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# Using Machine Learning Methods to Predict Bias in Nuclear Criticality Safety Simulations

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## 1. Introduction

For many real-world applications in radiation transport where simulations are compared to experimental measurements, like in nuclear criticality safety, the bias (simulated - experimental  $k_{eff}$ ) in the calculation is an extremely important metric used for code validation. The objective of this project is to accurately predict the bias of MCNP6 [1] criticality calculations using machine learning (ML) algorithms, with the intention of creating a tool that can complement those currently in use in the nuclear criticality safety community. In the latest release of MCNP6, the Whisper tool [2] is available for criticality safety analysts and includes a large catalogue of experimental benchmarks, sensitivity profiles, and nuclear data covariance matrices. This data, coming from 1100+ benchmark cases, is used in this study of ML algorithms for criticality safety bias predictions.

The standard method of evaluating a ML model is by cross validation [3], which works by splitting up the data set into a certain number of subsets (called folds), and evaluating the model on one fold while training on the others. This is done for every possible combination until every fold has been evaluated, with the other folds acting as training data. The mean squared error (MSE) and root mean squared error (RMSE) from each round is averaged to calculate a more representative value of model prediction performance.

## 2. Methods

The sensitivity vectors generated by MCNP6, which describe how  $k_{eff}$  is impacted by the nuclear data of a given application, are chosen as the features, due to the assumption that they inherently carry enough information to characterize a system. The sensitivity vector for each isotope-reaction is broken into 44 energy bins and there are 2040 individual isotope-reaction pairs, so each test case has 89,760 sensitivity features associated with it. The models were also evaluated on a modified set of sensitivity vectors, where the sensitivity values for each isotope-reaction pair are summed over all energies. Along with the sensitivity vectors, the models were also trained on  $k_{sim}$ , which is generated along with the sensitivity vectors in MCNP6. Decision tree machine learning algorithms from Scikit-Learn [3] were used in this study, primarily due to their superb accuracy and simplicity.

## 3. Results

The three best performing regression models used in the present work are Adaboost, Random Forest, and Extra Trees [3], and the performance statistics from cross validation can be found summarized in Table I. The mean standard deviation of experimental  $k_{eff}$  measurements for the benchmarks used in this study is 0.00328, and the mean absolute error is below that for all of the models. Which means that on average the error on the predicted bias is less than the uncertainty of the experimental  $k_{eff}$  measurements.

Model	Mean Absolute Error	Root Mean Squared Error
Adaboost (L)	0.00083	0.00161
Random Forest (L)	0.00210	0.00355
Extra Trees (L)	0.00279	0.00340
Adaboost (S)	0.00077	0.00146
Random Forest (S)	0.00212	0.00296
Extra Trees (S)	0.00256	0.00346

Table I: Statistics for decision tree models from 10 fold cross validation. (S = 2,065, and L = 90,817 features)

A very useful feature of decision trees is that they can calculate the importance of each feature to the estimated value. The importance can be thought of as the influence of each isotope-reaction on whether bias is present. Since the features are broken into 44 energy groups, the importance of each isotope-reaction pair can be analyzed at the energy level, and this provides insight into what cross sections or physics models should be improved in MCNP6 to reduce bias. The top five most important reactions separated by energy group can be found in Table II.

Thermal (0 - 0.625 ev)	Intermediate (1.0 ev - 0.1 Mev)	Fast (0.4 Mev - 20 Mev)
6000.80c n,gamma, 0.014562	92233.80c n,gamma, 0.018457	92233.80c fission, 0.015264
92233.80c total nu, 0.011437	92233.80c fission, 0.015724	92233.80c inelastic, 0.013543
92233.80c n,gamma, 0.010641	92233.80c total nu, 0.012844	92233.80c n,gamma, 0.012739
92234.80c n,gamma, 0.009479	92234.80c n,gamma, 0.011945	92233.80c total nu, 0.012644
1001.80c n,gamma, 0.009069	94239.80c n,gamma, 0.011687	9019.80c inelastic, 0.010355

Table II: Top five relative importances of each isotope-reaction by energy group to the Random Forest regressor on calculating bias. These importances make physical sense: capture at low energies, capture and fission for actinides at intermediate energies, inelastic scattering and fission at high energies.

#### 4. Conclusions

Decision tree algorithms have been observed to be very accurate in predicting bias using the sensitivity vectors and  $k_{sim}$  as features. Additionally, the feature importances are able to illuminate the isotopes and reactions that are leading to a divergence between MCNP6 and experimental  $k_{eff}$  values. Research is currently underway to apply the predictions of these models with other interesting applications within nuclear criticality safety.

#### Acknowledgements

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#### References

- [1] J.T. Goorley, *et al.*, "Initial MCNP6 Release Overview," *Nuclear Technology*, **180**, 298 (2012).

- [2] B.C. Kiedrowski, F.B. Brown, *et al.*, “Whisper: Sensitivity/Uncertainty-Based Computational Methods and Software for Determining Upper Subcritical Limits,” *Nucl. Sci. Eng.*, **181**, 14 - 47 (2015).
- [3] Pedregosa, Fabian and Varoquaux, *et al.*, “Scikit-learn: Machine learning in Python,” *Journal of Machine Learning Research*, **12**, 2825–2830, (2011).