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Title: Using Machine Learning Methods to Predict Bias in Criticality Safety Simulations

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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

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Background - Computational Bias

Upper Subcritical Limit (USL)

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

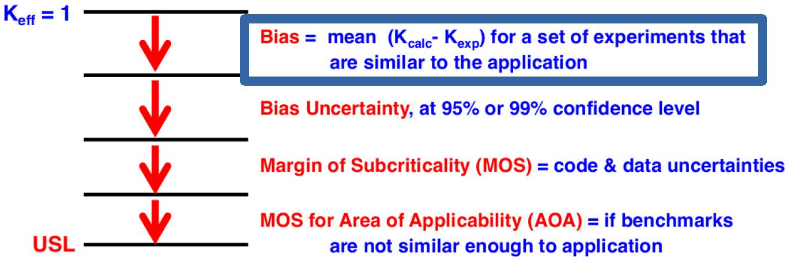


Image obtained from LANL Whisper presentation.

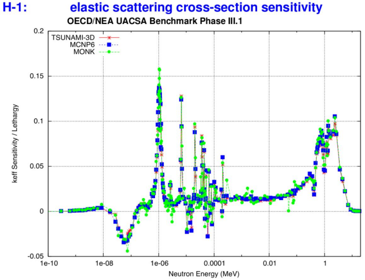
Background - Whisper

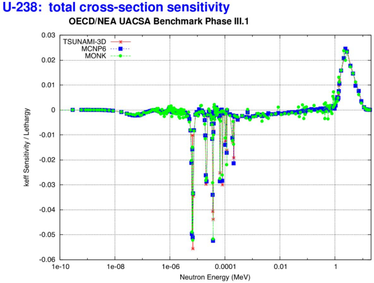
- Statistical analysis code used to determine USL
  - Uses **sensitivity profiles** from continuous energy MCNP6
  - Uses covariance data for nuclear cross sections
  - Finds applications that are neutronically similar to application of interest
- Features:
  - Calculates bias and bias uncertainty using extreme value theory
  - Calculates margin for nuclear data uncertainty using generalized linear least squares method
- Contains:
  - 1,100 benchmarks with experimental and simulated k_{eff}
  - Metal, composite, and solution experiments containing Pu and U

Background - Sensitivity Profiles

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

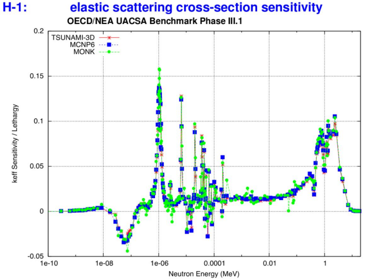
$$S_{k,x} = \frac{\Delta k / k}{\Delta x / x}$$

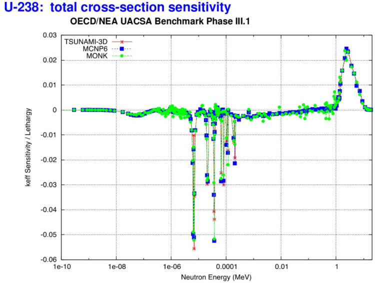




Background - Sensitivity Profiles

- 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

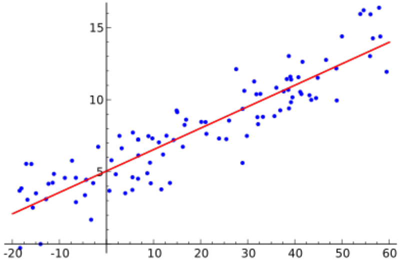


Image obtained from Wikipedia's Linear Regression page

Classification

- Identifying group membership

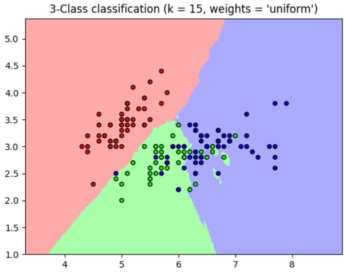


Image obtained from https://sebastianraschka.com/faq/docs/evaluate-a-model.html

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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

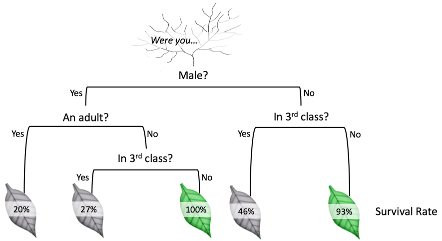
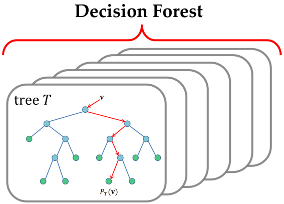


Image obtained from
https://algobeans.com/2016/07/27/decision-trees-tutorial

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

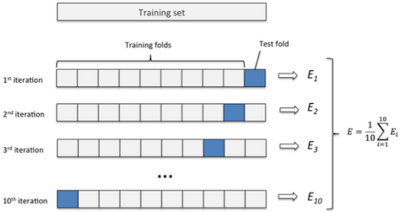
- k_{sim}
  - Generated with the sensitivity vectors from MCNP6
  - Strong linear relationship between bias and k_{sim}

- Predicting:
  - Bias (k_{sim} - k_{exp})
  - k_{exp}

Methods - Training and Validating

Model Evaluation

- Ten fold cross-validation



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Model Complexity

- Minimize model error

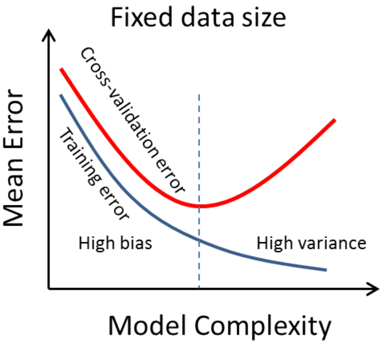
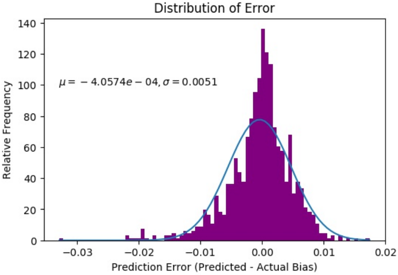
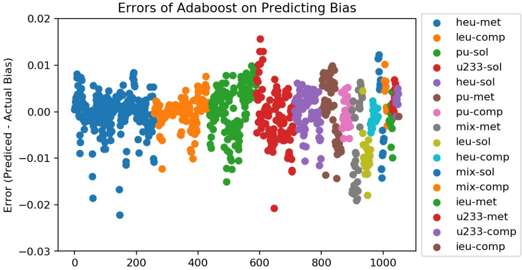


Image obtained at https://stats.stackexchange.com/questions/69549/

Results - Sensitivity Vectors as Features

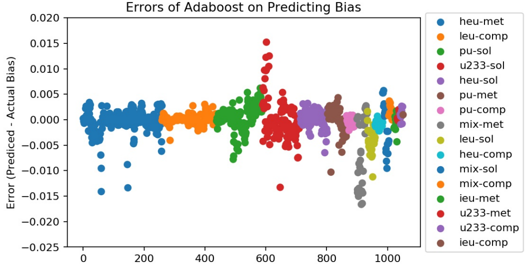
- Are sensitivity profiles sufficient to characterize the problem?
- Beginning to model the relationship
- MSE = 2.723E-5, RMSE = 0.00521, MAE = .00374

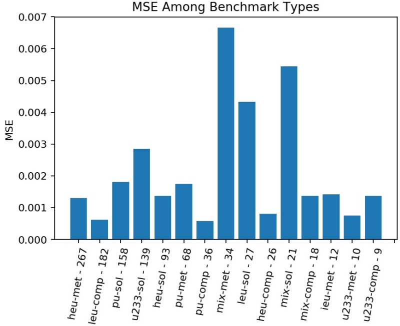




Results - Adaboost Predicting Bias

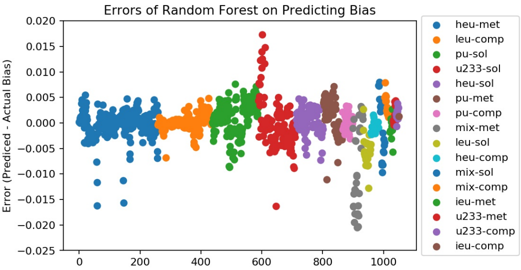
- Accurate for cases with high number of benchmarks
- Higher errors for Pu - composite, HEU composite, and MOX solutions.
- MSE = 9.106E-6, RMSE = 0.00301, MAE = .00177

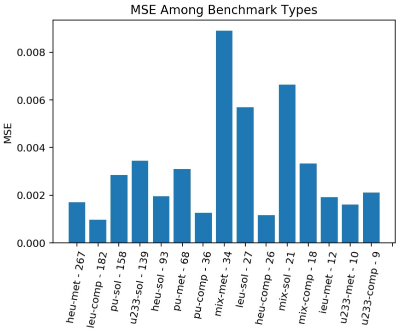




Results - Random Forest Predicting Bias

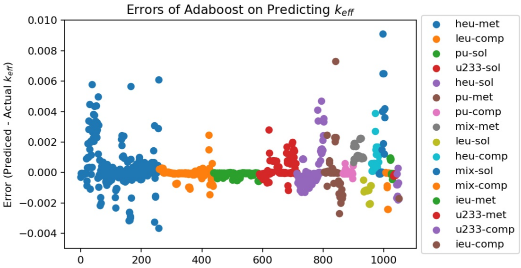
- Slightly less accurate than Adaboost
- Higher errors for same cases
- MSE = 1.498E-5, RMSE = 0.00387, MAE = .00248

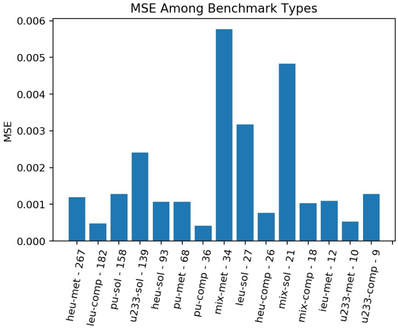




Results - Adaboost Predicting k_{meas}

- 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

Model	Mean Absolute Error	Root Mean Squared Error
Adaboost (Bias)	0.00142	0.00261
Random Forest (Bias)	0.00216	0.00348
Neural Network (Bias)	0.00492	0.00725
Adaboost (k_{meas})	0.00062	0.00129
Random Forest (k_{meas})	0.00079	0.00136
Whisper (Bias)	0.00906	0.01329
GLLSM (k_{meas})	0.00645	0.00959

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

Isotope Reaction	Relative Importance
92233.80c n,gamma	0.046818
92232.80c total nu	0.045100
92232.80c fission	0.039334
92234.80c n,gamma	0.035280
6000.80c n,gamma	0.032351
92234.80c fission	0.031656
92234.80c total nu	0.030931
92232.80c n,gamma	0.027735
6000.80c n,alpha	0.025528
6000.80c inelastic	0.024418

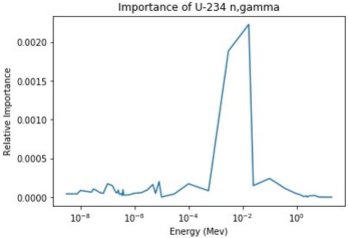
Results - Feature Importances

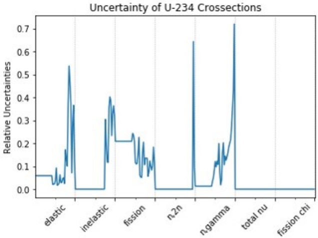
- Break down importance by energy
- Again U 234 has three reactions in top 10

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
poly.20t inelastic, 0.008879	6000.80c n,gamma, 0.008924	6000.80c elastic, 0.009997
be.20t elastic, 0.008204	**94239.80c total nu, 0.008325**	**92233.80c fission chi, 0.008758**
94239.80c n,gamma, 0.007522	**94239.80c fission, 0.008208**	**92234.80c total nu, 0.008494**
94239.80c fission, 0.007427	6000.80c elastic, 0.007817	**92234.80c fission, 0.008008**
9019.80c n,gamma, 0.007201	**92232.80c total nu, 0.006668**	1001.80c elastic, 0.007938

Results - Feature Importances

- U-234 n-gamma reaction
- Leu-comp-therm-079-010
- U-234 makes up 0.0074% of rod
- k_{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

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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

Awknowledgements

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Thank you!
Questions?