Poster number:P4

The optical potential for neutron-nucleus scattering derived by Bayesian optimization

Content of talk

○Background: Nuclear data evaluation with machine learning
○Framework: Nuclear reaction model
Bayesian optimization
An example of optimization by machine learning
○Result: Prediction of cross section by machine learning(^{54}Fe)
○Summary & Future work

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Nuclear data evaluation and machine learning

○ Nuclear data plays an important role in various scientific fields.

○ In order to produce nuclear data for practical applications,
it is essential to handle the huge amount of experimental data.

- Evaluate the reliability and accuracy of experimental data, and make a selection.
- Interpolation and extrapolation of experimental data using theoretical models

○ Recent development in data science will bring about significant breakthrough in,
there is a possibility that nuclear data evaluation.

A E Lovell, A T Mohan and P Talou, J. Phys. G, Vol. 47, 114001 (2020)
H. Iwamoto, J. Nucl. Sci. Tech. 57, 932 (2020)

Goal: Generating nuclear reaction data by machine learning

By using Bayesian optimization, we determine the optical potential for nucleon-nucleus scattering and predict the cross section at energies where experimental data is not available.

Framework: Nuclear reaction model

〇Nuclear reaction model : Coupled Channel Optical Model

$$\left(\left[\frac{d^2}{dr^2}-\frac{l_c(l_c+1)}{r^2}+k_c{}^2\right]u_c(r)-\sum_{c'}V_{cc'}u_{c'}(r)\right)=0$$

u_c: Wave function of scattered wave (radial direction)

c : Reaction channel $(\{l_c, j_c, n_c\})$

$V_{cc'}$: Optical potential(Between c and c' channels)

$$V(r)=-V_R(E)f_R+i\left[4W_Da_D\frac{d}{dr}f_D(r)-W_Vf_V(r)\right]+[Coul]+[LS]$$

$$V_R(E)=(V_R^0+V_R^{DISP}e^{-\lambda_RE})\cdots \qquad W_D=\left[W_D^{DISP}+(-1)^{Z'+1}C_{wiso}\frac{N-Z}{A}\right]e^{-\lambda_DE}\cdots$$

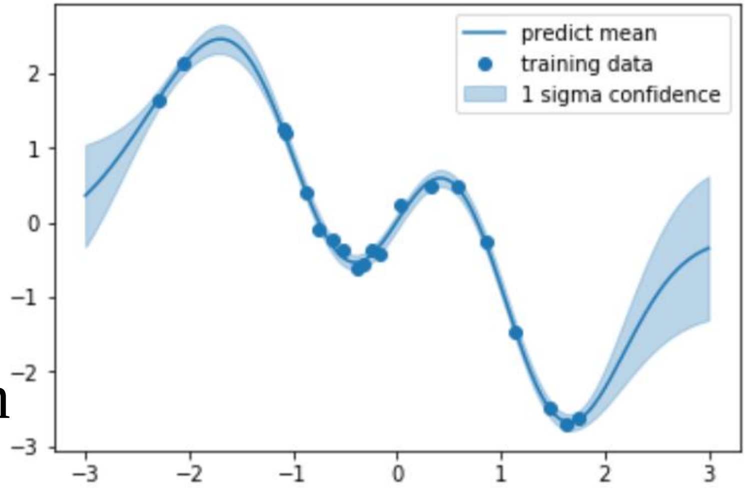
$$f_R(r)=\frac{1}{1+exp(\frac{r-R_R}{a_R})} \qquad R_R=r_RA^{1/3}$$

We solve coupled channel equations using CCONE
O. Iwamoto et al., Nucl. Data. Sheets 131, 259 (2016)

Framework : Bayesian optimization

○ Bayesian optimization with Gaussian process regression

– A model that estimates a function $y = f(x)$ from inputs x and output y variables, and find the minimum value of the objective function



○Objective function describes the deviation between experimental data and theoretical calculation.

$$f(x) = \sum_{cross\ \ section} \left\{ \frac{1}{N} \sum_{N} \left(\frac{\sigma_{exp}^{(i)}}{\Delta\sigma_{exp}^{(i)}} \log_{10} \frac{\sigma_{th}^{(i)}(x)}{\sigma_{exp}^{(i)}} \right)^2 \right\}$$

○ Determine the potential parameters x to minimize the Objective function y .

x :Parameter of optical potential
y :Evaluation function

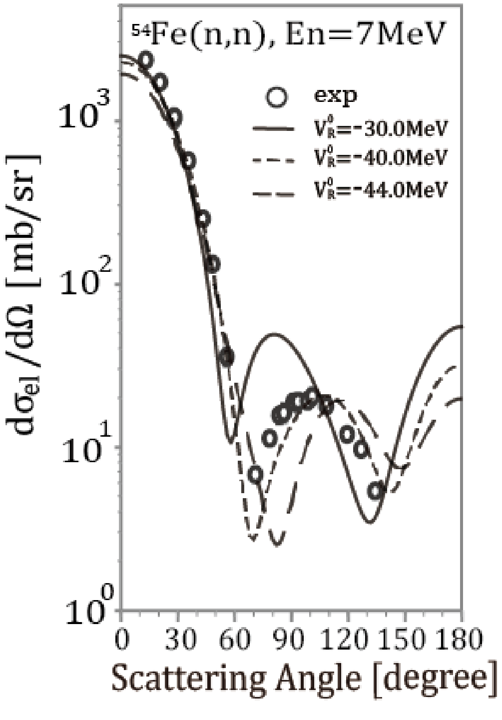
We use GPyOpt as Library of Gaussian process regression

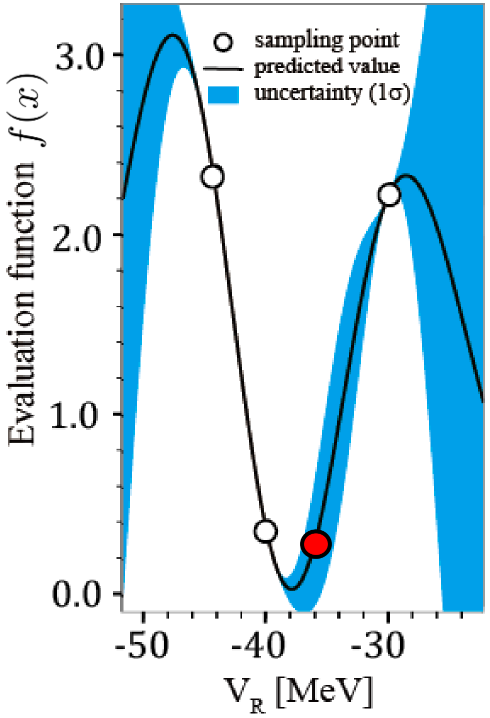
https://sheffieldml.github.io/GPyOpt/

Framework : An Example of optimization by machine learning

Estimate the evaluation function about optical parameter V_R^0 by Gaussian process regression from the sampling results.
Calculate the evaluation function for V_R^0, where the large uncertainty and the small predicted value.

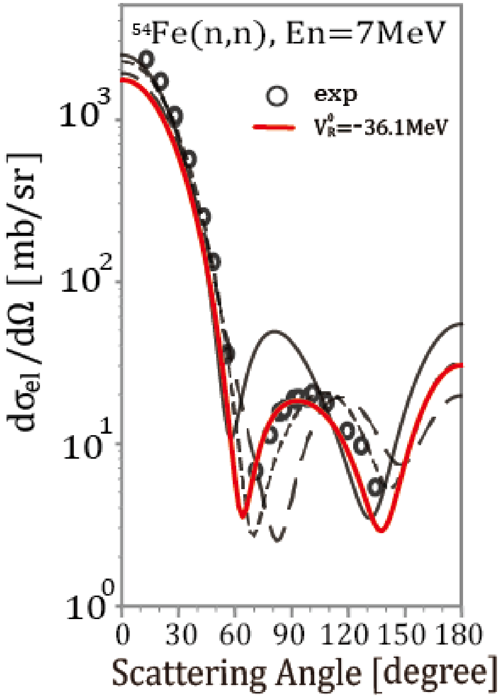
$$f(x) = \sum_{cross\ \ section} \left\{ \frac{1}{N} \sum_{N} \left(\frac{\sigma_{exp}^{(i)}}{\Delta\sigma_{exp}^{(i)}} \log_{10} \frac{\sigma_{th}^{(i)}(x)}{\sigma_{exp}^{(i)}} \right)^2 \right\}$$

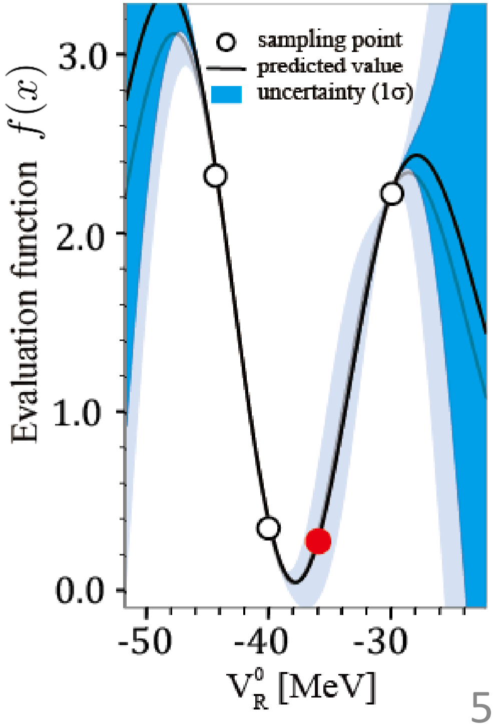




Sampling red point

Update Prediction





Result: Prediction of cross section by machine learning(^{54}Fe)

7 and 12 MeV data are used for fitting, and based on it, 8.5 and 24 MeV data are predicted.

This procedure enables an accurate generation of nuclear reaction data.

$$V_R(E) = (V_R^0 + V_R^{DISP} e^{-\lambda_R E}) \cdots$$

$$W_D = \left[W_D^{DISP} + (-1)^{Z'+1} C_{wiso} \frac{N-Z}{A} \right] e^{-\lambda_D E} \cdots$$

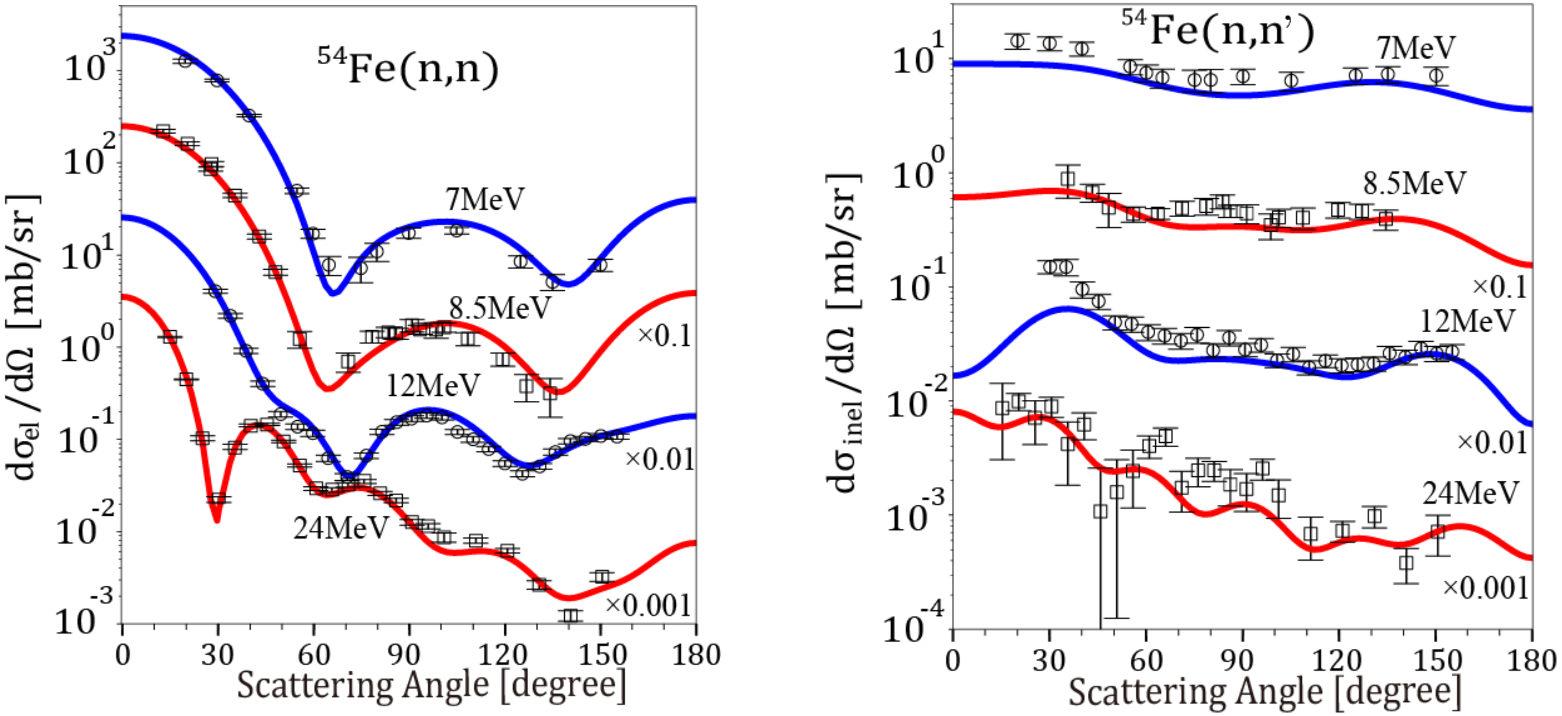
$$f_R(r) = \frac{1}{1 + exp(\frac{r - R_R}{a_R})} \qquad R_R = r_R A^{1/3}$$

Fitting Results

Experimental data used for training

Predicted cross section

Corresponding experimental data



Summary & Future work

Summary

- Reproduce experimental data by fitting the optical potential using Bayesian optimization.

- Cross sections estimated from a small number of sample data reproduce the test data well.

Future work

- We aim to predict the energy dependence of the parameters without assuming a function.