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<th>Using Machine Learning Methods to Predict Bias in Criticality Safety Simulations</th>
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Using Machine Learning Methods to Predict Bias in Criticality Safety Simulations

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Introduction

• Objectives
• Motivations
• Nuclear Background
• Machine Learning Background
• Methodology
• Results
• Conclusion
• Future work
Objectives

1. Accurately predict the bias of MCNP6 criticality calculations using machine learning algorithms
   • Using ensembles of decision trees
2. Identify which isotope reactions lead to bias
   • Using feature importances from decision trees
3. Determine if $k_{eff}$ sensitivity profiles from MCNP6 are good features for machine learning
Motivations

- Bias \((k_{sim} - k_{exp})\) is extremely important for criticality safety
  - Used for calculating upper subcritical limits
- Knowing what isotope reactions are leading to bias informs what physics models or data can be improved
- ML algorithms are great for problems where traditional approaches provide no solution
  - Can model extremely complicated relationships, and provide insights about large data sets
Background - Computational Bias

Upper Subcritical Limit (USL)

- A calculated $K_{\text{eff}} < 1.0$ is not sufficient to ensure subcriticality
- Must account for bias uncertainties in the calculational method

Image obtained from LANL Whisper presentation.
Background - Whisper

• Statistical analysis code used to determine USL
  • Uses sensitivity profiles from continuous energy MCNP6
  • Uses covariance data for nuclear cross sections
  • Finds applications that are neutronically similar to application of interest

• Features:
  • Calculates bias and bias uncertainty using extreme value theory
  • Calculates margin for nuclear data uncertainty using generalized linear least squares method

• Contains:
  • 1,100 benchmarks with experimental and simulated $k_{\text{eff}}$
  • Metal, composite, and solution experiments containing Pu and U
Background - Sensitivity Profiles

- How sensitive is $k_{\text{eff}}$ to uncertainty in some parameter?
- Defined as the ratio of relative change in a response to a relative change in a system parameter:

$$S_{k,x} = \frac{\Delta k / k}{\Delta x / x}$$
Background - Sensitivity Profiles

- Magnitude is proportional to its impact of the system’s effective multiplication
- The sign of the sensitivity coefficient gives the direction that k would change
- The sensitivity coefficient has the property of being additive
Machine Learning is the field of study that gives computers the ability to learn from data without being explicitly programmed.
Machine Learning Tasks

**Regression**
- Predict a target numeric variable

**Classification**
- Identifying group membership

Image obtained from Wikipedia's Linear Regression page

Image obtained from https://sebastianraschka.com/faq/docs/evaluate-a-model.html
Decision Trees

• A tree like model of decisions based on features
• All features are considered to split the data
• Splits are chosen that minimize a cost function (MSE)
• More important features are found near the top

Image obtained from https://algobeans.com/2016/07/27/decision-trees-tutorial
Ensembles of Decision Trees

- **Random Forest**
  - Each tree is trained on a random subset of the training instances
  - Using a random subset of features from the total feature set

- **Adaboost**
  - Iterative process where new predictors pays more attention to the cases that the previous predictors made errors on
  - Pays more attention to the difficult cases
Methods - Features and Targets

- Sensitivity Profiles
  - Inherently carry enough information to characterize a system
  - Can be used to find patterns that influence bias

- $k_{sim}$
  - Generated with the sensitivity vectors from MCNP6
  - Strong linear relationship between bias and $k_{sim}$

- Predicting:
  - Bias ($k_{sim} - k_{exp}$)
  - $k_{exp}$
Methods - Training and Validating

Model Evaluation

- Ten fold cross-validation

Model Complexity

- Minimize model error

![Diagram showing ten fold cross-validation](https://sebastianraschka.com/faq/docs/evaluate-a-model.html)

![Diagram showing model complexity and error trade-off](https://stats.stackexchange.com/questions/69549/)

Image obtained from https://sebastianraschka.com/faq/docs/evaluate-a-model.html

Image obtained at https://stats.stackexchange.com/questions/69549/
Results - Sensitivity Vectors as Features

- Are sensitivity profiles sufficient to characterize the problem?
- Beginning to model the relationship
- \( \text{MSE} = 2.723\times10^{-5}, \text{RMSE} = 0.00521, \text{MAE} = 0.00374 \)
Results - Adaboost Predicting Bias

- Accurate for cases with high number of benchmarks
- Higher errors for Pu - composite, HEU composite, and MOX solutions.
- MSE = 9.106E-6, RMSE = 0.00301, MAE = .00177
Results - Random Forest Predicting Bias

- Slightly less accurate than Adaboost
- Higher errors for same cases
- \( \text{MSE} = 1.498 \times 10^{-5}, \text{RMSE} = 0.00387, \text{MAE} = 0.00248 \)
Results - Adaboost Predicting $k_{meas}$

- Increased accuracy - same units as bias
- Different error profile
- MSE = 1.668E-6, RMSE = 0.00129, MAE = .00062
Results - Performance Statistics

- Models that predict $k_{meas}$ perform much better
- Average experimental uncertainty for $k_{meas}$ is 0.003

<table>
<thead>
<tr>
<th>Model</th>
<th>Mean Absolute Error</th>
<th>Root Mean Squared Error</th>
</tr>
</thead>
<tbody>
<tr>
<td>Adaboost (Bias)</td>
<td>0.00142</td>
<td>0.00261</td>
</tr>
<tr>
<td>Random Forest (Bias)</td>
<td>0.00216</td>
<td>0.00348</td>
</tr>
<tr>
<td>Neural Network (Bias)</td>
<td>0.00492</td>
<td>0.00725</td>
</tr>
<tr>
<td>Adaboost ($k_{meas}$)</td>
<td>0.00062</td>
<td>0.00129</td>
</tr>
<tr>
<td>Random Forest ($k_{meas}$)</td>
<td>0.00079</td>
<td>0.00136</td>
</tr>
<tr>
<td>Whisper (Bias)</td>
<td>0.00906</td>
<td>0.01329</td>
</tr>
<tr>
<td>GLLSM ($k_{meas}$)</td>
<td>0.00645</td>
<td>0.00959</td>
</tr>
</tbody>
</table>

Table 1: Statistics for the machine learning models from 10 fold cross validation, GLLSM, and Whisper. The top ML models are predicting bias, and the middle are predicting $k_{meas}$. 
Results - Feature Importances

- Obtained from random forest regressor
- Mostly actinides and other elements common in dataset
- Some unexpected elements like U-234

<table>
<thead>
<tr>
<th>Isotope Reaction</th>
<th>Relative Importance</th>
</tr>
</thead>
<tbody>
<tr>
<td>92233.80c n,gamma</td>
<td>0.046818</td>
</tr>
<tr>
<td>92232.80c total nu</td>
<td>0.045100</td>
</tr>
<tr>
<td>92232.80c fission</td>
<td>0.039334</td>
</tr>
<tr>
<td>92234.80c n,gamma</td>
<td>0.035280</td>
</tr>
<tr>
<td>6000.80c n,gamma</td>
<td>0.032351</td>
</tr>
<tr>
<td>92234.80c fission</td>
<td>0.031656</td>
</tr>
<tr>
<td>92234.80c total nu</td>
<td>0.030931</td>
</tr>
<tr>
<td>92232.80c n,gamma</td>
<td>0.027735</td>
</tr>
<tr>
<td>6000.80c n,alpha</td>
<td>0.025528</td>
</tr>
<tr>
<td>6000.80c inelastic</td>
<td>0.024418</td>
</tr>
</tbody>
</table>
Results - Feature Importances

• Break down importance by energy
• Again U 234 has three reactions in top 10

<table>
<thead>
<tr>
<th>Thermal (0 - 0.625 ev)</th>
<th>Intermediate (1.0 ev - 0.1 Mev)</th>
<th>Fast (0.4 Mev - 20 Mev)</th>
</tr>
</thead>
<tbody>
<tr>
<td>6000.80c n, gamma, 0.014562</td>
<td>92233.80c n, gamma, 0.018457</td>
<td>92233.80c fission, 0.015264</td>
</tr>
<tr>
<td>92233.80c total nu, 0.011437</td>
<td>92233.80c fission, 0.015724</td>
<td>92233.80c inelastic, 0.013543</td>
</tr>
<tr>
<td>92233.80c n, gamma, 0.010641</td>
<td>92233.80c total nu, 0.012844</td>
<td>92233.80c n, gamma, 0.012739</td>
</tr>
<tr>
<td>92234.80c n, gamma, 0.009479</td>
<td>92234.80c n, gamma, 0.011945</td>
<td>92233.80c total nu, 0.012644</td>
</tr>
<tr>
<td>1001.80c n, gamma, 0.009069</td>
<td>94239.80c n, gamma, 0.011687</td>
<td>9019.80c inelastic, 0.010355</td>
</tr>
<tr>
<td>poly.20t inelastic, 0.008879</td>
<td>6000.80c n, gamma, 0.008924</td>
<td>6000.80c elastic, 0.009997</td>
</tr>
<tr>
<td>be.20t elastic, 0.008204</td>
<td></td>
<td></td>
</tr>
<tr>
<td>94239.80c n, gamma, 0.007522</td>
<td>94239.80c total nu, 0.008325</td>
<td>92233.80c fission chi, 0.008758</td>
</tr>
<tr>
<td>94239.80c fission, 0.007427</td>
<td>94239.80c fission, 0.008208</td>
<td>92234.80c total nu, 0.008494</td>
</tr>
<tr>
<td>9019.80c n, gamma, 0.007201</td>
<td>6000.80c elastic, 0.007817</td>
<td>92234.80c fission, 0.008008</td>
</tr>
<tr>
<td></td>
<td>92232.80c total nu, 0.006668</td>
<td>1001.80c elastic, 0.007938</td>
</tr>
</tbody>
</table>
Results - Feature Importances

- U-234 n-gamma reaction
- Leu-comp-therm-079-010
- U-234 makes up 0.0074% of rod
- $k_{\text{eff}}$ n-gamma sensitivity is 12.58% of the average
- Pattern of low concentration and high sensitivity importance seen in other cases as well
Conclusion

- Sensitivity vectors are excellent features for ML algorithms
- ML algorithms estimate bias very accurately for criticality simulations
- Feature importances imply what iso-rxns are important to predicting bias
- These methods should be explored for applications
Future Work

- Incorporating conservatism into models (NCS angle)
- Applying these methods to reactors
- Investigate high importance reactions
- Continued optimization of models and incorporating neural networks
Acknowledgements

- This work was supported by the DOE Nuclear Criticality Safety Program, funded and managed by the National Nuclear Security Administration for the Department of Energy, and performed at Los Alamos National Laboratory.

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Thank you!
Questions?