1 X_2}{10000}))} \tag{15}$$

where $(\omega_0, \omega_1, \omega_2, \omega_3)$ are assumed to follow the following noninformative prior distribution:

$$\omega_k \sim Normal(0, 100) \quad (k = 0, 1, 2, 3) \tag{16}$$

3.2.2. Calculation Flow

Numerical experiments were conducted as the same steps a) to f) in Section 3.1.2.

3.2.3. Results and Discussion

The relationship between the Bayes generalization loss and the number of data points added is shown in Figure 5. The results of 100 independent experiments with different random number seeds are shown in this figure as box plots. For comparison, the results of conventional methods [1,5] using the functional variance and the empirical loss are also shown in this figure.

As shown in this figure, the Bayes generalization loss was lowest on average when WAIC was used to design experiments. Therefore, the proposed method is considered to effectively reduce the prediction uncertainty of fracture when the number of experimental data is limited.

There were outliers regardless of the number of data points added for all the cases using WAIC, the functional variance, and the empirical loss. Upon investigating the additional data in the cases where these outliers occurred, the binary data regarding fracture/non-fracture tended to differ from the binary predictions made by the predictive model. In other words, due to the probabilistic fluctuations of the samples, rare datasets that differed from the predictions were generated, resulting in a lack of improvement in prediction accuracy and a significant deterioration in the Bayes generalization loss.

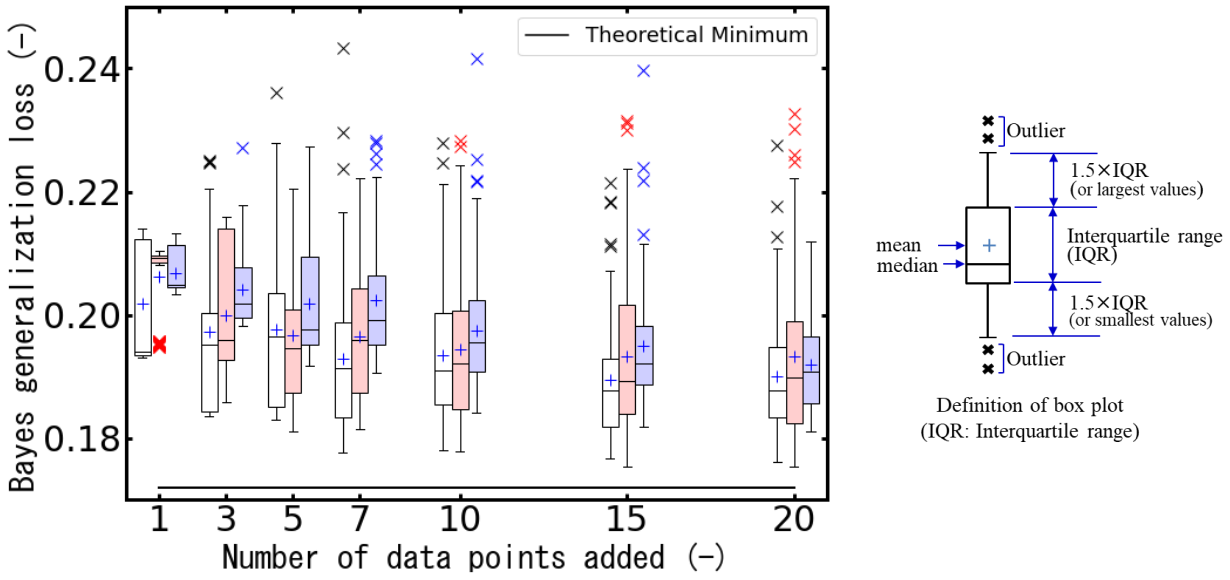

Figure 5. Relationship between the Number of Data Added and Bayes Generalization Loss
(White: WAIC; Red: Functional Variance; Blue: Empirical loss)

4. CONCLUSION

The purpose of this research is to develop a method to effectively reduce the prediction uncertainty of fuel fracture using a limited experimental data. To achieve this, we proposed a Bayesian updating method using an information criterion WAIC and conducted numerical experiments to evaluate its effectiveness.

Numerical experiments were conducted for the following two cases: one where the true model and the predictive model share the same mathematical structure (Case 1) and one where they have different mathematical structures (Case 2). In Case 1, when the number of newly added data points was relatively small (fewer than ~10), minimizing empirical loss, as proposed in a previous study, most effectively reduced the Bayes generalization loss, which is a measure of the accuracy of fracture predictions. This result aligns with the mathematical fact that minimizing empirical loss also minimizes the KL divergence between the true model and the predictive model. In Case 2, the proposed method using WAIC most effectively reduced the Bayesian generalization loss. Therefore, the proposed method enables more valuable experiments on average and can reduce the uncertainty in fracture prediction in realistic situations where the true model is unknown. This indicates that the proposed method can predict fuel fracture stably with higher accuracy and less uncertainty, even when the experimental data are limited.

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