Transactions of the Korean Nuclear Society Autumn Meeting
Changwon, Korea, October 24-25, 2024

Epistemic Uncertainty in Deep Learning Models and Its Application to Simulation Optimization and Consequence Parameter Trend Predictions for Dynamic Risk Assessment

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***Keywords :** Deep learning, Epistemic Uncertainty, Dynamic Risk Assessment, Parameter Trend Prediction

1. Introduction

Risk assessment of nuclear power plants (NPPs) is classically performed with representative accident scenarios involving conservative, static and binary assumptions about event sequences and success criteria. However, these assumptions may overlook dynamic factors that can change the accident progression, such as delayed operator response and partial operation of safety systems. In the case of multiple units with shared components and passive safety systems with natural power sources, these dynamic factors may need to be considered more explicitly in the assessment.

To this end, so-called dynamic safety (risk) assessments, which takes the dynamic factors into account more consciously, have been proposed to complement the static approaches with representative scenarios. Typically, these assessments decompose a single representative scenario into multiple ones according to the variances of dynamic factors. Consequently, a clear challenge of these assessments is that the number of scenarios to be simulated increases exponentially. This challenge imposes a computational burden because each scenario should be simulated by computationally expensive physical models, such as thermal-hydraulic (TH) system codes. For instance, in the dynamic risk assessments performed by Kubo et al., more than 100,000 scenarios were considered according to the initiation time of the reactor coolant pump seal loss-of-coolant accident and the failure times of the emergency diesel generators, safety injections and offsite power restoration [1].

To alleviate this burden, two approaches have been intensively investigated: a fast-running surrogate and an adaptive sampling. A fast-running surrogate is to simulate the scenarios with rapid data-driven models instead of costly physical models. Due to its ability to capture complex patterns, deep learning has been widely used as the surrogate model [2, 3]. Adaptive sampling, on the other hand, is an approach to reduce the number of scenarios to be simulated. To do this, sampling approaches typically employ an iterative sampling process with a metamodel, where the model training and model-guided sampling are repeated [4-6].

However, both approaches have limitations. For a fast-running surrogate, training data-driven models requires simulation results of substantial scenarios as a training data. As a result, it can pose another simulation burden. For adaptive sampling, the consequences of unsampled scenarios, including the trends of critical plant parameters, are not revealed. In addition, the previously proposed adaptive sampling methods use classical machine learning models as metamodels, which makes it difficult to apply to more than millions of scenarios due to the high time complexity.

To address these limitations, we propose a novel platform to reduce the computational burden of simulating massive dynamic scenarios. Given dynamic scenarios, this approach first optimizes the scenarios to be simulated using a previously developed deep learning-based adaptive sampling algorithm. Then, another deep learning model is trained to predict the trends of unsimulated scenarios based on the trends of simulated ones.

The proposed platform utilizes the epistemic uncertainty in deep learning models and this paper will mainly focus on how this uncertainty is exploited. Section 2 provides a brief overview of epistemic uncertainty in deep learning and how it can be quantified. Section 3 introduces the novel platform to reduce the computational burden of dynamic risk assessment. Section 4 explains how epistemic uncertainty has been applied in this platform to improve the efficiency and consistency of the simulation optimization results and to provide a prediction interval (PI) of the trend predictions. Section 5 concludes the paper.

2. Epistemic Uncertainty in Deep learning

There are two primary sources of uncertainty in deep learning: aleatoric and epistemic. Aleatoric uncertainty accounts for the randomness inherent in the data itself, while epistemic uncertainty represents the ignorance in the model's knowledge, especially when only a limited data is given. Figure 1 illustrates the difference between aleatoric and epistemic uncertainties.

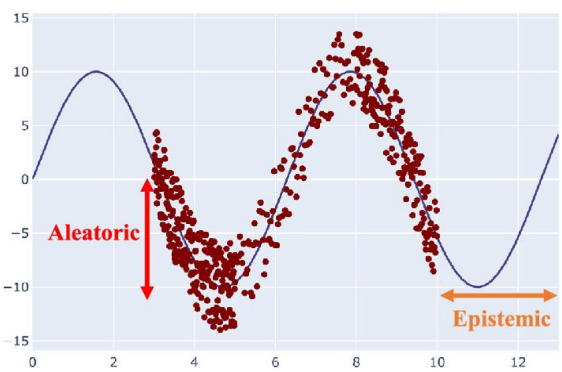

Fig. 1. Aleatoric and epistemic uncertainties.

Monte Carlo dropout (MC dropout) is a cost-effective approximation of the epistemic uncertainty in deep learning [7]. It is widely used due to its practicality in applying to deep learning without major modifications, The first step for applying it is to activate a dropout during the training phase. A dropout is a regularization technique to prevent model overfitting. As the name suggests, it randomly drops a fraction of neurons for each training trial, as shown in the Figure 2.

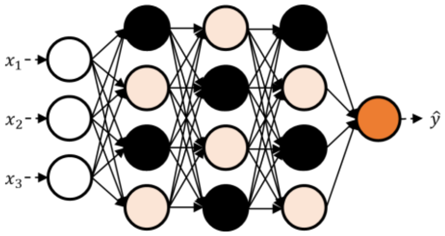

Fig. 2. A deep learning model with dropout

In the inference phase, MC dropout activates the dropout and makes multiple predictions for a given input with different dropout configurations. If the model has sufficient knowledge about a given input, it will produce consistent outputs. Conversely, if the model has limited knowledge, it will produce variant outputs according to the dropout configurations. By measuring the variance of the outputs, the epistemic uncertainty can be quantified.

3. Deep Learning-Based Platform for Dynamic Risk Assessment

In this research, we propose a novel deep learning-based platform for dynamic risk assessment, named a deep learning-based optimized simulation and consequence estimation with neural network uncertainty (DOSCENT). It consists of a deep learning-based algorithm for simulation optimization (i.e., deep learning-based searching algorithm of informative limit surfaces/scenarios/states [Deep-SAILS]) proposed in the authors' previous work [8], and a deep learning-based parameter trend prediction model, named consequence estimation with neural network uncertainty (CENT).

To overcome the limitations of an adaptive sampling and a fast-running surrogate, we sequentially integrate the surrogate and sampling and introduce deep learning and its epistemic uncertainty. Figure 3 illustrates how the DOSCENT works for given dynamic scenarios. First, DOSCENT selectively simulates the scenarios as guided by Deep-SAILS. Then, using the optimized simulations, DOSCENT trains a deep learning model to predict the trends of the critical parameters for the non-simulated scenarios. Both Deep-SAILS and CENT utilizes epistemic uncertainty in deep learning to improve the sampling efficiency and provide a PI in trend prediction. The details of the utilization of the uncertainty are discussed in the following section.

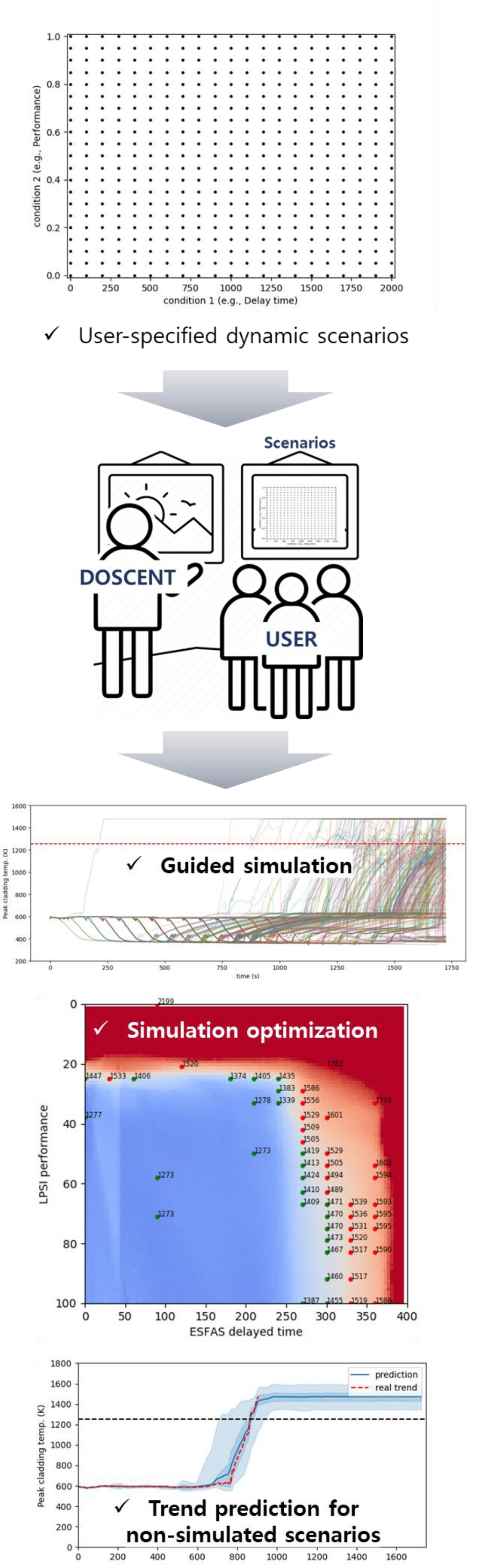

Fig. 3. Promising results of DOSCENT including simulation optimization and trend predictions for non-simulated scenarios.

4. Utilization of Epistemic Uncertainty

4.1 Simulation Optimization

Deep-SAILS is an iterative process that identifies limit surfaces (i.e., boundary between success and failure scenarios) and intensively simulates the scenarios close to the surfaces. Figure 4 shows the flowchart of Deep-SAILS. The process first simulates heuristically selected scenarios or extreme scenarios that configured by the highest and lowest values of the dynamic factors. Based on the simulation results, a deep learning model is trained to predict the outcome (e.g., peak cladding temperature) of given scenario conditions. Next, the algorithm selects the scenarios to be simulated based on the predictions for the unsimulated scenarios. This process continues until most of the scenarios selected in the current stage have been selected in the previous stages, indicating that the algorithm is converging. More details about Deep-SAILS can be found in [8].

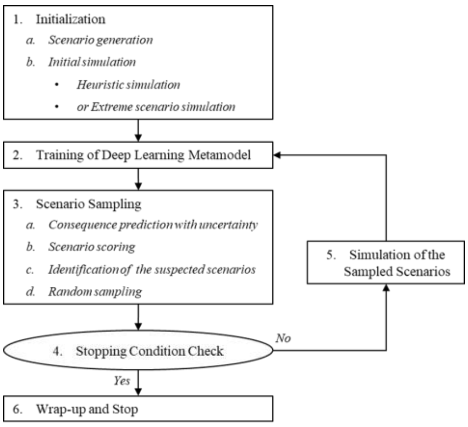

Fig. 4. Algorithm flow chart of Deep-SAILS [8]

In this algorithm, epistemic uncertainty is used to improve sampling efficiency. Figure 5 shows the scenario scoring function [9] of Deep-SAILS. The numerator is an absolute deviation between the predicted outcome and the failure criteria, and the scenarios with lower scores are sampled preferentially. This is a typical scoring function employed by various adaptive sampling methods [4-6].

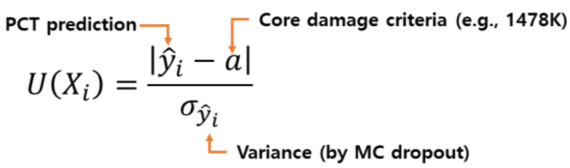

Fig. 5. U-learning function [9] for scoring the scenarios.

The idea of Deep-SAILS is to divide deviations with epistemic uncertainty. Since this uncertainty is associated with lack of knowledge, it helps to sample the scenarios more homogeneously by giving more weight to the scenarios from less sampled regions. Figure 6 presents the results of the case study with and without the uncertainty [8]. Deep-SAILS with uncertainty information identified the success and failure of the scenarios with higher accuracy compared to the algorithm without uncertainty. Another notable point is that the algorithm runs with uncertainty produce consistent results compared to the runs without uncertainty.

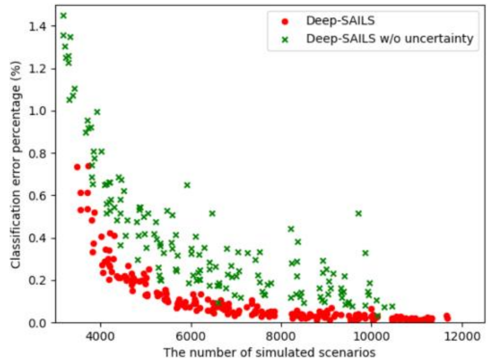

Fig. 6. The percentage of error in classifying the success and failure of entire scenarios (40,250 scenarios were assumed) when simulating different numbers of scenarios. Green dots are the result without uncertainty information and red dots are the result with uncertainty information (i.e., Deep-SAILS) [8].

4.2 Consequence Estimation

As mentioned above, a clear disadvantage of adaptive sampling methods is that most scenarios remain unsimulated and therefore the consequences, including time variations of important parameters, of these scenarios cannot be known. To overcome this limitation, DOSCENT uses deep learning to estimate the consequence of unsimulated scenarios. The training data is the optimized simulation result guided by Deep-SAILS.

The challenge of consequence estimation lies in the lack of knowledge due to preferential simulation. For instance, when there are many simulated scenarios similar to a given unsimulated scenario, accurate predictions can be made. However, when there are no simulated scenarios near the given unsimulated scenario, predictions carry high uncertainty. Furthermore, predictions can also have high uncertainty when the conditions of the given unsimulated scenario fall within a region of rapid change. As this issue is inevitable, CENT addresses this issue by revealing the uncertainty in trend predictions.

Figure 7 shows the structure of the deep learning model of the CENT. It consists of a latent predictor, which outputs the latent vector (z) for a given scenario condition, and the decoder, which reconstructs the parameter trend from the estimated latent vector.

In the training phase, the predictor learns the latent vectors of the training data (i.e., the trends of the critical parameters) while activating the MC dropout. When given an unsimulated scenario, the latent predictor will output relatively consistent vectors (red dots) regardless

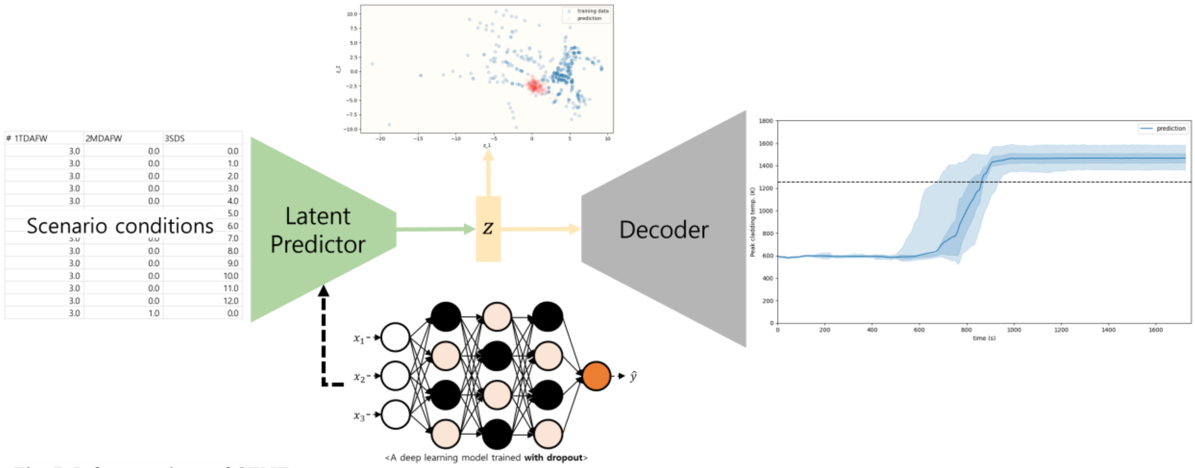

Fig. 7. Inference phase of CENT

of different dropout configurations if the given condition is similar to the training data. The parameter trend reconstructed from these vectors will also be consistent and have a narrow PI, as shown in Figure 8.

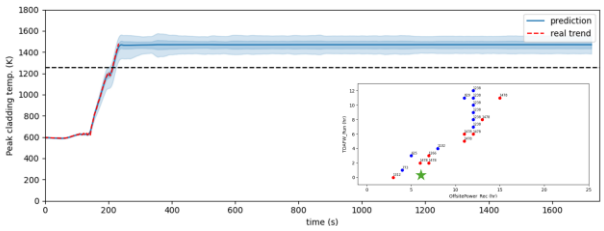

Fig. 8. Trend prediction for low uncertainty scenario. The blue line is the point-estimated trend prediction, and the shaded areas corresponding to the 98% and 60% PI, and the red-dotted line is the real trend given by the TH simulation.

In contrast, if the given condition is relatively much different from the training data, the latent vector predictions will vary with the dropout configurations, and the reconstructed trend will have a wide PI, as shown in Figure 9. It should be noted that even if the given condition is similar to the training data, a PI can be wide if the condition is on a region with rapid changes in the parameter trends.

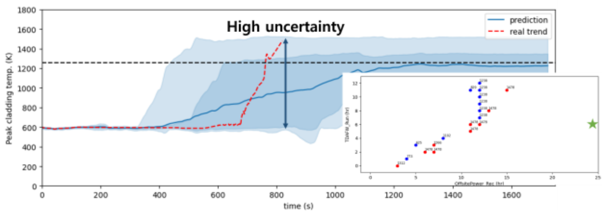

Fig. 9. Trend prediction for high uncertainty scenario.

5. Conclusion

In this research, we developed DOSCENT to reduce the computational burden associated with dynamic risk assessment and employed epistemic uncertainty in deep learning models to improve the sampling efficiency of simulation optimization and provide a PI in consequence parameter trend prediction. Currently, DOSCENT has been integrated into the TH system codes and is being used to analyze the dynamic scenarios.

ACKNOWLEDGEMENT

This work was supported by the National Research Foundation of Korea (NRF) grant funded by the Korea government (MSIT) (No. RS-2022-00143695)

REFERENCES

[1] Kubo, K., et al., Quasi-Monte Carlo sampling method for simulation-based dynamic probabilistic risk assessment of nuclear power plants. Journal of Nuclear Science and Technology, 2022. 59(3): p. 357-367.
[2] Ryu, S., et al., Probabilistic deep learning model as a tool for supporting the fast simulation of a thermal–hydraulic code. Expert Systems with Applications, 2022. 200: p. 116966.
[3] Chae, Y.H., et al., Development of a data-driven simulation framework using physics-informed neural network. Annals of Nuclear Energy, 2023. 189: p. 109840.
[4] Zheng, X., et al., Dynamic probabilistic risk assessment of nuclear power plants using multi-fidelity simulations. Reliability Engineering & System Safety, 2022. 223: p. 108503.
[5] Alfonsi, A., et al., Dynamic PRA: an Overview of New Algorithms to Generate, Analyze and Visualize Data. Vol. 109. 2013.
[6] Matsushita, M., T. Endo, and A. Yamamoto, Development of a reduced order model for severe accident analysis codes by singular value decomposition aiming probabilistic safety margin analysis. Journal of Nuclear Science and Technology, 2020. 57(5): p. 573-589.
[7] Gal, Y. and Z. Ghahramani, Dropout as a Bayesian Approximation: Representing Model Uncertainty in Deep Learning, in Proceedings of The 33rd International Conference on Machine Learning, B. Maria Florina and Q.W. Kilian, Editors. 2016, PMLR: Proceedings of Machine Learning Research. p. 1050--1059.
[8] Bae, J., J.W. Park, and S.J. Lee, Limit surface/states searching algorithm with a deep neural network and Monte Carlo dropout for nuclear power plant safety assessment. Applied Soft Computing, 2022. 124: p. 109007.
[9] Echard, B., N. Gayton, and M. Lemaire, AK-MCS: An active learning reliability method combining Kriging and Monte Carlo Simulation. Structural Safety, 2011. 33(2): p. 145-154.