Unique Questions and Answers Revealed in Automated Resonance Fitting and Demonstrated on Ta-181

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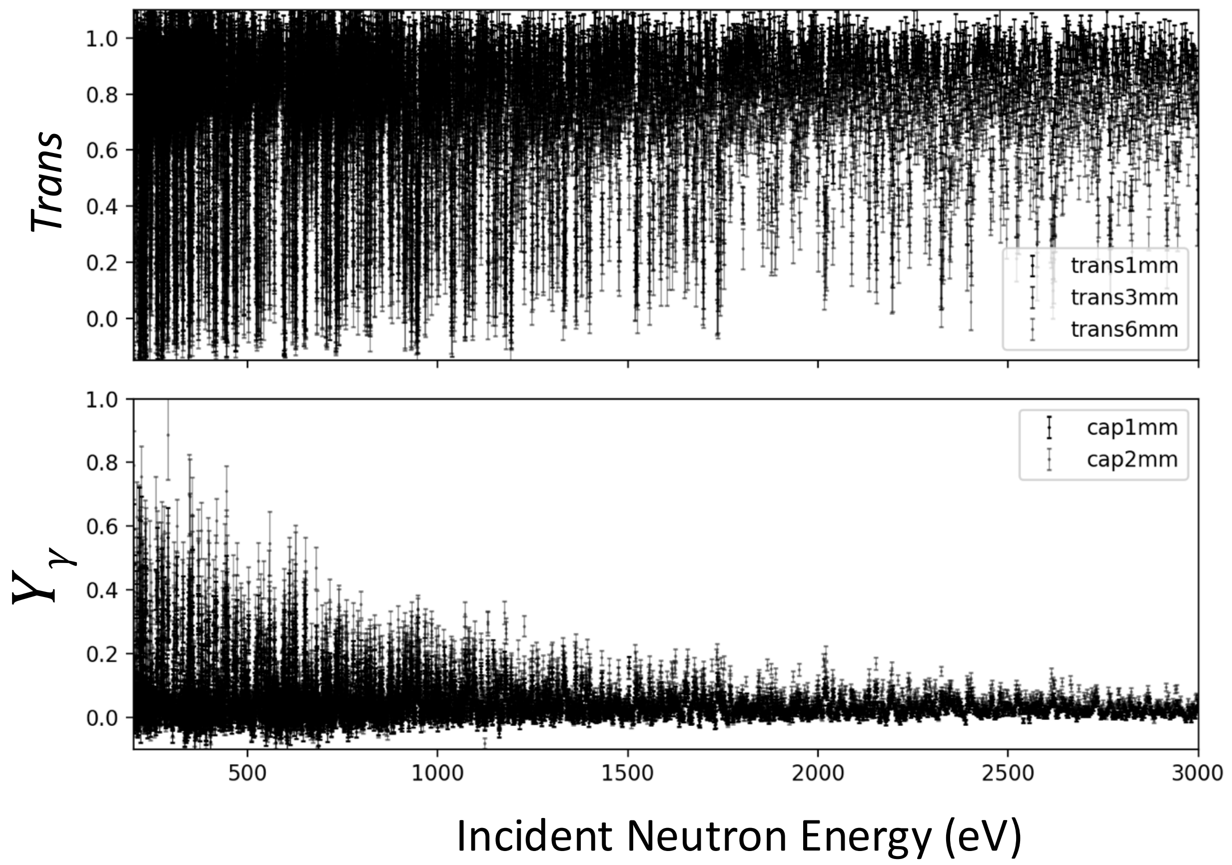
Unique Questions and Answers Revealed in Automated Resonance Fitting and Demonstrated on Ta-181

1. Does differential data have information on the spin group of resonances?
2. Quantitatively assess the impact of the PPP correction for Data Covariance Matrix
3. Smooth deterioration of evaluation performance approaching the URR

Can automation help?

- Manual effort and reproducibility
- Prior evaluations
- Uncertainty quantification

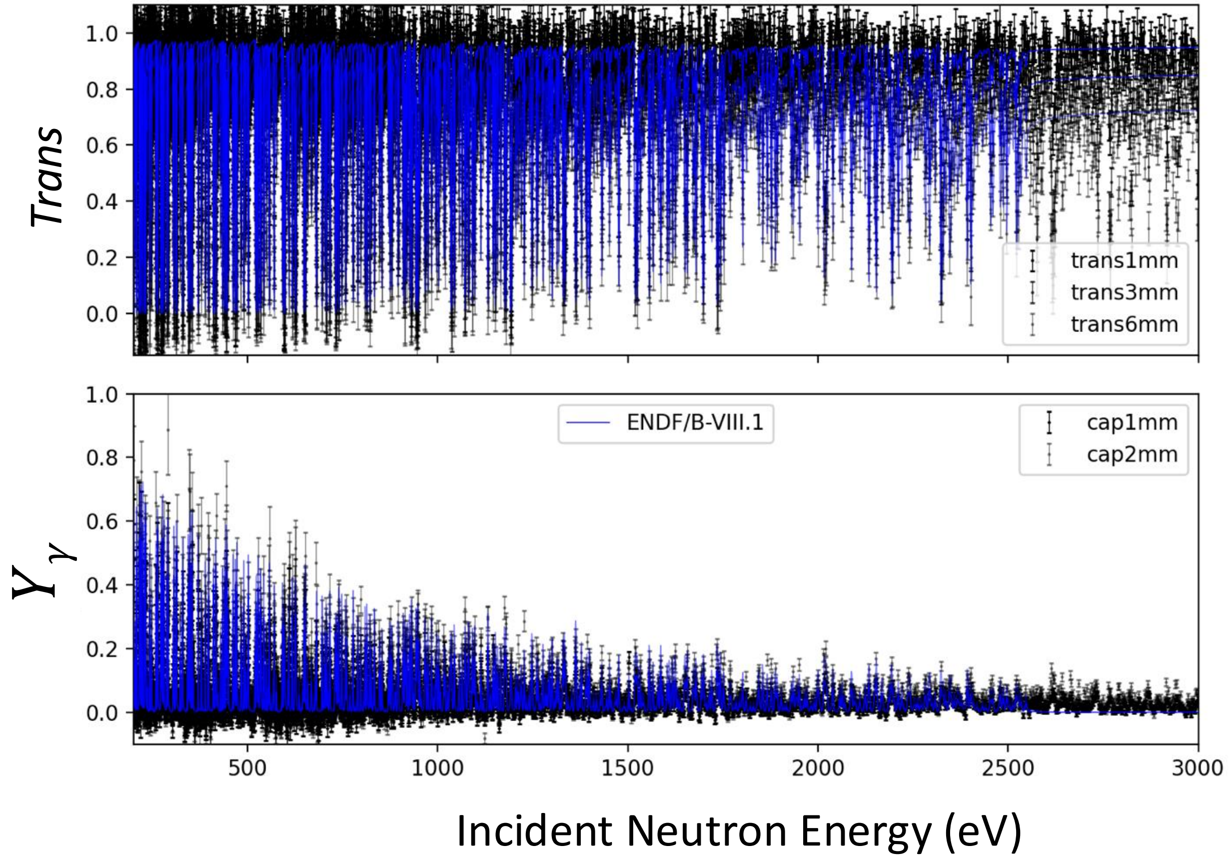
Composite observables used to infer resonance parameters



Challenges in resonance parameter inference

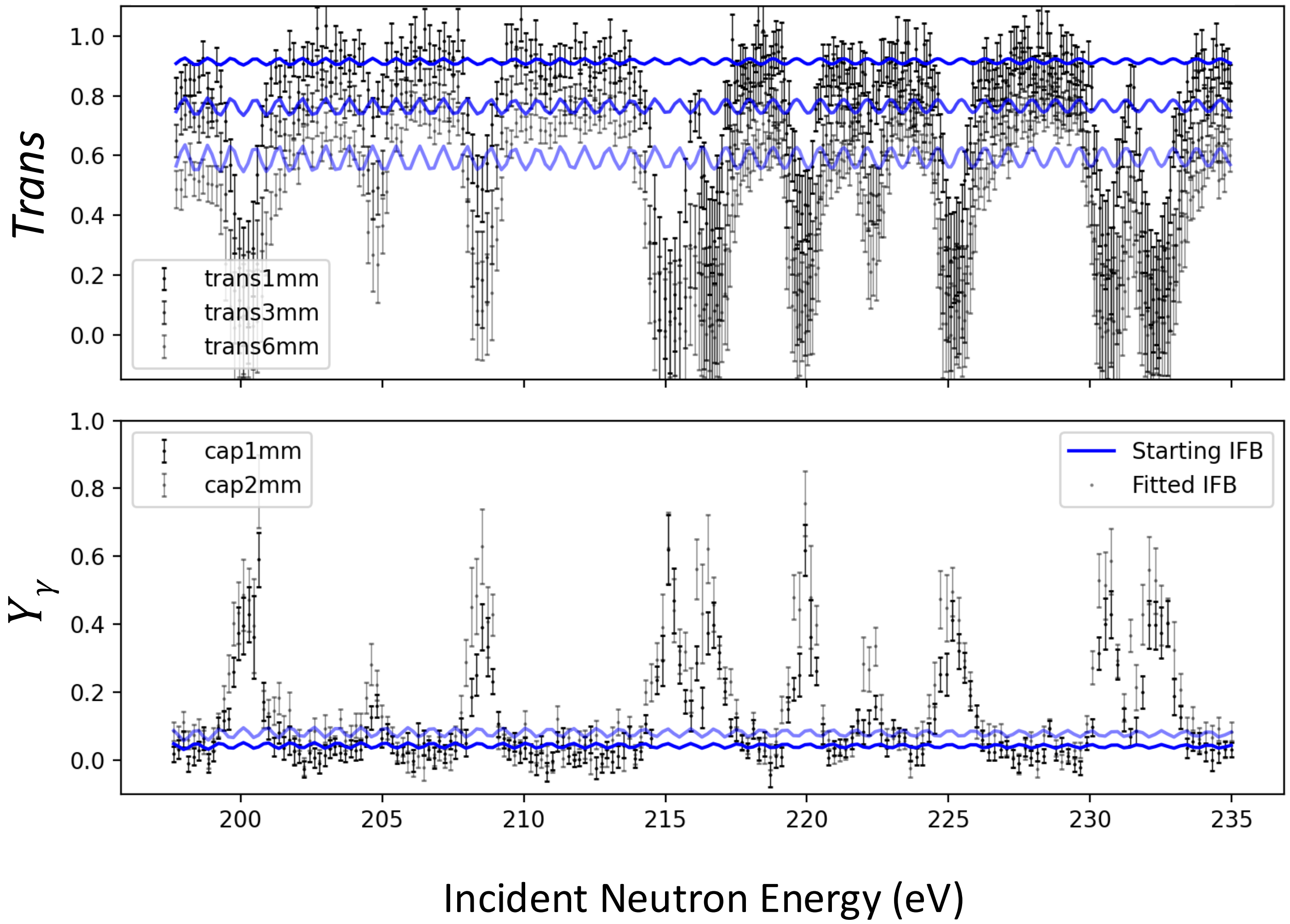
- Manual effort and reproducibility
- Prior evaluations
- Uncertainty quantification

Composite observables used to infer resonance parameters



1. Design initial feature bank

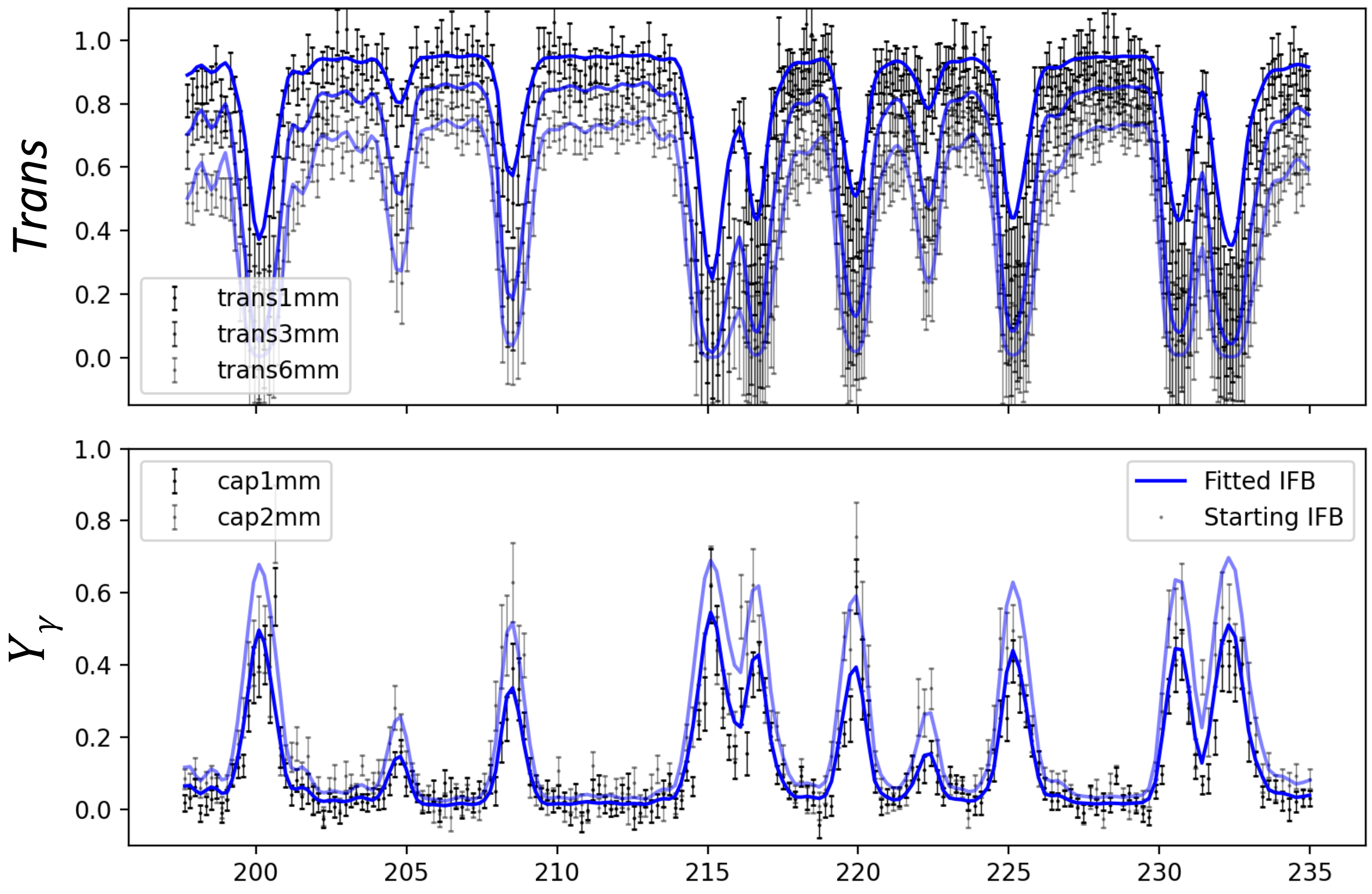
Composite observables used to infer resonance parameters



Automated parameter inference

1. Design initial feature bank
2. Non-linear optimization

Composite observables used to infer resonance parameters

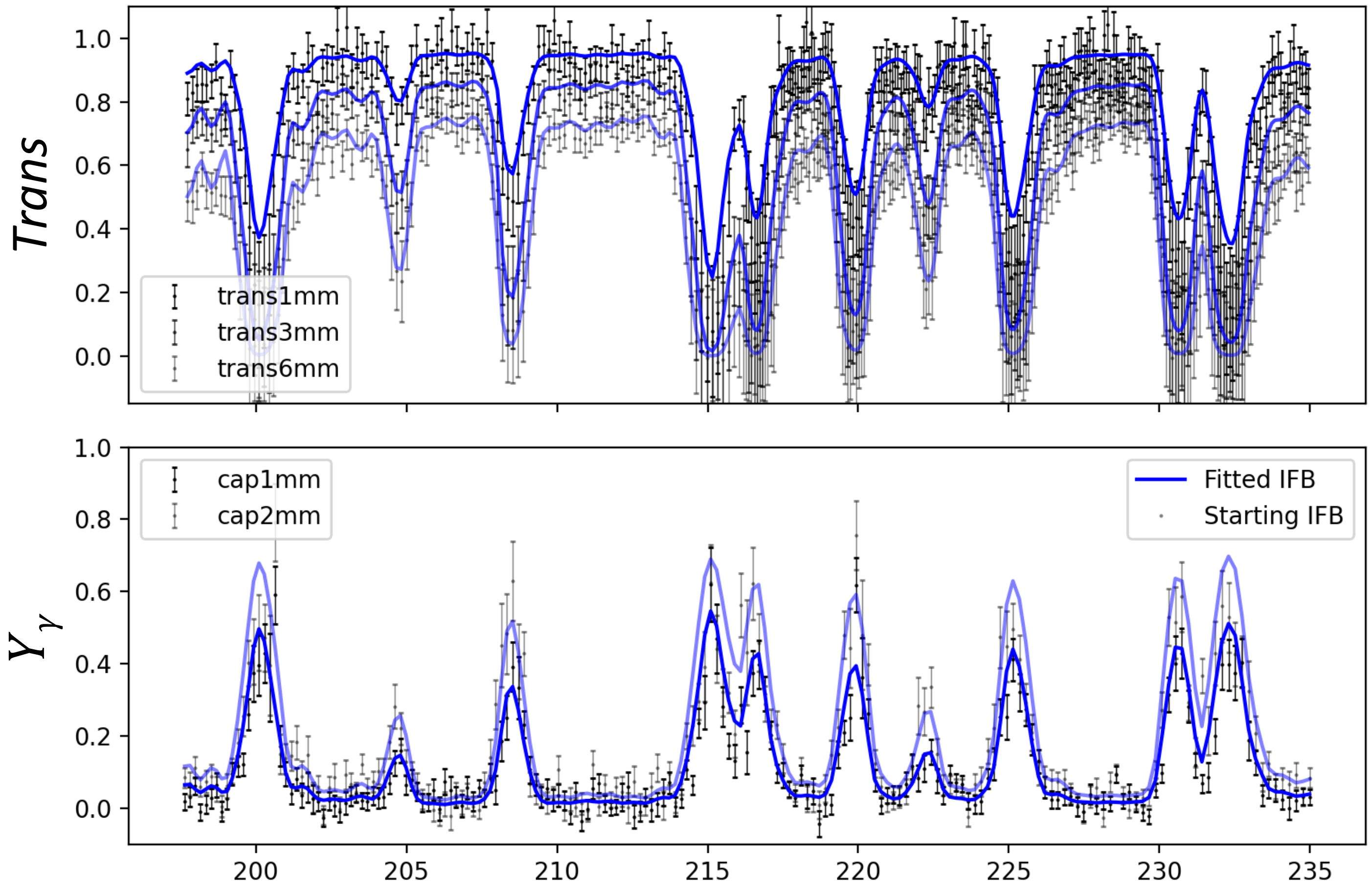


Incident Neutron Energy (eV)

Automated parameter inference

1. Design initial feature bank
2. Non-linear optimization
3. Stepwise variable selection

Composite observables used to infer resonance parameters



Incident Neutron Energy (eV)

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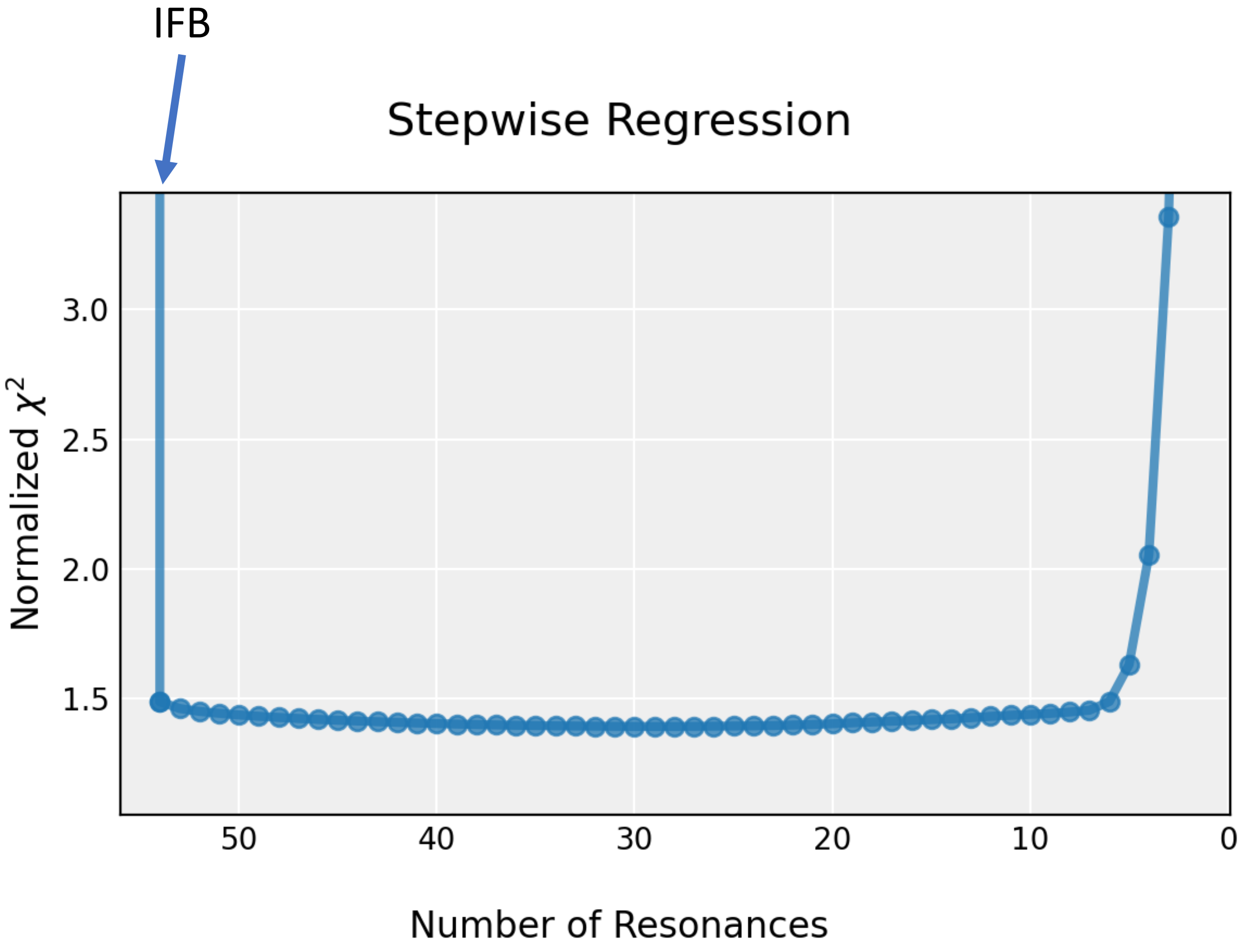
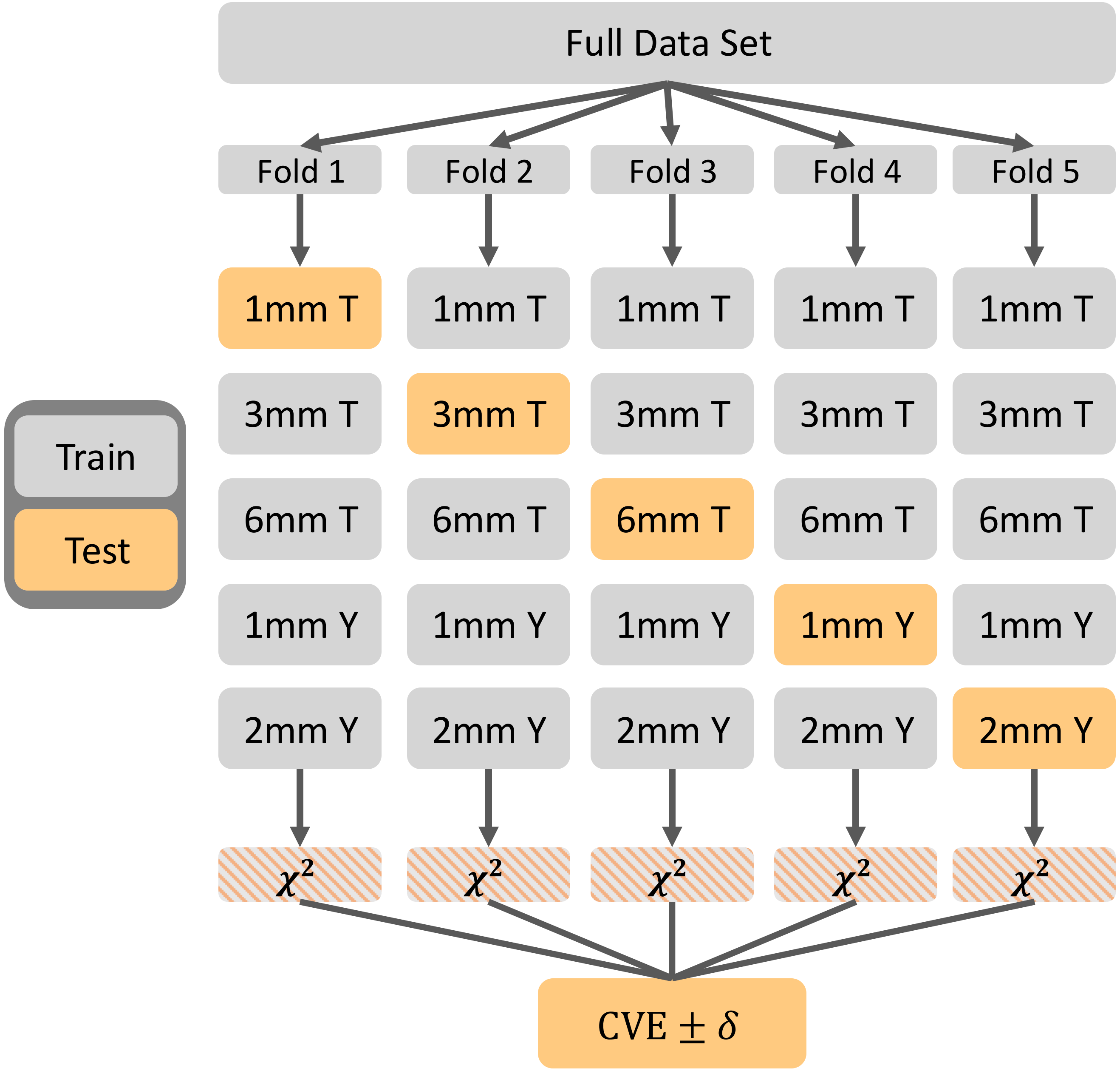
Automated parameter inference

1. Design initial feature bank
2. Non-linear optimization
3. Stepwise variable selection



Automated parameter inference

1. Design initial feature bank
2. Non-linear optimization
3. Stepwise variable selection
4. Cross validation for model selection



Automated parameter inference

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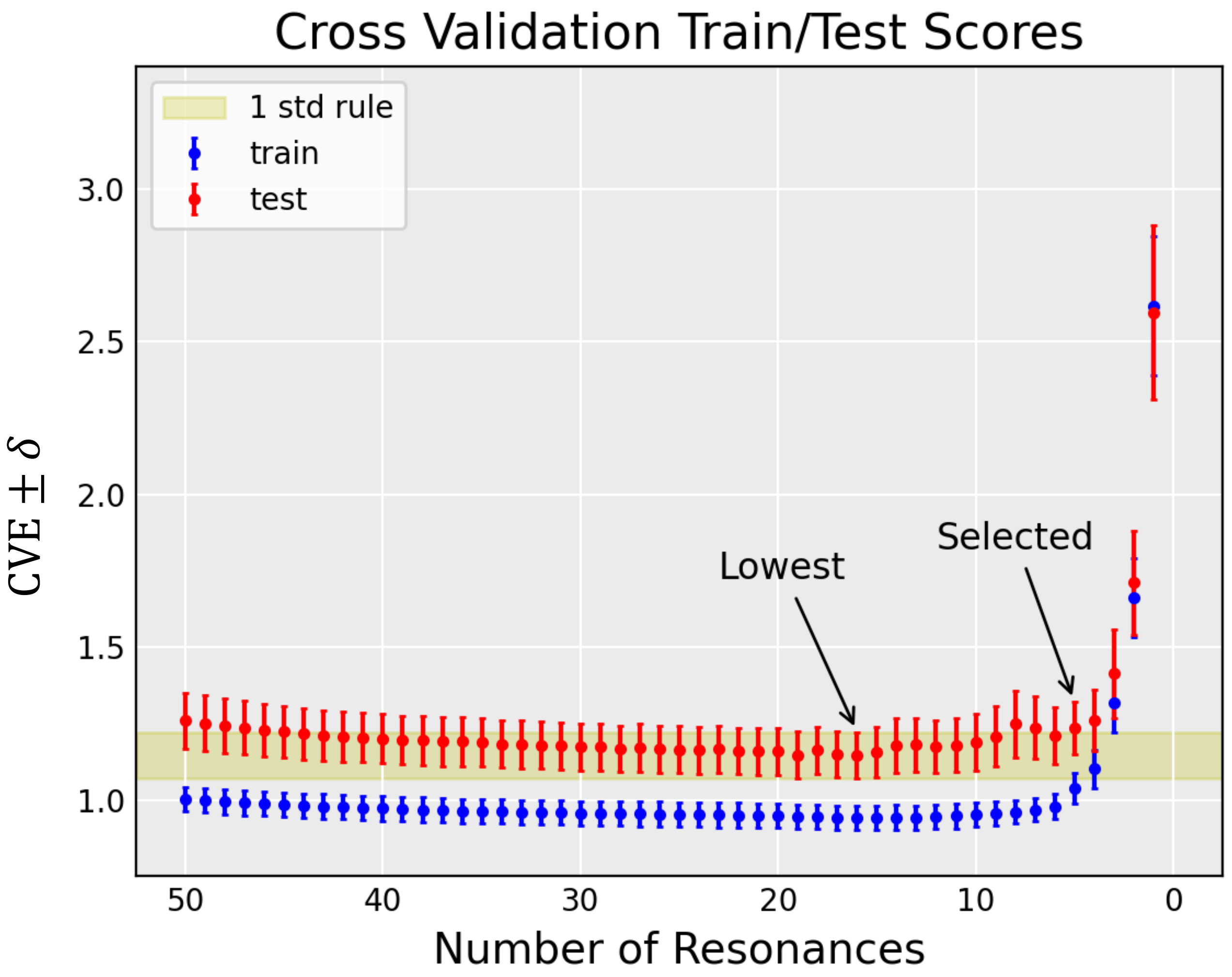

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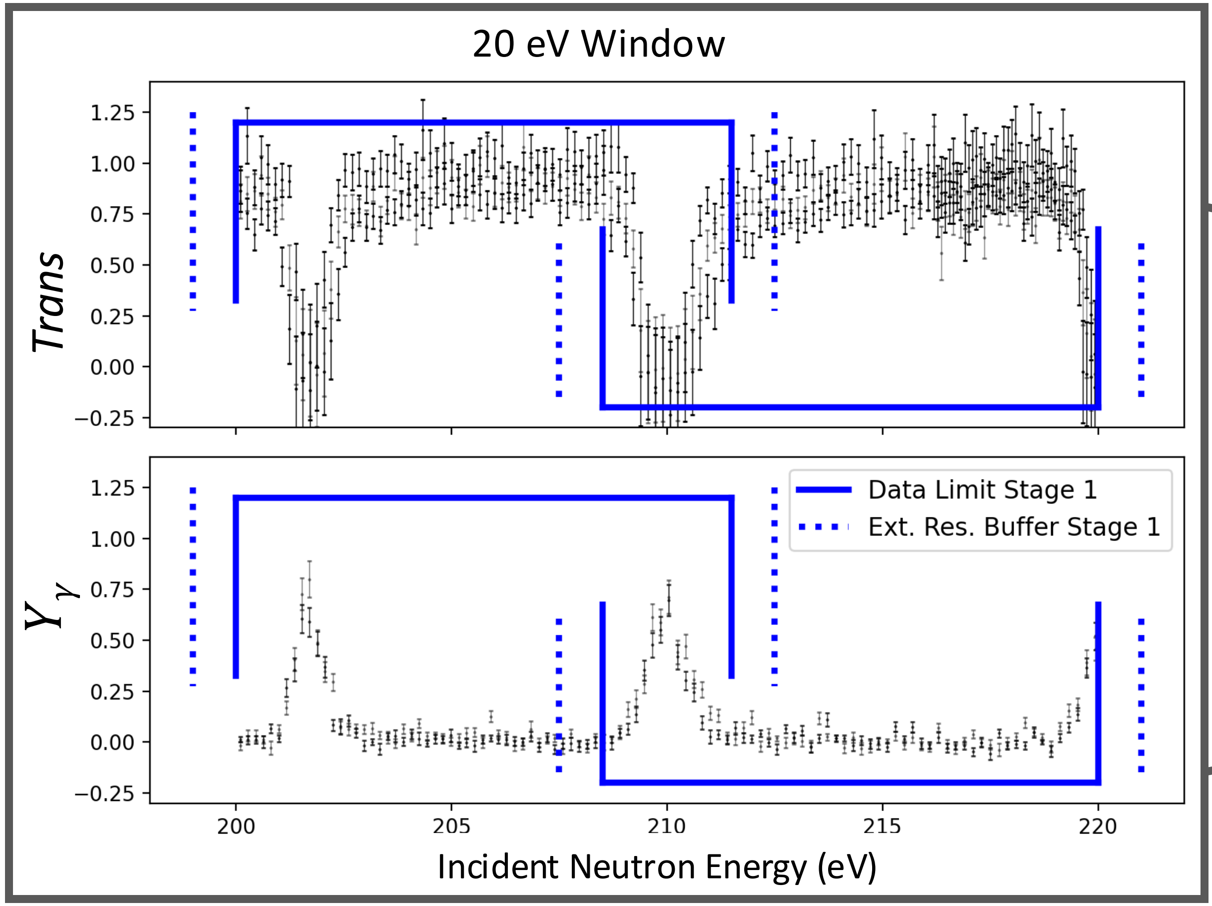
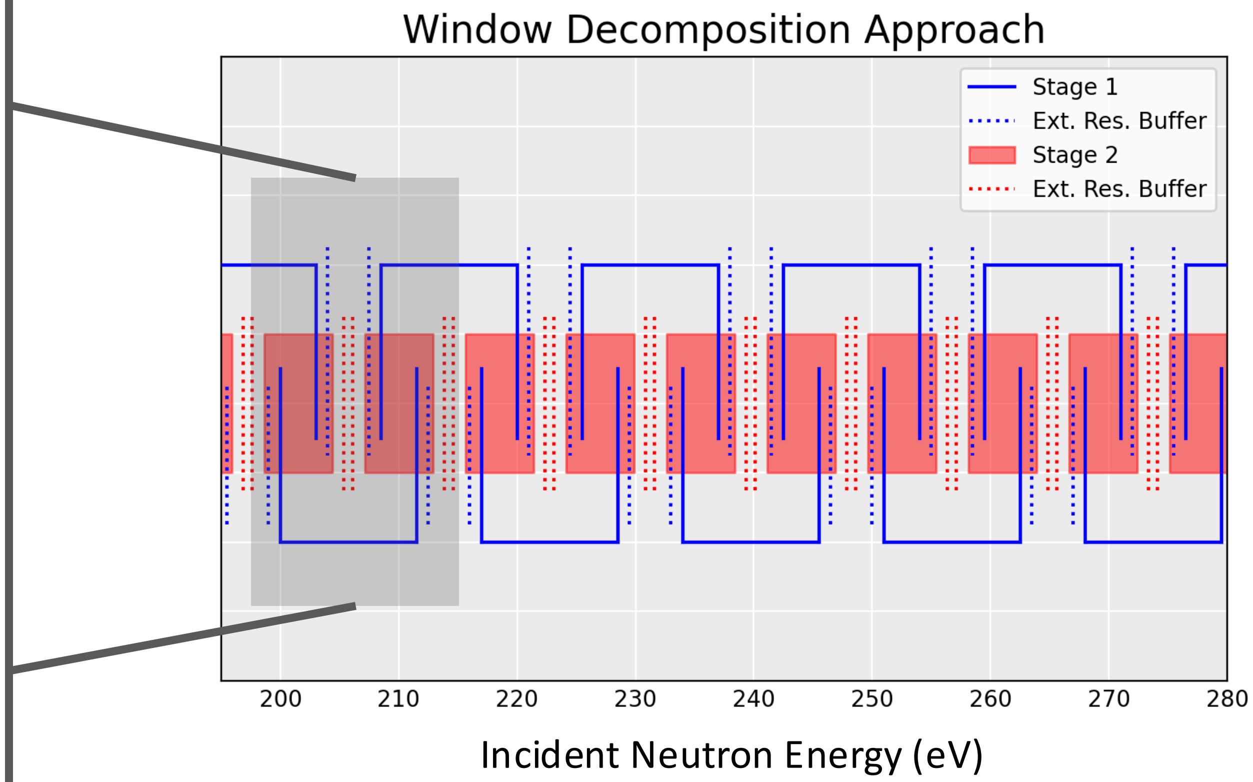
Solved in overlapping windows





AutoFit "Hyperparameters"

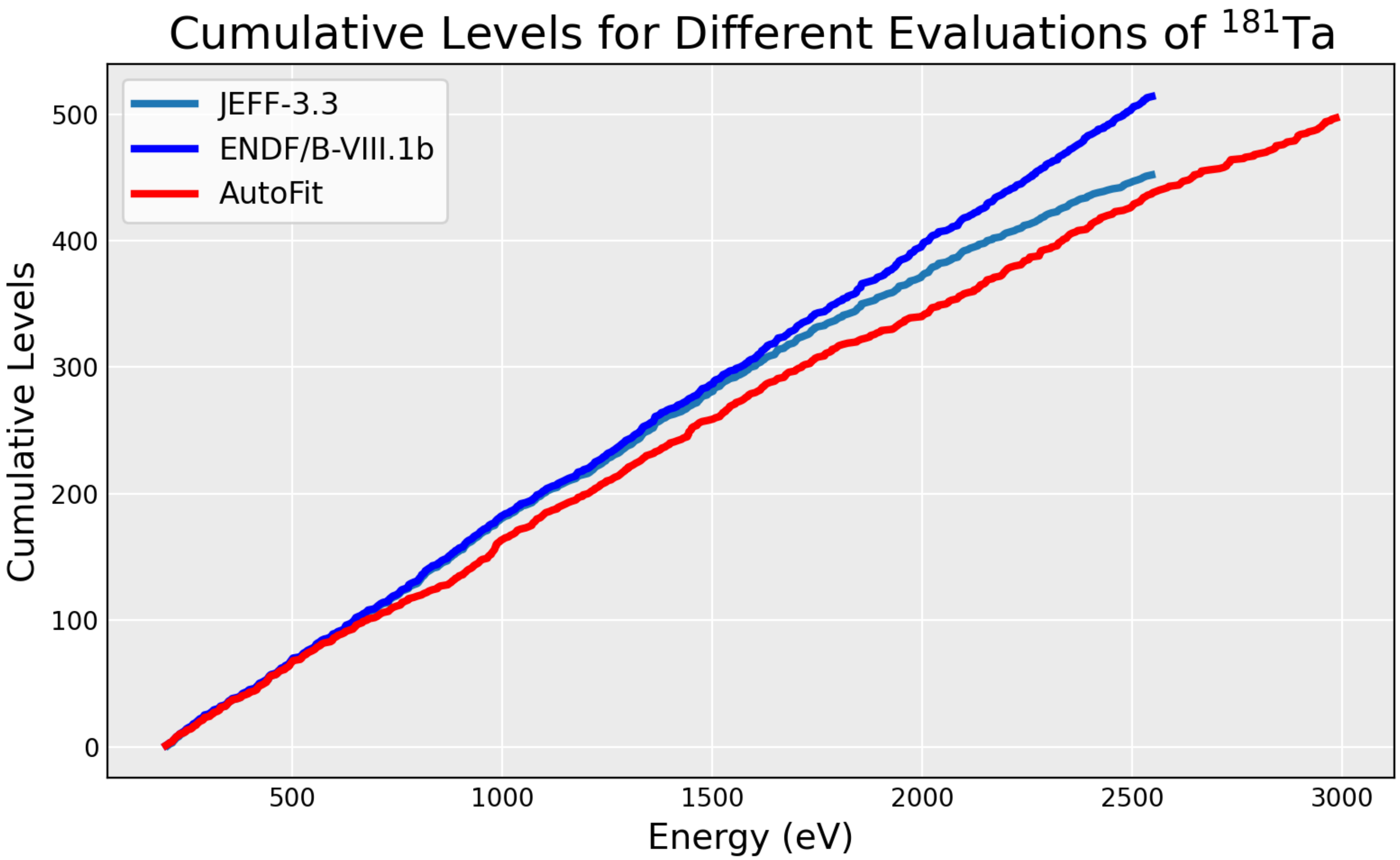
- Few inputs ⇨ reproducible estimates
- Intuition for good settings
- Initial feature bank can integrate with prior knowledge

Parameter	Setting
Initial feature bank design	$\Delta E_\lambda = Q_{\mathrm{W}}(0.01)$
	$\Gamma_\gamma = \langle \Gamma_\gamma \rangle$
	$\Gamma_n = Q_{\mathrm{PT}}(0.1)$
Fitting precision	$\frac{\Delta\chi^2}{N_{\mathrm{d}}} < 0.01$
Stepwise greediness	Low
CV window size	20 eV

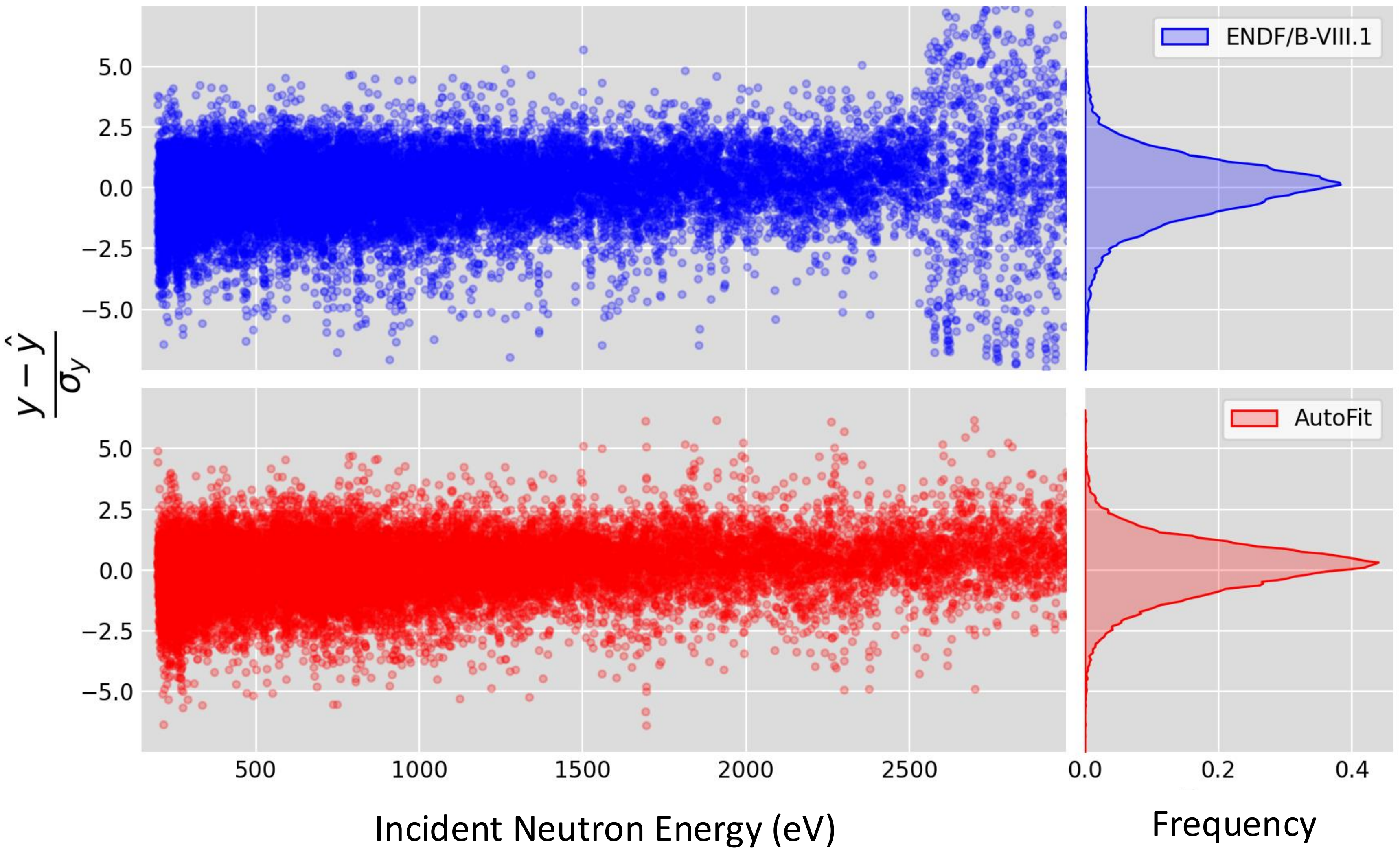
Differences in evaluation methods

	AutoFit	ENDF/B-VIII.1
Spin group selection	χ^2	Atlas/resonance statistics
Fitting method	Simultaneous	Sequential
Small fake resonances added	No	Yes
Datasets used in 200-2550eV	5	6
Fit Γ_γ	Average +/- 2%	Average +/- 2%
Prior evaluation	None	JEFF-3.3

AutoFit prefers parsimonious models



Normalized Residuals For Different Fitting Approaches

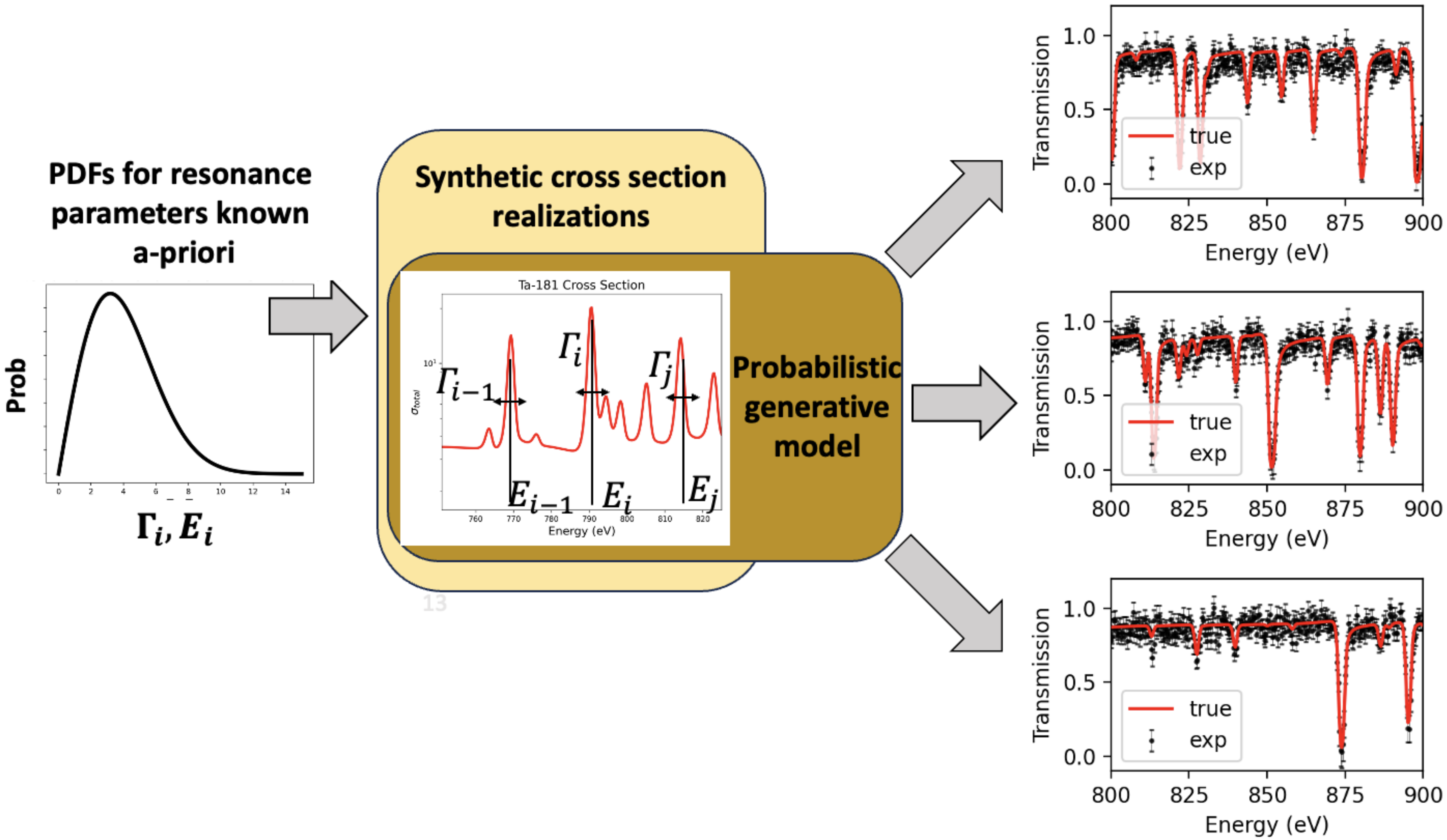


χ^2 calculated below 2500 eV

Fitting Method	χ^2/N_{data}
AutoFit	1.354
ENDF/B-VIII.1	1.698
ENDF/B-VIII.1 Fit	1.581

Synthetic Data Testing Framework

Sampled Resonance Ladders

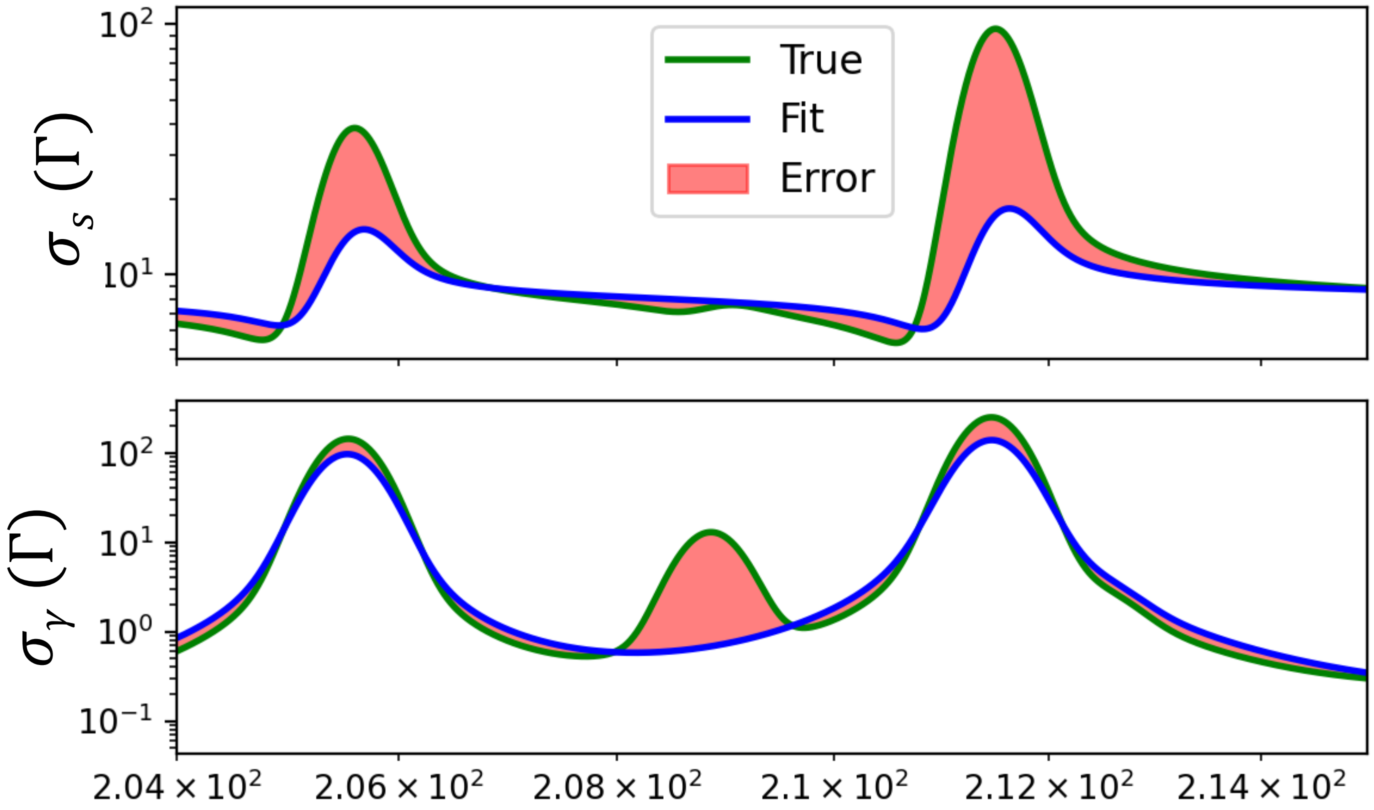


$$\text{True} = \sigma_{\text{rxn}}(\Gamma_{\text{True}})$$

$$\text{Fit} = \sigma_{\text{rxn}}(\Gamma_{\text{Fit}})$$

- Root Mean Squared Error (RMSE)

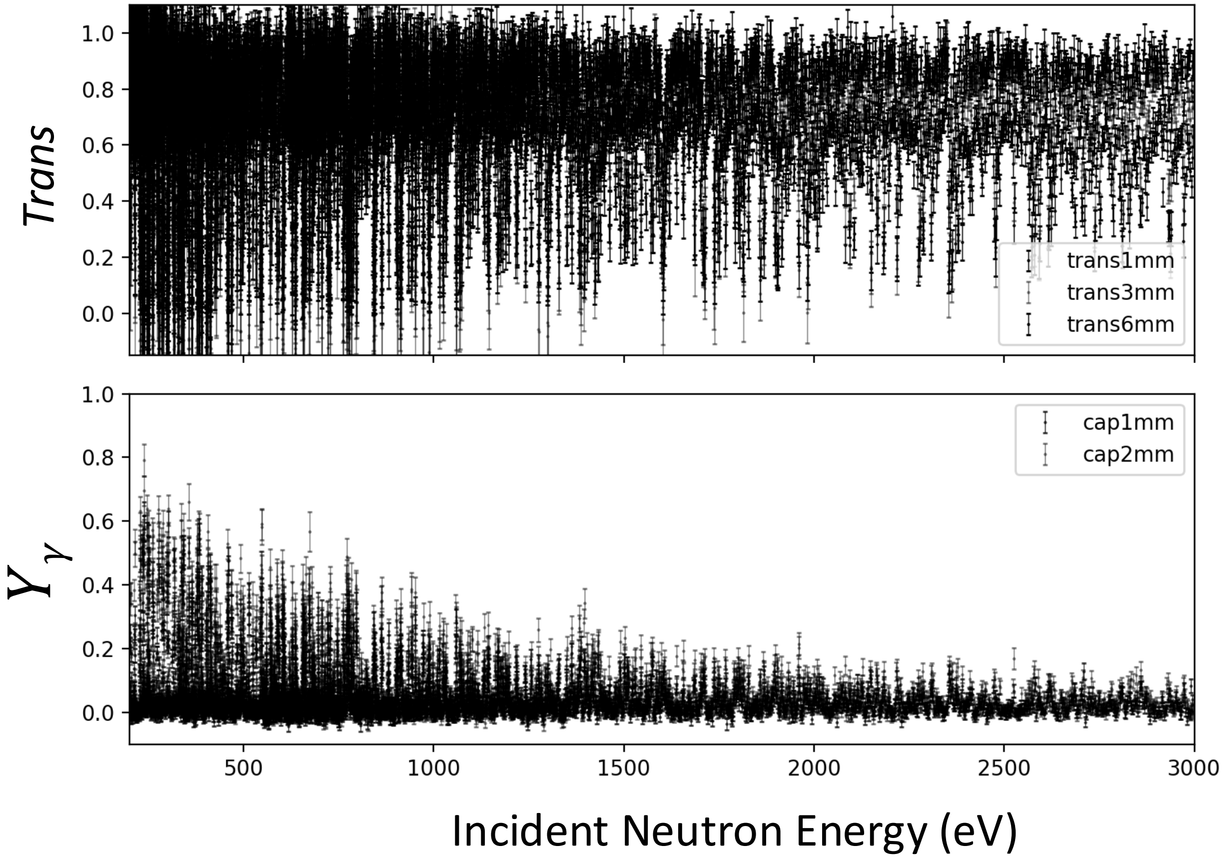
Doppler Broadened Reaction Cross Sections



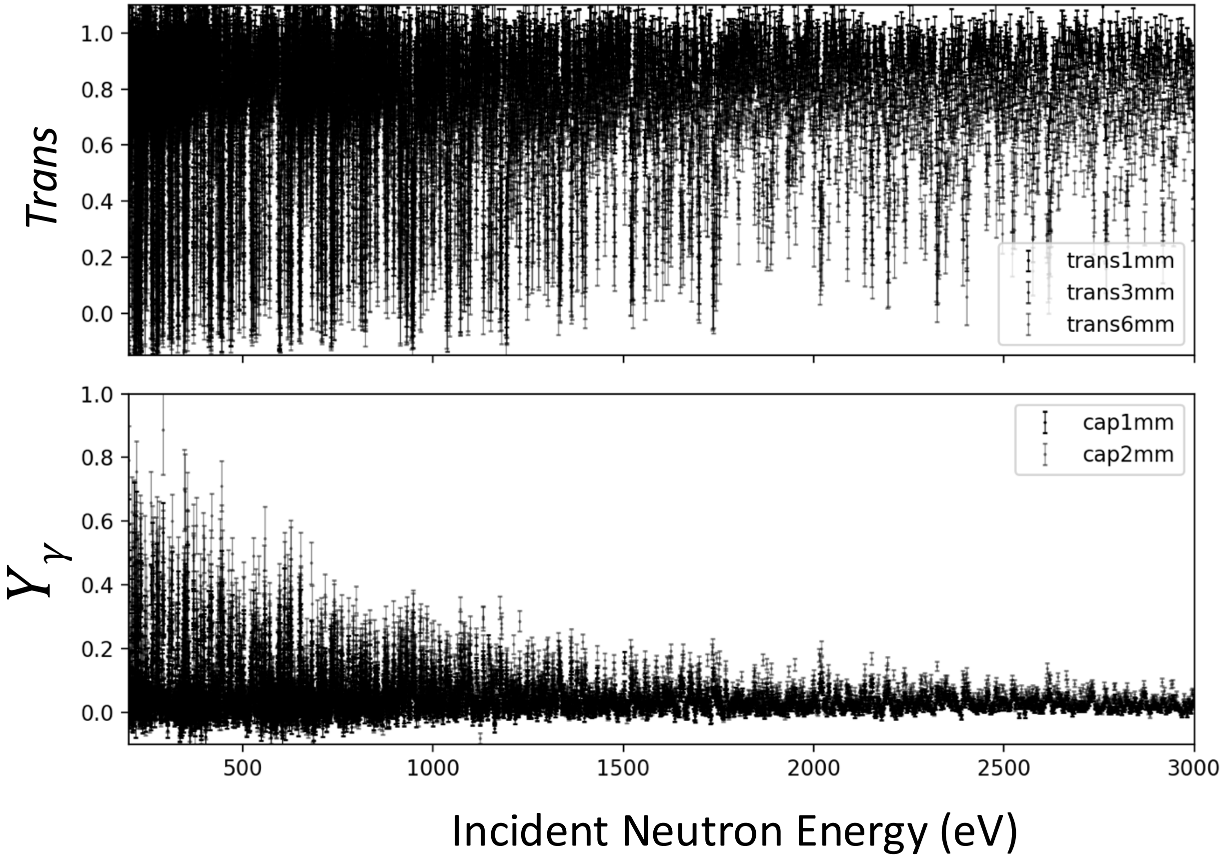
Incident Neutron Energy (eV)

Generative Models Developed Mimicking Actual Measurements

5 Measurements Synthetically Generated



5 Measurements by Brown, et al.



What questions does this allow us to ask?

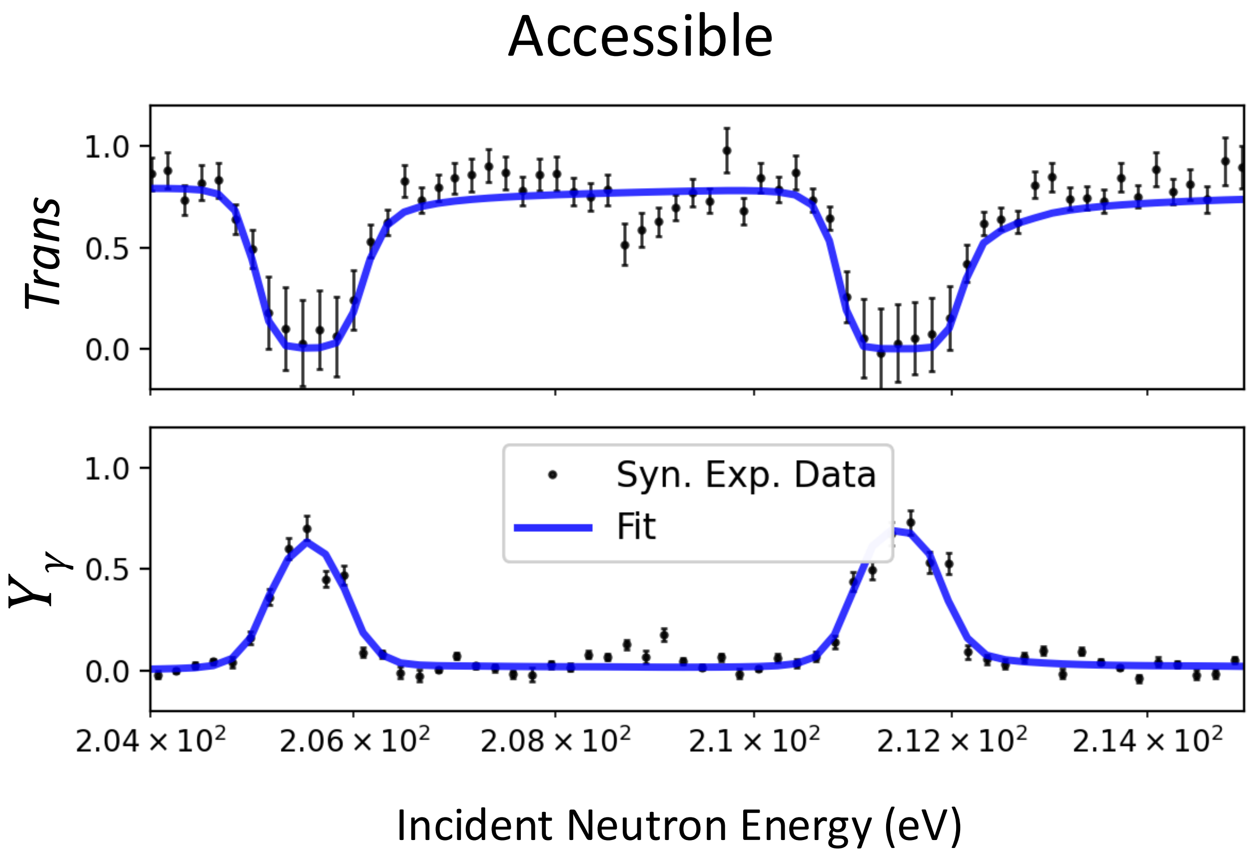
Different Regression Objectives

$$\mathrm{LS} = (D - T)^T (D - T)$$

$$\mathrm{WLS} = (D - T)^T V^{-1} (D - T)$$
$$\text{where}: \ V_{i \neq j} = 0$$

$$\chi^2_{\mathrm{D}} = (D - T)^T V^{-1} (D - T)$$

$$\chi^2_{\mathrm{T}} = (D - T)^T V(T)^{-1} (D - T)$$



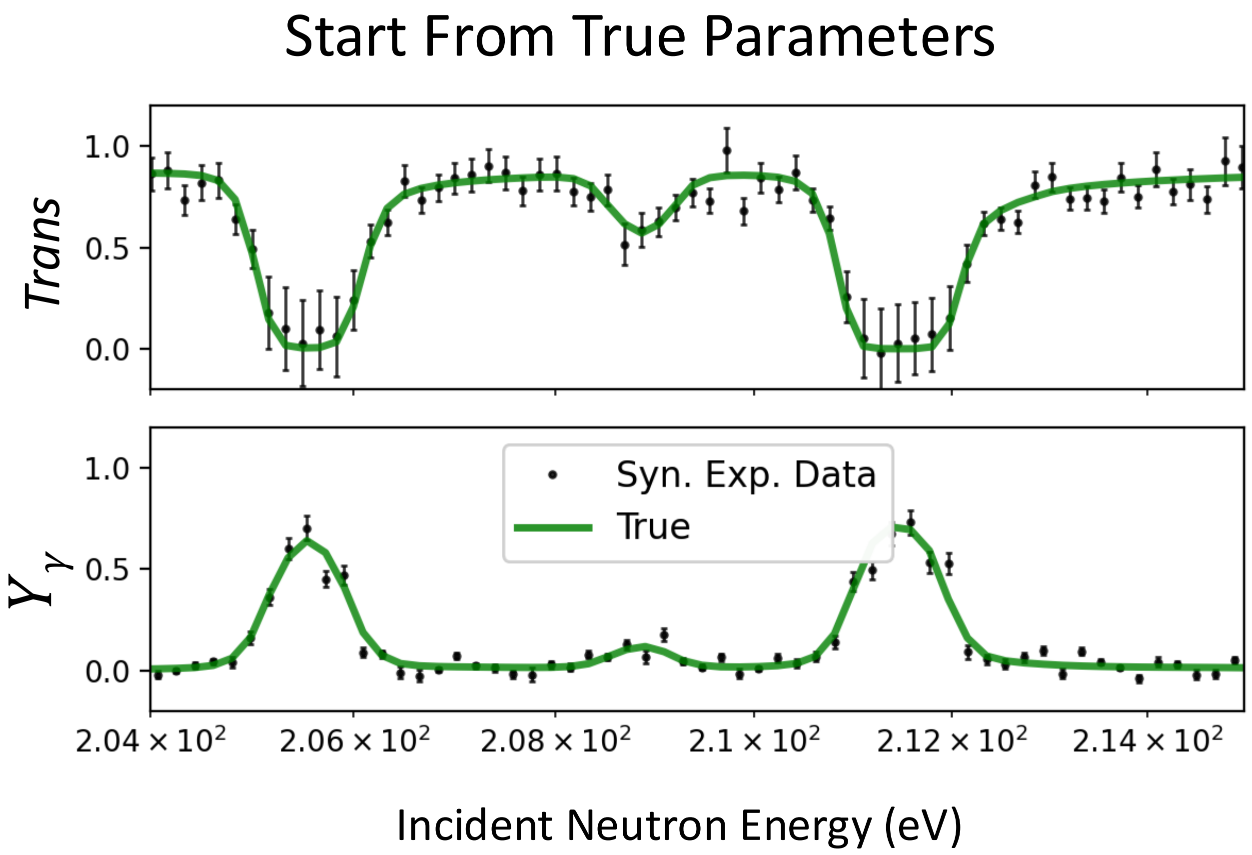
Start From True Parameters

$$\mathrm{LS} = (D-T)^T(D-T)$$

$$\mathrm{WLS} = (D-T)^T V^{-1}(D-T)$$
$$\text{where}: \; V_{i\neq j} = 0$$

$$\chi^2_{\mathrm{D}} = (D-T)^T V^{-1}(D-T)$$

$$\chi^2_{\mathrm{T}} = (D-T)^T V(T)^{-1}(D-T)$$



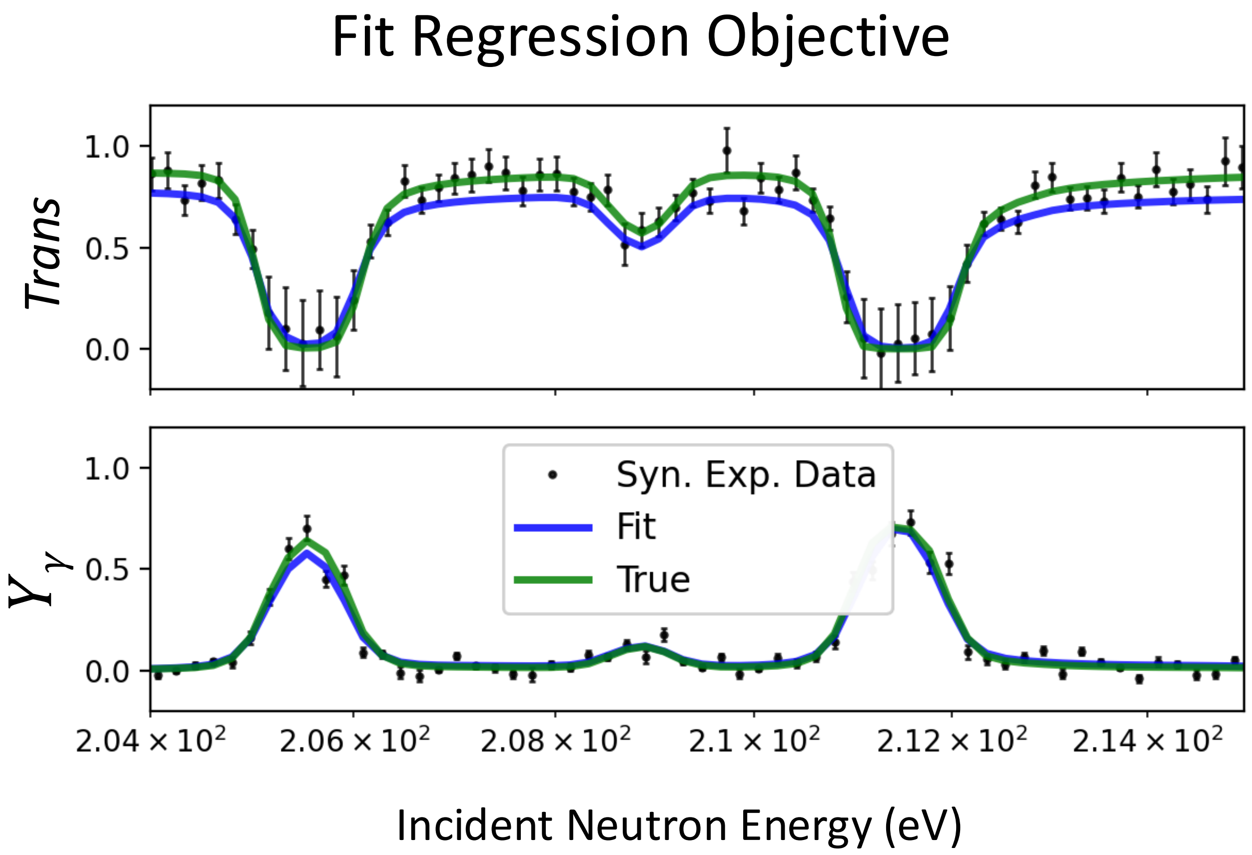
Fit Regression Objective

$$\mathrm{LS} = (D - T)^T (D - T)$$

$$\mathrm{WLS} = (D - T)^T V^{-1} (D - T)$$
$$\text{where}: \; V_{i \neq j} = 0$$

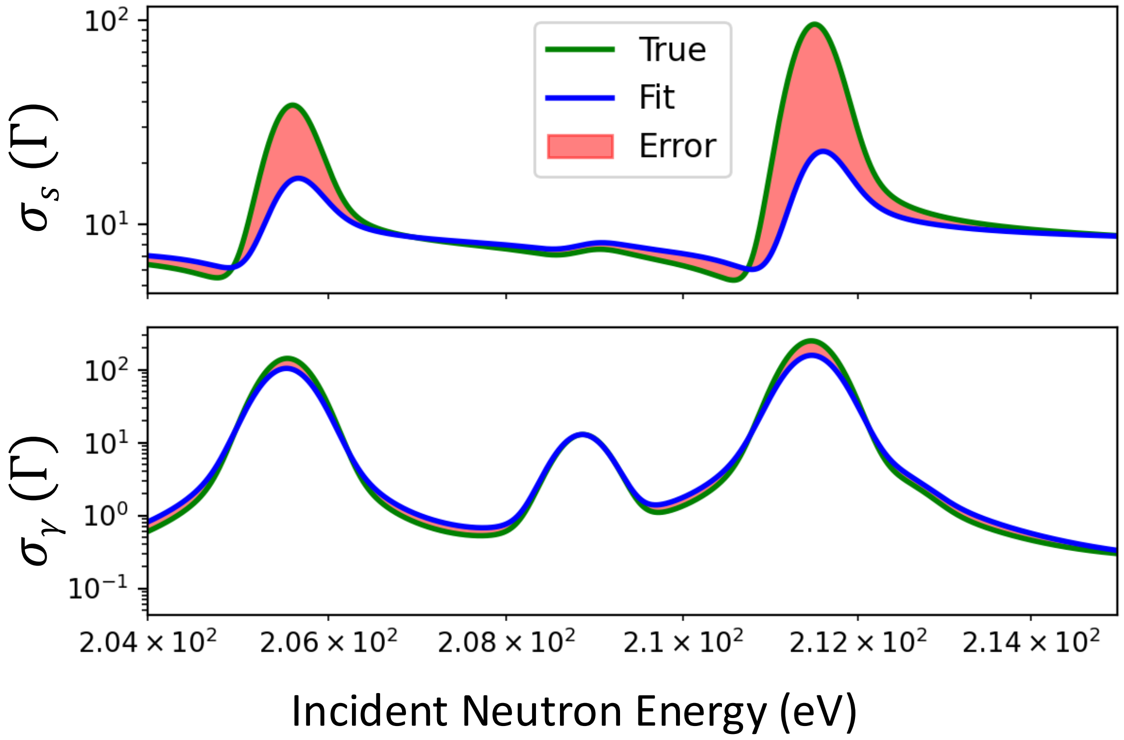
$$\chi^2_{\mathrm{D}} = (D - T)^T V^{-1} (D - T)$$

$$\chi^2_{\mathrm{T}} = (D - T)^T V(T)^{-1} (D - T)$$

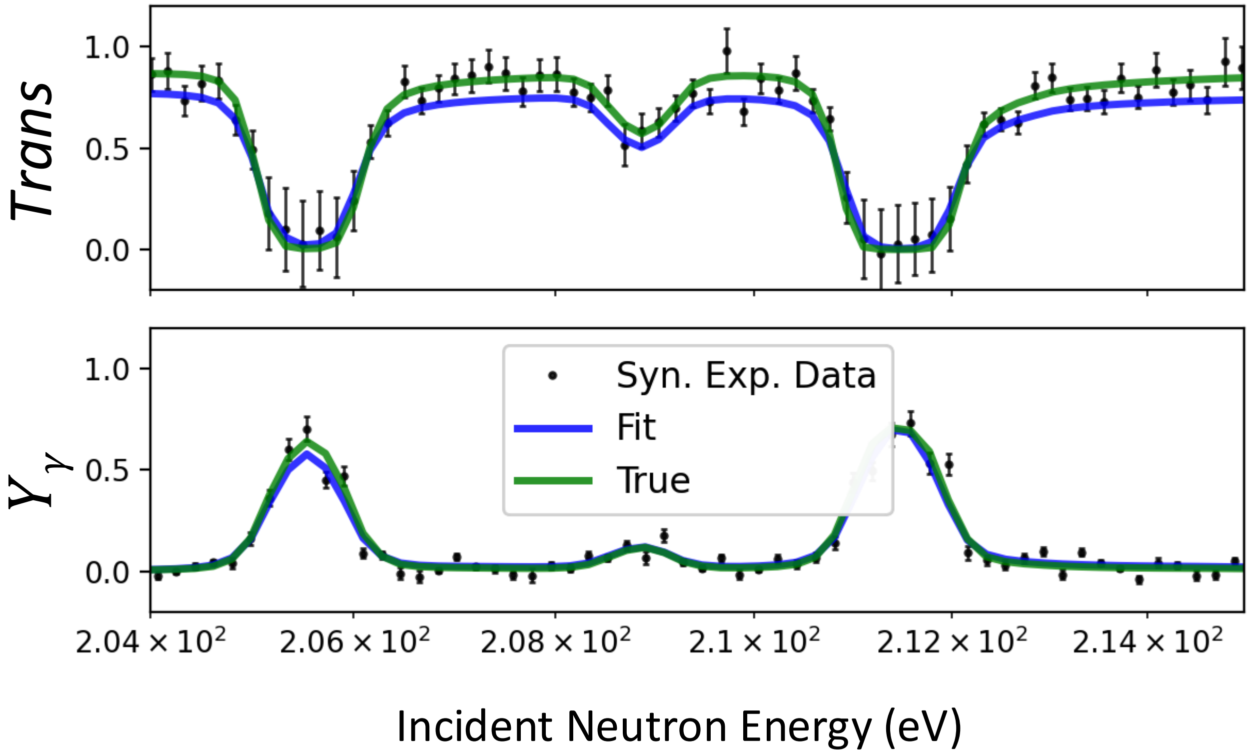


Inaccessible Objective = Metric

Compare Theoretical Objective

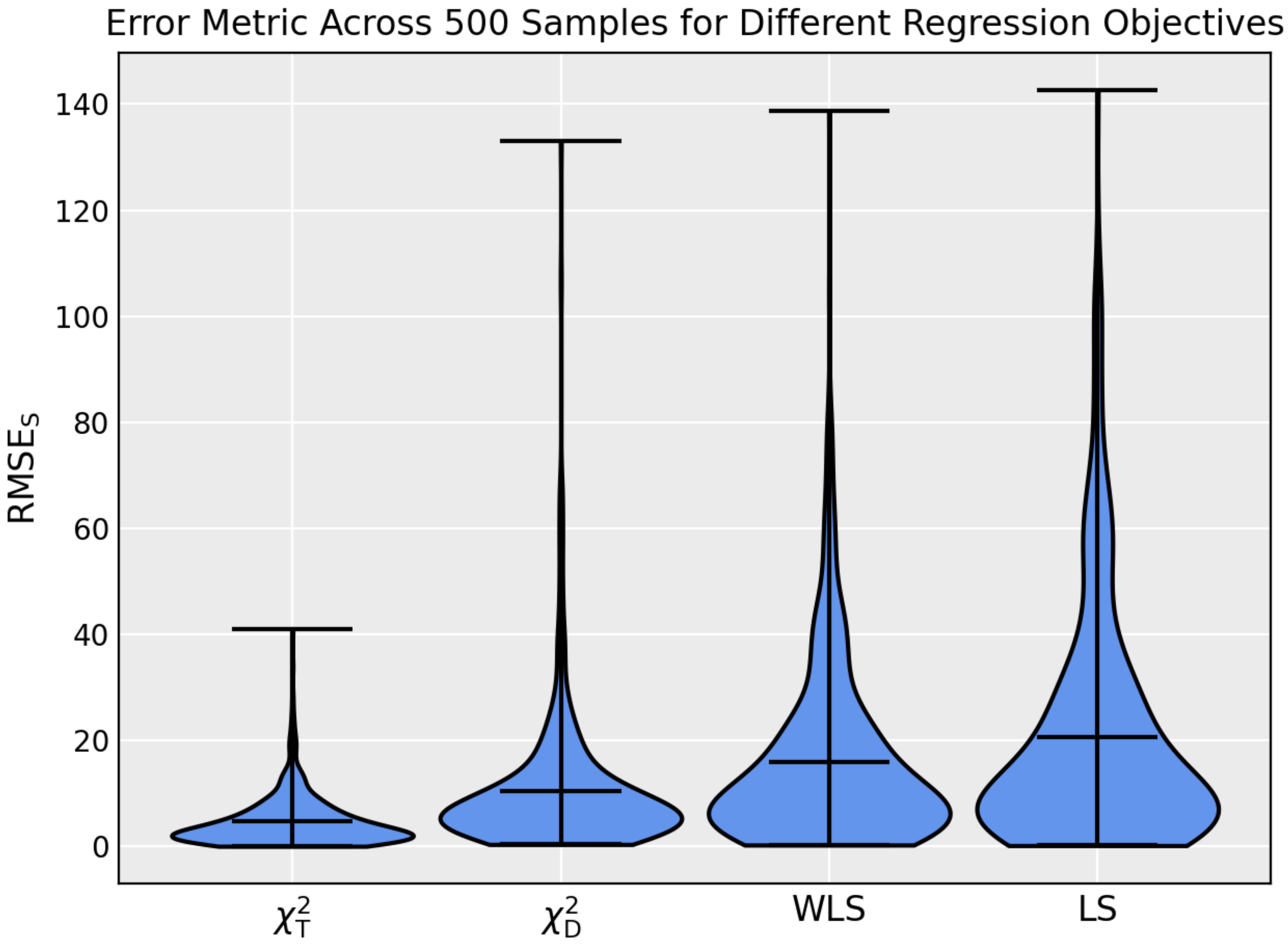


Fit Regression Objective



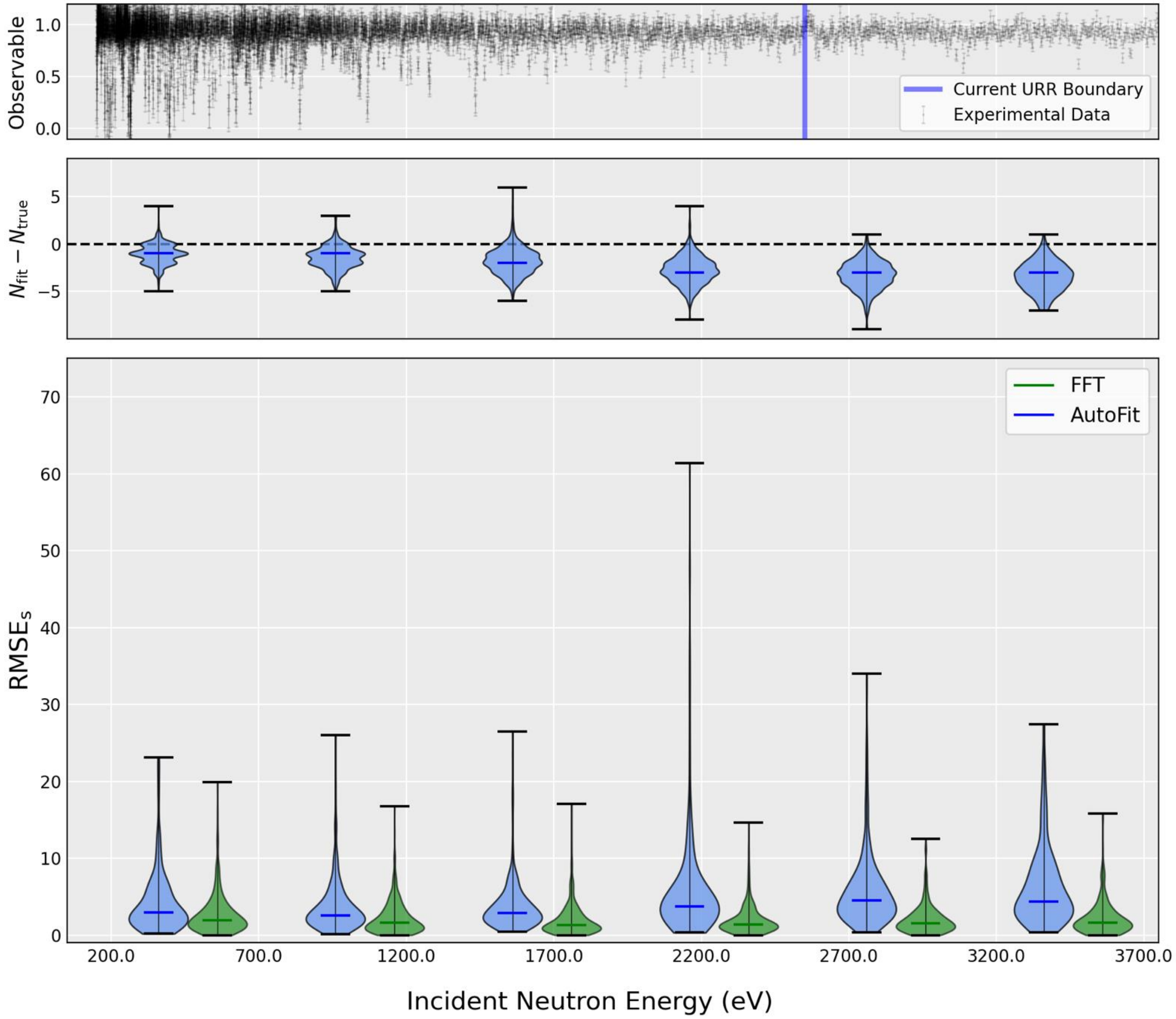
Repeated over 500 Samples

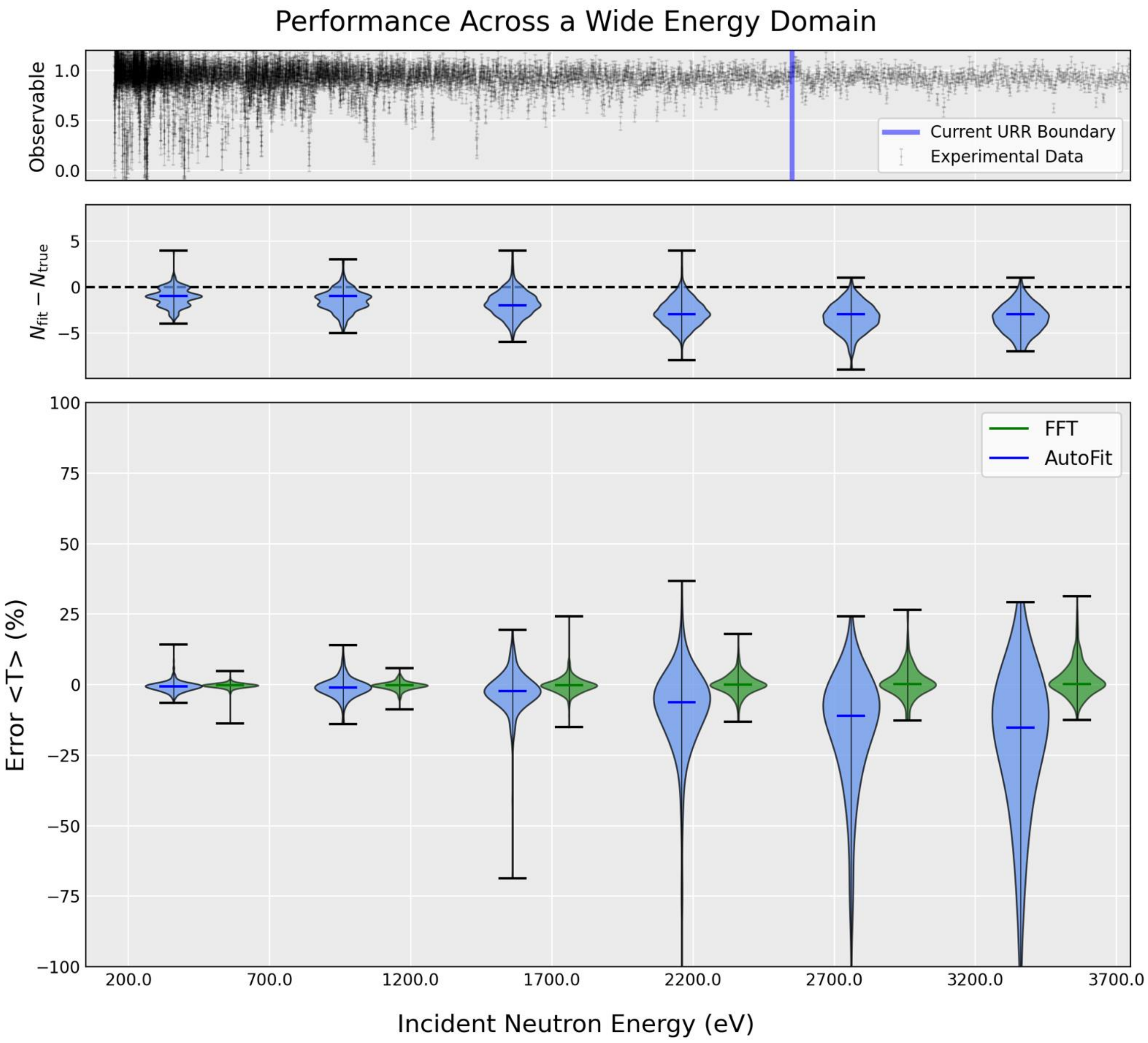
Surrogate Objective	RMSE (bn)	MAE (bn)
χ^2_{T}	6.68	1.40
χ^2_{D}	16.37	3.22
WLS	23.40	4.97
LS	30.88	6.74



URR Study

Performance Across a Wide Energy Domain




Performance Across a Wide Energy Domain
Observable
1.0
0.5
0.0
Current URR Boundary
Experimental Data
$N_{\mathrm{fit}} - N_{\mathrm{true}}$
5
0
−5
Error <T> (%)
100
75
50
25
0
−25
−50
−75
−100
FFT
AutoFit
200.0
700.0
1200.0
1700.0
2200.0
2700.0
3200.0
3700.0
Incident Neutron Energy (eV)

ATARI

AI/ML Tool for Automated Resonance Inference

Computational framework: ATARI

- Automated resonance inference is **reproducible** and **fast**
- Performance can be **tested** and **benchmarked**
- Constant PPP bias even if correlations are small
- Future work: resonance parameter statistics, uncertainty quantification

Ta-181 Analysis

- Minimal deterioration of **theoretical objective** approaching URR
- **Regression objective** is as-good-or-better that ENDF/B-VIII.1 evaluation
- Differential data has **some** spin information

NSSC

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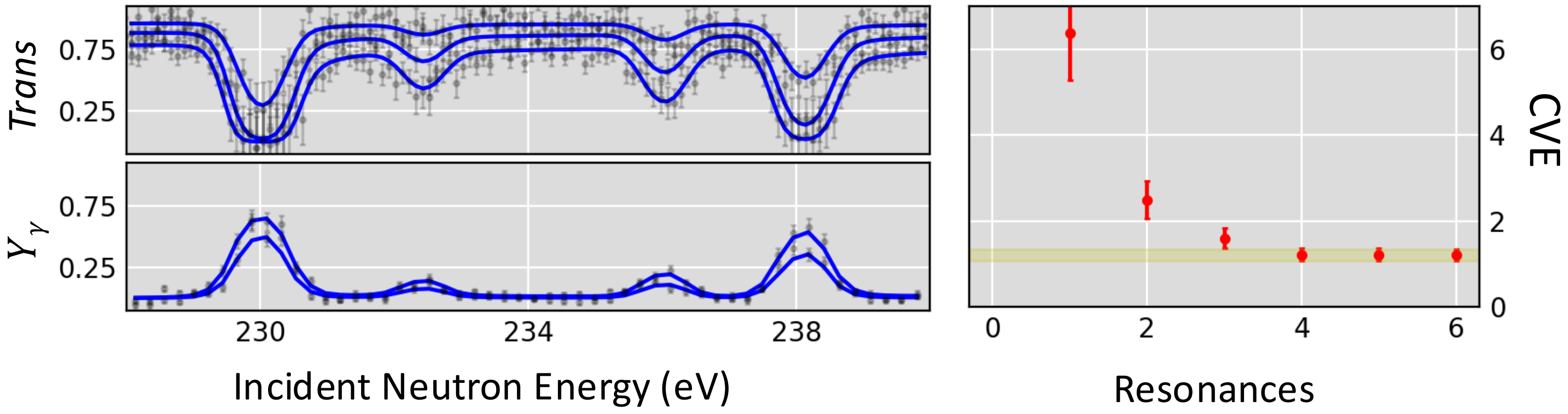
Impact of Window Size on CV-model selection



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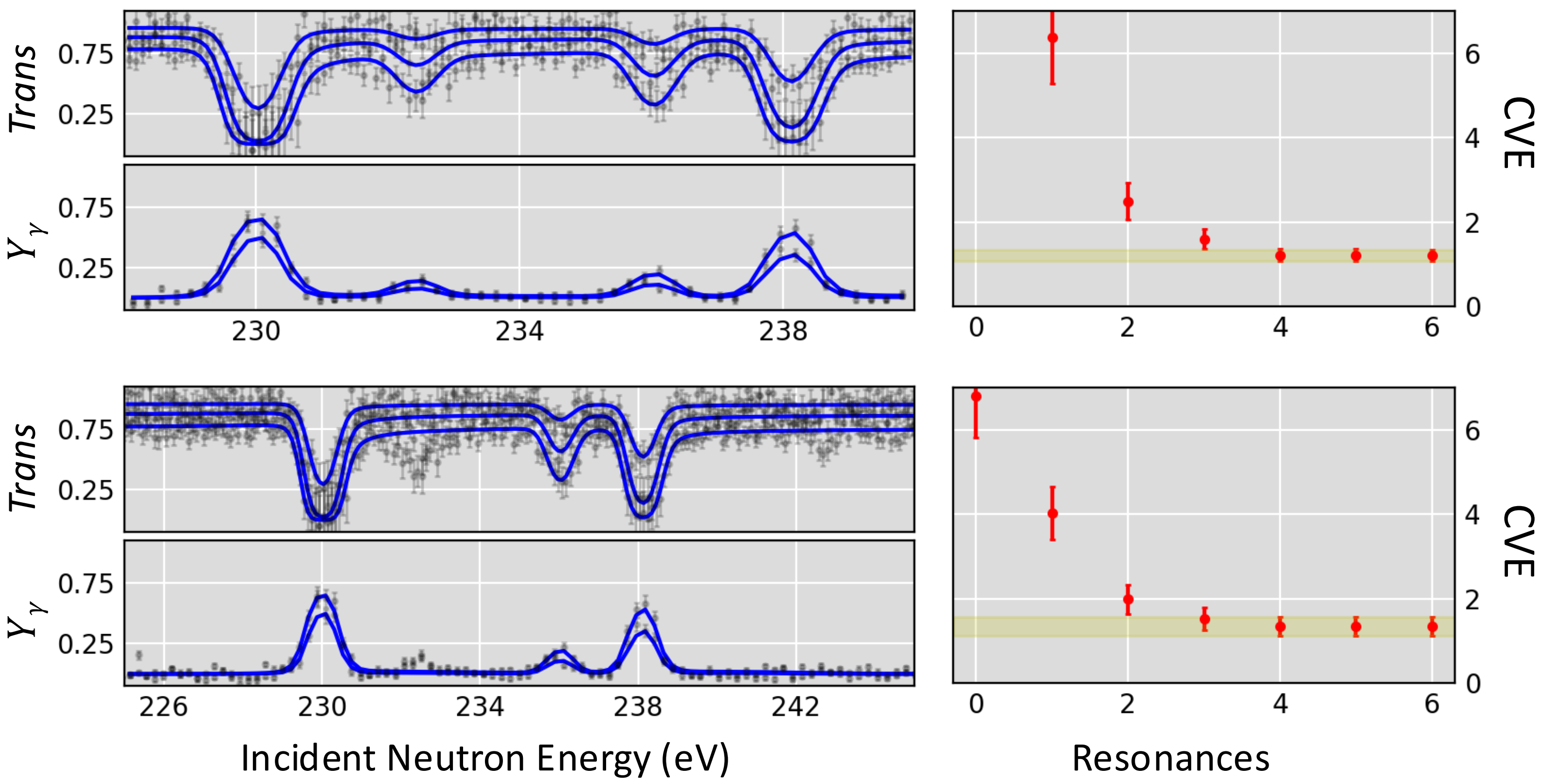

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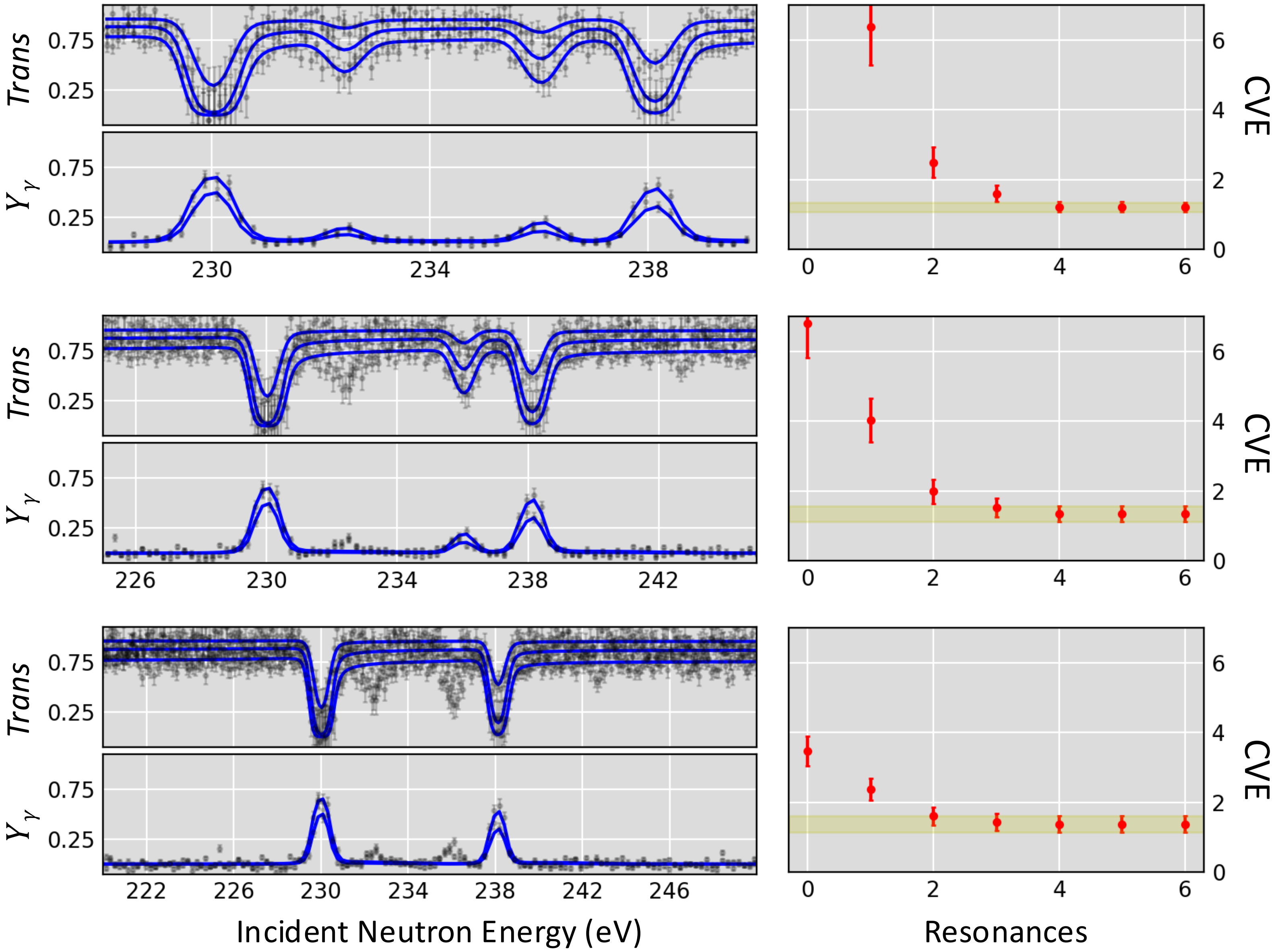
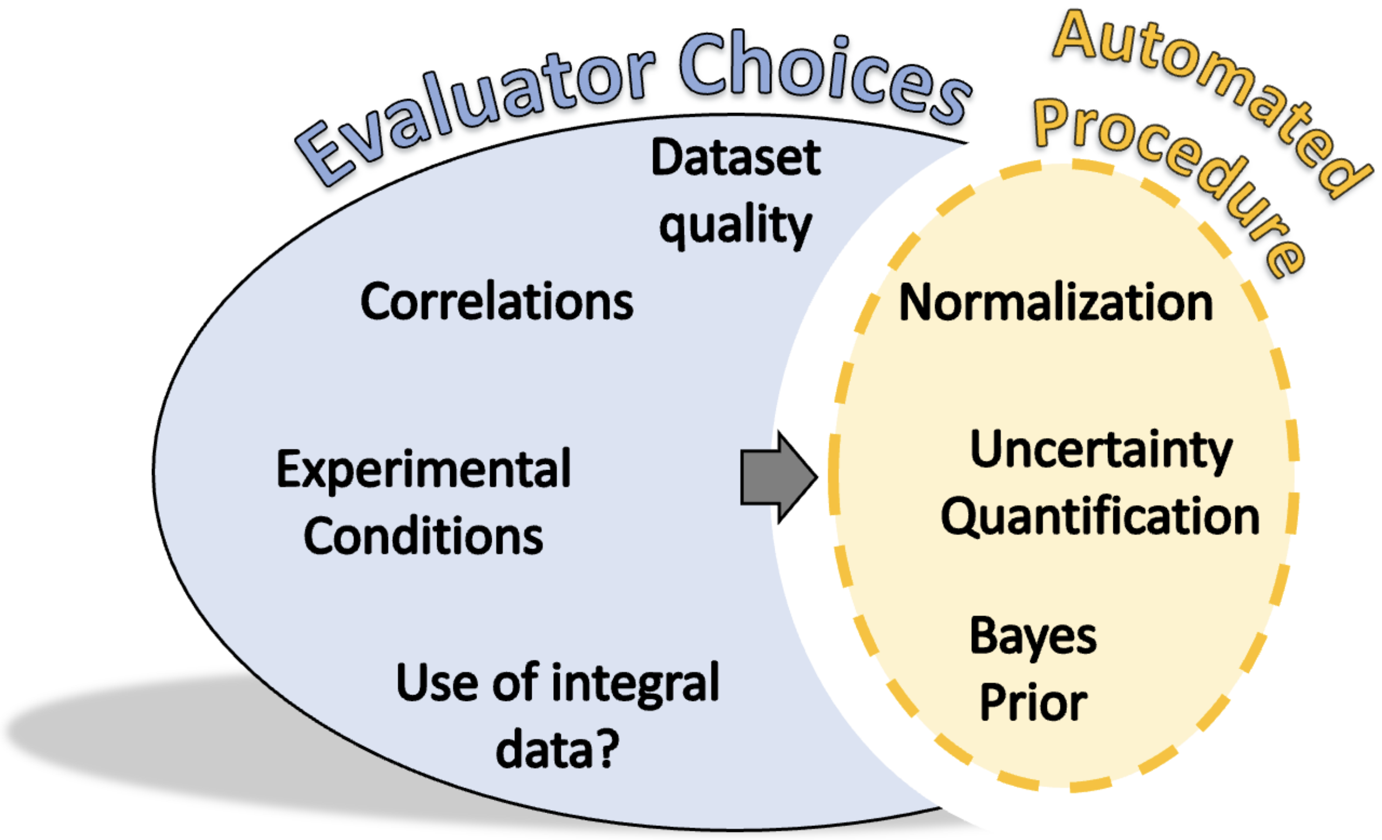


Automated parameter inference

1. Develop automated tool
   - Augment evaluators
2. Computational experiments
   - Benchmark tool
   - Improve tool
   - Learn new physics



Computational Framework