

Supplementary File S2. The sensitivity analysis results

1. Sensitivity analysis for the hyperparameters of lattice-physics dataset

Finding the valid range of hyperparameter values in DNNs is crucial, as it directly impacts the efficiency of the optimization process. Due to the unknown nature of valid values and ranges, sensitivity analysis focuses exclusively on non-categorical hyperparameters. These non-categorical hyperparameters include variables such as learning rate, validation split, number of nodes, and epochs. The selection to exclusively evaluate non-categorical hyperparameters is driven by their continuous nature, which makes them suitable for sensitivity analysis. On the other hand, categorical hyperparameters, such as activation functions and optimizers, are predefined with distinct values that are integral to the neural network architecture, allowing their exclusion from the sensitivity test.

By isolating non-categorical hyperparameters for investigation, we aim to gain insights into the impact of continuous adjustments on the performance of the system, contributing to a comprehensive understanding of its behavior. These sensitivity tests play a pivotal role in establishing valid ranges for subsequent optimization processes. Our focus in this context is to identify a hyperparameter range that guarantees a stable system state, thereby enhancing the reliability of the optimization process [1].

Once a specific non-categorical hyperparameter is adjusted, the others are fixed with the value displayed in Table S1. These fixed values and the test range are carefully selected based on the preliminary investigations. For example, the chosen number of hidden layers is two layers, the activation function is ReLU [2], and the optimizer is Adam [3]. All these sensitivity tests are conducted using 1000 uniform random samples within the test range in Table S1.

Table S1. The hyperparameters for sensitivity analysis

No	Quantity	Test range	Fixed value
1	Learning rate	0.0001 to 0.1	0.01
2	Number of hidden layers	2	2
3	Number of nodes per layers	0 to 200	128, 64
4	Validation split	0.05 to 0.85	0.1
5	Activator	ReLU	ReLU
6	Optimizer	Adam	Adam
7	Epochs	1 to 200	200

Learning rate sensitivity test

In deep neural networks, the learning rate is a hyperparameter that determines the step size of each iteration to move toward a minimum value of the loss function. A very high learning rate may not facilitate finding the minimum loss function and increases the uncertainty of the machine learning model. Conversely, a very low learning rate may take too long to converge and sometimes get stuck in an unexpected local minimum. In this case, we adjusted the learning rate from 0.0005 to 0.1 using a uniform random variable; the other hyperparameters such as the number of hidden layers, number of nodes per layer, validation split, activation functions, optimizer, and number of epochs are fixed as shown in Table S1. The Mean square error (MSE) value was used to track the DNN's predictions and can be calculated using the following equation:

$$MSE = \frac{1}{m} \sum_{i=1}^m (t_i - \tilde{t}_i)^2 \quad (12)$$

where t is the predicted value and \tilde{t} is the actual value, and m is the number of datasets.

It can be observed that when the learning rate is higher than approximately 0.06, the accuracy of DNNs significantly fluctuates, leading to the unacceptable prediction of DNNs. This phenomenon gradually reduced when the learning rate decreased to approximately 0.02. Therefore, a learning rate higher than 0.02 is strongly not recommended for this problem (see Fig. S1).

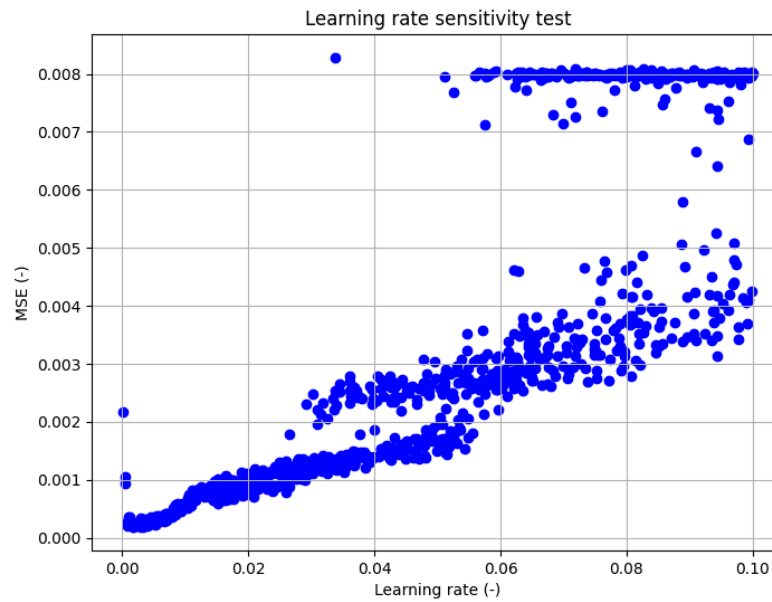


Figure S1. Learning rate sensitivity test results

Validation split test

The validation split involves partitioning the dataset into a training set and a validation set, enabling the assessment of our machine learning model's performance during the training process. The validation split value represents the percentage ratio between the training data and the validation dataset. It has been observed that setting the validation split value excessively high can result in an inadequate training dataset, increasing the uncertainty of the model. Conversely, a very small validation split may lead to insufficient validation of the DNN's predictions. Figure S2 illustrates that the valid range for the validation split value lies between 0.05 and 0.5. However, it was revealed that maintaining this value as fixed throughout the optimization process is essential to ensure a sufficient and consistent validated dataset, guaranteeing the stable accuracy of the DNN predictions.

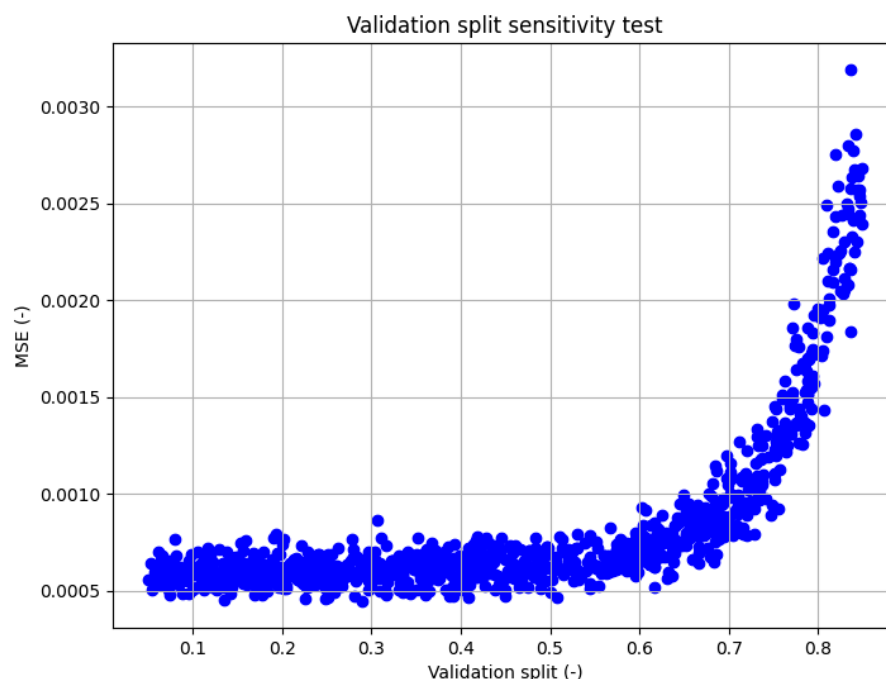


Figure S2. Validation split sensitivity test results

Number of nodes per hidden layers test

This test is to roughly identify the valid range of the number of nodes for the two-hidden layer case by adjusting their number of nodes, independently. Therefore, the results can be constructed by the combination of a random number of nodes in each layer, which is a so-called dual sensitivity test. In this dual sensitivity test, we utilized the MSE-1 as a metric to measure the accuracy of the DNN predictions. The

blue zone in Figure S3 indicates the very bad ML predictions due to the high value of MSE. As a result, it is recommended that the number of nodes should be generally greater than 30 for each layer to obtain acceptable accuracy.

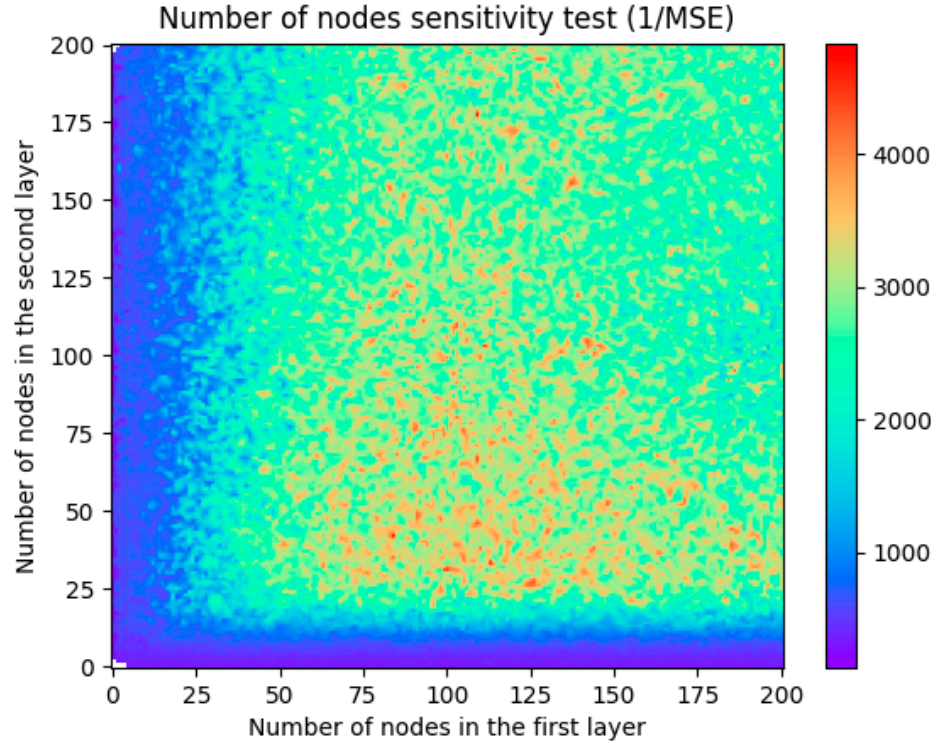


Figure S3. Number of nodes sensitivity test results

Number of epochs

The term "epochs" represents the number of iterations over the training dataset during which a DNN learns and updates its parameters to enhance its predictions. Therefore, the valid value of epochs should be an integer number (\mathbb{Z}^+). The optimal number of epochs depends on factors such as the complexity of the problem, the size of the dataset, and the architecture of the neural network. In this sensitivity test, we adjusted the epochs under 1 to 200. Consequently, the results indicated that the number of epochs should be higher than 50 (see Fig. S4). However, it can be observed that there are still some noisy results even after 50 epochs. To mitigate this bias, we implemented the ModelCheckpoint in Keras [4] during the training process. This allowed us to store the best accuracy achieved, ensuring that the best candidate could always be obtained despite the presence of noise. As a result, we treated the number of epochs as a fixed value (epochs = 200) during the optimization process and did not consider it as a hyperparameter requiring adjustment.

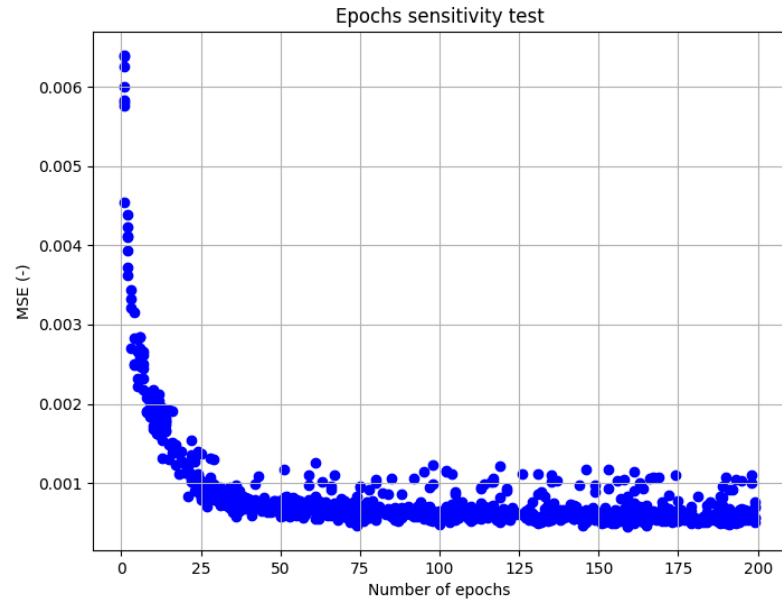


Figure S4. Number of epochs sensitivity test

2. Sensitivity analysis for the hyperparameters of the public datasets

The selected initial range for sensitivity analysis were presented in Table S2.

Table S2. The hyperparameters for sensitivity analysis

No	Quantity	Test range	Fixed value
1	Learning rate	0.00001 to 0.1	0.001
2	Number of hidden layers	2	2
3	Number of nodes per layers	1 to 200	100, 100
4	Activator	ReLU	ReLU
5	Optimizer	Adam	Adam
6	Batch size	1 to 200	50
7	Epochs	1 to 200	100

2.1 Boston Housing dataset

Learning rate sensitivity test

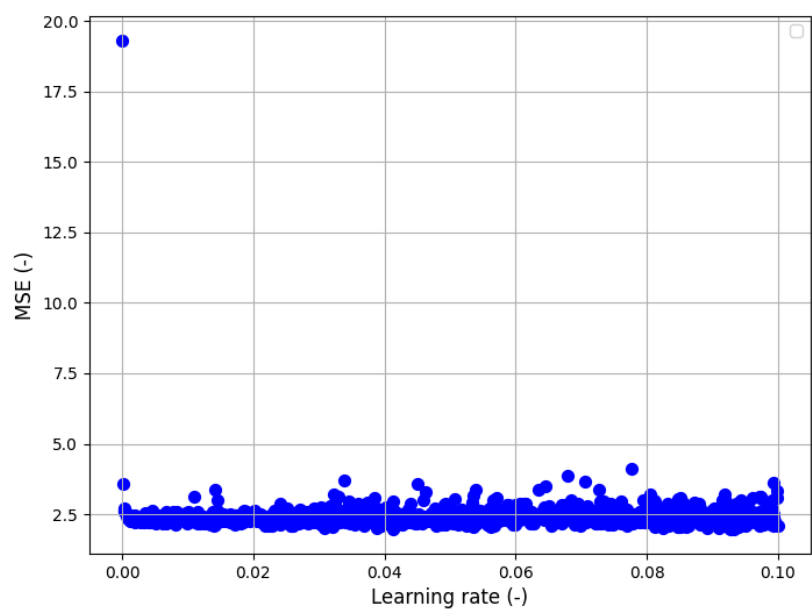


Figure S5. Learning rate sensitivity test

Batch size test

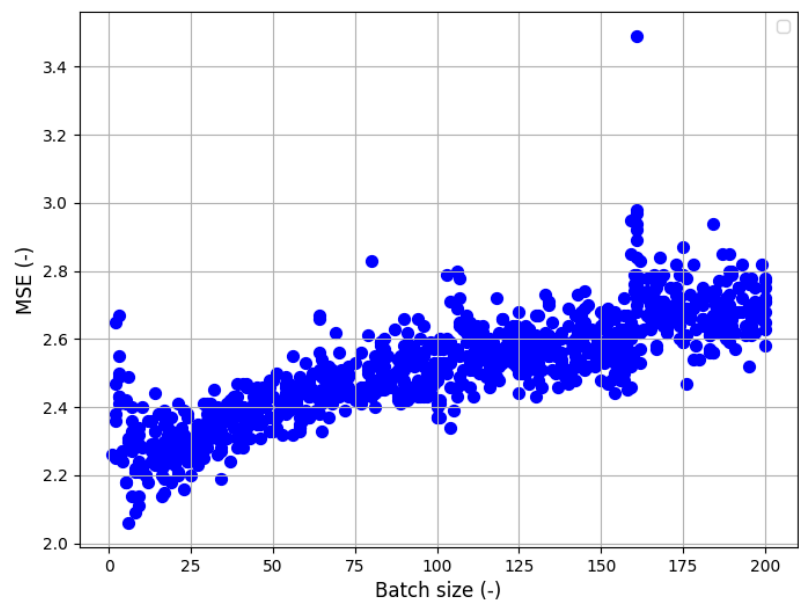


Figure S6. Batch size sensitivity test

Epochs test

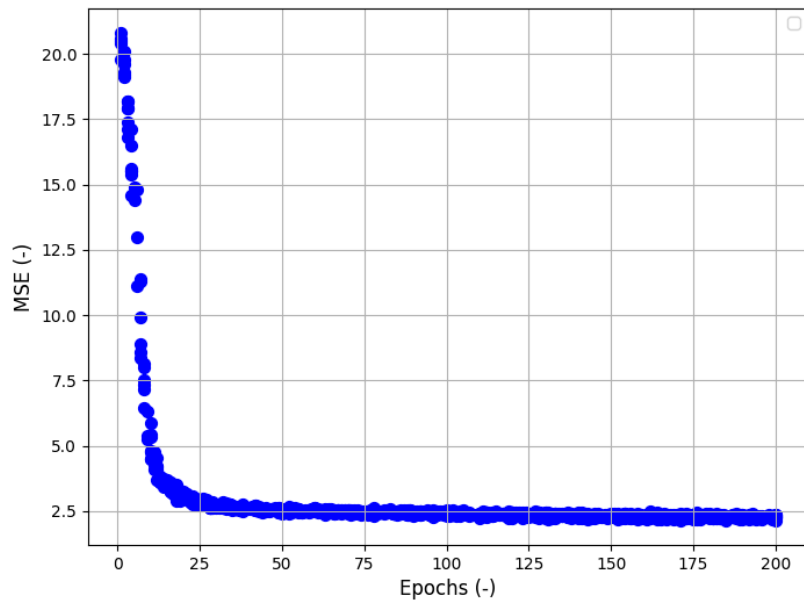


Figure S7. Number of epochs sensitivity test

Number of nodes test

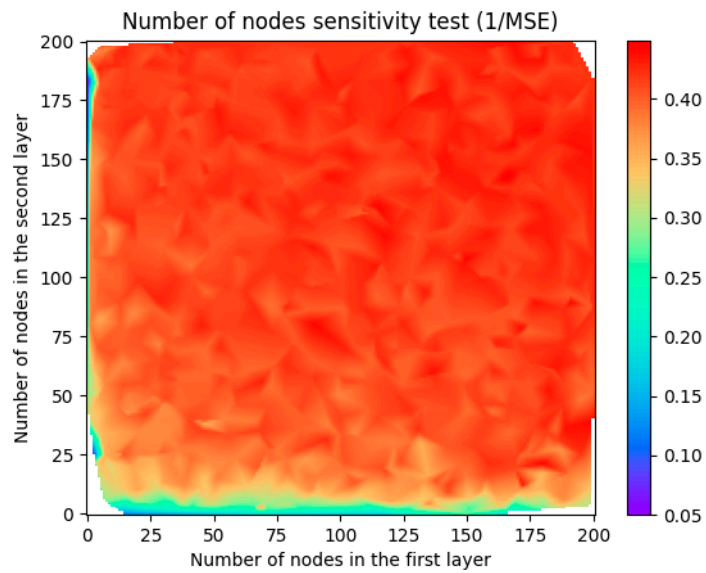


Figure S8. Number of nodes sensitivity test

2.2 CHF dataset

Learning rate sensitivity test

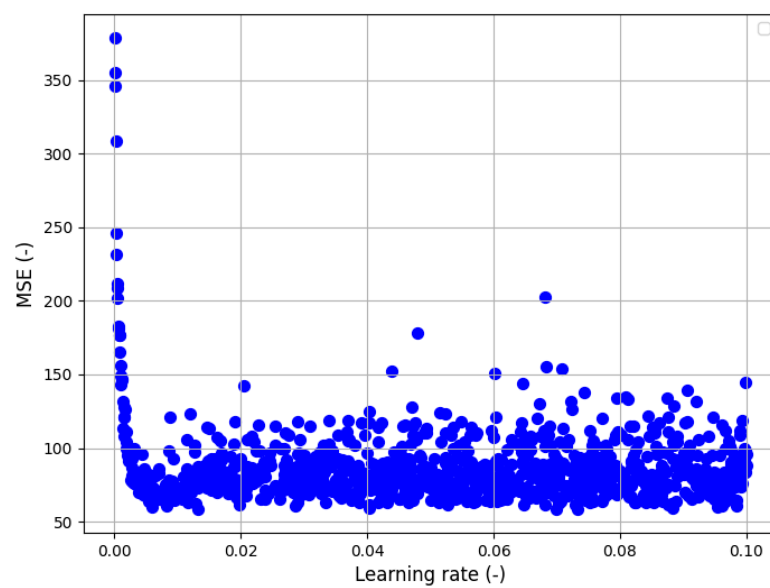


Figure S9. Learning rate sensitivity test

Batch size test

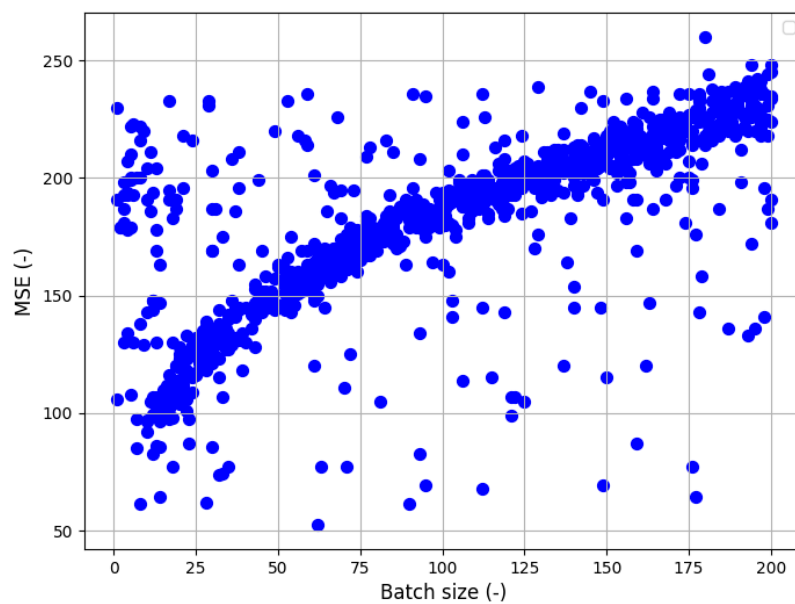


Figure S10. Batch size sensitivity test

Epochs test

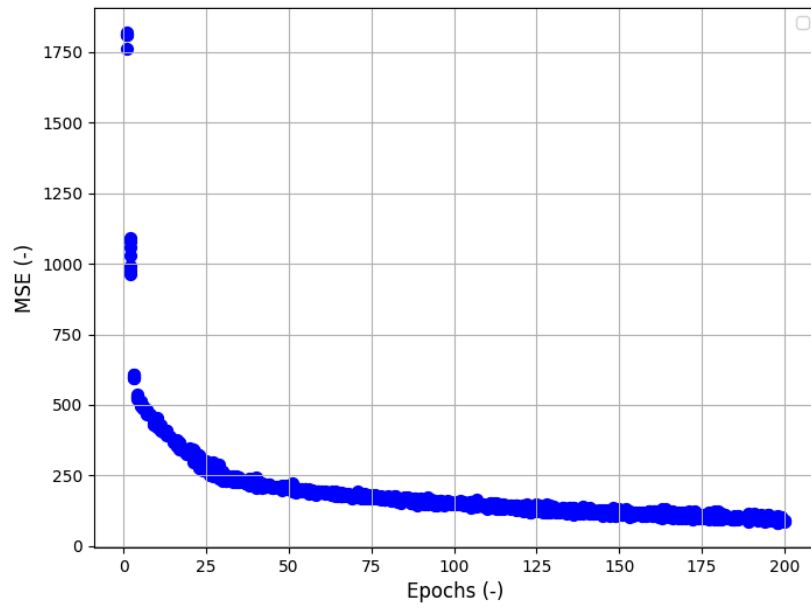


Figure S11. Number of epochs sensitivity test

Number of nodes test

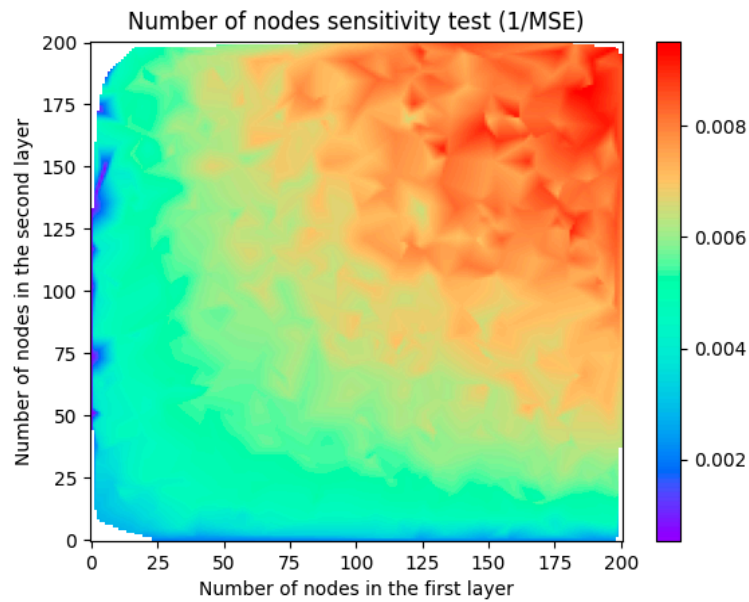


Figure S12. Number of nodes sensitivity test

2.3 Concrete compressive strength (CCS) dataset

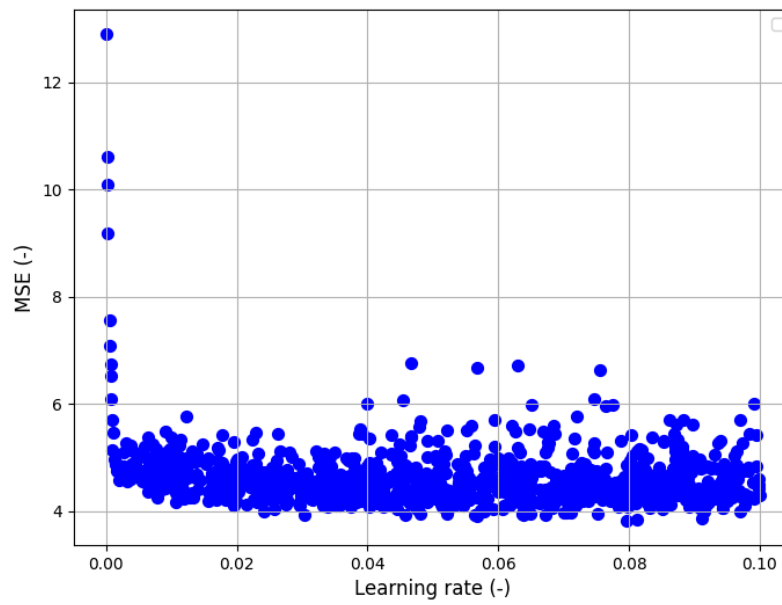


Figure S13. Learning rate sensitivity test

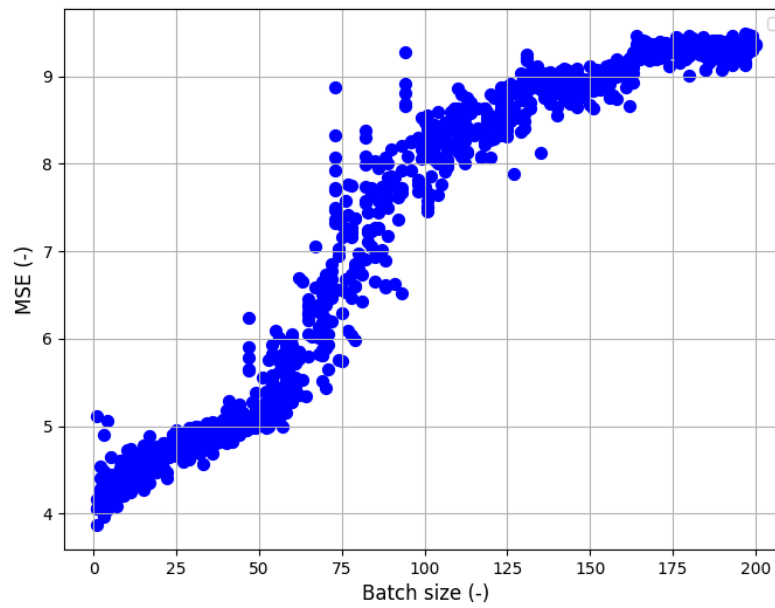


Figure S14. Batch size sensitivity test

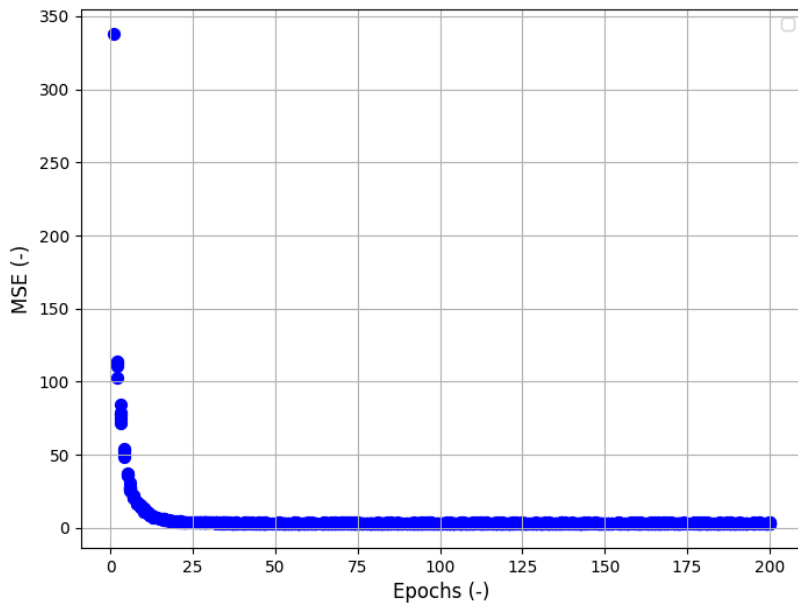


Figure S15. Epochs sensitivity test

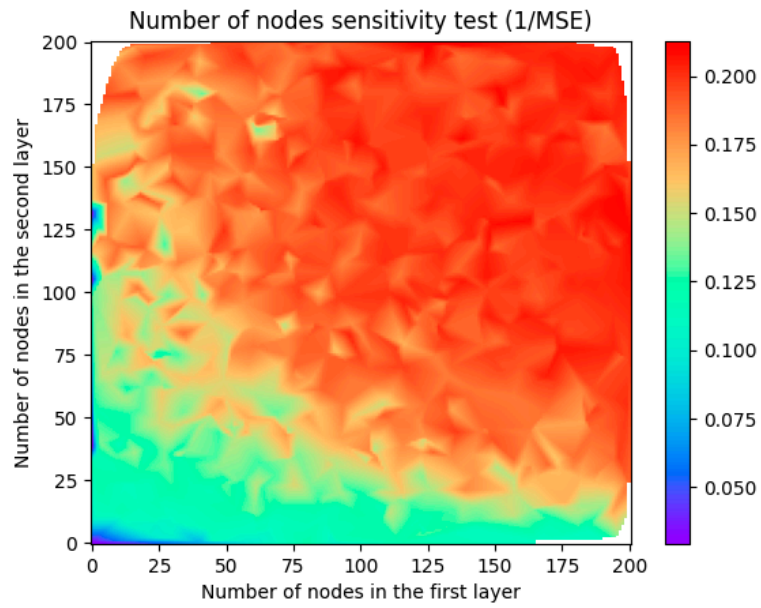


Figure S16. Number of nodes sensitivity test

2.4 Combined Cycle Power Plant (CCPP) dataset

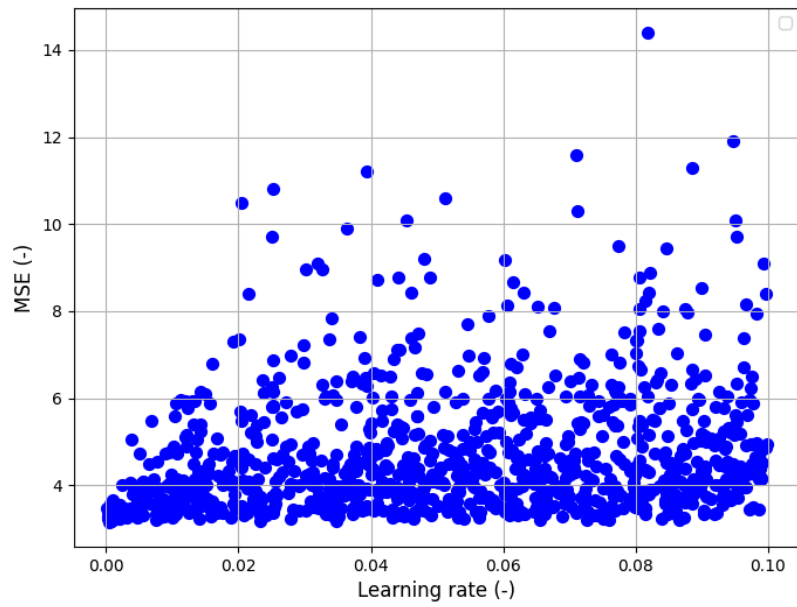


Figure S17. Learning rate sensitivity test

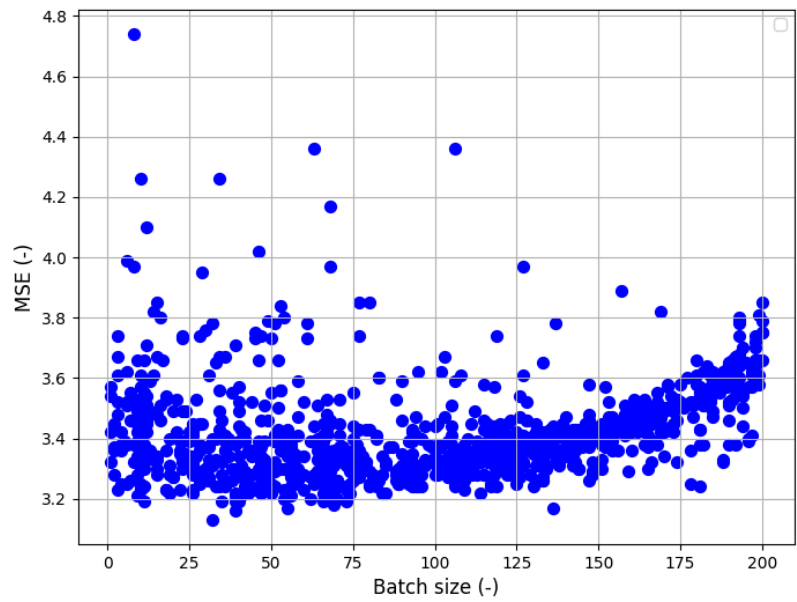


Figure S18. Batch size sensitivity test

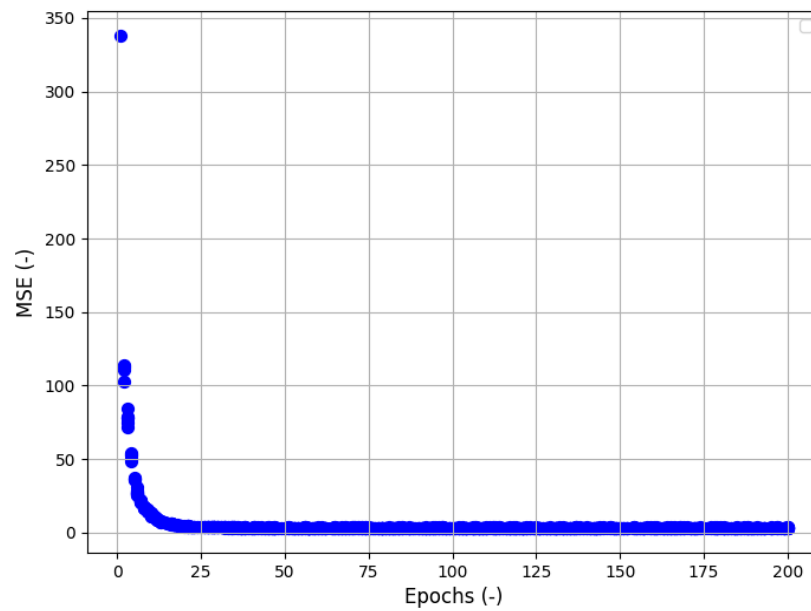


Figure S19. Epochs sensitivity test

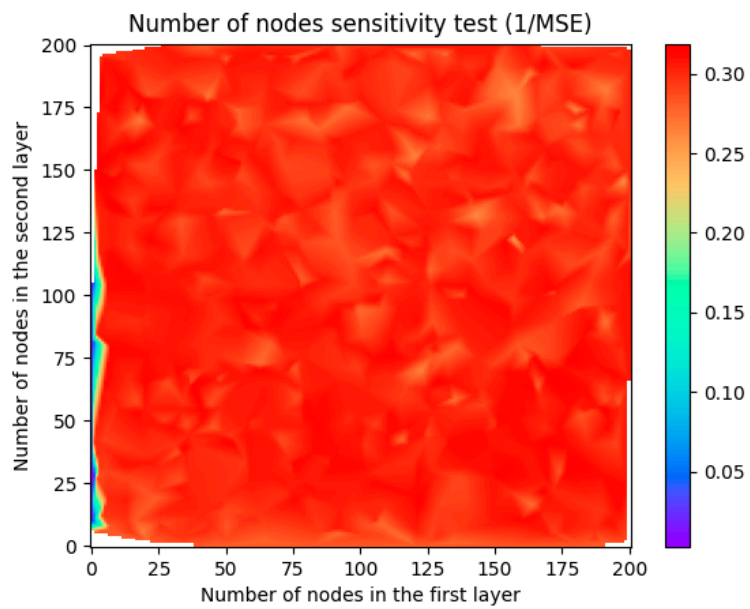


Figure S20. Number of nodes sensitivity test

2.5 Gas Turbine CO and NO_x Emission (NOX) dataset

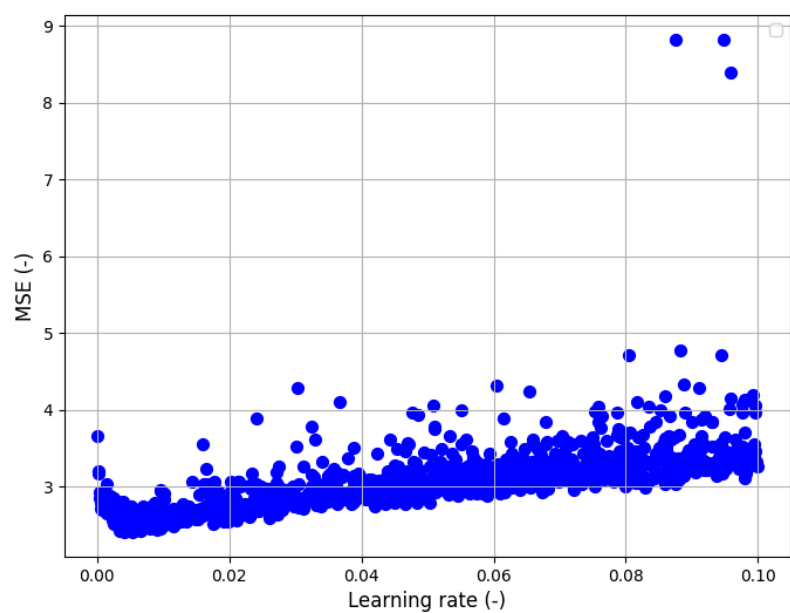


Figure S21. Learning rate sensitivity test

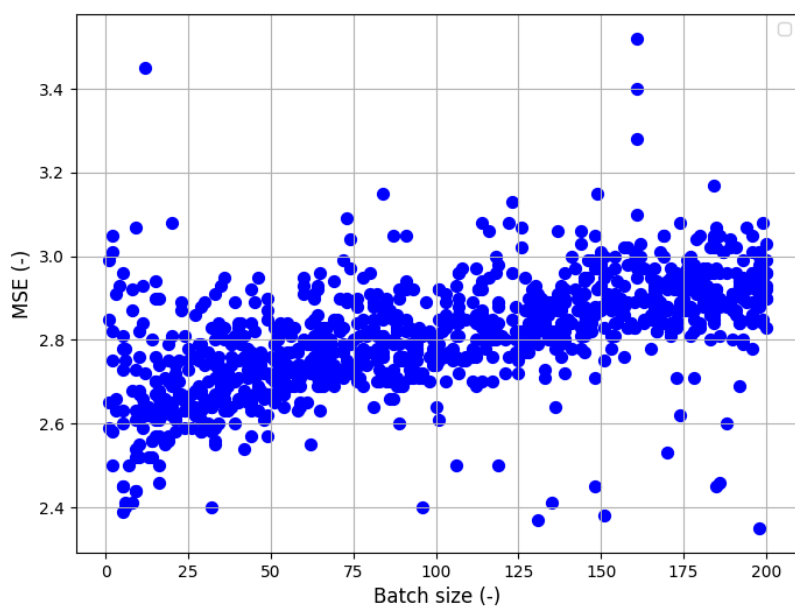


Figure S22. Batch size sensitivity test

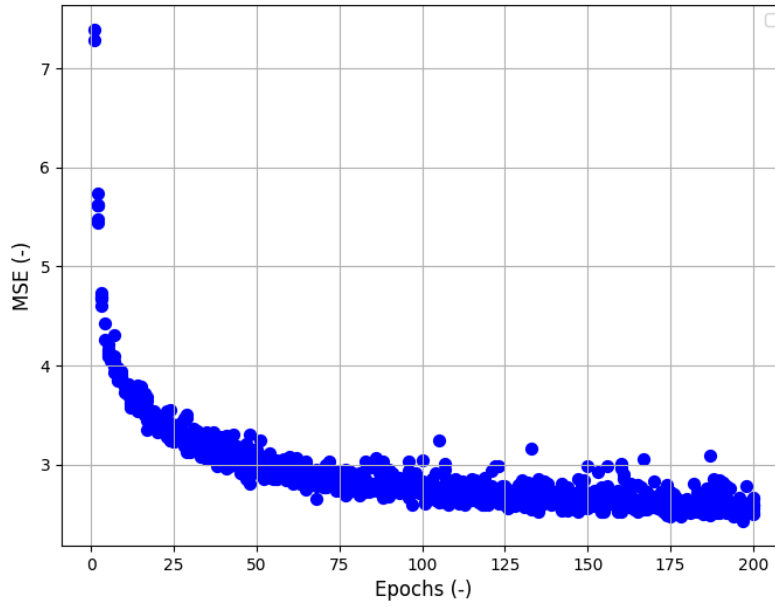


Figure S23. Epochs sensitivity test

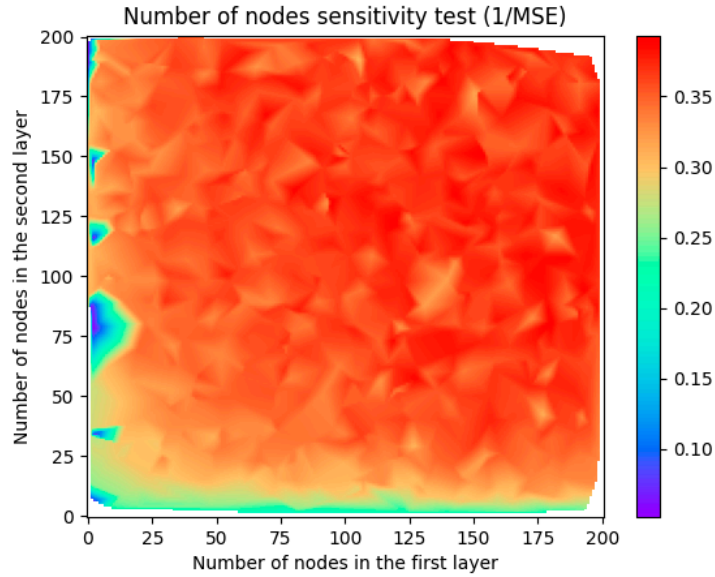


Figure S24. Number of nodes sensitivity test

In this investigation, the hyperparameters to be selected to optimize such as learning rate, number of epochs, batch size, and number of nodes in the hidden layers of the DNN model. The selected ranges of hyperparameters in Table S3 for all datasets are carefully evaluated based on this sensitivity test. The total number of sample is 1000 for all sensitivity tests.

Table S3. The selected ranges of hyperparameters for all public datasets

No	Quantity	BH	CHF	CCS	CCPP	NOX
1	Learning rate	1E-5 to 1E-2	5E-3 to 2E-2	1E-2 to 4E-2	2E-3 to 2E-2	5E-3 to 2E-2
2	Number of hidden layers	2	2	2	2	2
3	Number of nodes per layers	25 to 200	100 to 200	100 to 200	25 to 200	25 to 200
4	Epochs	50 to 200	50 to 200	25 to 200	50 to 200	100 to 200
5	Activator	ReLU	ReLU	ReLU	ReLU	ReLU
6	Optimizer	Adam	Adam	Adam	Adam	Adam
7	Batch size	1 to 50	1 to 50	1 to 25	100 to 150	25 to 50

References

- [1] Nguyen Huu Tiep, Kyung-Doo Kim, Jaeseok Heo, Chi-Woong Choi, and Hae-Yong Jeong. "A newly proposed data assimilation framework to enhance predictions for reflood tests." Nuclear Engineering and Design 390 (2022).
- [2] Nair Vinod, and Geoffrey E. Hinton. "Rectified linear units improve restricted boltzmann machines." Proceedings of the 27th international conference on machine learning (ICML-10). 2010.
- [3] Kingma Diederik P., and Jimmy Ba. "Adam: A method for stochastic optimization." International Conference on Learning Representations (ICLR). 2014.
- [4] Documentation, Keras. "Keras Documentation." <https://keras.io/api/> (2022). (Accessed on 30.10.2024)