Application of Gaussian Process Regression for Total Kinetic Energy in Neutron-Induced Fission

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Introduction

Total Kinetic Energy (TKE) is one of the key observables in fission. It is challenging to obtain both theoretical and experimental data. Theoretical calculations require significant computational resources and time, while experimental data are available only for a limited number of incident energies. Machine learning offers a potential alternative by enabling the prediction of TKE curves for a given isotope and incident energy. This work investigates the use of Gaussian Process Regression (GPR) for TKE prediction. The model is trained on data generated by the General Description of Fission Observables (GEF), a semi-empirical computational tool for fission simulation.

Background

Total Kinetic Energy (TKE)

- TKE is the sum of the kinetic energies of the two fission fragments immediately after scission.
- It is dominated by the Coulomb repulsion, which depends on the effective distance between the fragments.
- A smaller correction arises from the pre-scission kinetic energy of the fragments.

Gaussian Process Regression (GPR)

- GPR is a non-parametric Bayesian regression method.
- It uses kernel functions to capture data structure and make predictions.
- A GP defines a probability distribution over functions and provides uncertainty estimates along with its predictions.

Methodology

Model Development

- TKE data are generated with the GEF code.
- The data are extracted, transformed into input features and scaled.
- The available isotope–incident energy cases are split into training (80%) and test (20%) subsets.
- Kernel selection and hyperparameter optimization result in a Matern + RBF kernel as the best-performing configuration.
- Model generalization is evaluated on an independent validation dataset, including comparisons between ^{240}Pu predictions and experimental data.

Feature Importance

- SHAP values are used to quantify the contribution of each feature to the model predictions, based on the Shapley values from cooperative game theory.

Training isotopes	^{229}Th, ^{230}Pa, ^{234}U, ^{236}U, ^{237}Np, ^{239}Pu, ^{243}Am, ^{248}Cm, ^{251}Cf, ^{255}Fm
Validation isotopes	^{235}U, ^{240}Pu
Incident energies	0.025 eV, 5 MeV, 10 MeV, 15 MeV, 20 MeV
Training points	4500
Kernel combination	Matern + RBF

Results

Results are shown for the training isotope ^{236}U and validation isotopes ^{235}U, ^{240}Pu at different incident energies. A WhiteKernel (WK) variant is included to improve numerical stability and uncertainty estimation.

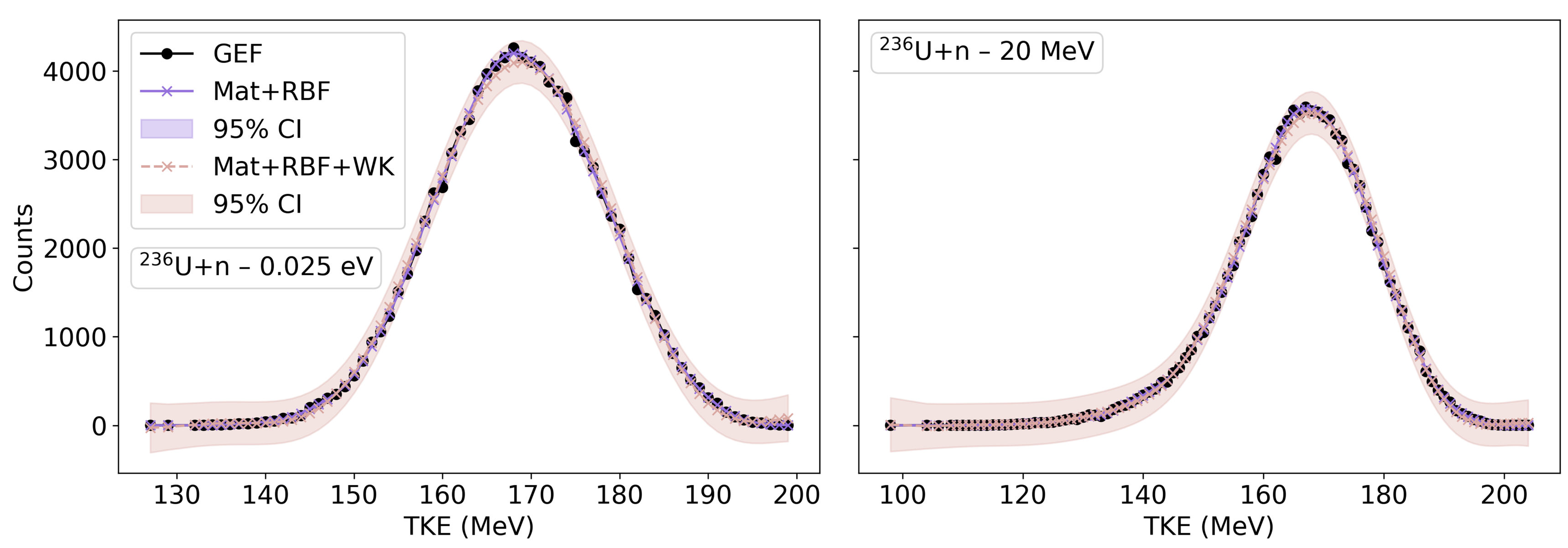

Figure 1: TKE distributions for training target nucleus ^{236}U

- The model reproduces the overall TKE shape, indicating good generalization.
- The absence of fine-scale fluctuation fitting suggests no signs of overfitting.
- The WK introduces non-zero uncertainty bands and slightly modifies the mean predictions near the peaks.

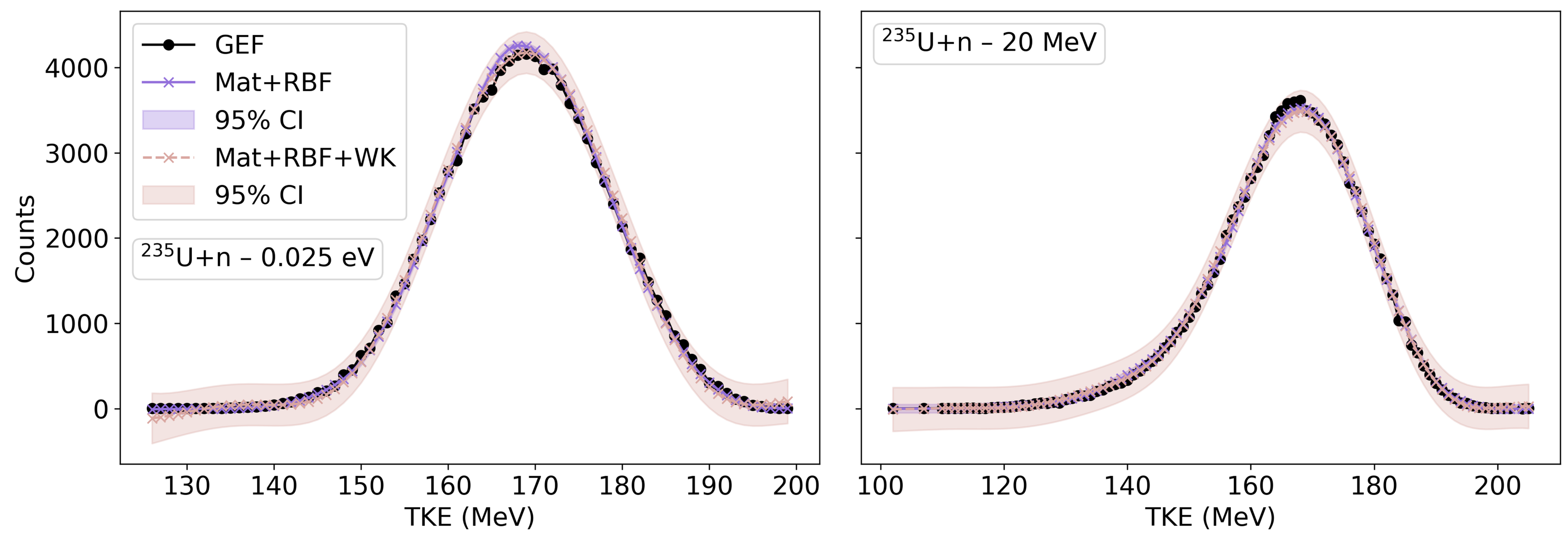

Figure 2: TKE distributions for validation target nucleus ^{235}U

- The model captures the overall TKE shape with minor deviations from the reference data.
- The baseline model shows overly narrow confidence intervals, indicating overconfidence.
- The WK improves uncertainty calibration while preserving the mean predictions.

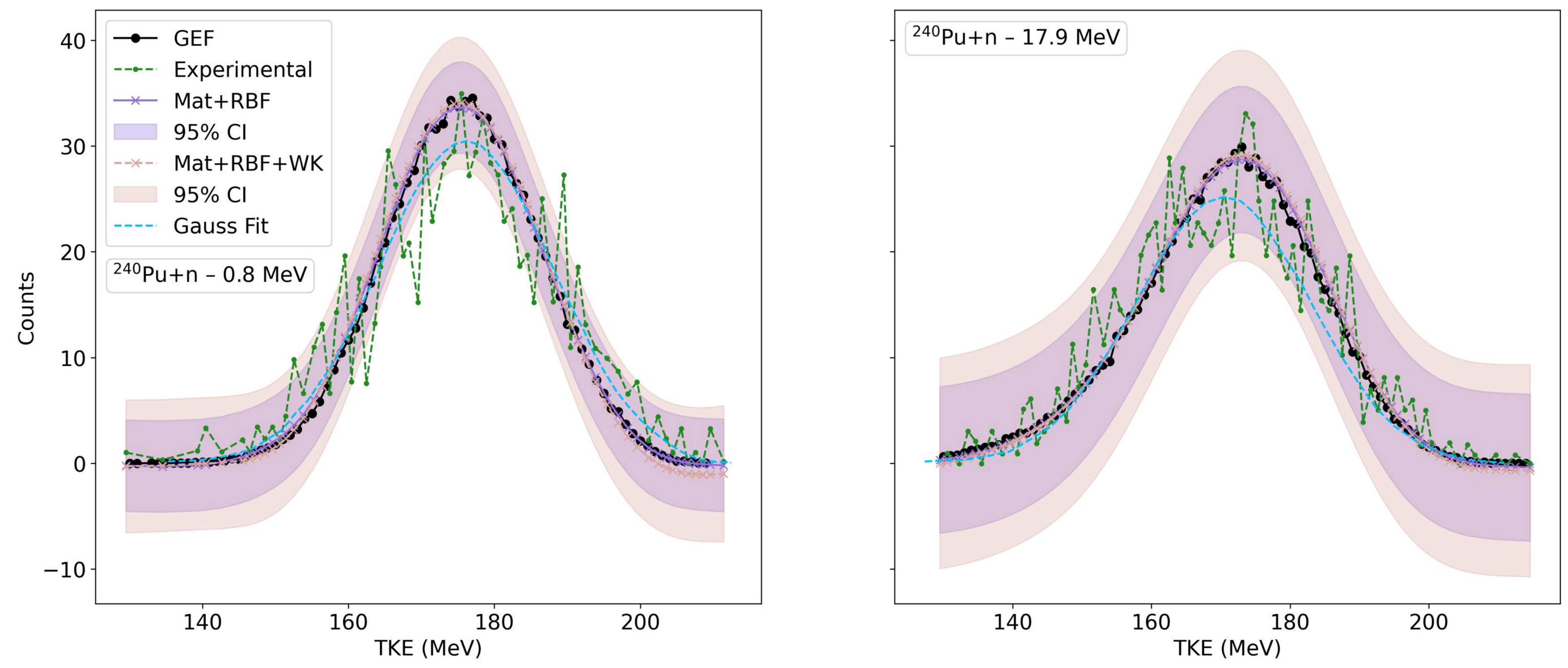

Figure 3: Comparison of GPR, GEF and experimental data for target nucleus ^{240}Pu

- Model predictions and GEF data are scaled to match the experimental counts for comparison.
- Predictions follow the overall trend of both GEF and experimental data.
- Experimental fluctuations are larger due to energy binning (0.55–1.01 MeV and 11.68–24.21 MeV) and measurement uncertainties.

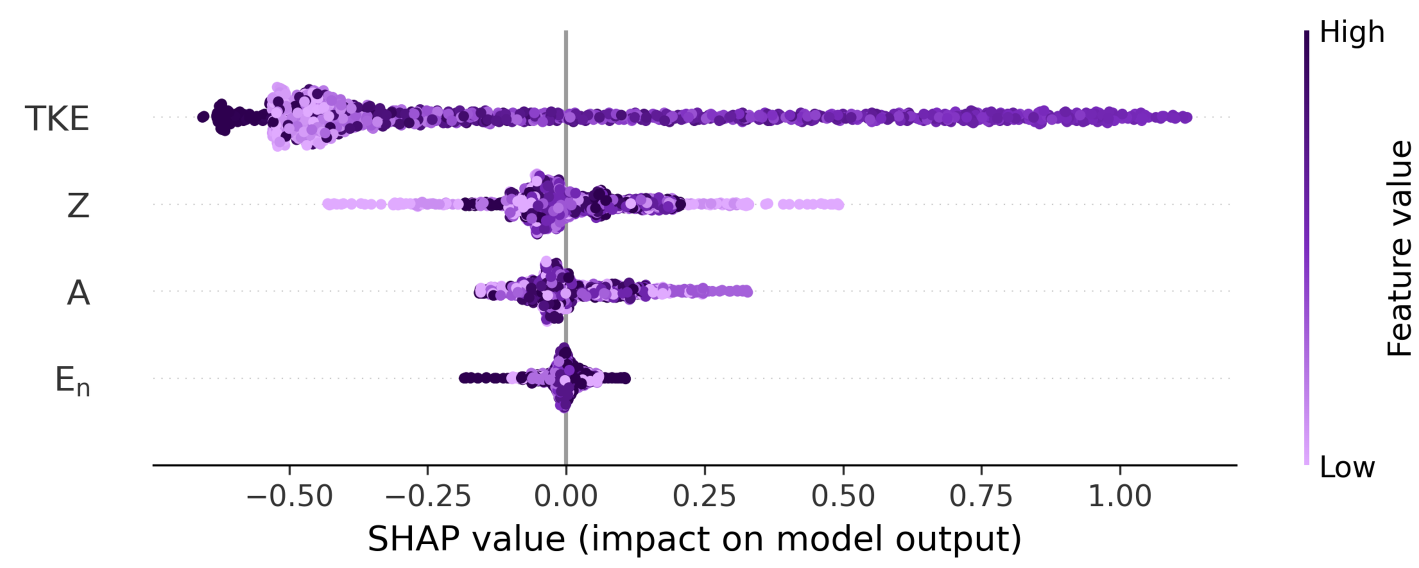

Figure 4: Feature importance for the Matern + RBF GPR model

- SHAP values are consistent across models with and without WK, so only the Matern + RBF model is shown.
- TKE is the dominant feature influencing the predicted counts.
- Z and A exhibit moderate influence.
- E_n has a weak contribution to the predictions.

Conclusion

- Gaussian Process Regression successfully reproduces the overall shape of the TKE curves and generalizes well to unseen isotopes and incident energies.
- The addition of the WhiteKernel increases the confidence interval and reduces the overconfidence of the model, while the predicted means remain largely unchanged.
- Comparisons with experimental data for isotope ^{240}Pu show that the model captures the main trends of the measured distributions.

References

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