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Title: Applying Machine Learning Techniques to Understand Nuclear Data Areas of Interest

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Applying Machine Learning Techniques to Understand Nuclear Data Areas of Interest

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2018 Nuclear Data Week
CSEWG Meeting
Brookhaven National Laboratory

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Outline

- **Motivation**
- **Background**
  - MCNP6 / Sensitivity Profiles, Criticality Safety & Whisper-1.1
- **k_{eff} Bias Predictions & Feature Importance**
- **Criticality Benchmark Clustering**
- **Nuclear Data Adjustment**
- **Reality**
- **Conclusions & Future Work**

Motivation

- **Make use of large collection of (already existing) data to understand where deficiencies in nuclear data & critical experiments may reside**
- **Use new MCNP6 / Whisper-1.1 features**
- **Data from ICSBEP handbook and DICE database can be utilized**
- **Machine learning is current “hot topic”**
  - Explore these methods to hopefully learn something new that can be used to supplement expert knowledge and judgement
  - Very interested and motivated summer student (P. Grechanuk, OSU)
- **For criticality safety, we may want to explore new methods to:**
  - Find similarity between applications and experiments
  - Calculate bias for a new application
  - Provide feedback to the nuclear data community

Background

Background

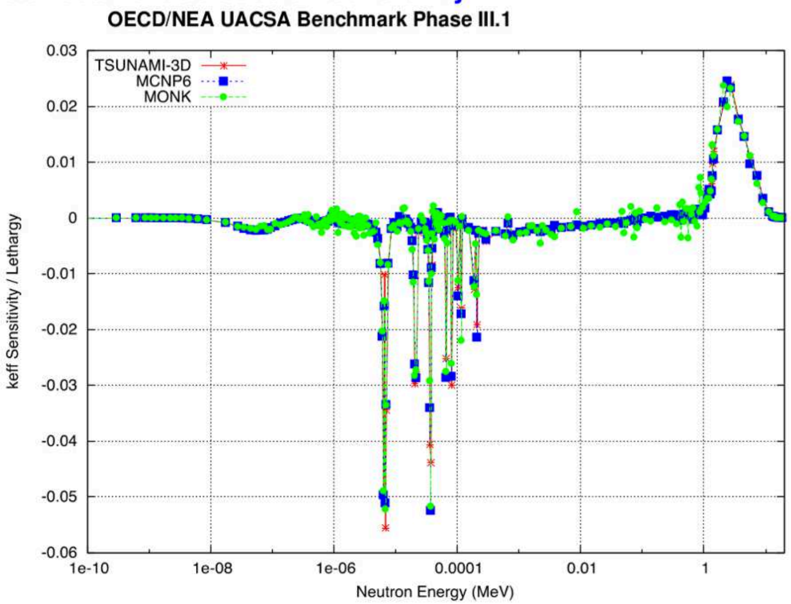
MCNP6 / Sensitivity Profiles

- **Use MCNP6 perturbation/sensitivity features**
  - Can compute profiles of k_{eff} – nuclear data sensitivity profiles
  - How does a relative change in the cross section impact k_{eff} of the system?

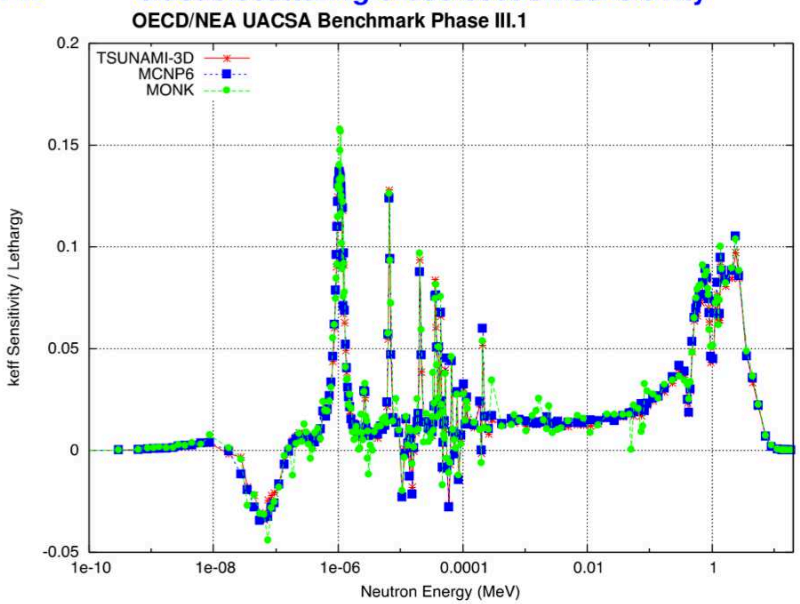
$$S_{k,\sigma} = \frac{\Delta k / k}{\Delta \sigma / \sigma}$$

  - For a single system, these (energy-dependent) profiles are unique

U-238: total cross-section sensitivity



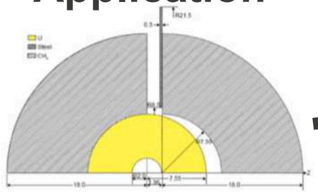
H-1: elastic scattering cross-section sensitivity

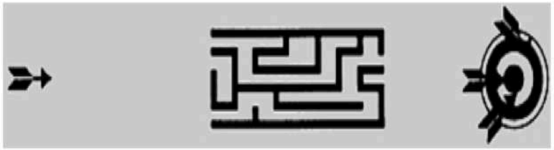


Background

Criticality Safety / Whisper-1.1

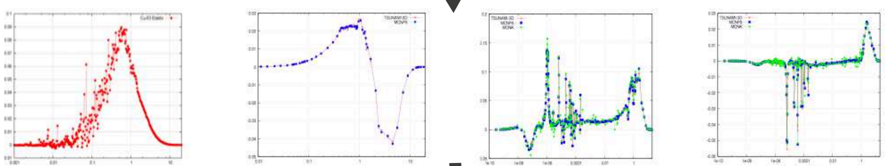
Application





MCNP6
Monte Carlo
Criticality Calculation

Nuclear Cross-section Data



Application Sensitivity Profile

Nuclear Cross-section Covariance Data

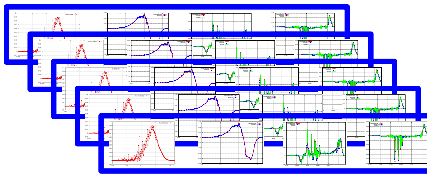
SU-based Analysis

Whisper

Pattern matching – application sensitivity profile vs catalog

Select similar experiments

Statistical analysis to determine bias & uncertainty & extra margin



Catalog of sensitivity profiles for 1000s of experiments

USL
Upper Subcritical Limit
for criticality safety analysis

How Can Machine Learning Methods be Applied to Support Nuclear Data?

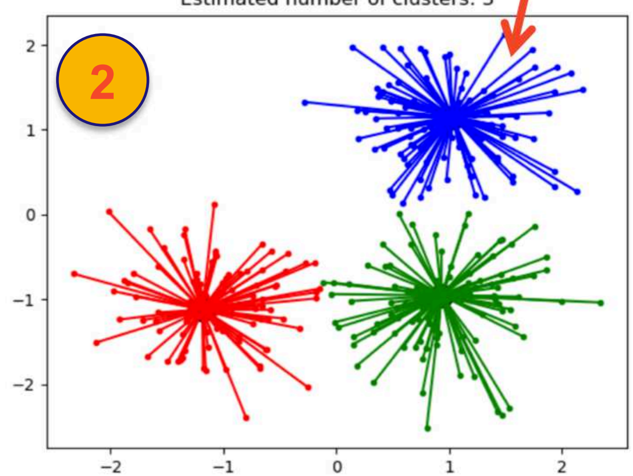
- **Need Data to Feed the Machine Learning Methods**
  - Whisper-1.1 provides:
    - Statistical analysis methods to determine baseline USLs
    - Covariance data for nuclear cross-sections (use is limited)
    - Most importantly, a catalogue of 1100+ ICSBEP benchmarks
      - Each benchmark contains sensitivity profiles for
        a) each isotope in the benchmark (~170 unique isotopes across the catalogue)
        b) 12 reactions per isotope
        c) 44 energy bins per reaction
      - Total of nearly ~90,000 unique isotope-reaction-energy sensitivity coefficients

- **Questions**
  - Using only the sensitivity profiles, for an unknown application, can machine learning methods help in …
    - predicting bias (calculation – experiment)? (regression)
    - finding similar benchmarks? (clustering)
    - adjusting cross sections to reduce biases? (optimization)

k_{eff} Bias Predictions & Feature Importance

Machine Learning

- Machine learning algorithms can be used to find "hidden" patterns in data that are not necessarily obvious
- Can be used to **cluster** data or to build a **regression** model



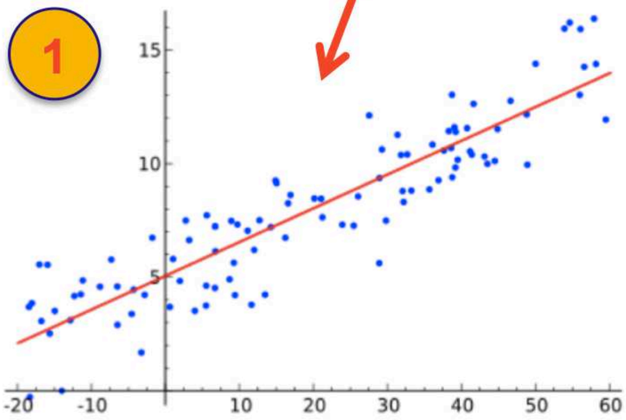


Image obtained from Wikipedia's Linear Regression page

Some nomenclature:
features = x

- In this case, we want to "predict" something: **given x, what is f(x)?**

1 The **first** objective is to predict k_{eff} bias (calculation – experiment)

Machine Learning

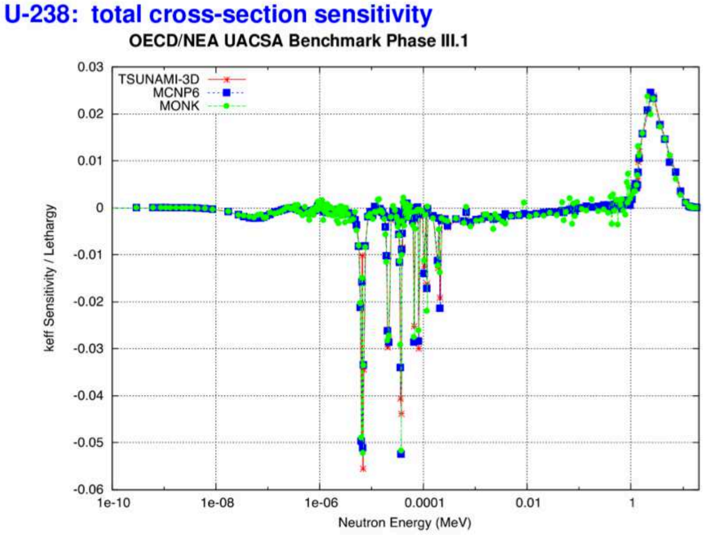
k_{eff} Bias Prediction

- **Prediction of Bias using Sensitivity Profiles**
  - Sensitivity profiles are readily available, $S^i_{k,\sigma}$
  - Bias, B, known for Whisper benchmarks,

$$B_i = k^i_{calc} - k^i_{exp}$$

  - Goal is to predict bias:

$$B_i \approx f(S^i_{k,\sigma})$$



- **Regression Trees**
  - A tree-like model of decisions based on the features
  - All features are considered to split the data
  - Splits are chosen to minimize a cost function (i.e. mean-square error)

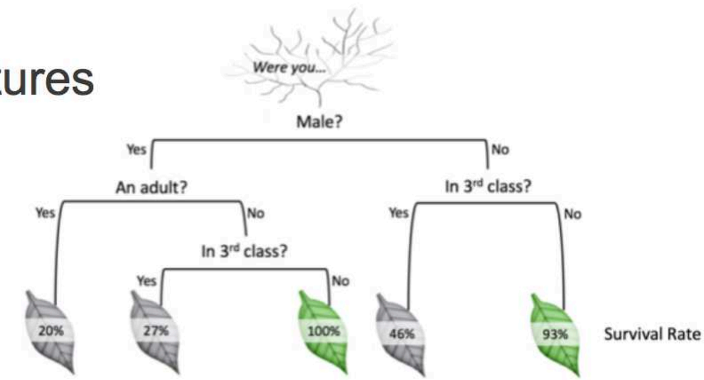


Image obtained from https://algobeans.com/2016/07/27/decision-trees-tutorial

- **Random Forest**
  - Ensemble of regression trees
  - Random subset of data in each trees and subset of features in each split

Machine Learning

k_{eff} Bias Prediction Results

- With the bias known for all of the Whisper-1.1 catalogue cases, the generalized model predictions (comparison of known bias to predicted bias) are promising

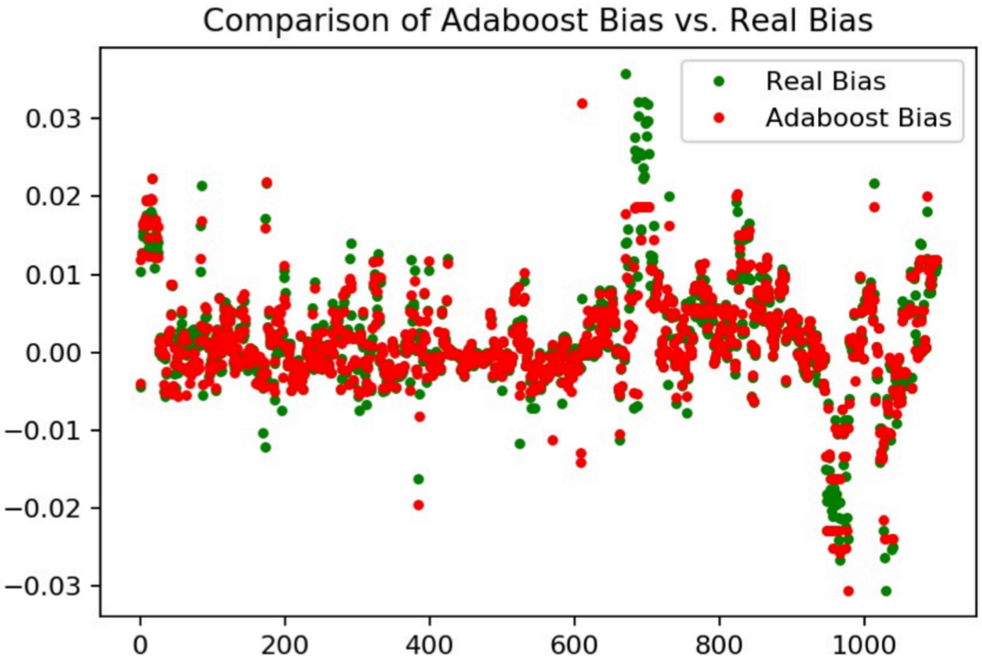
- This leads us to believe that sensitivity profiles, given that they are unique for each individual benchmark case, can be used to as a feature in machine learning methods to prediction the bias in a similar system of interest

- What else can be learned from the machine learning methods?

Bias Accuracy Metrics

Model	RMSE	MAE
Random Forest (I)	0.00499	0.00350
AdaBoost (I)	0.00498	0.00352
Random Forest (D)	0.00572	0.00397
AdaBoost (D)	0.00537	0.00374

I=energy-integrated sensitivities
D=energy-dependent sensitivities



Machine Learning

k_{eff} Bias Prediction Feature Importance

- **From the machine learning methods, feature importance can be used to identify what nuclear data is cause for bias predictions**
- **Shapley Additive exPlanation (SHAP) metric for feature importance**
  - For each benchmark, estimate the additive contribution to the predicted bias for each feature
  - For global importance, assess the mean absolute additive contribution across observations
  - "A Unified Approach to Interpreting Model Predictions" Lundberg, Lee (2017)

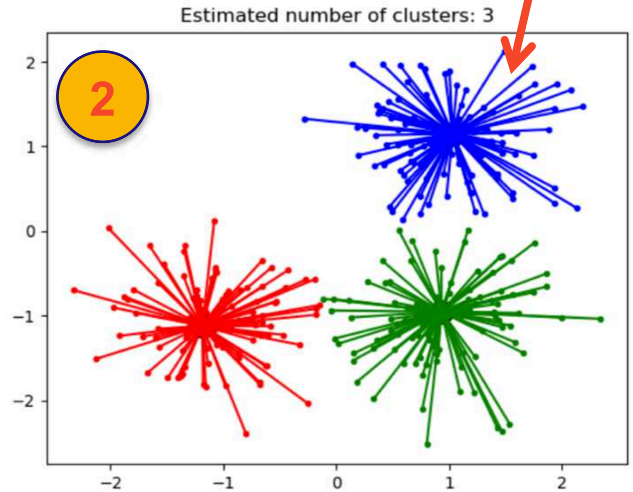
Top 10 Important Features using the SHAP metric on a bias model constructed from only ^{233}U solution benchmarks

Isotope	Reaction	Energy
^{19}F	elastic	2.48 – 3.00 MeV
^{19}F	elastic	1.40 – 1.85 MeV
^{27}Al	elastic	0.55 – 3.00 keV
^{19}F	inelastic	3.00 – 4.80 MeV
^{19}F	inelastic	1.85 – 2.35 MeV
^{19}F	n,gamma	25.0 – 100. keV
^{235}U	nu,total	30.0 – 100. eV
^{19}F	elastic	400. – 900. keV
^{235}U	nu,total	10.0 – 30.0 eV
^{235}U	nu,total	100. – 550. eV

Criticality Benchmark Clustering

Machine Learning

- Machine learning algorithms can be used to find “hidden” patterns in data that are not necessarily obvious
- Can be used to cluster data or to build a regression model



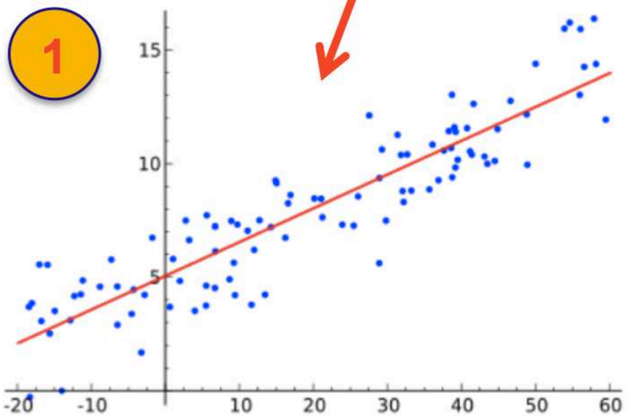


Image obtained from Wikipedia's Linear Regression page

Some nomenclature:
features = x

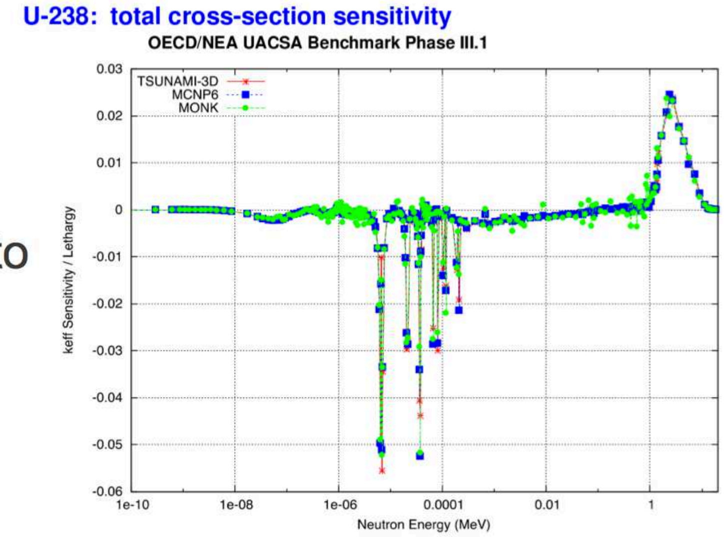
- In this case, we want to group together similar benchmarks: **given x, what group (cluster) do I belong to?**

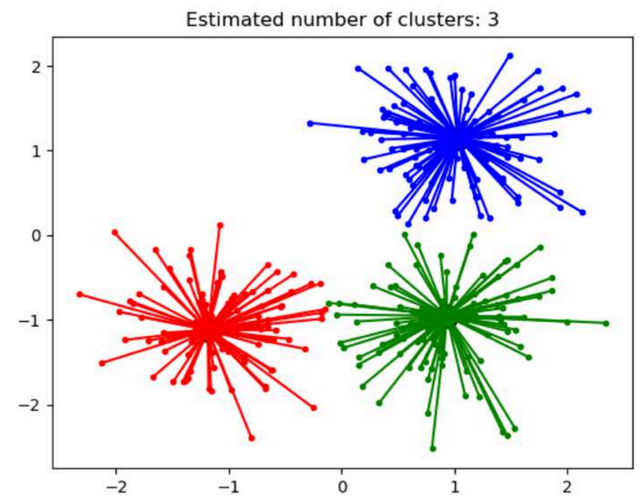
2 The **second** objective is to cluster together similar benchmarks

Machine Learning

Criticality Benchmark Clustering

- **Clustering is used to find inherent relationships in the data**
  - Objects in the same cluster are more similar to each other than those in other clusters
  - Used to find groups of benchmarks that have similar sensitivity profiles, $S^i_{k,\sigma}$
- **Affinity propagation works the best on the sensitivities**
  - Based on the concept of message passing between clusters
  - Does not require number of clusters a priori
  - Finds 'exemplars' representative of the cluster
- **Goal is to observe how the machine learning clustering compares to the ICSBEP classification of benchmarks**

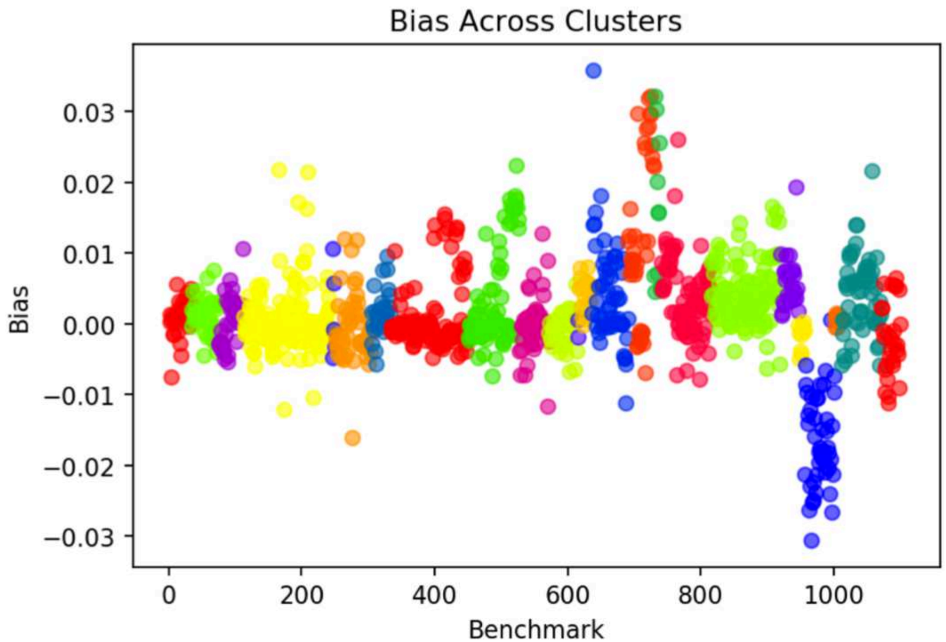




Machine Learning

Criticality Benchmark Clustering Results

- **Finds 24 clusters ranging in population from 2 to 133**
  - Segregated mainly based on materials present and spectrum



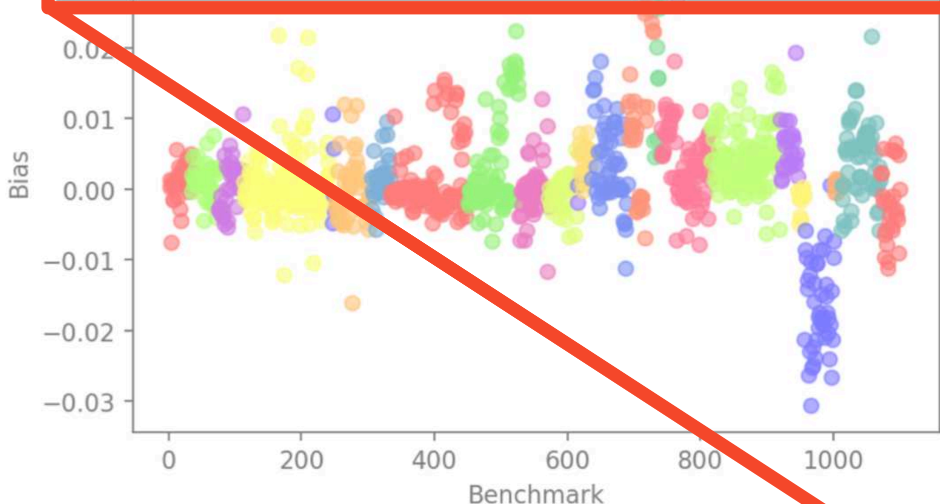
- **Can these clusters be used in some way?**

Cluster	Number of Cases	Benchmark Types
0	33	heu-met-fast
1	41	heu-met-fast, heu-met-mixed
2	38	heu-met-fast
3	133	heu-met-fast
4	5	heu-met-inter
5	54	heu-sol-therm, leu-comp-therm, u233-comp-therm
6	29	heu-met-fast, ieu-met-fast
7	117	leu-comp-therm, heu-comp-therm, heu-met-therm
8	77	heu-comp-therm, leu-comp-therm, heu-sol-therm
9	44	leu-comp-therm, heu-sol-therm
10	43	heu-sol-therm, leu-sol-therm
11	2	mix-comp-fast
12	20	mix-met-fast
13	54	pu-sol-therm, mix-sol-therm, mix-comp-therm
14	39	pu-comp-mixed, pu-sol-therm
15	11	pu-comp-mixed, pu-met-fast
16	75	pu-met-fast, mix-met-fast
17	105	pu-sol-therm, mix-sol-therm, mix-comp-therm
18	26	pu-sol-therm, mix-sol-therm,
19	10	u233-met-fast
20	45	u233-sol-therm, u233-sol-inter
21	10	u233-sol-therm
22	60	u233-sol-therm
23	29	u233-sol-therm, u233-comp-therm

Machine Learning

Criticality Benchmark Clustering Results

Cluster	Number of Cases	ICSBEP Benchmark Type
19	10	u233-met-fast
20	45	u233-sol-therm, u233-sol-inter
21	10	u233-sol-therm
22	60	u233-sol-therm
23	29	u233-sol-therm, u233-comp-therm



Cluster	Number of Cases	Benchmark Types
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2	38	heu-met-fast
3	133	heu-met-fast
12	20	mix-met-fast
13	54	pu-sol-therm, mix-sol-therm, mix-comp-therm
14	39	pu-comp-mixed, pu-sol-therm
15	11	pu-comp-mixed, pu-met-fast
16	75	pu-met-fast, mix-met-fast
17	105	pu-sol-therm, mix-sol-therm, mix-comp-therm
18	26	pu-sol-therm, mix-sol-therm,
19	10	u233-met-fast
20	45	u233-sol-therm, u233-sol-inter
21	10	u233-sol-therm
22	60	u233-sol-therm
23	29	u233-sol-therm, u233-comp-therm

- Can these clusters be used in some way?

Machine Learning

Clustering Applications

- **Can train and test on a few clusters at a time**
  - Well populated classes of benchmarks skew the overall model
  - Training and testing on a subset of the data leads to a more specialized and accurate model
    - This has been done (results not shown here)
  - More accurate model ↔ More accurate feature importance

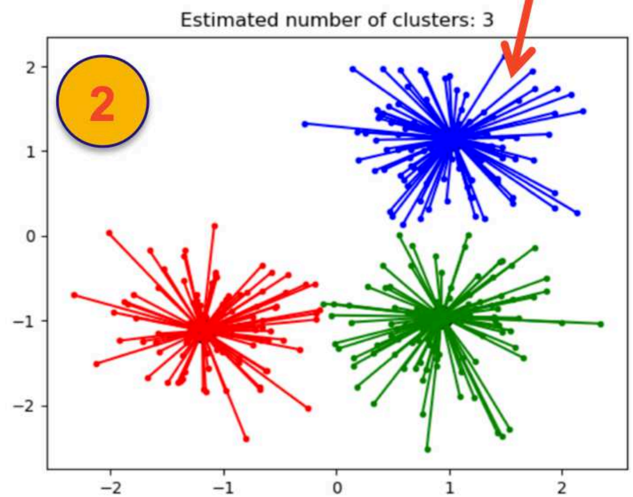
- **Can use clustering to find similar benchmarks for:**
  - Benchmark selection for statistical analysis in Whisper
    - Use in place of c_k (correlation coefficient) as similarity measure
  - Finding regions in sensitivity space that are sparse (more benchmarks needed, see cluster #11 with mix-comp-fast on previous slide)

- **When looking at the nuclear data adjustment methods (on the following slides), a model based on a few clusters is used**

Nuclear Data Adjustment

Machine Learning

- **Machine learning algorithms can be used to find "hidden" patterns in data that are not necessarily obvious**
- **Can be used to cluster data or to build a regression model**



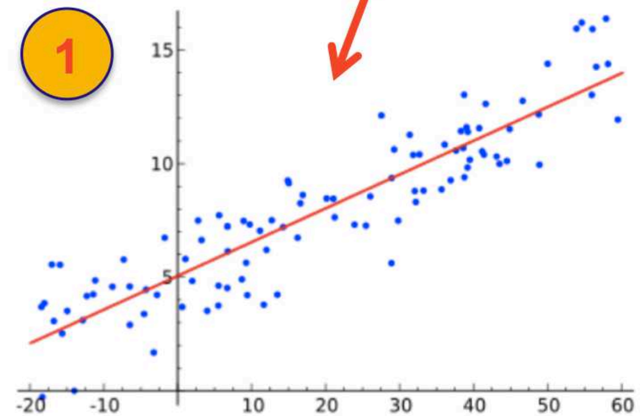


Image obtained from Wikipedia's Linear Regression page

Some nomenclature:
features = x

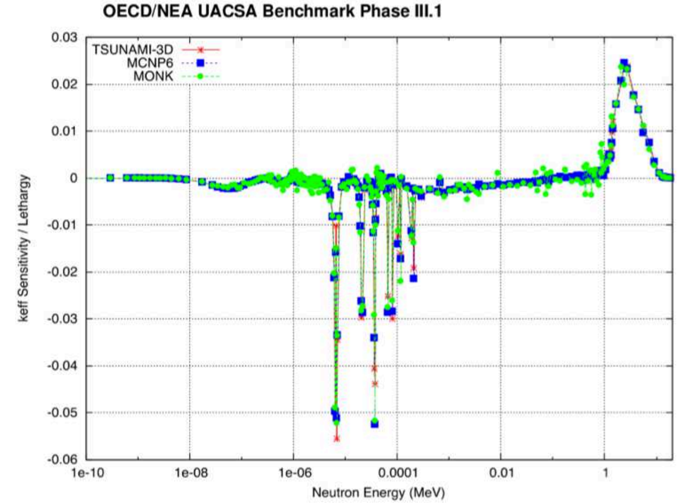
- **In this case, the objective is to optimize cross section perturbations using information from both 1 and 2**

Machine Learning

Nuclear Data Adjustment

- **Using the sensitivities, $S^{i}_{k,\sigma}$ - cross sections can be adjusted in order to reduce k_{eff} bias**
  - Can be done by Generalized Linear Least Squares Method (GLLSM)
  - GLLSM used in Whisper to calculate MOS_{data}

U-238: total cross-section sensitivity



- **Look at only U^{233} solution clusters**

20	45	u233-sol-therm, u233-sol-inter
21	10	u233-sol-therm
22	60	u233-sol-therm
23	29	u233-sol-therm, u233-comp-therm

- **Build a random forest model to predict the k_{eff} bias within these clusters**

- **Find the most important features to predicting the bias**

Isotope	Reaction	Energy
^{19}F	elastic	2.48 – 3.00 MeV
^{19}F	elastic	1.40 – 1.85 MeV
^{27}Al	elastic	0.55 – 3.00 keV
^{19}F	inelastic	3.00 – 4.80 MeV
^{19}F	inelastic	1.85 – 2.35 MeV
^{19}F	n,gamma	25.0 – 100. keV
^{235}U	nu,total	30.0 – 100. eV
^{19}F	elastic	400. – 900. keV
^{235}U	nu,total	10.0 – 30.0 eV
^{235}U	nu,total	100. – 550. eV

- **Apply genetic algorithm to optimize perturbations of the most important features**

Machine Learning

Nuclear Data Adjustment

- **Applied genetic algorithm**
  - Minimize bias for specific clusters of benchmarks
  - Only perturb the most important cross sections to predicting bias

$$\Delta k^i_{calc} = k^i_{calc} S^i_{k,\sigma} \boxed{\frac{\Delta\sigma}{\sigma}}$$

- **Population:**
  - Array of potential perturbations (individuals)
  - Bounded by 3 standard deviations
  - Top **100** important reactions to predicting bias
    - Only top 10 important reactions shown in the table

Isotope	Reaction	Energy
^{19}F	elastic	2.48 – 3.00 MeV
^{19}F	elastic	1.40 – 1.85 MeV
^{27}Al	elastic	0.55 – 3.00 keV
^{19}F	inelastic	3.00 – 4.80 MeV
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^{235}U	nu,total	30.0 – 100. eV
^{19}F	elastic	400. – 900. keV
^{235}U	nu,total	10.0 – 30.0 eV
^{235}U	nu,total	100. – 550. eV

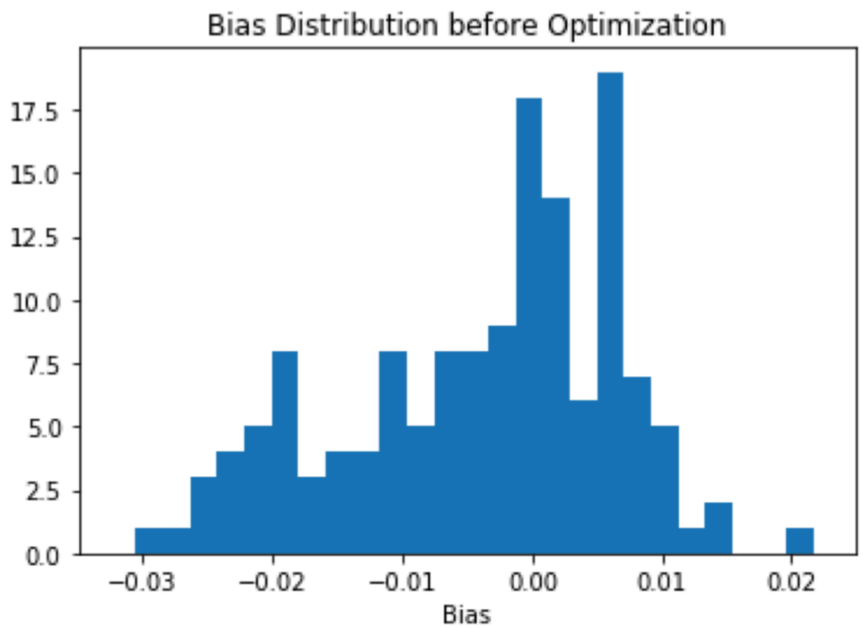
- **Fitness Function:**
  - Squared error between perturbed and experimental k_{eff} across all benchmarks

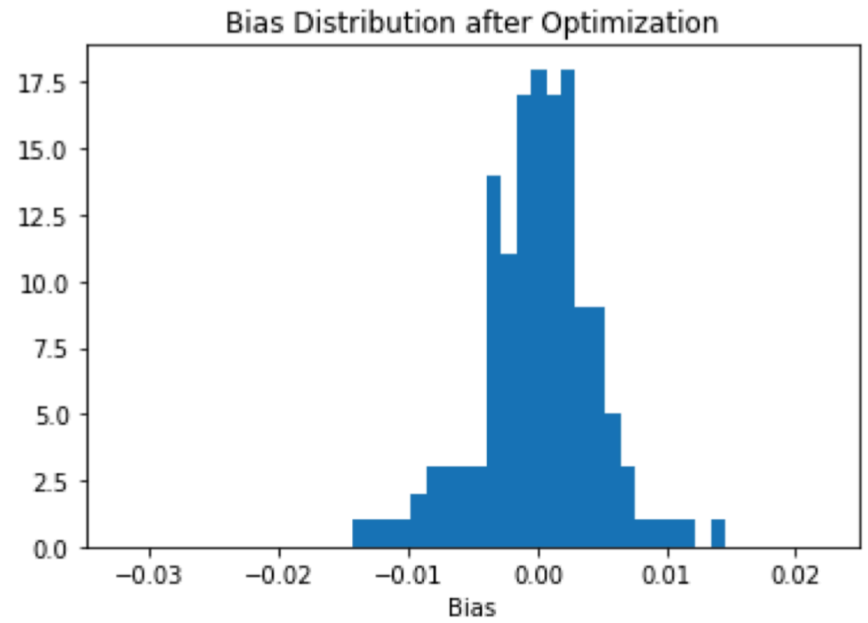
$$Cost = \sum_i^I \left(k^i_{pert} - k^i_{exp}\right)^2$$

Machine Learning

Nuclear Data Adjustment *Initial* Results

- **Distribution of k_{eff} bias for selected ^{233}U solution clusters is far more Gaussian after cross section perturbation optimization**





- **MAE reduced by 33.3% from 0.00842 to 0.00561**
- **RMSE reduced by 34.6 % from 0.01111 to 0.00723**

Machine Learning

Nuclear Data Adjustment *Initial* Results

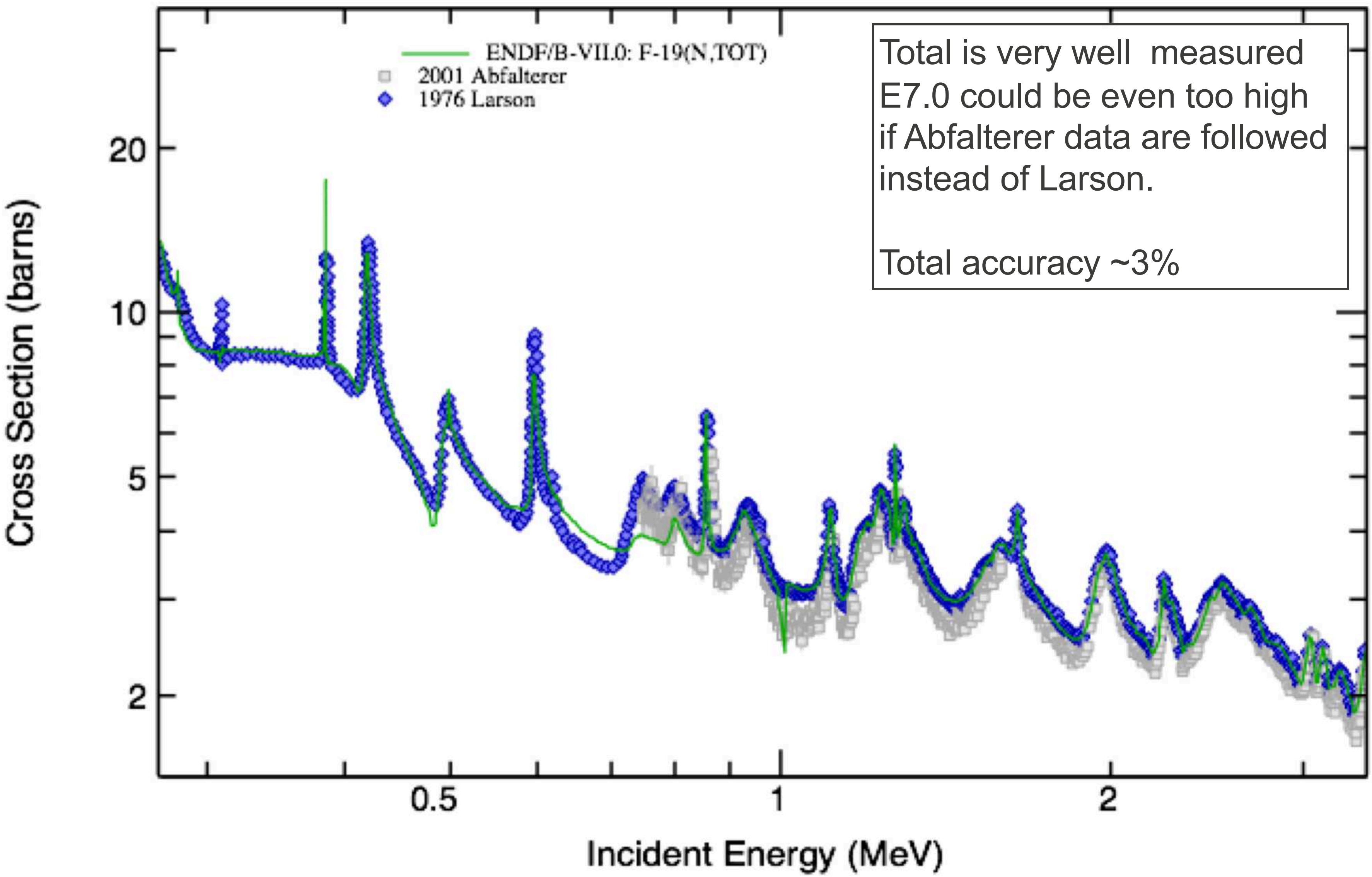
- **Adjusted Nuclear Data for top 10 important features**

Isotope	Reaction	Energy	GA Perturbation, $\Delta\sigma/\sigma$
^{19}F	elastic	2.48 – 3.00 MeV	0.27726
^{19}F	elastic	1.40 – 1.85 MeV	0.24301
^{27}Al	elastic	0.55 – 3.00 keV	-0.02295
^{19}F	inelastic	3.00 – 4.80 MeV	0.37294
^{19}F	inelastic	1.85 – 2.35 MeV	0.33434
^{19}F	n,gamma	25.0 – 100. keV	-0.07822
^{235}U	nu,total	30.0 – 100. eV	0.00047
^{19}F	elastic	400. – 900. keV	0.18738
^{235}U	nu,total	10.0 – 30.0 eV	-0.00285
^{235}U	nu,total	100. – 550. eV	0.00309

- **Are these suggested nuclear data perturbations realistic?**

Reality

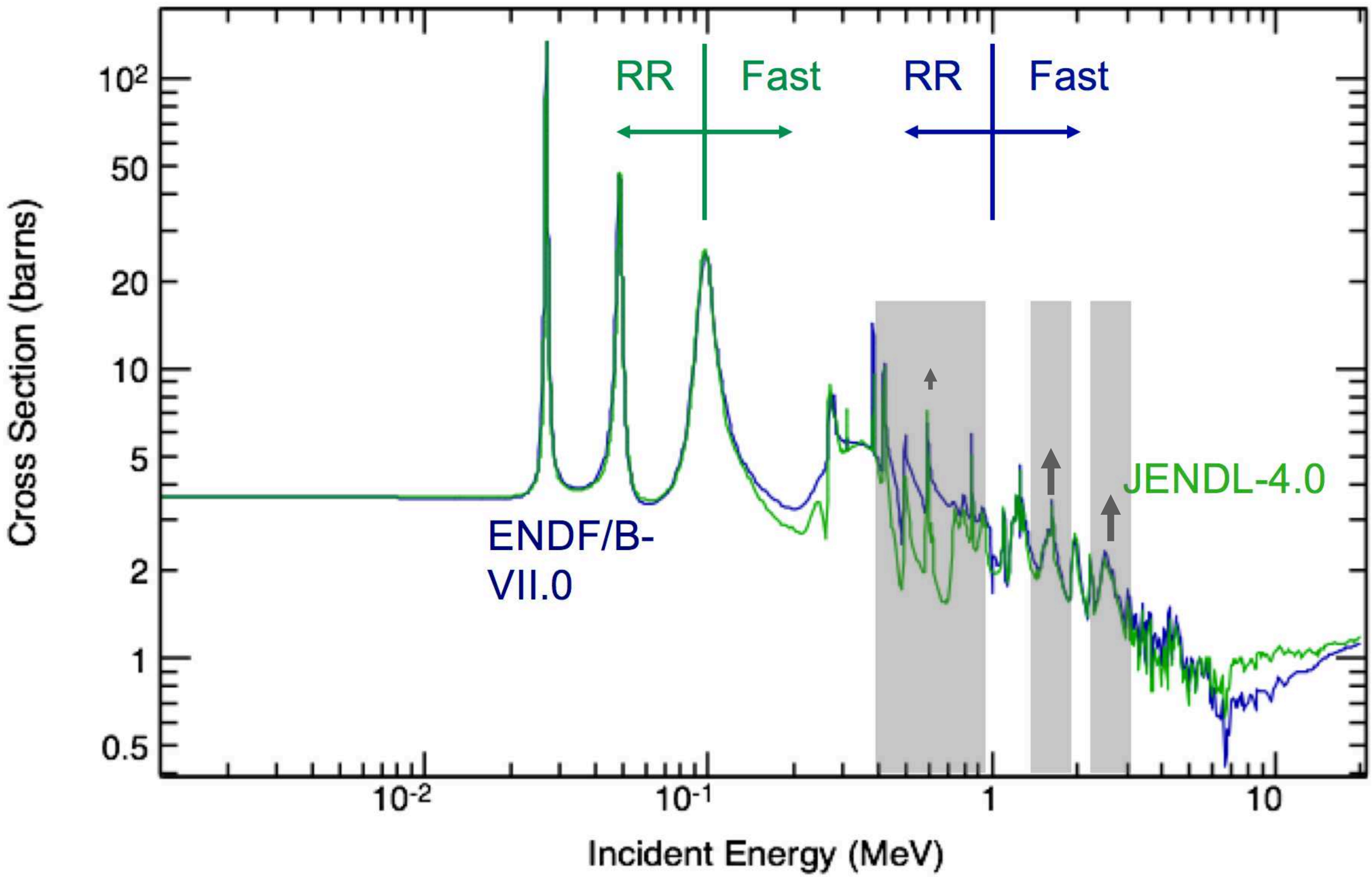
^{19}F Total & exp. data (zoomed)



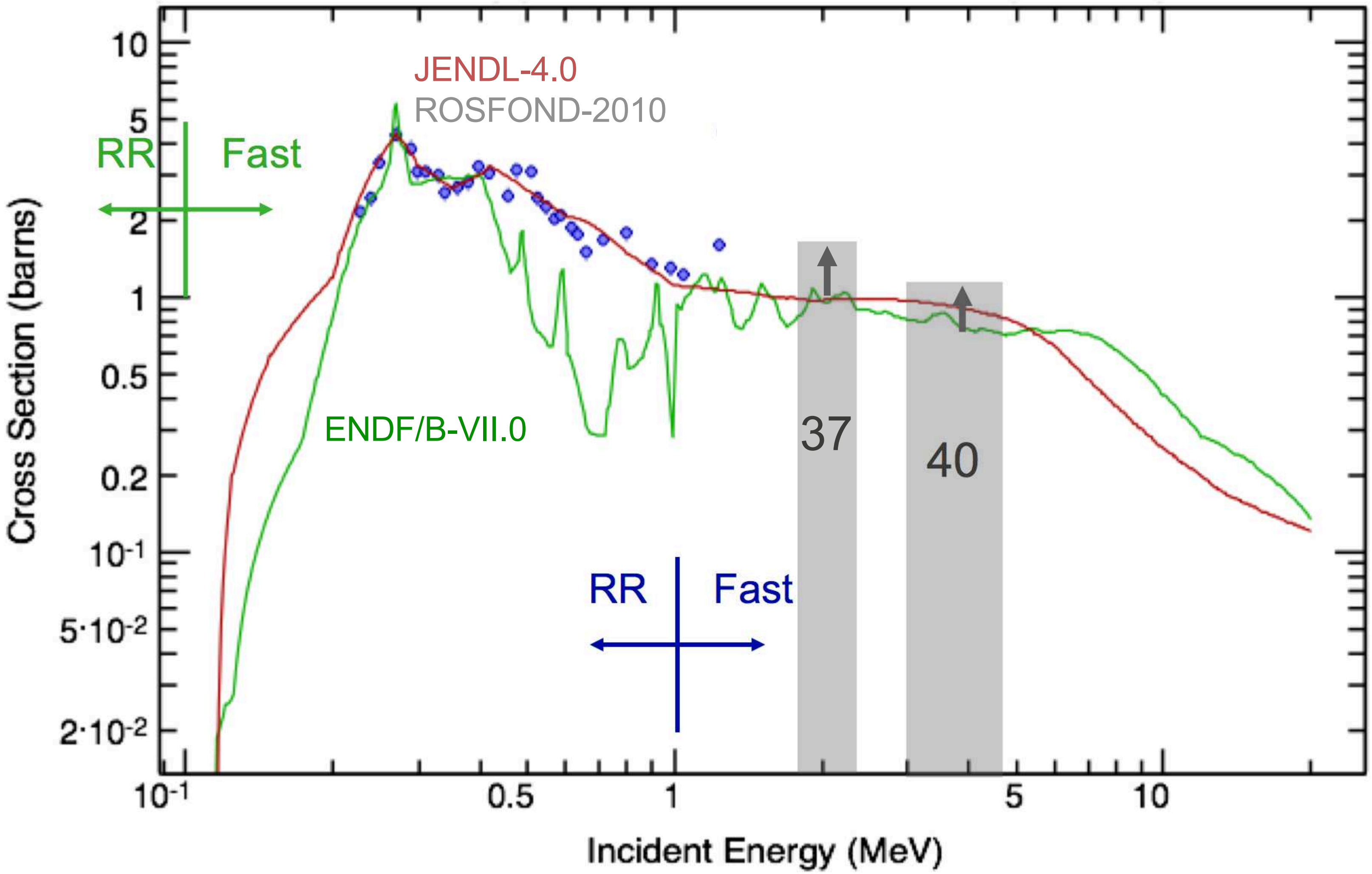
Total is very well measured
E7.0 could be even too high
if Abfalterer data are followed
instead of Larson.

Total accuracy ~3%

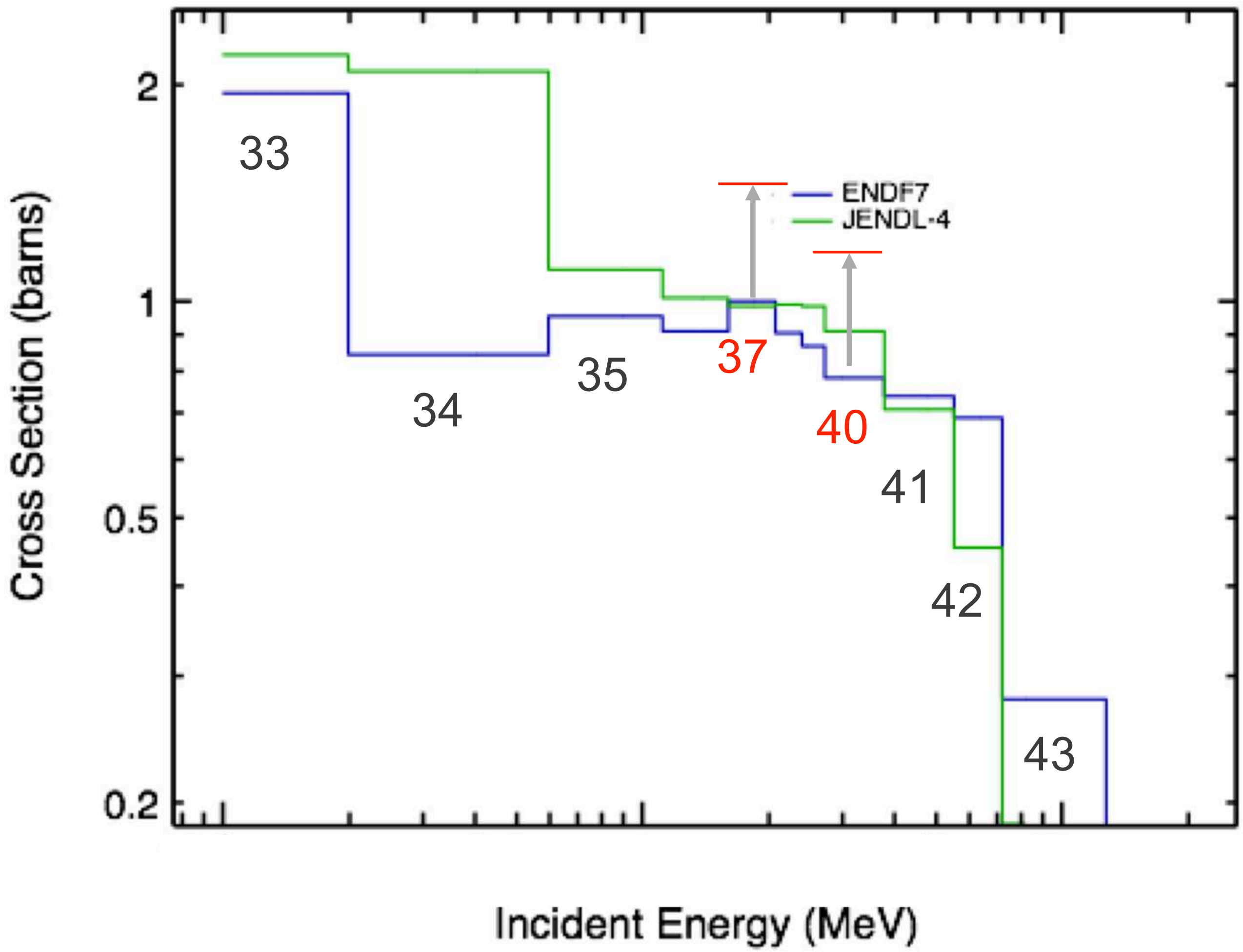
^{19}F elastic - ML proposes increases by ~18-27%



^{19}F inelastic - ML proposes increases 33 & 37%



^{19}F Inelastic (grouped)



Unitarity problem in adjusted ENDF/B-VII.0 XS (barns)

^{19}F Reactions

	Energy Groups				
	34	36	37	39	40
Tot.	4.870	3.203	2.865	2.700	2.063
Ela.	3.306	2.716	1.877	2.194	1.103
Inel.	2.092	1.013	1.318	0.986	1.248
Cap.	0.000	0.000	0.000	0.000	0.000
Sum-Tot	0.528	0.526	0.330	0.479	0.289
Sum/Tot	1.108	1.164	1.115	1.178	1.140

Adjusting Cross Sections – Results U233 Cluster

Isotope	Reaction	Energy	GA Perturbation, $\Delta\sigma/\sigma$
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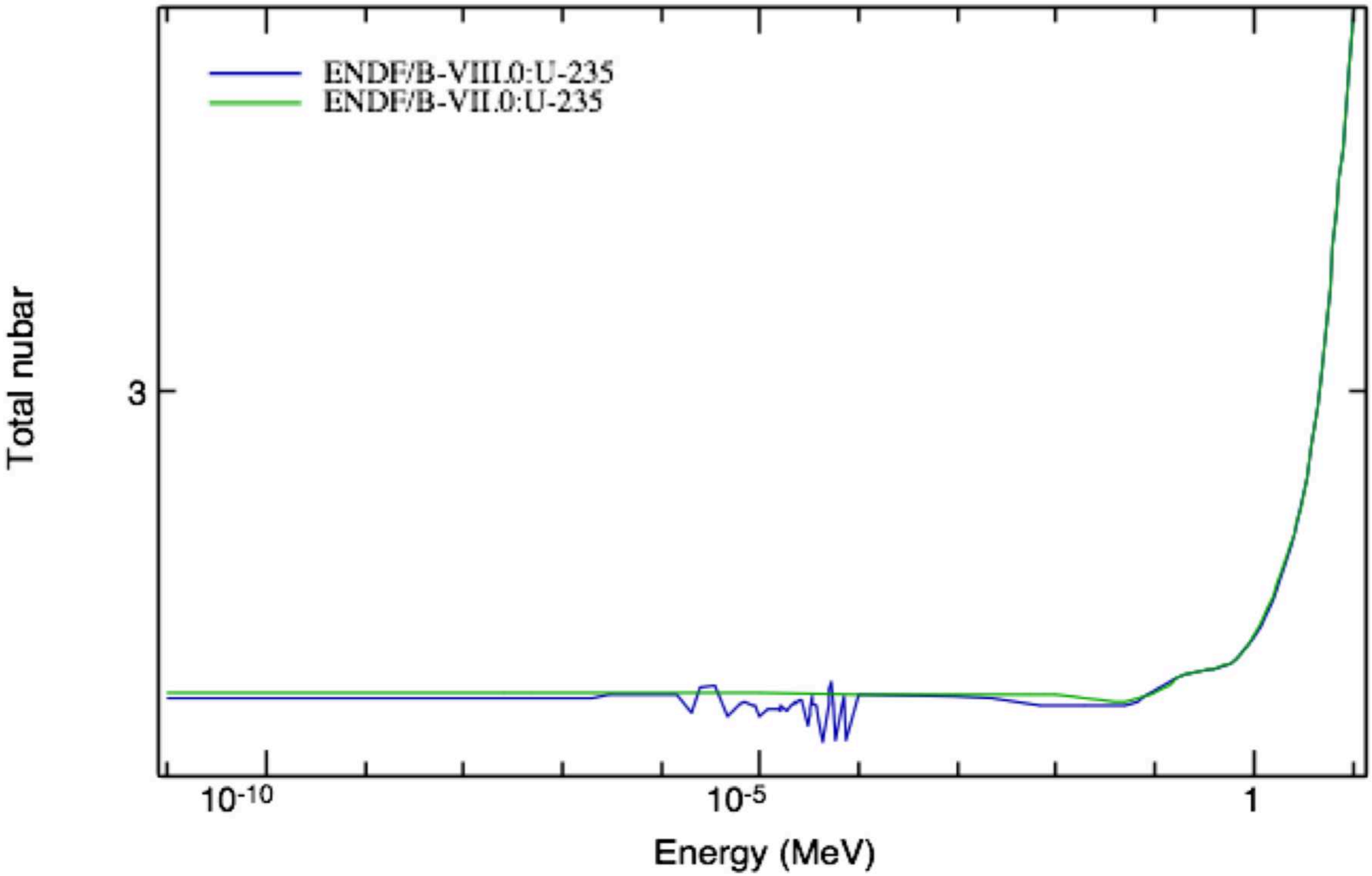
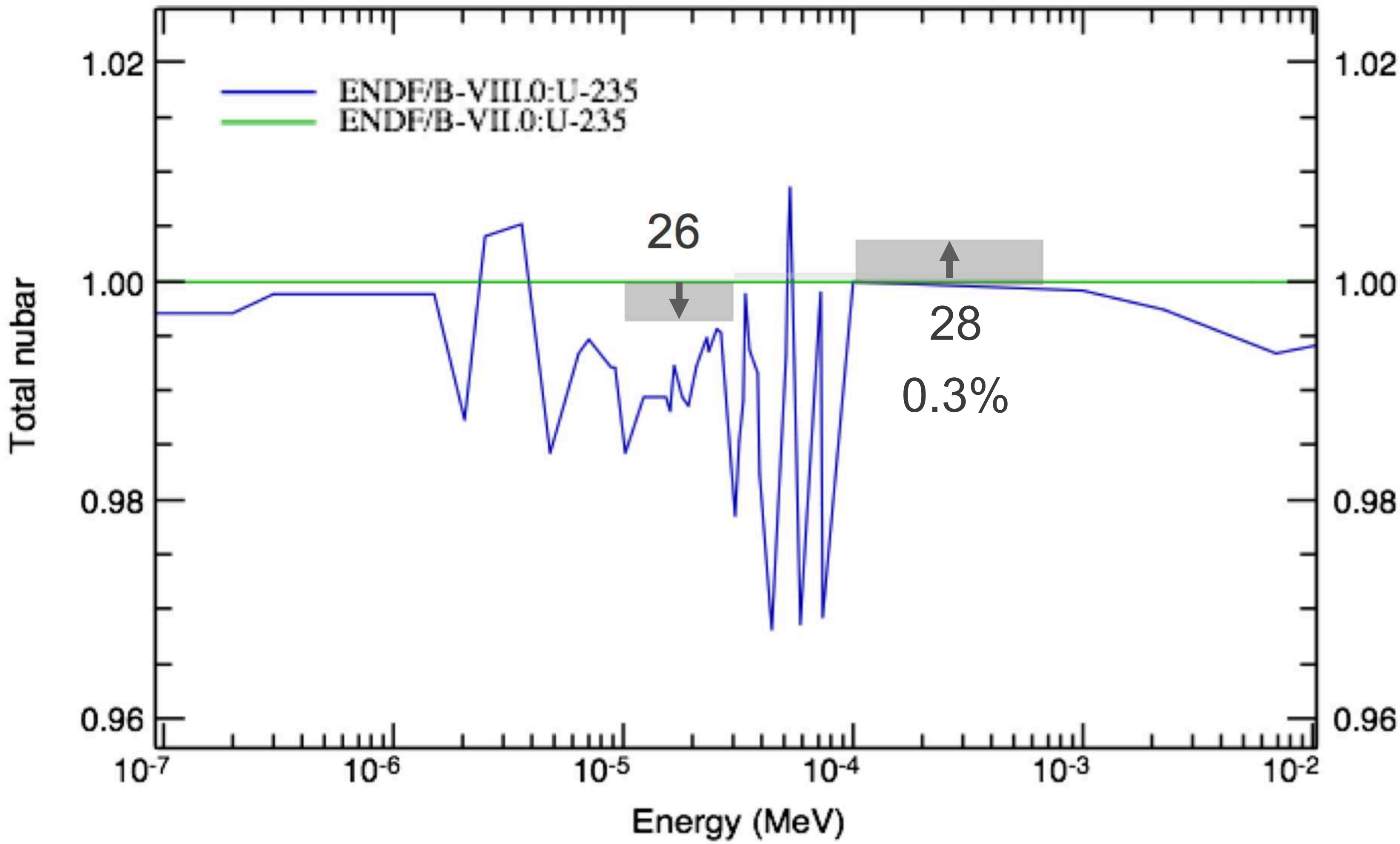
^{235}U	nu,total	$10.0 - 30.0$ eV	-0.00285
^{235}U	nu,total	$100. - 550.$ eV	0.00309

^{235}U nu-bar - difference between E7.0 and E8.0



^{235}U nu-bar - E8.0 to E7.0 ratio and ML proposed change



Conclusions

- **Using MCNP6 capabilities to calculate nuclear data sensitivity profiles along with the Whisper-1.1 catalogue of 1100+ criticality safety benchmarks, several Machine Learning methods were applied to predict k_{eff} bias, cluster similar benchmarks together and optimize perturbations to important cross sections.**

- **There is no physical support for the proposed changes in the current ENDF/B ^{19}F evaluation, but…**
  - ML have pointed out to the file that needs a reevaluation.
  - ^{235}U nu-bar results are interesting - ML got right the region which has been changed in ENDF/B-VIII.0. One change is consistent with E8, the second is irrelevant, the third in not confirmed by E8.

- **ML (as any other adjustment) might not be reliable if the prior is wrong.**

Future Work

- **Need to examine all of the Machine Learning results more closely, especially the *initial* nuclear data adjustment results**
  - Comparison to GLLSM is needed
  - Inclusion of the nuclear data covariances should be investigated (bounding by 3 standard deviations is likely not appropriate)
- **Using more features of the benchmarks could be explored to see if they can help in clustering benchmarks or finding systematic outliers**
- **To get the full story on ^{19}F, still need to investigate ways to include:**
  - physics (unitarity)
  - covariance's
  - angular distributions haven't been used in ML but might play a role

Questions?