Generating scattering data using Gaussian process regression†

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Recently, several studies[1,2] have employed machine learning algorithms to improve the accuracy of nuclear data evaluation and reduce the production cost. Herein, we introduce a framework which combines Gaussian process regression (GPR) with a nuclear reaction model code, *i.e.*, 'CCONE'.[3,4] The framework determines model parameters required by CCONE to reproduce and predict nuclear reaction data.

Figures 1 and 2 demonstrate how the proposed framework works. In this example, we used the experimental data of neutron elastic scattering on ^{54}Fe at incident energies of $E = 6$, 10, 15, and 17 MeV as input.[5] In the first step, by combining CCONE and Bayesian optimization with the Gaussian process (BO-GP), we optimize the depth of the real part of the optical potential, which is denoted by $v_R^0(E)$, to reproduce these data. The obtained optimal values of $v_R^0(E)$ at each energy is plotted by open circles in Fig. 1.

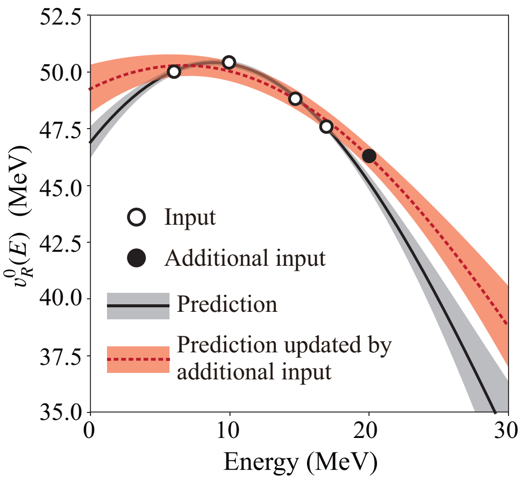

Fig. 1. Open circles show the optimal values of $v_R^0(E)$ at $E = 6$, 10, 15 and 17 MeV obtained by BO-GP. With these input, GPR predicts $v_R^0(E)$ as shown by solid line with shadowed area. With additional input at $E = 20$ MeV denoted by filled circle, GPR updates the prediction as shown by dotted line with shadowed area.

In the second step, using optimal values as inputs, $v_R^0(E)$ as a function of E is predicted by GPR, as denoted by the solid line with a shadowed area in Fig. 1.

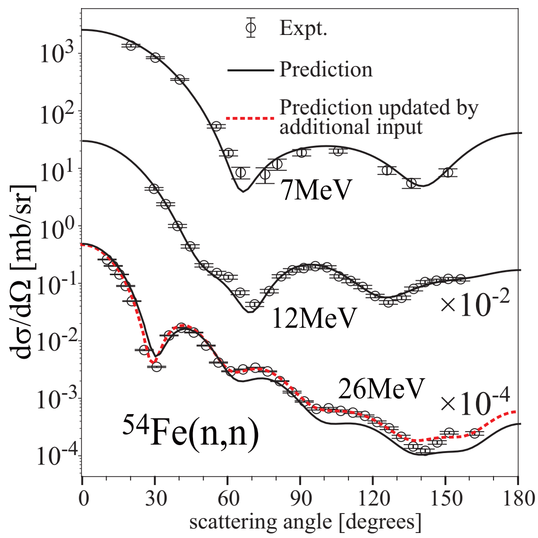

Fig. 2. Predicted and observed angular distributions of ^{54}Fe(n, n) at the incident energies of $E = 7$, 12, and 26 MeV.

Then, using CCONE and the predicted value of $v_R^0(E)$, our framework predicts unknown cross sections. Figure 2 shows the comparison of the prediction results for $E = 7$, 12, and 26 MeV with the actual experimental data. The framework works quite effectively to predict data at $E = 7$ and 12 MeV, which correspond to the interpolation of the known data. Even in the case of the extrapolation of the known data, *i.e.*, $E = 26$ MeV, it can perform a plausible prediction.

This framework can investigate how new experimental data improve prediction. Herein, we add a new data set at $E = 20$ MeV, and calculate the optimal $v_R^0(E)$ at this energy, as denoted by the filled circle in Fig. 1. With this additional input, GPR can enhance the prediction of $v_R^0(E)$, as denoted by the dashed line with a shadowed area. With this enhanced $v_R^0(E)$, the cross section at $E = 26$ MeV is calculated as plotted as a dotted line in Fig. 2, where we see considerable improvement in backward angles.

The development of this framework is in progress, and we expect that it will generate accurate nuclear reaction databases enhanced with a large amount of experimental data produced at RIBF.

References

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5) All experimental data are collected from EXFOR database.

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