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Probabilistic Neural Network Approach for Critical Heat Flux Prediction with Uncertainty Quantification

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1. Introduction

In the light water reactors, accurate prediction of the thermal-hydraulic phenomena accompanying two-phase flow is paramount as they dominate the system behavior during design basis accidents and design extension conditions. Among the various two-phase flow phenomena, the critical heat flux (CHF) is recognized as one of the most important criteria as it primarily determines the fuel rod integrity. However, the complex nature of the CHF including its triggering mechanism, and limitations of applicable instrumentations are contributing to the remarkable uncertainties in the models and correlations based on physical assumptions and regression features. To resolve the uncertainties of the existing CHF models/correlations, new prediction approaches applying for the machine learning techniques are being suggested because the machine learning models have excellent analysis capability figuring out the complex patterns between the input and output variables based on the nonlinear regression features, i.e., bulk weight/bias matrix. A wide range of the machine learning architectures have been constructed as an augmented prediction tool for the CHF [1-3] successfully demonstrating the improved prediction capability compared to the existing prediction methods, such as look-up table [4] and correlations [5, 6], however, it is challenging to use them as an engineering feature because quality assurance and regulation methodology about the machine learning techniques is still not established due to the methodological absence evaluating the uncertainty of the machine learning models. Therefore, a probabilistic neural network technique, which can provide the uncertainty information regarding their prediction, can be a potential approach to evaluate its predictive capability in both aspects of the developer and regulator. In this paper, Bayesian neural network based on the variational inference, facilitating the CHF prediction and its uncertainty quantification, is proposed describing their predictive performance and prospect.

2. Methods

Typically, the neurons in the deep neural network (DNN) models consist of the weight and bias in the form of certain point values. Because the trained DNN has a fixed weight and bias matrix, its prediction uncertainty is hard to quantify. Although explainable artificial intelligence (XAI) methods and physics-informed neutral networks (PINN) [7, 8] are being applied to reduce the 'black-box' characteristics, reliability of the DNN is still being debated due to the difficulty in models' uncertainty quantification. Therefore, probabilistic DNN were suggested as an alternative for the conventional DNNs. The fundamental concept of the probabilistic DNNs is constructing the architecture in a variable (distribution) weight and bias matrix, based on the variational inference [9].

2.1 Bayesian Neural Network (BNN)

In the system of random variables where X and Z represent the observed variable and hidden variable, respectively, the conditional probability density $p(X|Z)$, referred to as likelihood. From Bayesian theorem, the posterior probability density can be computed as:

$$p(Z|X) = \frac{p(X|Z)p(Z)}{p(X)} \tag{1}$$

Although the evidence ($p(X)$) can be computed as integration of the likelihood ($p(X|z)$) and prior ($p(z)$) for an instance z, the integration is not computable in general because the hidden variable Z has high dimension. Therefore, the posterior is inferred by a variational distribution ($q^*(Z)$), which is an arbitrary distribution. This variational inference is performed by Kullback-Leibler (KL) Divergence, which calculates the difference between the variational distribution and posterior [10].

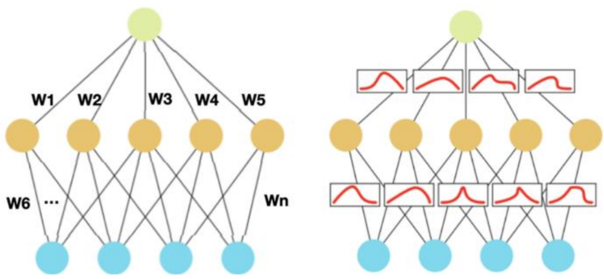

Fig. 1. Comparison of (a) conventional DNN and (b) BNN [11]

In the BNN, the relationship (posterior) between weight/bias and input/output variables is estimated by the variational inference based on the KL-Divergence as shown in Fig. 1. Because the weight/bias in the BNN is a form of probabilistic distribution, the model will provide the prediction in the form of certain distribution. As a result, the uncertainty of the neural network can be quantified based on the distribution. Therefore, a BNN model is developed in this study for the CHF prediction with providing the uncertainty information about the prediction.

2.2 Dataset

The CHF database (total 22,532 data) is established by collecting the experimental data from open literatures including AECL 2006 CHF look-up table [4] to train and test the probabilistic DNN models. The input features are classified as tube inner diameter (d_i, 0.002~0.016 m), heated length (L_h, 0.05~2 m), system pressure (p, 1~200 bar), mass flux (G, 10~7900 kg/m^2-s), exit quality (x_{exit}, -0.5~1.0), and inlet subcooling ($\Delta T_{in,sub}$, 0~150 °C). As shown in Fig. 3, the mass flux, exit quality, inlet subcooling, and system pressure exhibit the wide distributions as mentioned order.

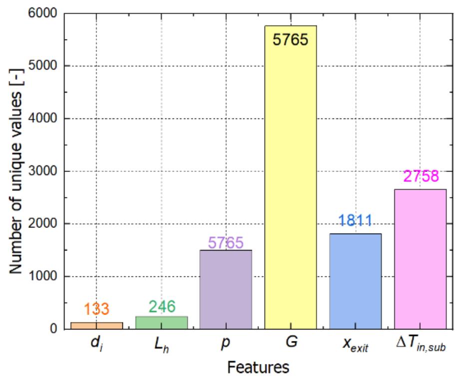

Fig. 2. Number of unique values in the train dataset according to individual input features

2.3 Model Description

The BNN is built in the Tensorflow platform and the details in the model (architectures and hyperparameters) are summarized in Table I.

Table I: BNN model summary

Parameters	Description or value
Architecture	6-256-256-256-128-1
Activation function	ReLu
Data scaling	StandardScaler
Batch size	64
Optimizer	RMSprop
Learning rate	0.001
Loss function	Mean squared error
Validation	5-fold cross-validation
Early stopping	100 epochs in a row
Number of epochs	1000
Size of dataset	Train (Random 80% of 22,532 samples)
	Test (Random 20% of 22,532 samples)

The dense variational, which is a module implementing the probabilistic weight (weight distribution), is applied for the first hidden layer consisting of 256 neurons and the rest three layers (256-256-128) are modeled as conventional dense layer.

3. Results and Discussion

The performance of trained BNN is evaluated with root-mean squared error (RMSE) and regression coefficient (R^2) as Eqs. (2) and (3). The RMSE and R^2 score of the trained BNN model regarding the test dataset with 500 iterations are 147.58 kW/m^2 and 0.8867, respectively. As shown in Fig. 3 (red dots in Fig. 3 denote the mean value of the predicted CHF by the trained BNN for 500 iterations), the trained BNN shows good prediction capability excluding the relatively high CHF values (> 6000 kW/m^2).

$$RMSE = \sqrt{\frac{1}{n}\sum_{i=1}^{N}\left(y_{\exp,i} - y_{pred,i}\right)^2} \quad (2)$$

$$R^2 = 1 - \frac{\sum_{i=1}^{n}\left(y_{\exp,i} - y_{pred,i}\right)^2}{\sum_{i=1}^{n}\left(y_{\exp,i} - \bar{y}_{\exp,i}\right)^2} \quad (3)$$

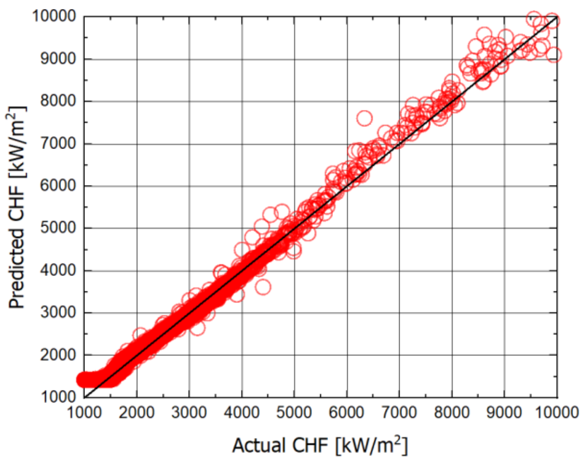

Fig. 3. Histograms for pressure, mass flux, and exit quality

To evaluate the trained BNN performance in figuring out the relationship between the individual input features and CHF, the mean values and 95% confidence intervals of the BNN's CHF predictions with respect to the pressure, mass flux, and exit quality. As shown in Figs. 4~6, the BNN model successfully provides the ensembled prediction (mean) and uncertainty (standard deviation) for the input features. It should be noted that the predictions are conducted with arbitrary dataset (variation of a single input feature and remaining other feature values as a constant) due to the high dimension of the input dataset.

The mean value of the 500 predictions by the constructed BNN model, depicted as a solid line, increases with mass flux, and decreases with system pressure, and exit quality.

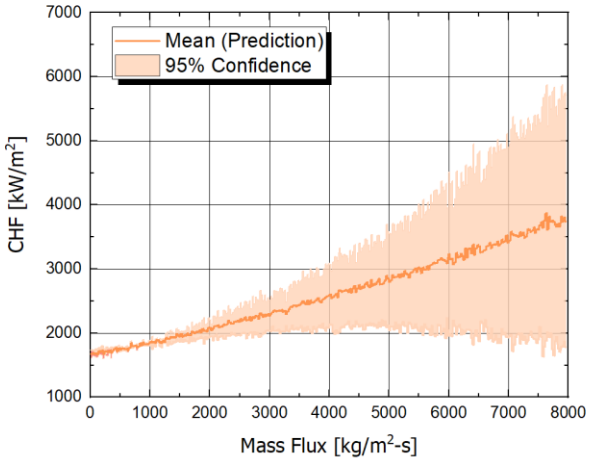

Fig. 4. Variations of mean and 95% confidence intervals of the CHF prediction by the BNN with respect to mass flux (constant d_i=0.004 m, p=100 kPa, and x_{exit}=0.8)

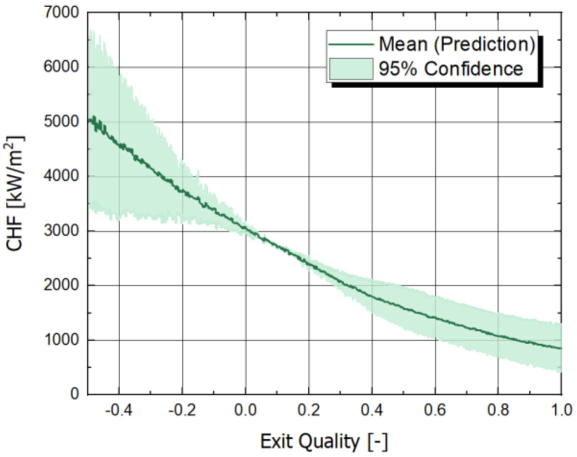

Fig. 5. Variations of mean and 95% confidence intervals of the CHF prediction by the BNN with respect to exit quality (constant d_i=0.004 m, p=100 kPa, and G=100 kg/m^2-s)

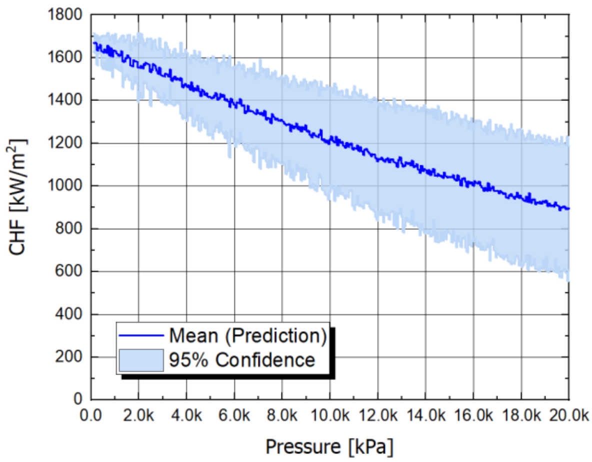

Fig. 6. Variations of mean and 95% confidence intervals of the CHF prediction by the BNN with respect to system pressure (constant d_i=0.004 m, G=100 kg/m^2-s and x_{exit}=0.8)

Because this tendency is also generally observable in 2006 CHF look-up table and analysis of the train dataset, it could be concluded that the trained BNN model has a physical insight in the CHF prediction according to the input features.

The standard deviation of the CHF prediction by the BNN model increases as the mas flux increases as shown in Fig. 4. As shown in Fig. 7, which plots the histograms for the individual input features of the dataset, the number of data exponentially decreases as the mass flux increases. Therefore, the increase of prediction uncertainty with increasing the mass flux is attributed to the lack of dataset. The relationship between the BNN's prediction uncertainty and amount of the dataset could also be supported by Fig. 5. The uncertainty decays as the exit quality increases from the negative x_{exit} to the positive x_{exit}, while the uncertainty increases from x_{exit} = 0.3 to 1.0. From the comparison between the model uncertainty and data histogram, it could be found that the amount of data primarily dominates the uncertainty of the probabilistic neural network.

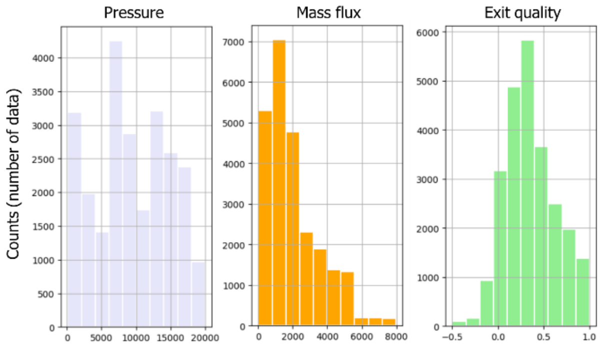

Fig. 7. Histograms for pressure, mass flux, and exit quality

On the other hand, the uncertainty of the prediction increases as the system pressure increases despite the dataset distribution with respect to the system pressure is relatively uniform compared to other features. The characteristics could be caused by two mechanisms; i) quantity (frequency) of the multivariable dataset, and ii) intensity of outlier in the dataset. The multivariable histogram demonstrates the number of data in a function of multiple variables. To analyze if the increased uncertainty as the increased system pressure results from the deficiency of the data in the given mass flux and exit quality condition, the 2D histograms consisting of pressure-mass flux, and pressure-exit quality are drawn as Fig. 8 because the mass flux and exit quality is remained as the constant value in Fig. 6.

As shown in Fig. 8, the amount of data decreases as the system pressure increases in the given mass flux and exit quality. Whereas the sufficient amount number of data exist in the x_{exit} = 0.8 for varied system pressure condition, there is insufficient data for the mass flux of 100 kg/m^2-s. In addition, the effect of the outlier in the dataset cannot be explored because the number of data is unsatisfactory for the pressure in the given mass flux and exit quality. Therefore, it is drawn that the increase of the uncertainty as the increase of the system pressure attributed to the low frequency of the dataset for the other features, especially for the mass flux.

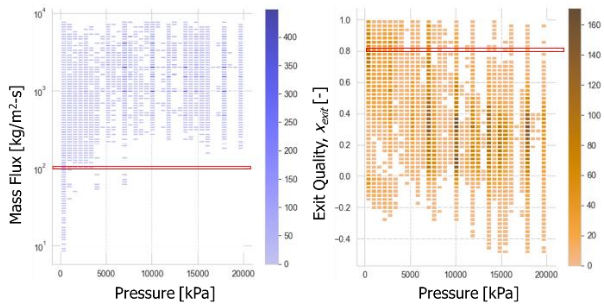

Fig. 8. 2D histograms; pressure versus mass flux and exit quality

Although the current BNN model exhibits relatively noticeable uncertainty in the data-deficient regimes, its prediction results are physically explainable and the uncertainty could be further reduced by optimizing its model architecture and hyperparameters. In addition, because the probabilistic neural network model provides the reasonable uncertainty information, which facilitates the quantitative quality assurance on the NN model, it will be preferable as an engineering feature in comparison with conventional neural networks having the weight/bias matrix in terms of point values. Thus, the probabilistic NN models will be a valuable approach in the reactor safety assessment by providing the better prediction capability and uncertainty band, which helps the making decisions of the operators, designers, and regulator.

4. Conclusions and Future works

To develop a deep neural network model, enabling the accurate prediction of CHF and uncertainty quantification of the constructed NN, a probabilistic NN (Bayesian NN) based on the variational inference was constructed with a total 22,532 dataset. The mean predictions of 500 iterations by the trained BNN model showed good predictions compared to the train and test dataset with a regression coefficient of 0.8867. In comparison with the conventional NN models, which have the point values of weights and biases, the uncertainty could be successfully demonstrated as the BNN provides the different values for each iteration. The uncertainty of the BNN model was closely related to the data distribution according to individual features and multivariable dataset. Therefore, further optimization of the model architecture, hyperparameter, and data augmentation will facilitate the application of the NN technique for the reactor safety assessment through the quantitative assurance of its performance.

In the future, the optimization work in aspects of the reorganization of the input features, model architecture, and combination with other probabilistic techniques, will be carried out to improve its performance. In addition, the predictive performance of the probabilistic NN models will be evaluated quantitatively compared to the existing models/correlations and conventional NN.

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