A Methodology for Verifiable Uncertainty Quantification

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Purpose

Current uncertainty quantification (UQ) methods have known limitations:

- inaccurate when model assumptions are violated
- error corrections depend on subject matter expertise

The nuclear data community needs repeatable, accurate UQ methods. This first requires a methodology for verifying any given UQ approach.

Purpose

Current uncertainty quantification (UQ) methods have known limitations:

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The nuclear data community needs repeatable, accurate UQ methods. This first requires a methodology for verifying any given UQ approach.

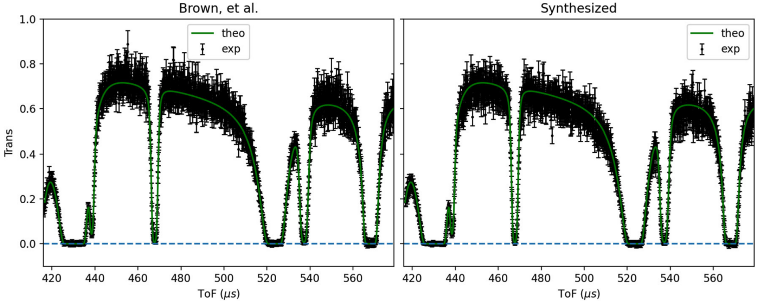
We propose a methodology which leverages high-fidelity synthetic data for verifying any candidate UQ approach.

Syndat: Reproducible Synthetic Data

Walton, Brown, Fritsch, *et al.* [1] provide

> *"a generative model for the experimental observables produced by a determined total cross section in a neutron time-of-flight (TOF) transmission experiment,"*

and accompanying open source code [2].



[1] N. Walton, J. Brown, W. Fritsch, D. Brown, G. Nobre, and V. Sobes, "Methodology for physics-informed generation of synthetic neutron time-of-flight measurement data," *Computer Physics Communications*, vol. 294, p. 108 927, 2024.

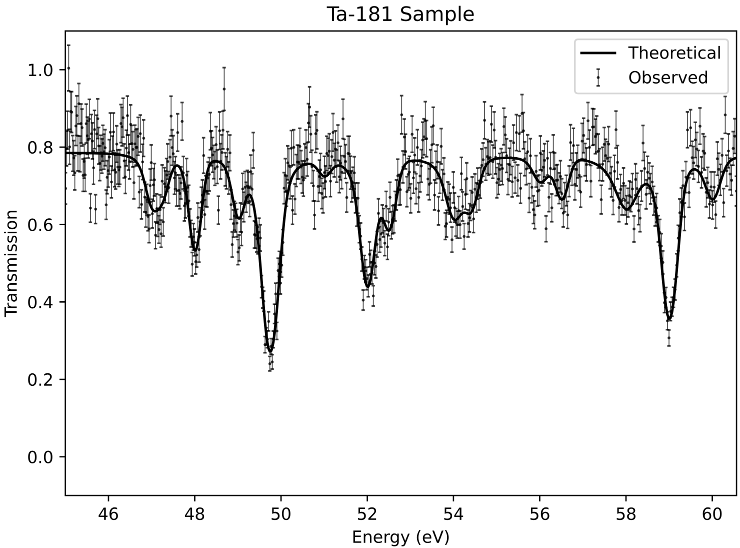
SAMMY UQ Limitations

Updated Users' Guide to SAMMY, Section IV.E.6:

> *"The posterior resonance parameter covariance matrix (RPCM) produced by SAMMY is a accurate representation of the uncertainties in the R-matrix evaluation. Nevertheless, uncertainties for evaluated cross sections reproduced by propagating the RPCM have historically been regarded as 'too small.'" [3]*

[3] N. M. Larson, "Updated users' guide for sammy: Multilevel r-matrix fits to neutron data using bayes' equations," ORNL, ORNL, Oak Ridge, TN, Tech. Rep. ORNL/TM-9179/R8, 2008, Section IV.E.6.

Ta-181 Example



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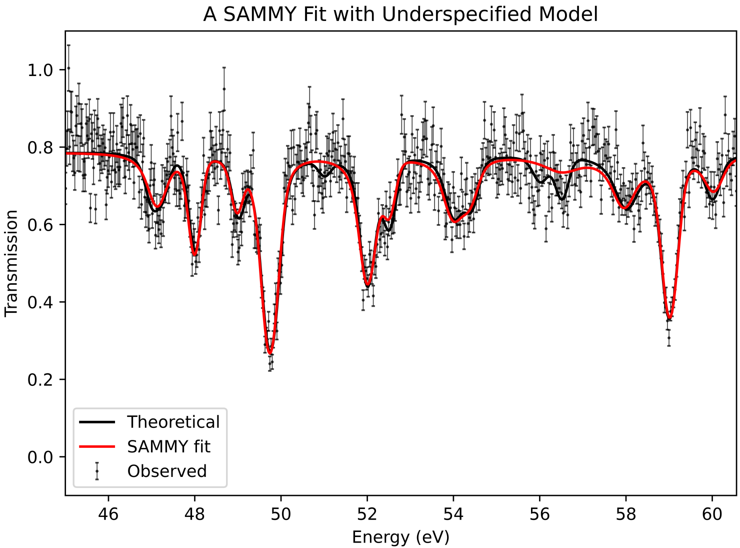

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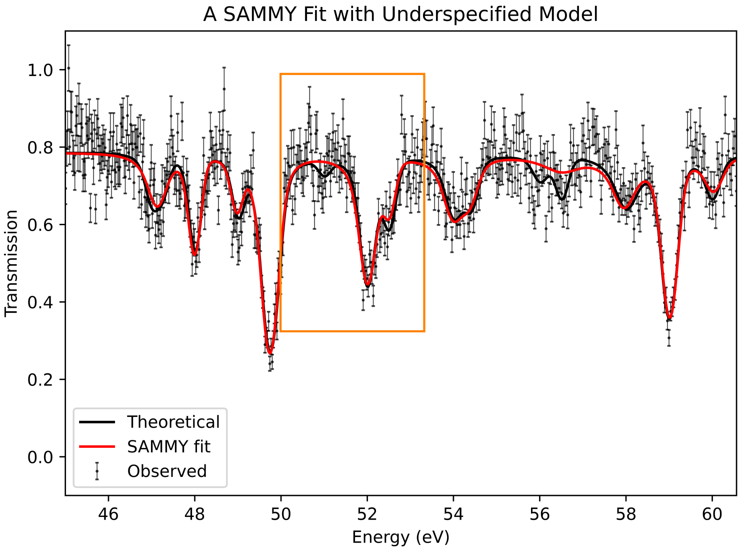

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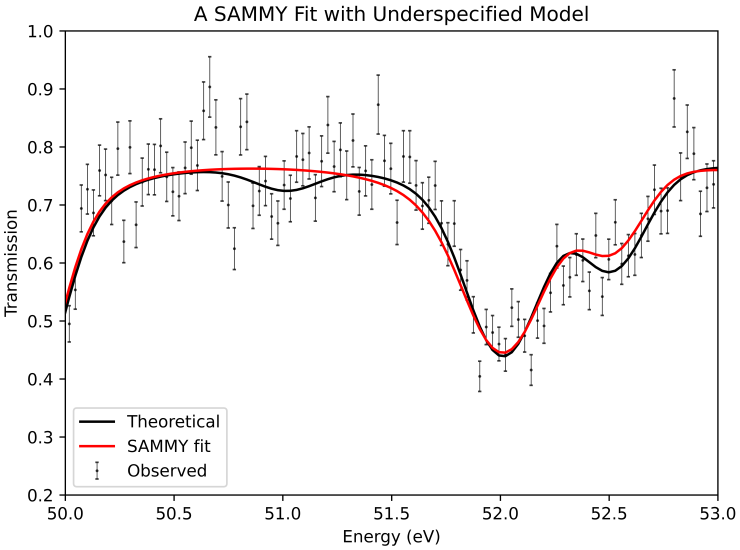

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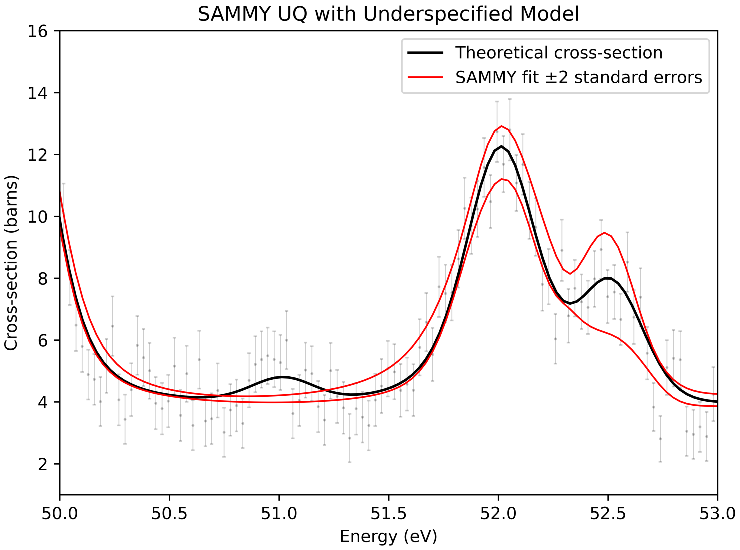

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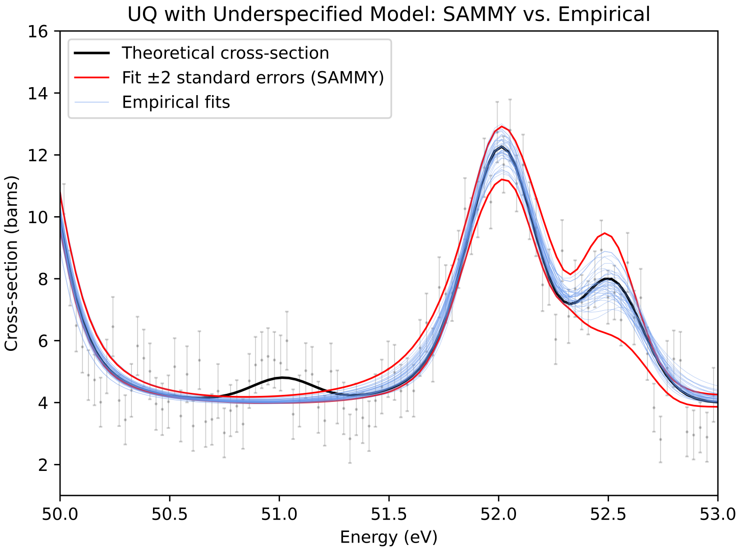

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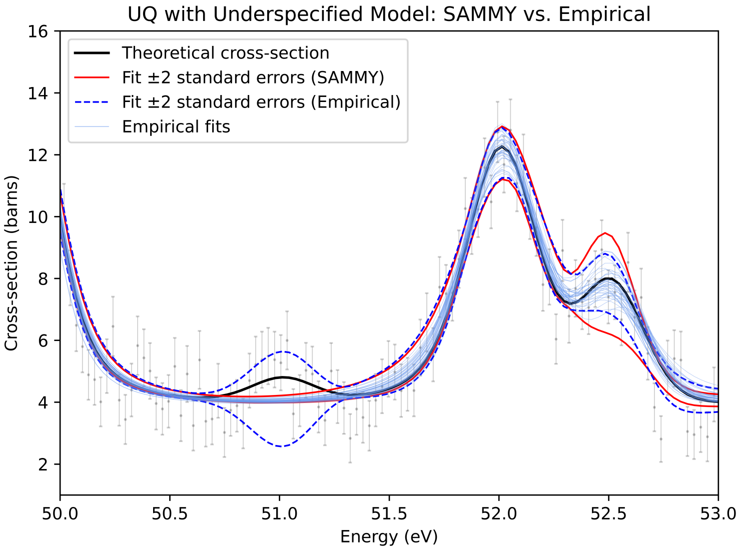

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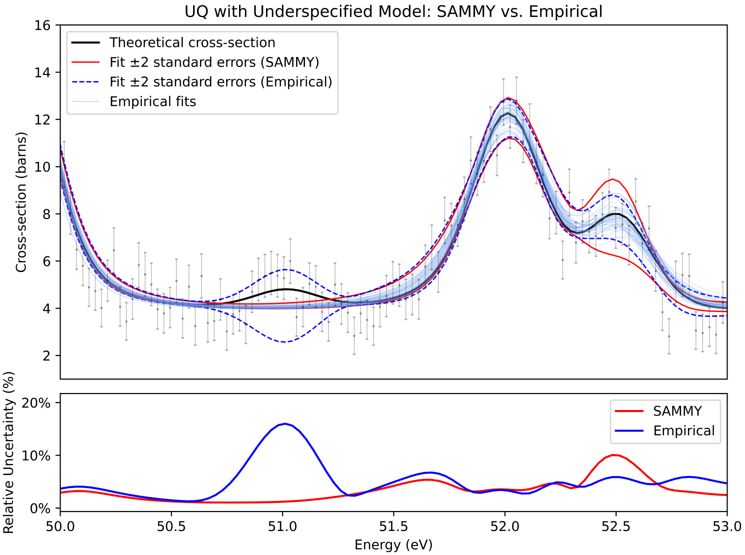

Pause and reflect

What have we shown?

- Use synthetic data to quantify the impact of model assumption violations on UQ accuracy.

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- Use synthetic data to quantify the impact of model assumption violations on UQ accuracy.

What's next?

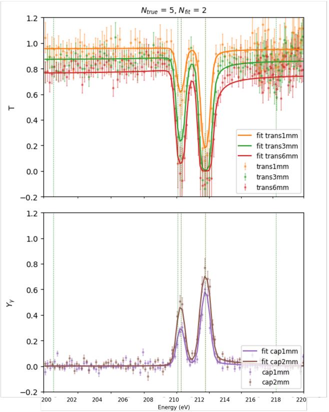
- Use synthetic data to develop a repeatable methodology for generating verifiably accurate UQ.

Automated Fitting

A sneak peek at AutoFit (see Noah Walton's talk tomorrow)...

- Dense feature bank of many resonances
- Iteratively step down model complexity and fit
- Use cross-validation to determine final model

Valuable information for UQ is contained in higher-order model fits.



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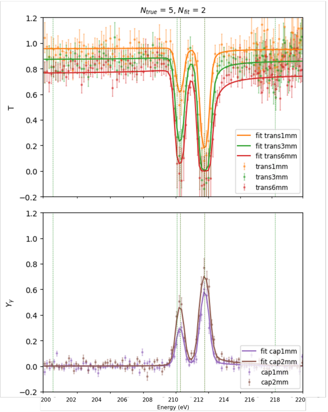
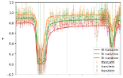


Key idea: SAMMY cross section cov matrices computed for Syndat samples can be used as features to machine learn parameters which can be applied to new data for improved UQ.

Process

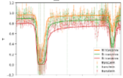
Training Data

$k_1 = 2$



$\longrightarrow C_1$

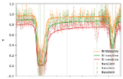
$k_2 = 3$



$\longrightarrow C_2$

⋮

$k_{10} = 11$



$\longrightarrow C_{10}$

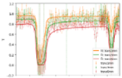
Learn parameters that map SAMMY covariances to empirical.

$$\hat{\beta}_{1:10} = \underset{\beta_{0:10}}{\operatorname{argmin}}(\|E - (\beta_0 + \beta_1 C_1 + \cdots + \beta_{10} C_{10})\|_2)$$

Process

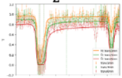
Training Data

$k_1 = 2$



$\longrightarrow C_1$

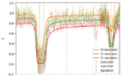
$k_2 = 3$



$\longrightarrow C_2$

⋮

$k_{10} = 11$



$\longrightarrow C_{10}$

Learn parameters that map SAMMY covariances to empirical.

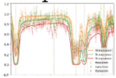
$$\hat{\beta}_{1:10} = \underset{\beta_{0:10}}{\operatorname{argmin}}(\|E - (\beta_0 + \beta_1 C_1 + \cdots + \beta_{10} C_{10})\|_2)$$

$$C_M = \_ + \_C_1 + \cdots + \_C_{10}$$

We want to improve the UQ accuracy by using information contained in SAMMY covariances for the test data.

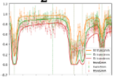
Test Data

$k_1 = 4$



$C_1 \longleftarrow$

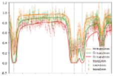
$k_2 = 5$



$C_2 \longleftarrow$

⋮

$k_{10} = 13$

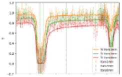


$C_{10} \longleftarrow$

Process

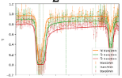
Training Data

$k_1 = 2$



$\longrightarrow C_1$

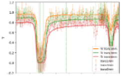
$k_2 = 3$



$\longrightarrow C_2$

⋮

$k_{10} = 11$



$\longrightarrow C_{10}$

Learn parameters that map SAMMY covariances to empirical.

$$\hat{\beta}_{1:10} = \underset{\beta_{0:10}}{\operatorname{argmin}}(\|E - (\beta_0 + \beta_1 C_1 + \cdots + \beta_{10} C_{10})\|_2)$$

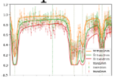
$$C_M = \hat{\beta}_0 + \hat{\beta}_1 C_1 + \cdots + \hat{\beta}_{10} C_{10}$$

Apply learned parameters on user data to obtain improved UQ.

Test Data

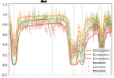
$k_1 = 4$

$C_1 \longleftarrow$



$k_2 = 5$

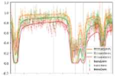
$C_2 \longleftarrow$



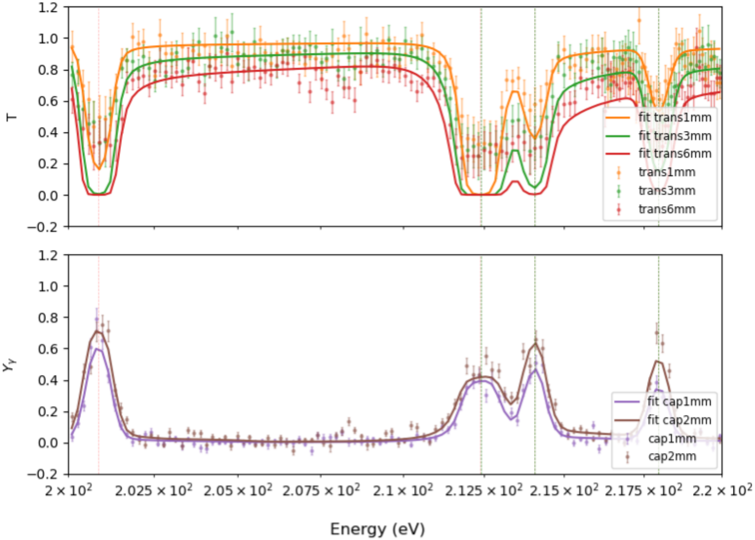
⋮

$k_{10} = 13$

$C_{10} \longleftarrow$

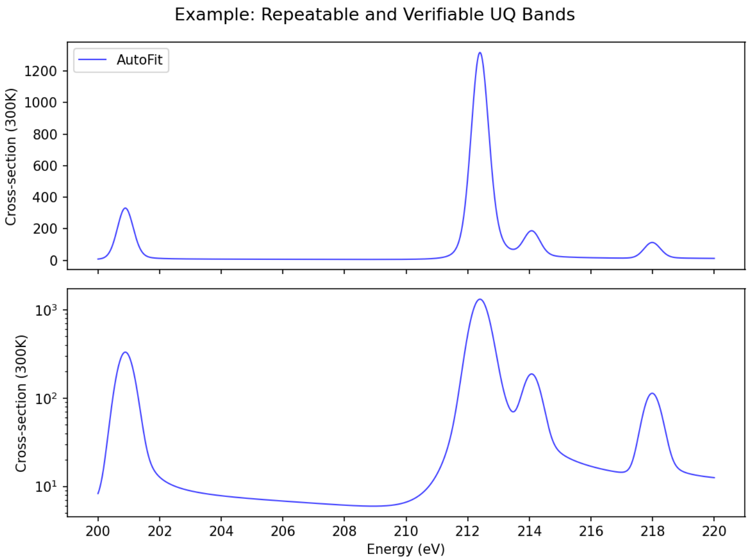


Example



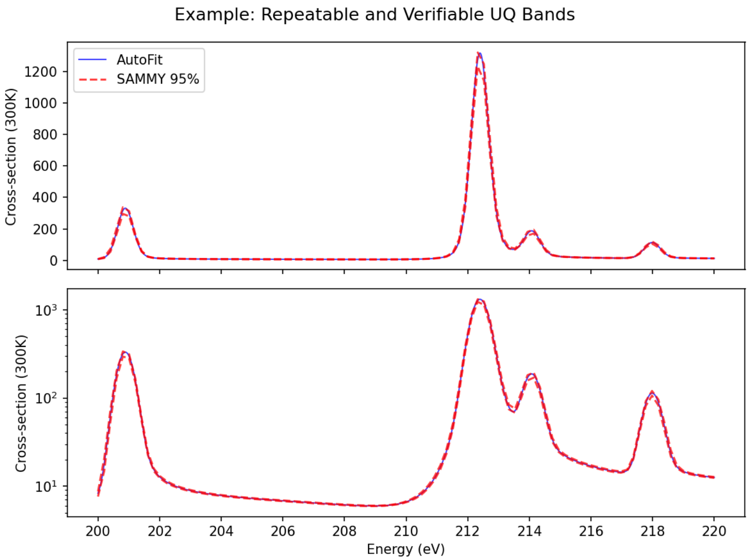
T
Y_γ
1.2
1.0
0.8
0.6
0.4
0.2
0.0
−0.2
fit trans1mm
fit trans3mm
fit trans6mm
trans1mm
trans3mm
trans6mm
fit cap1mm
fit cap2mm
cap1mm
cap2mm
2×10^2
2.025×10^2
2.05×10^2
2.075×10^2
2.1×10^2
2.125×10^2
2.15×10^2
2.175×10^2
2.2×10^2
Energy (eV)

Example



Example: Repeatable and Verifiable UQ Bands
AutoFit
Cross-section (300K)
1200
1000
800
600
400
200
0
10^3
10^2
10^1
200
202
204
206
208
210
212
214
216
218
220
Energy (eV)

Example



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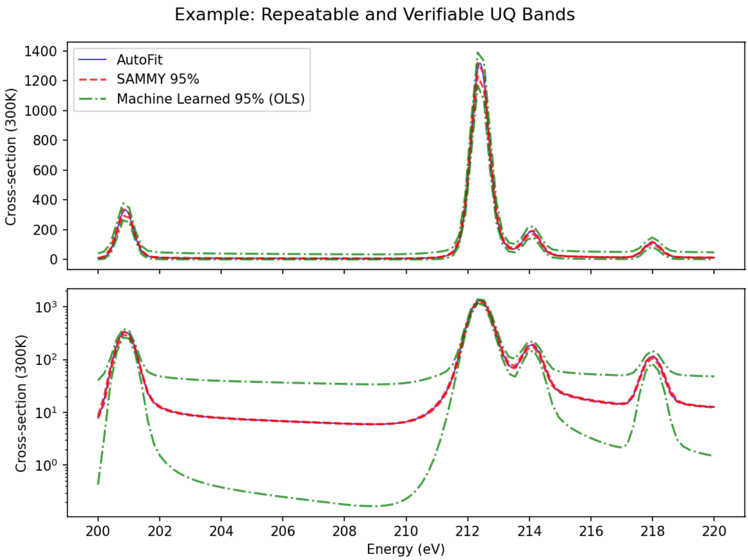
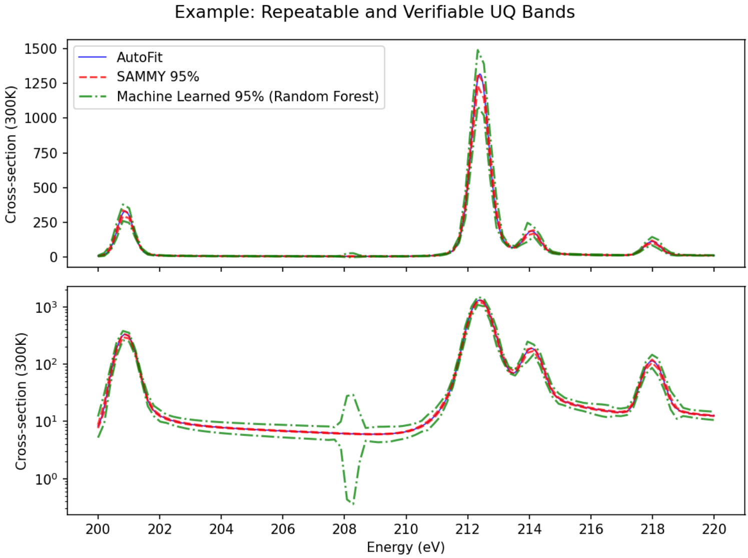
Example


Example: Repeatable and Verifiable UQ Bands
AutoFit
SAMMY 95%
Machine Learned 95% (OLS)
Cross-section (300K)
1400
1200
1000
800
600
400
200
0
10^3
10^2
10^1
10^0
200
202
204
206
208
210
212
214
216
218
220
Energy (eV)

Example



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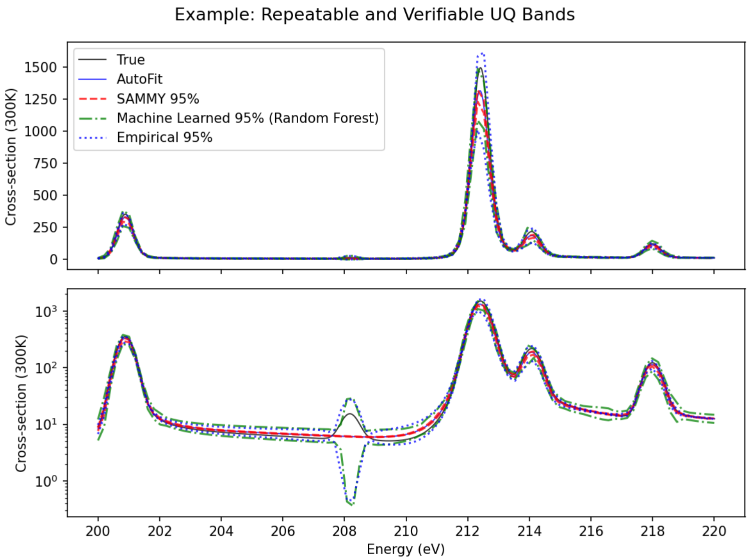
Example



Example: Repeatable and Verifiable UQ Bands
True
AutoFit
SAMMY 95%
Machine Learned 95% (Random Forest)
Empirical 95%
Cross-section (300K)
1500
1250
1000
750
500
250
0
Cross-section (300K)
10^3
10^2
10^1
10^0
200
202
204
206
208
210
212
214
216
218
220
Energy (eV)

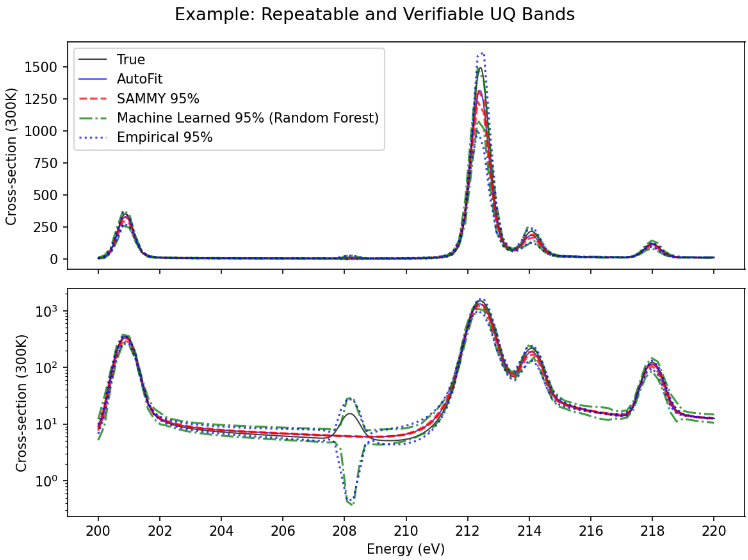
Conclusions

1. A train-then-test process using synthetic data allows us to verify the performance of any UQ approach.
2. Machine learning methods which combine SAMMY UQ output from higher-order models may produce more accurate UQ for cross-sections than standard SAMMY UQ.

Future work

- Identify best metric for evaluating a candidate UQ relative to empirical UQ.
- Further explore candidate models for improved UQ
- Develop process for stitching learned UQ across energy windows

Questions?



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References I

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