Towards rigorous and reproducible uncertainty quantification in resonance evaluation

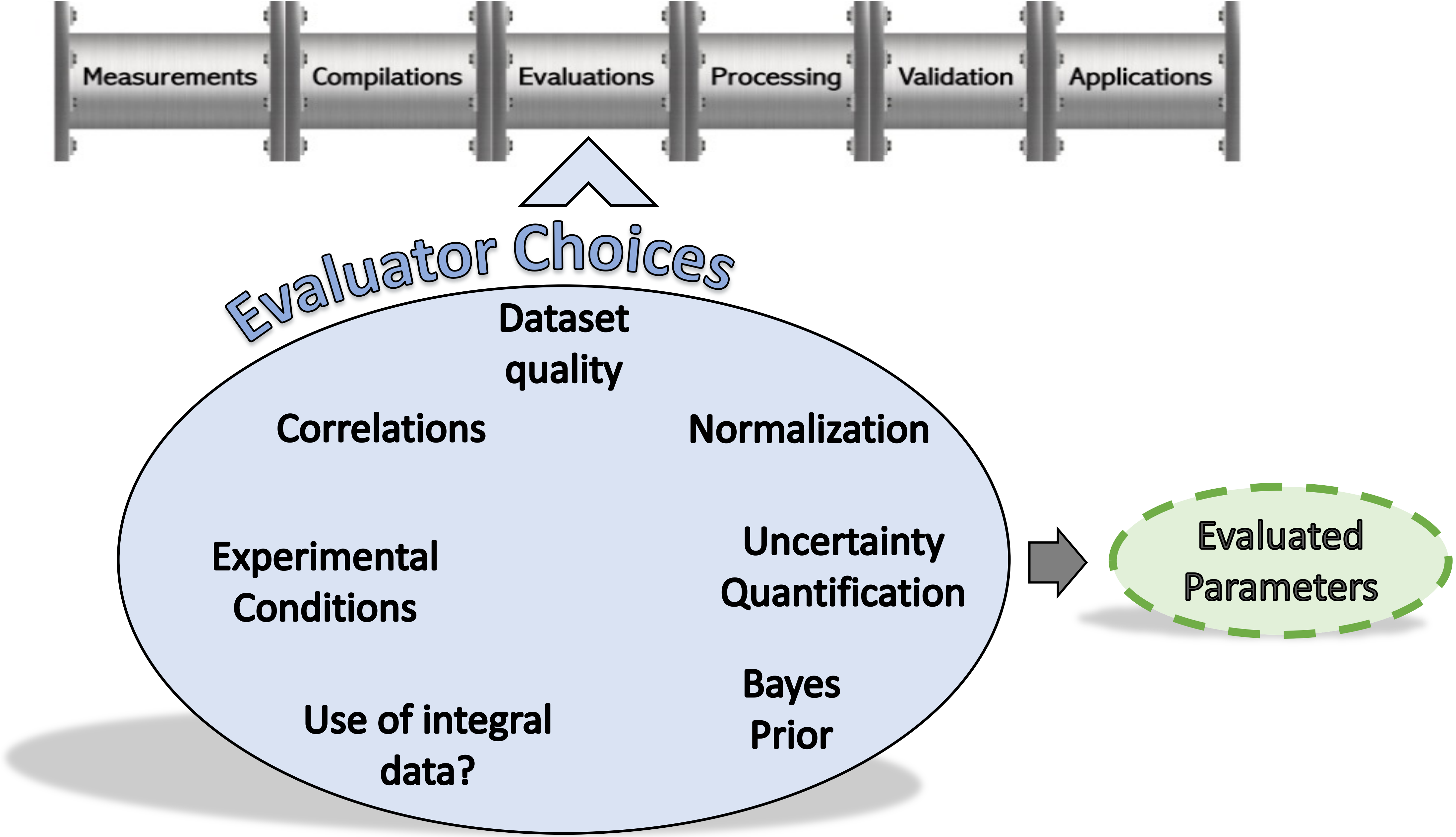
Noah Walton[1], Vladimir Sobes[1], Oleksii Zivenko[1], Jesse Brown[2], Jake Forbes[1], Cole Fritsch[1], Aaron Clark[1], Dave Brown[3] , Denise Neudecker[4] , Mike Grosskopf[4]

The University of Tennessee[1]

Oak Ridge National Laboratory[2]

Brookhaven National Laboratory[3]

Los Alamos National Laboratory[4]


Measurements
Compilations
Evaluations
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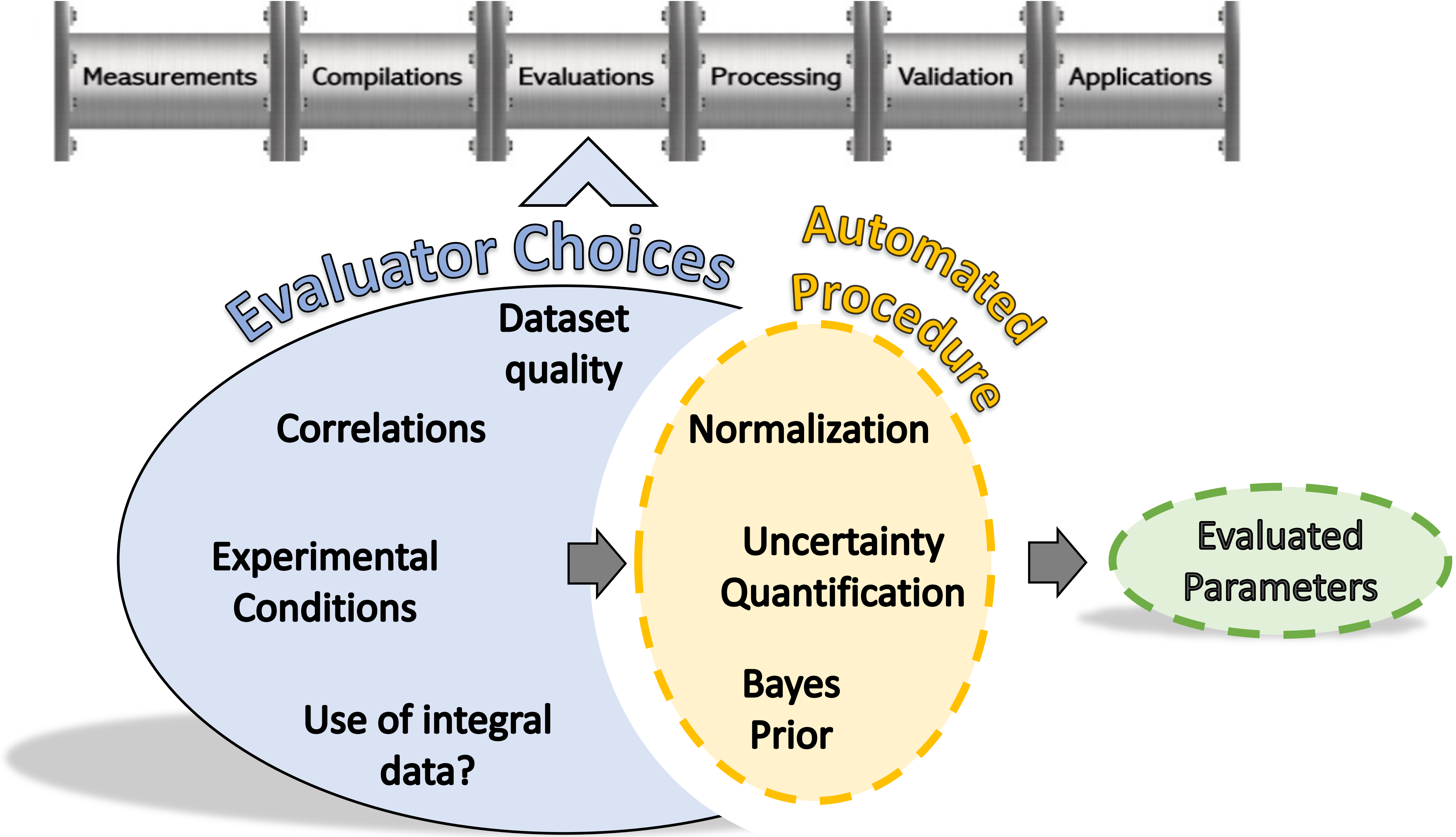
Evaluator Choices
Dataset quality
Correlations
Normalization
Experimental Conditions
Uncertainty Quantification
Use of integral data?
Bayes Prior
Evaluated Parameters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Use of integral data?
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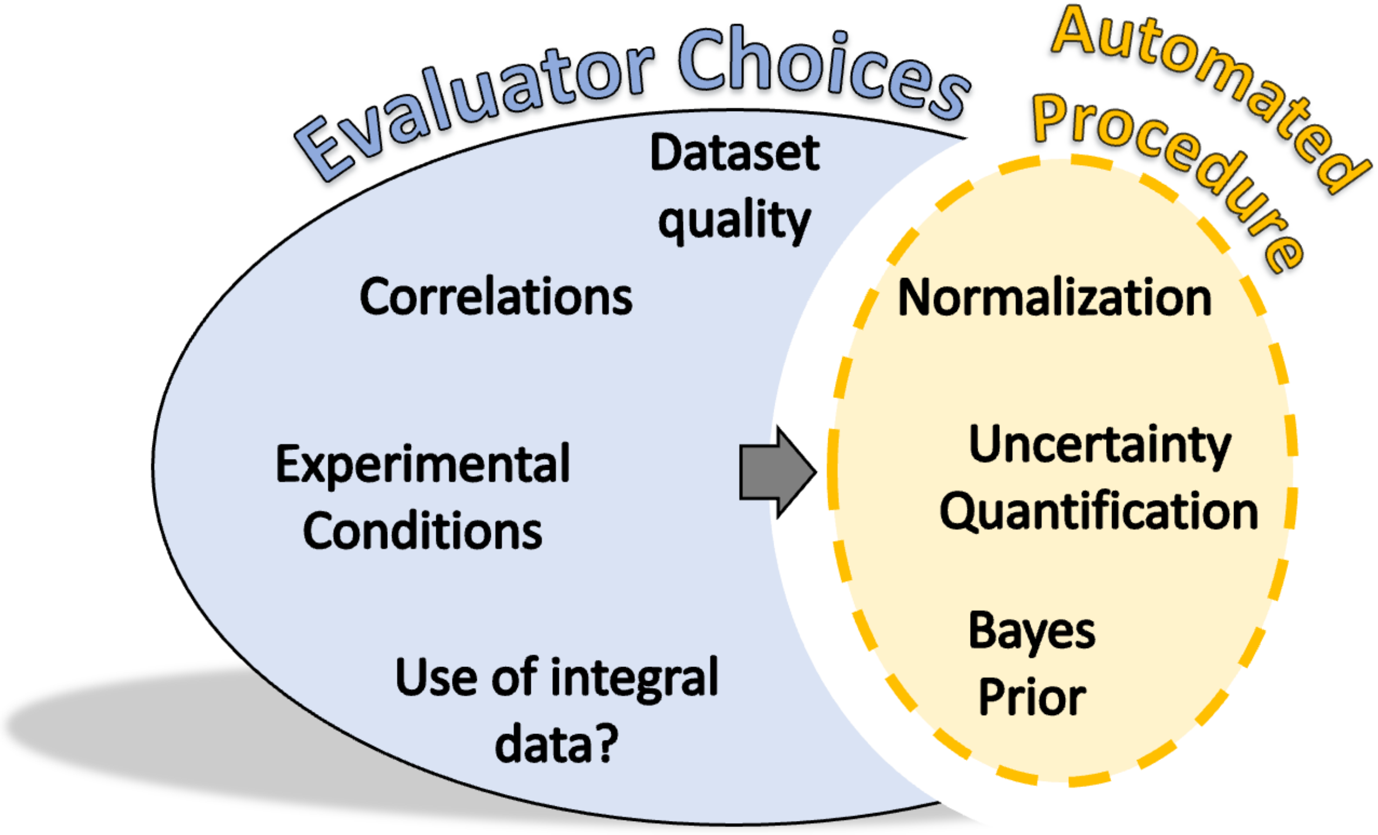
Evaluated Parameters

Two primary efforts

1. Develop automated tool
   - Augment evaluators

2. Computational experiments
   - Benchmark tool
   - Improve tool
   - Learn new physics



Automated Tool

Methods

- SAMMY
- Robust, non-linear least squares algorithm
- Feature selection

Results

- Accurate resonance I.D.
- No spin groups (yet)

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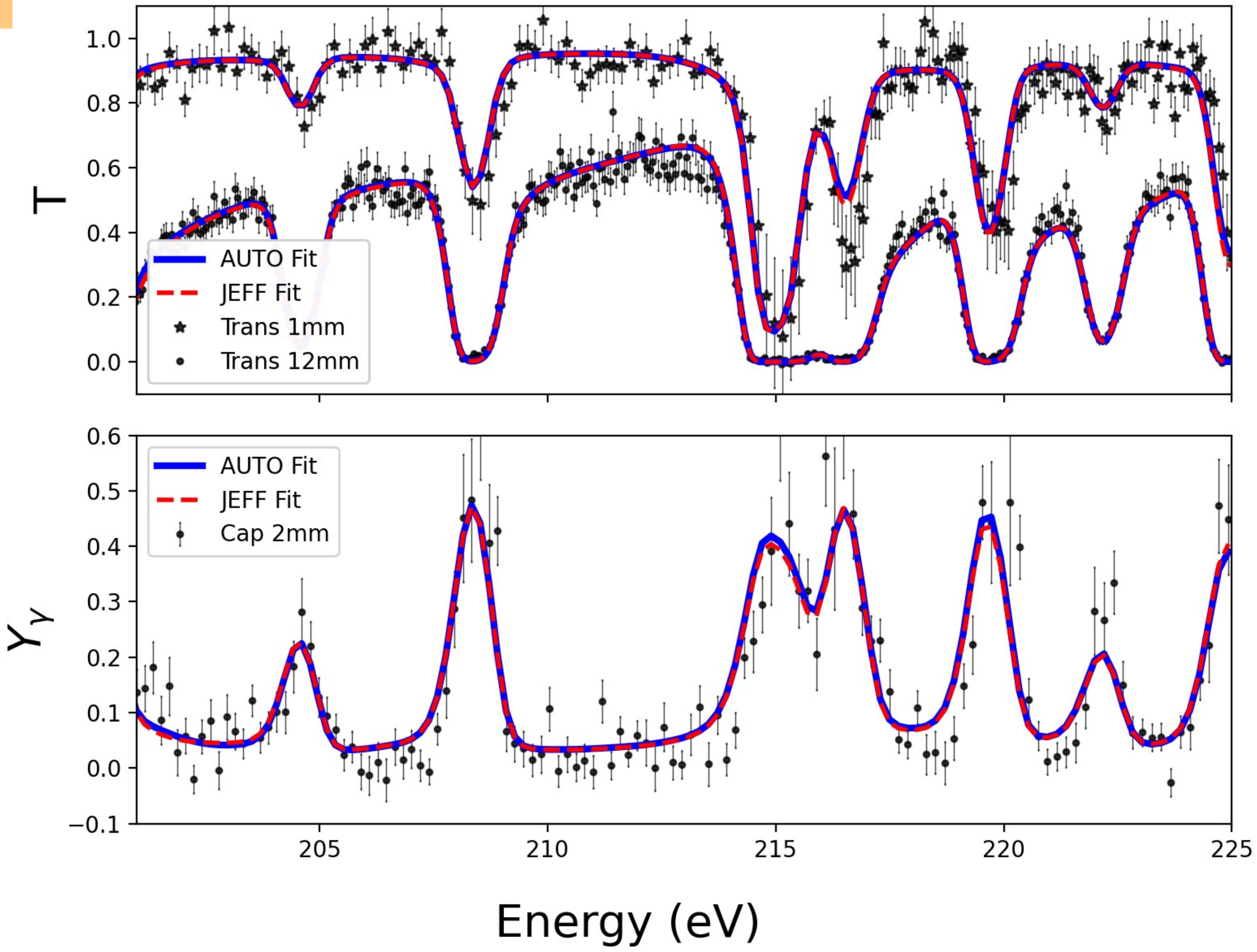
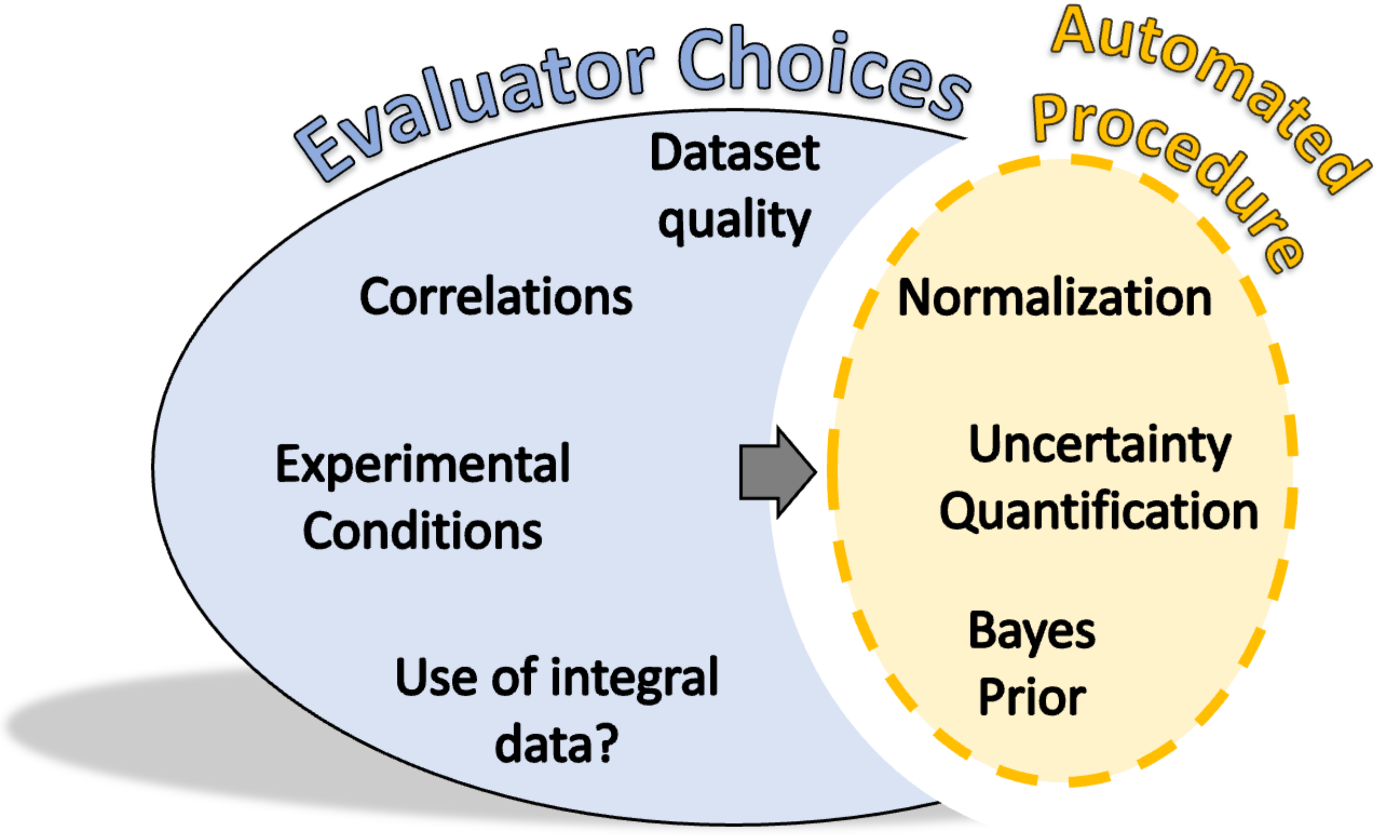


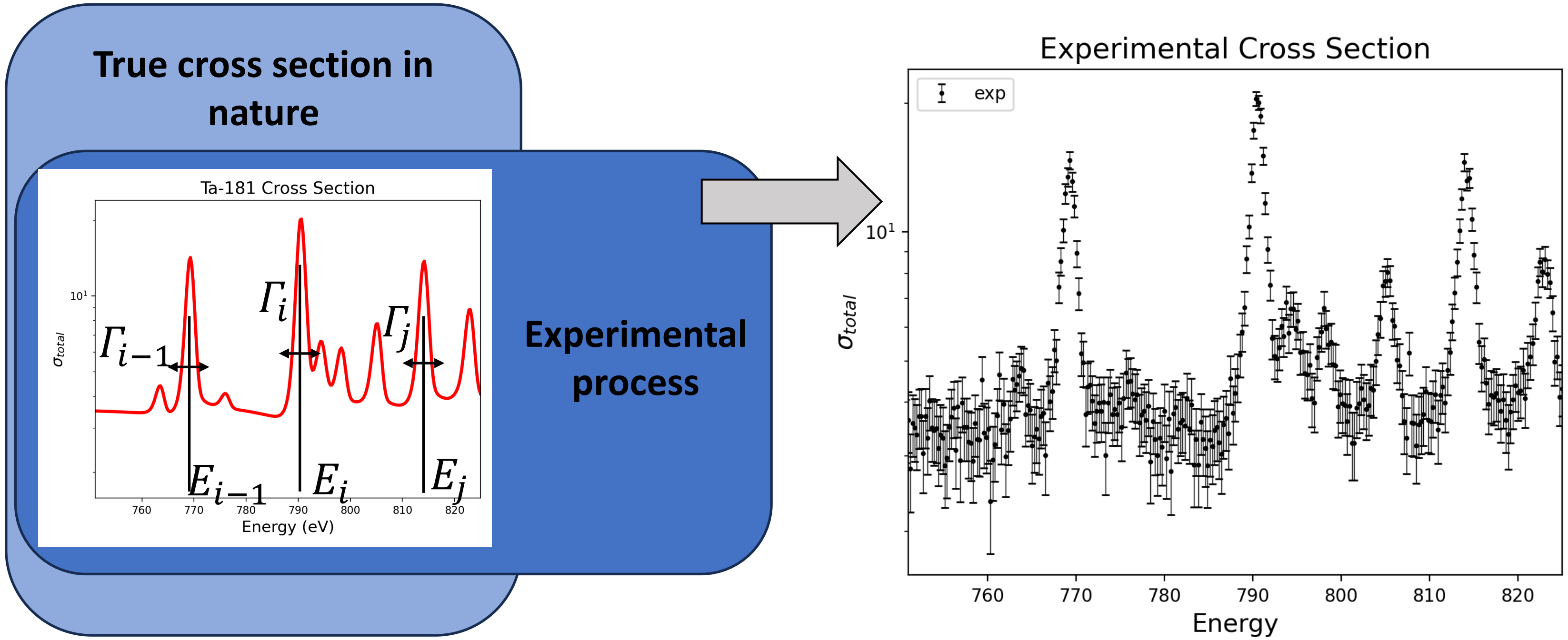
Goal

- Benchmark at differential level
- Improve performance
- Test choices & assumptions

ML Approach

- Synthetic data
- Transmission last year
- Capture yield this year




True cross section in nature
Ta-181 Cross Section
Γ_{i-1}
Γ_i
Γ_j
E_{i-1}
E_i
E_j
σ_{total}
10^1
760
770
780
790
800
810
820
Energy (eV)
Experimental process
Experimental Cross Section
exp
10^1
σ_{total}
760
770
780
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810
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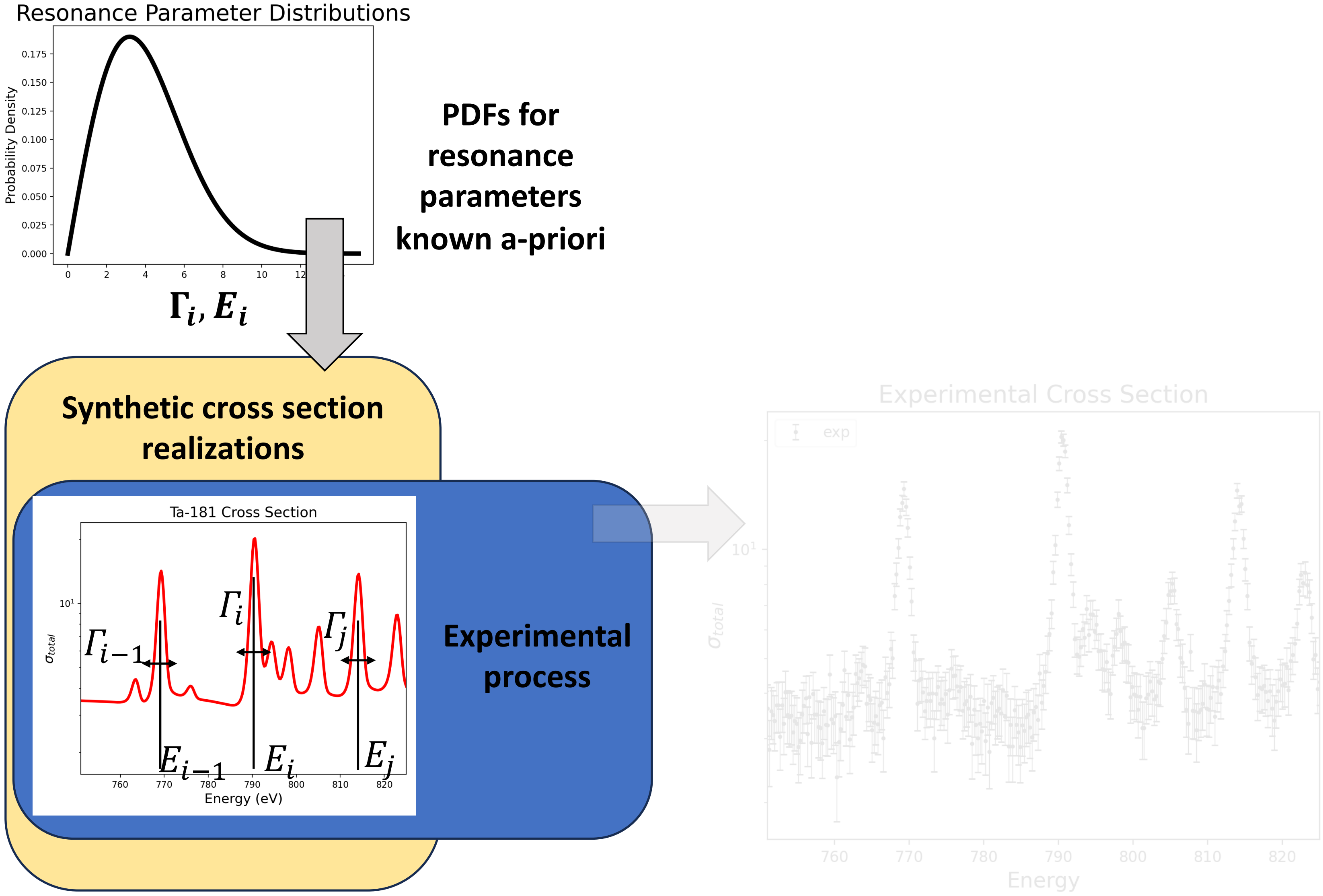
Energy


Resonance Parameter Distributions
Probability Density
Γ_i, E_i
PDFs for resonance parameters known a-priori
Synthetic cross section realizations
Ta-181 Cross Section
σ_{total}
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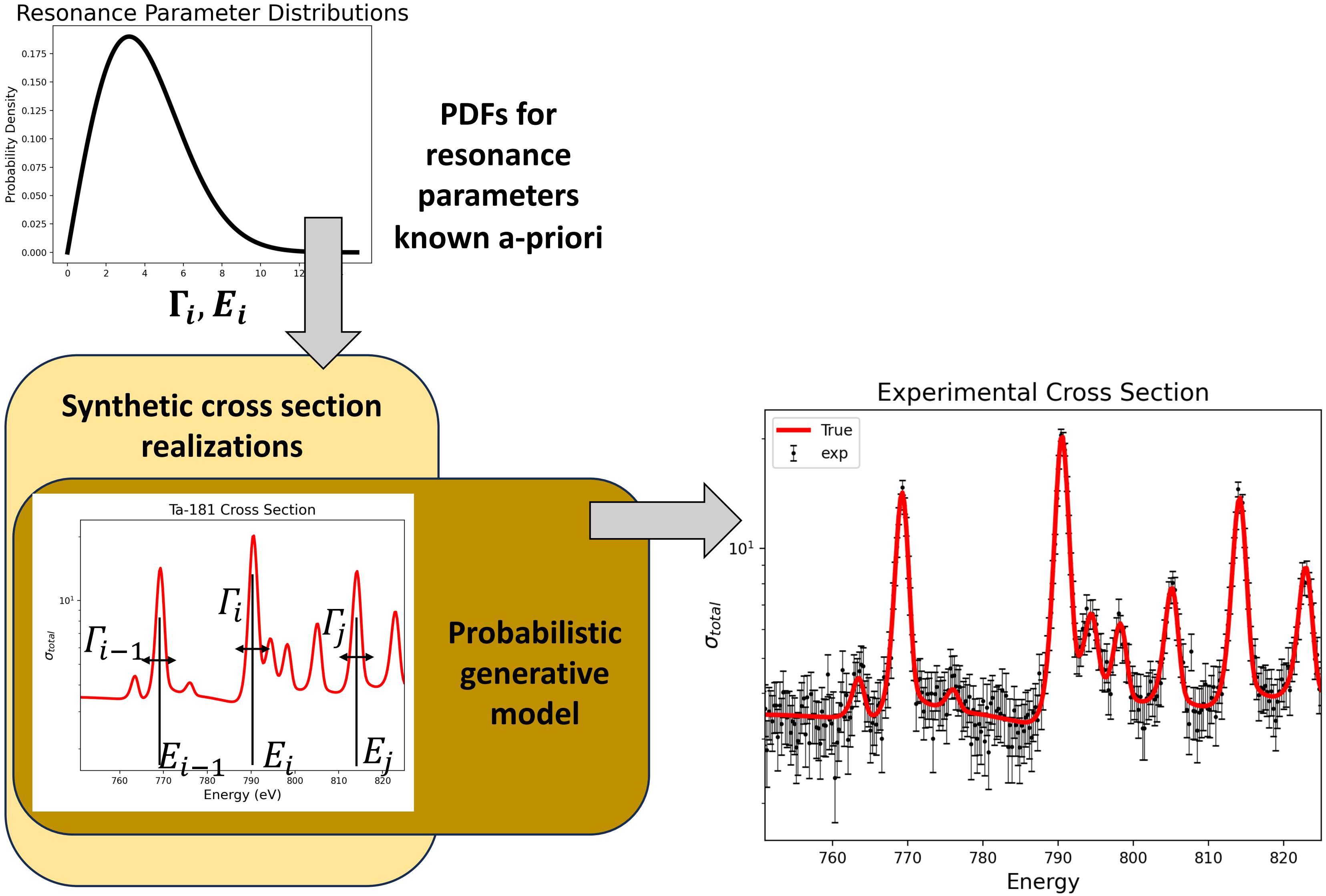
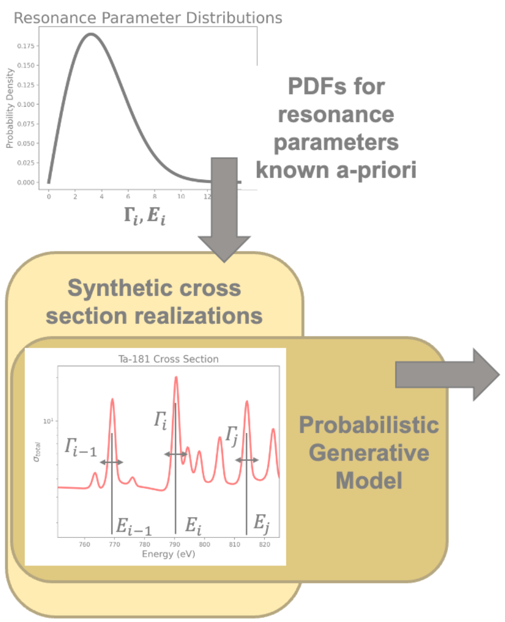
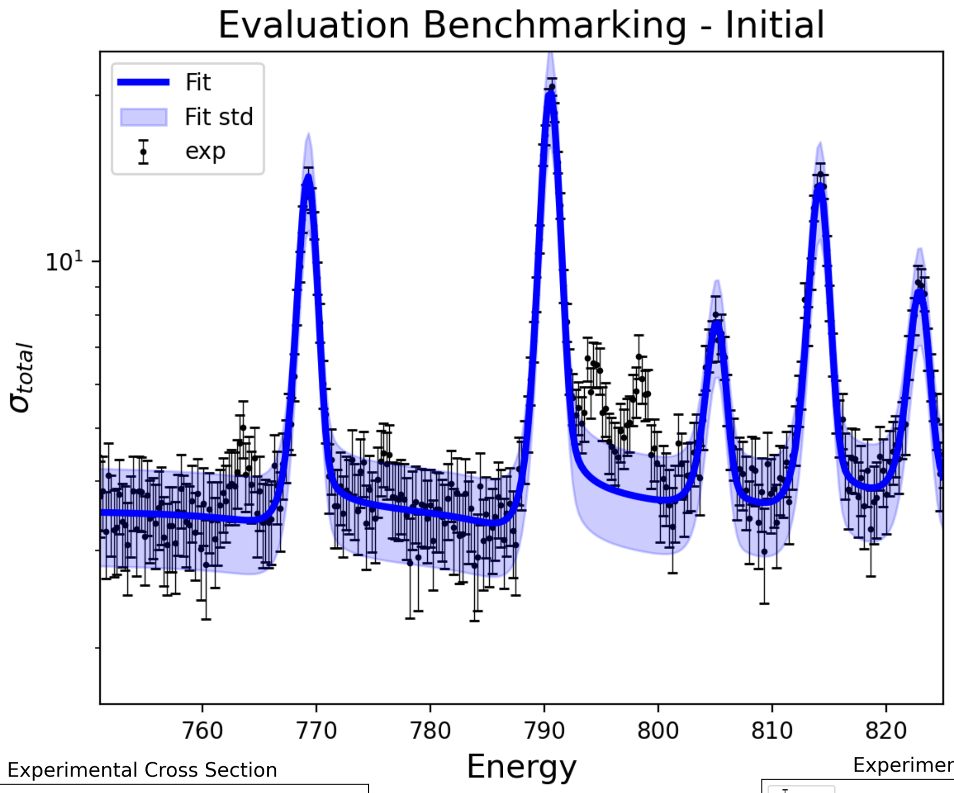
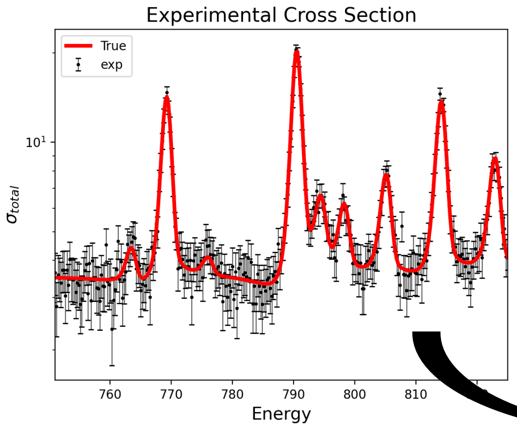


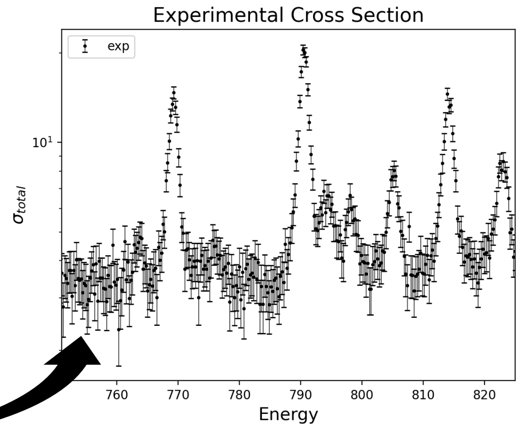
Walton, N.A.W., Brown, J., Fritsch, W., Brown, D., Nobre, G., Sobes, V., Methodology for physics-informed generation of synthetic neutron time-of-flight measurement data, *Computer Physics Communications,* Vol 294, 2024, 108927, ISSN 0010-4655, https://doi.org/10.1016/j.cpc.2023.108927.

Synthetic data generator



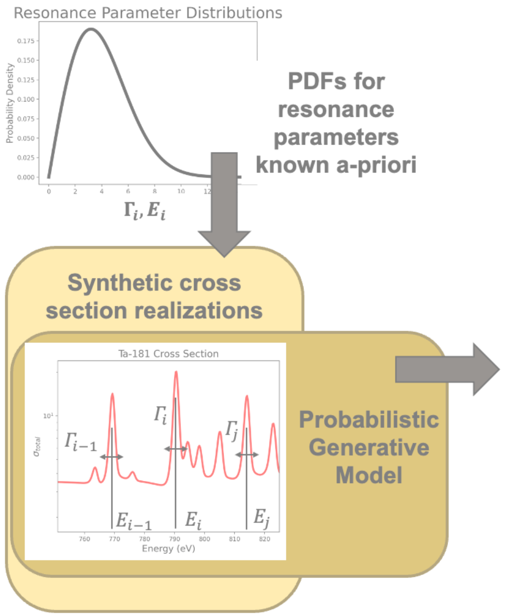


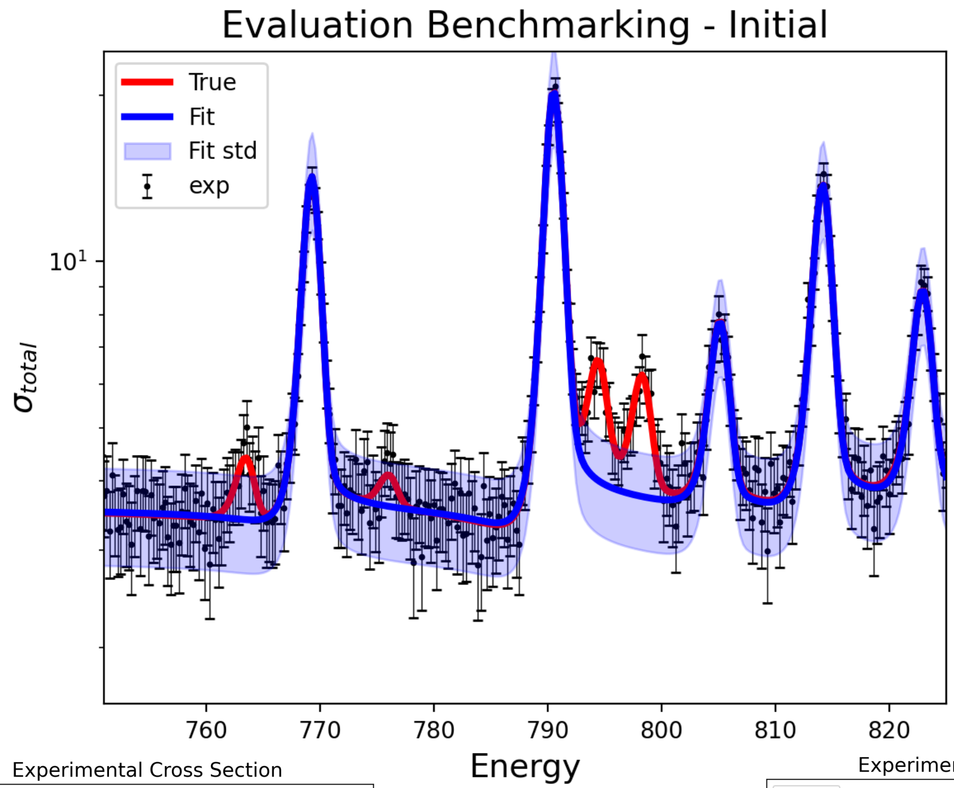


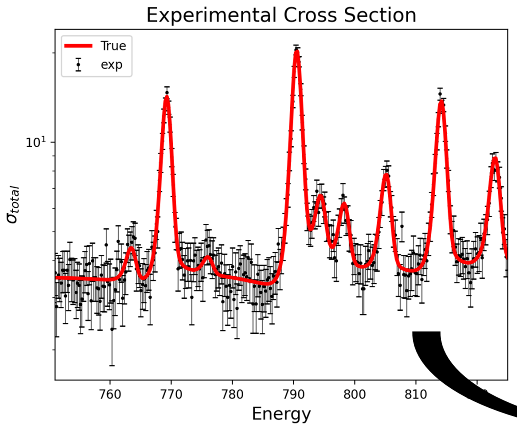


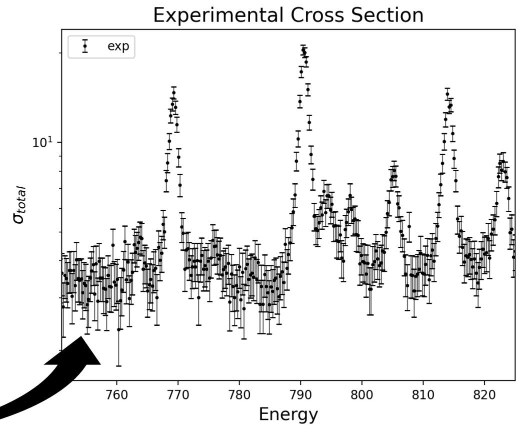
Automated procedure

Synthetic data generator



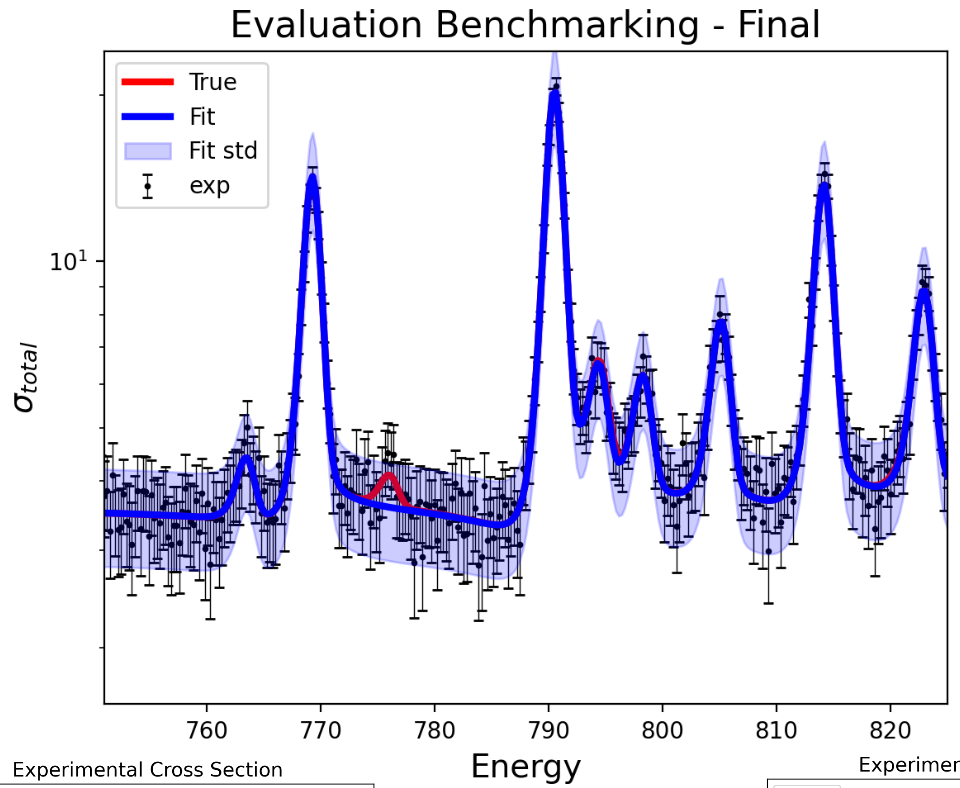






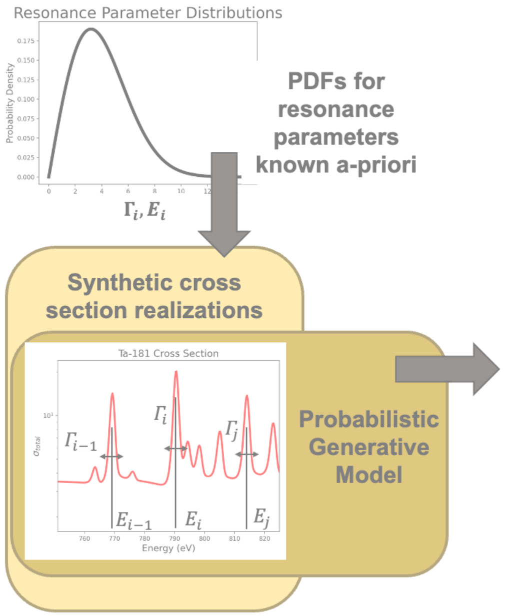
Automated procedure

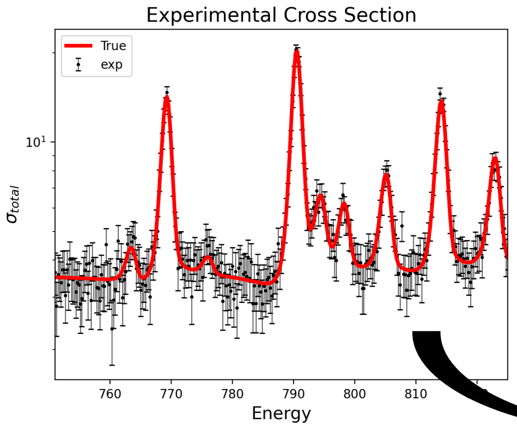
Learn hyperparameters optimize & benchmark accuracy

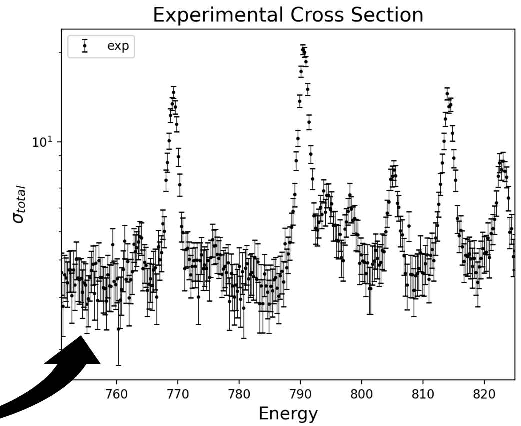


Automated procedure

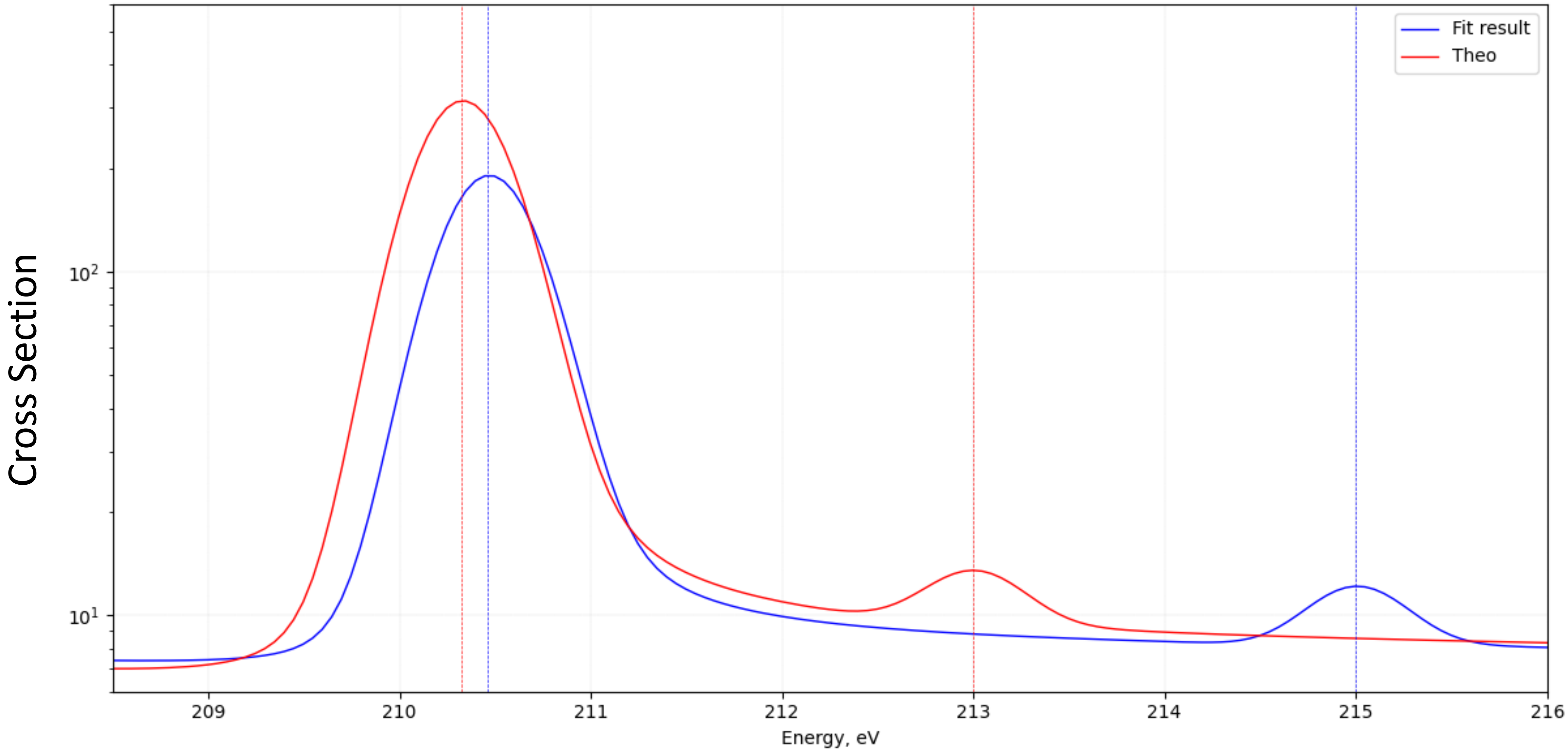
Synthetic data generator







Performance Metric



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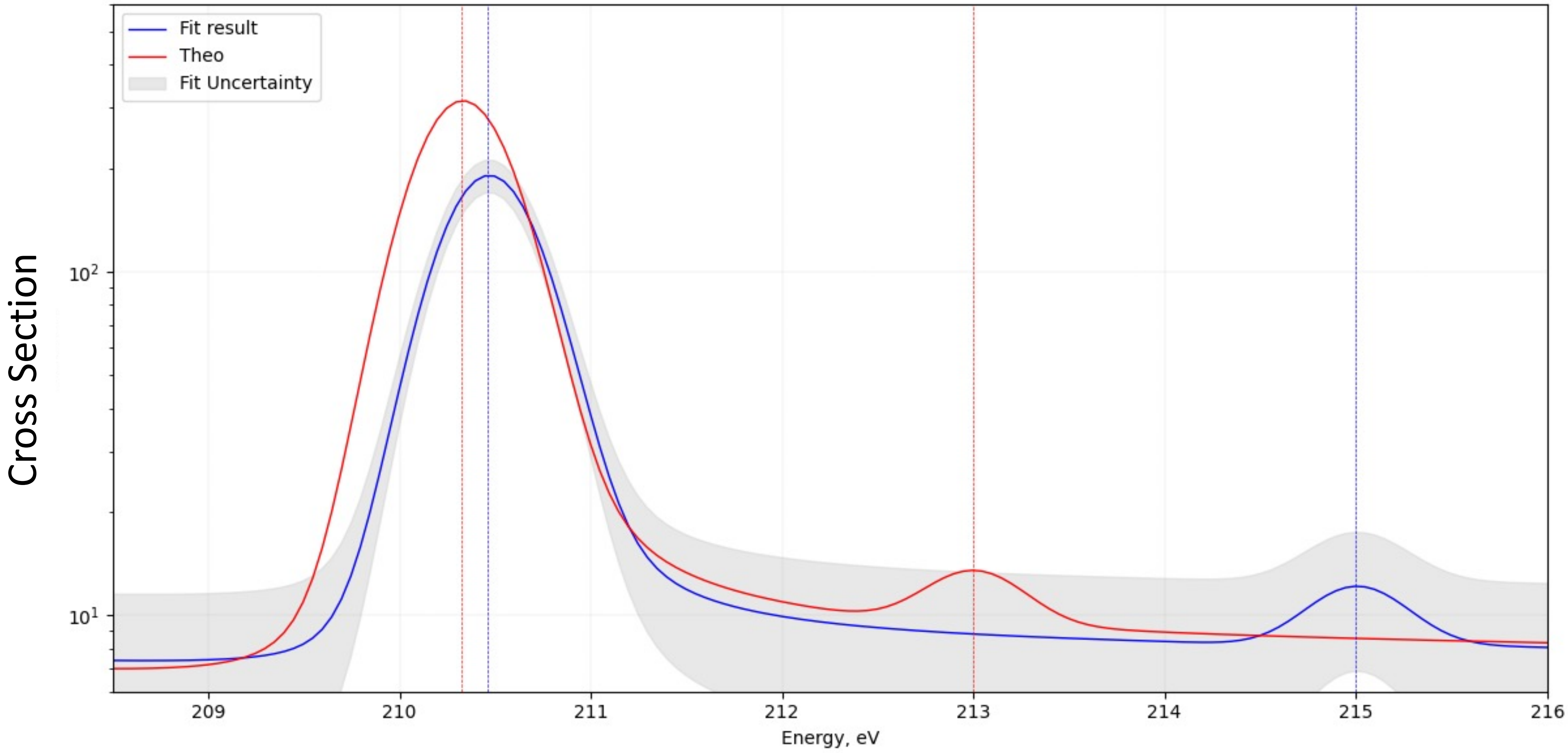

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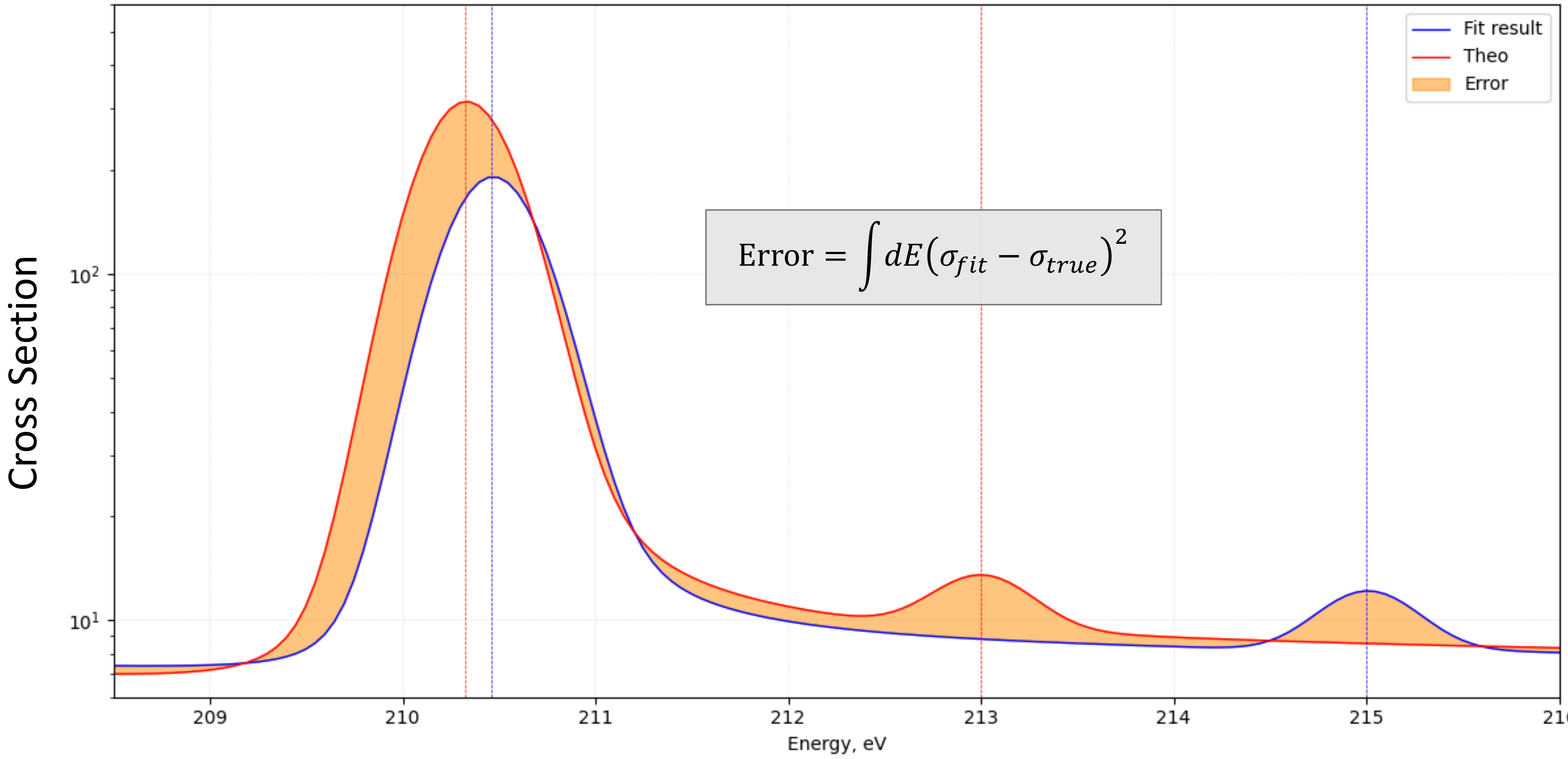
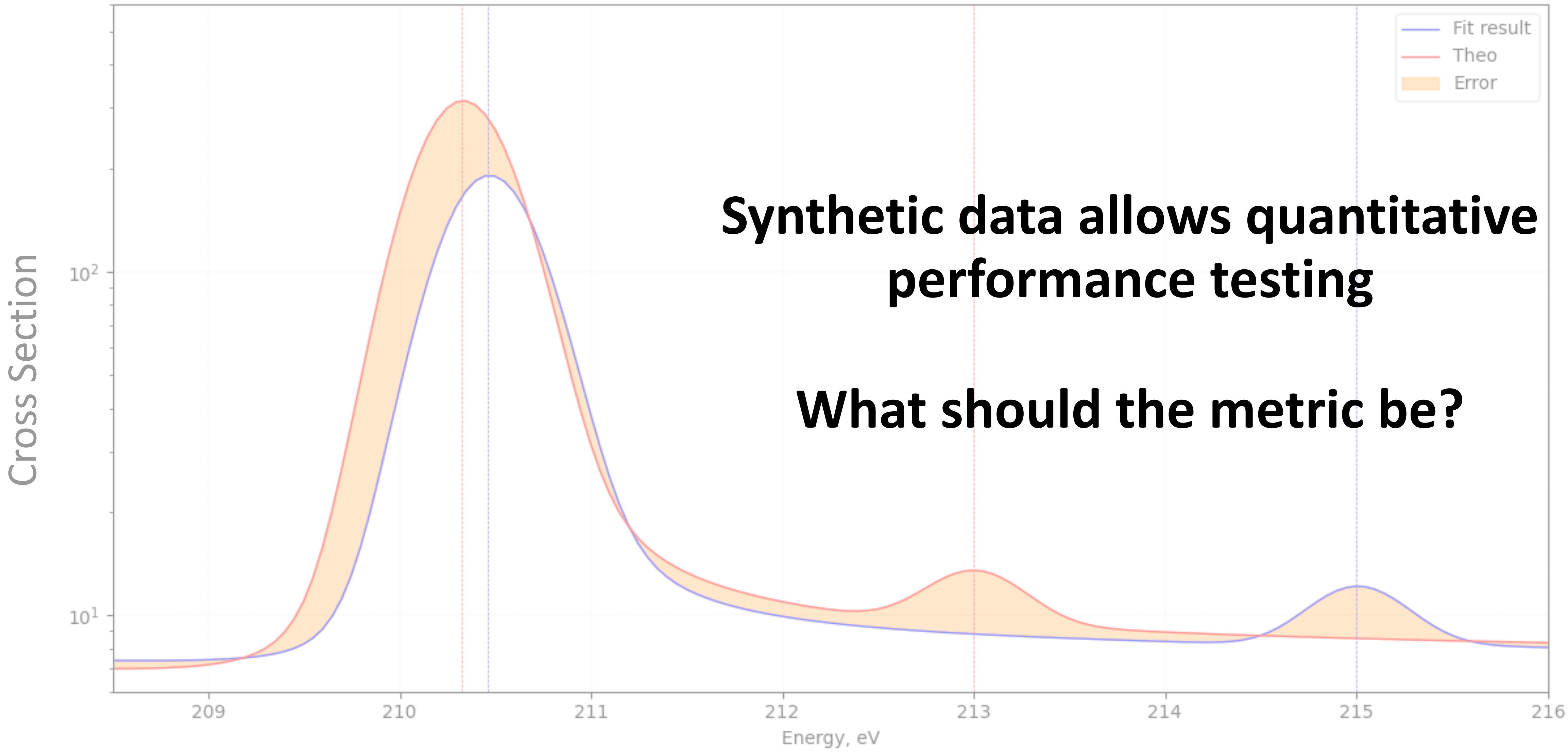


$$\text{Error} = \int dE\left(\sigma_{fit} - \sigma_{true}\right)^2$$

Performance Metric

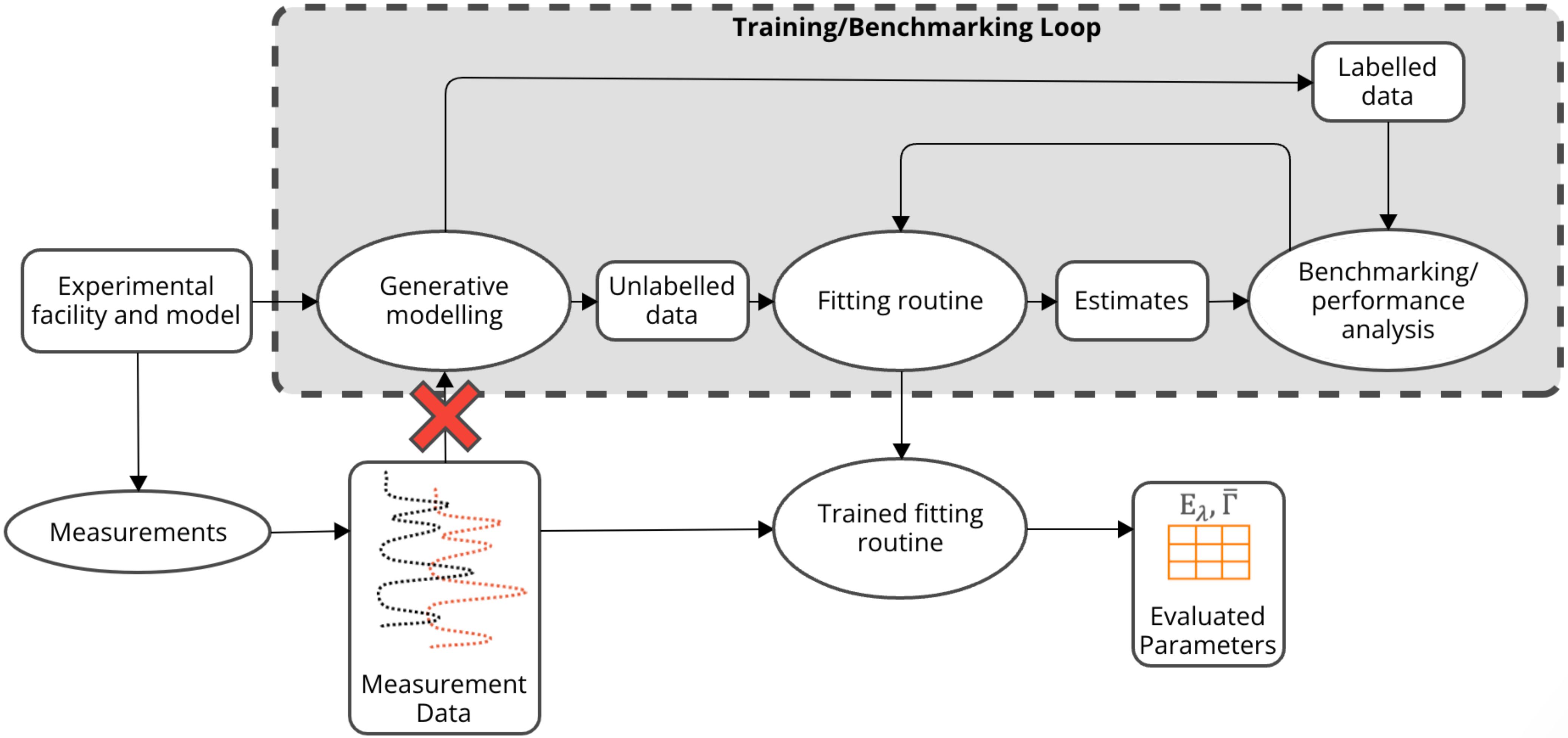


Synthetic data allows quantitative performance testing

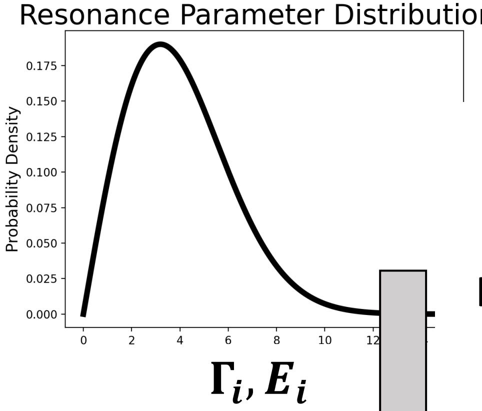
What should the metric be?

This material is based upon work supported by the Department of Energy National Nuclear Security Administration through the Nuclear Science and Security Consortium under Award Number DE-NA0003996.

Computational Framework

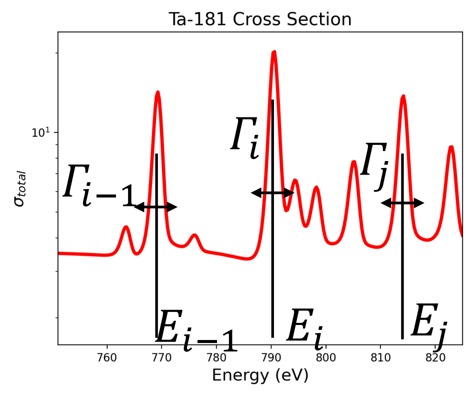


Developing a generative model for the resonance experiments

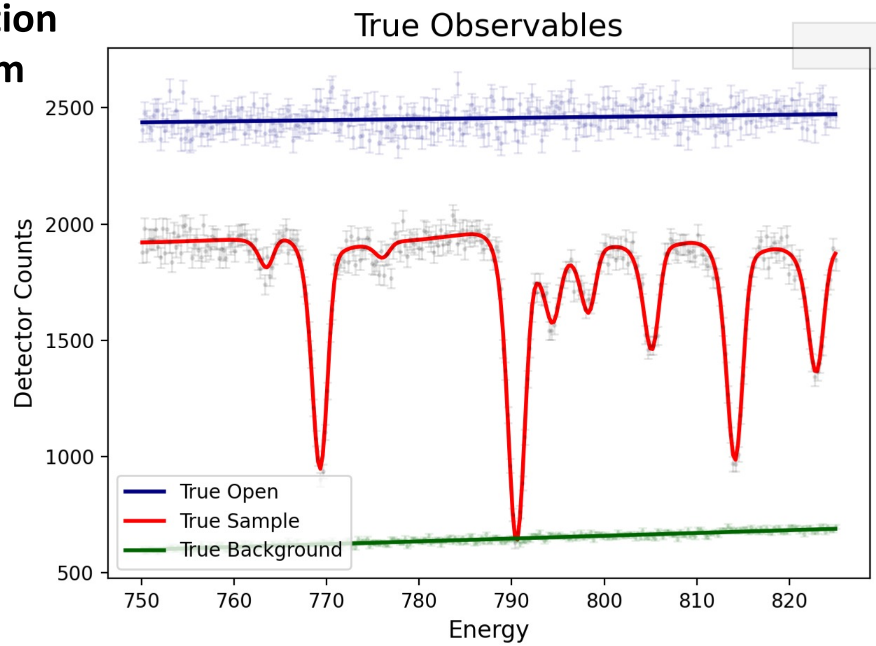


PDFs for resonance parameters known a-priori

Synthetic cross section realizations



Novel method for inverse reduction using random sampling



Data Reduction

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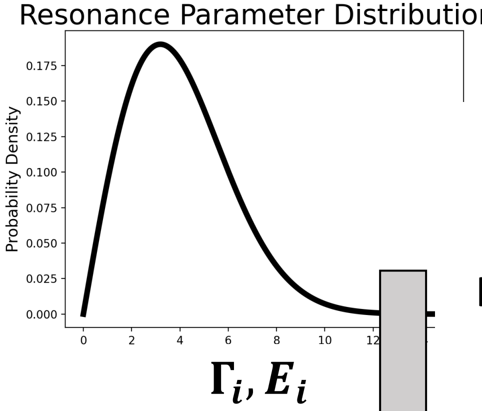

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Noise model given by counting statistics

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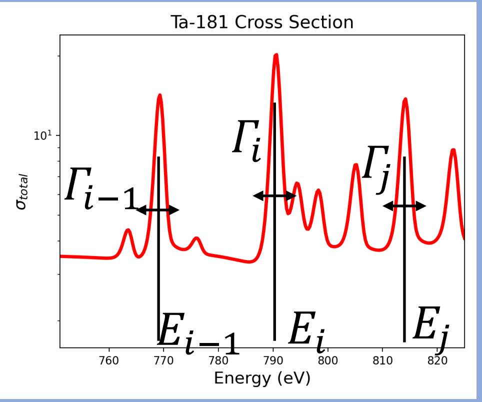

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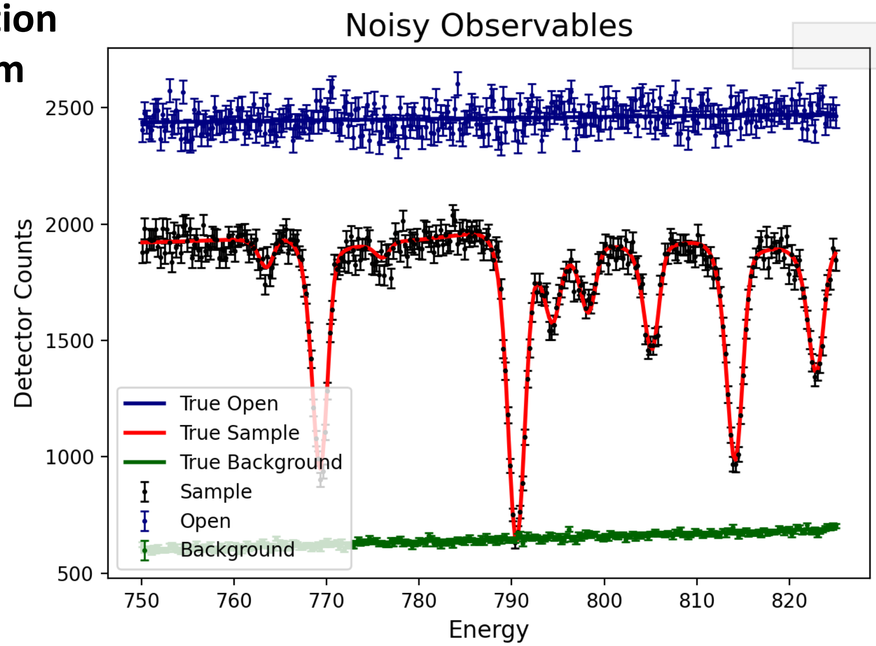

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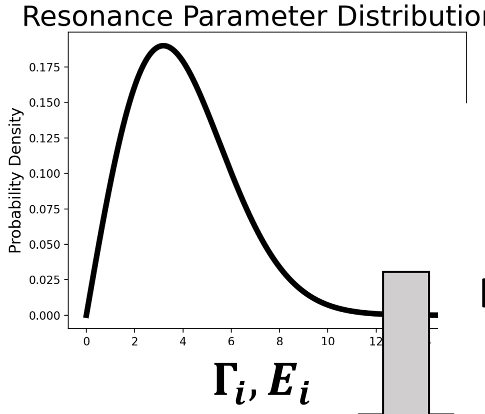

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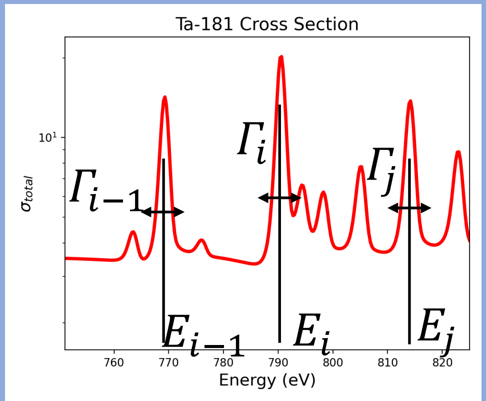

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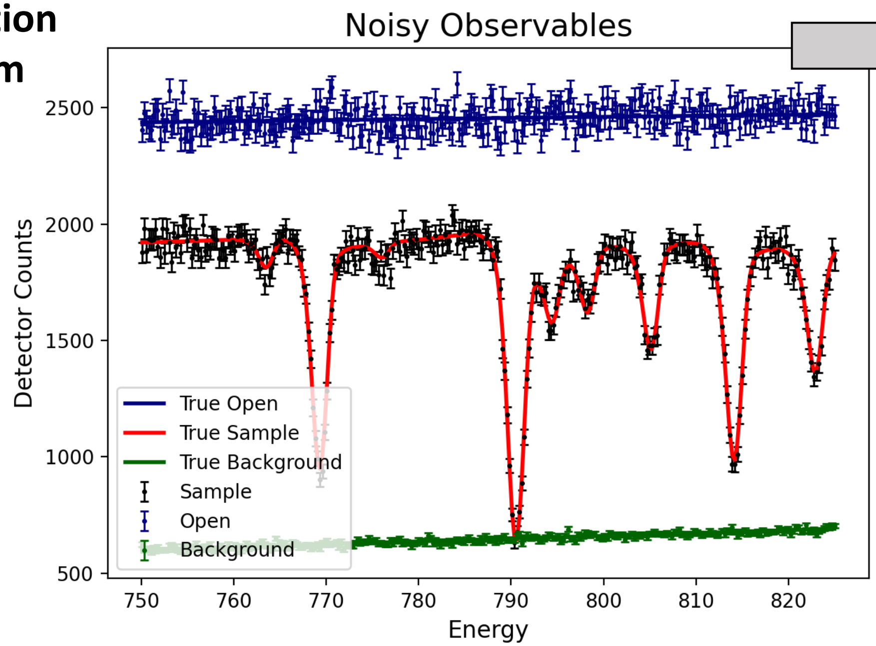
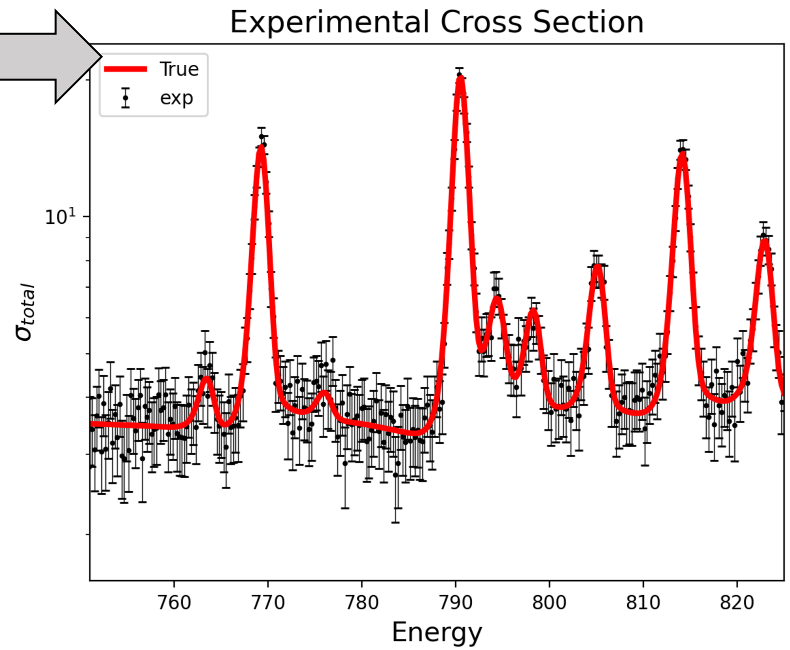
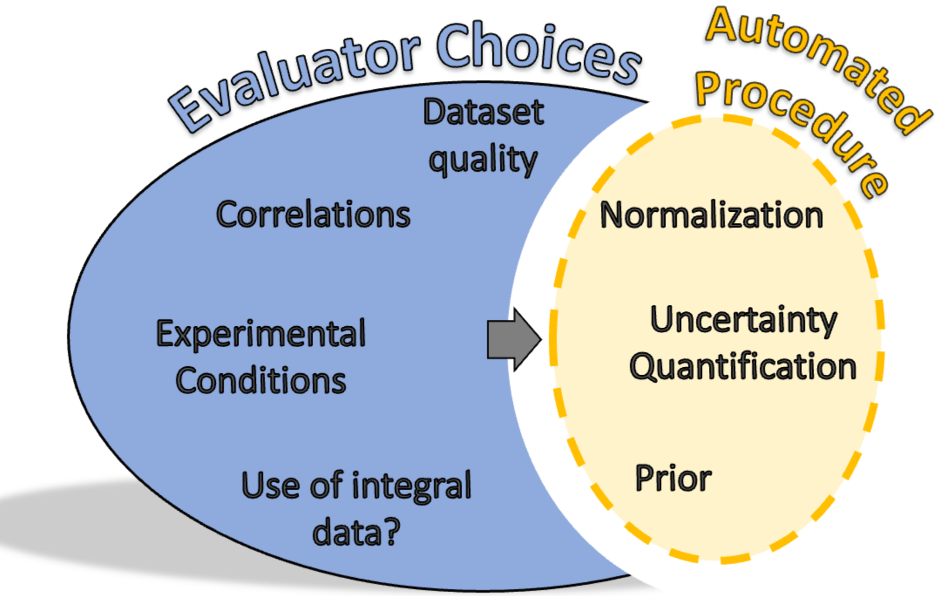
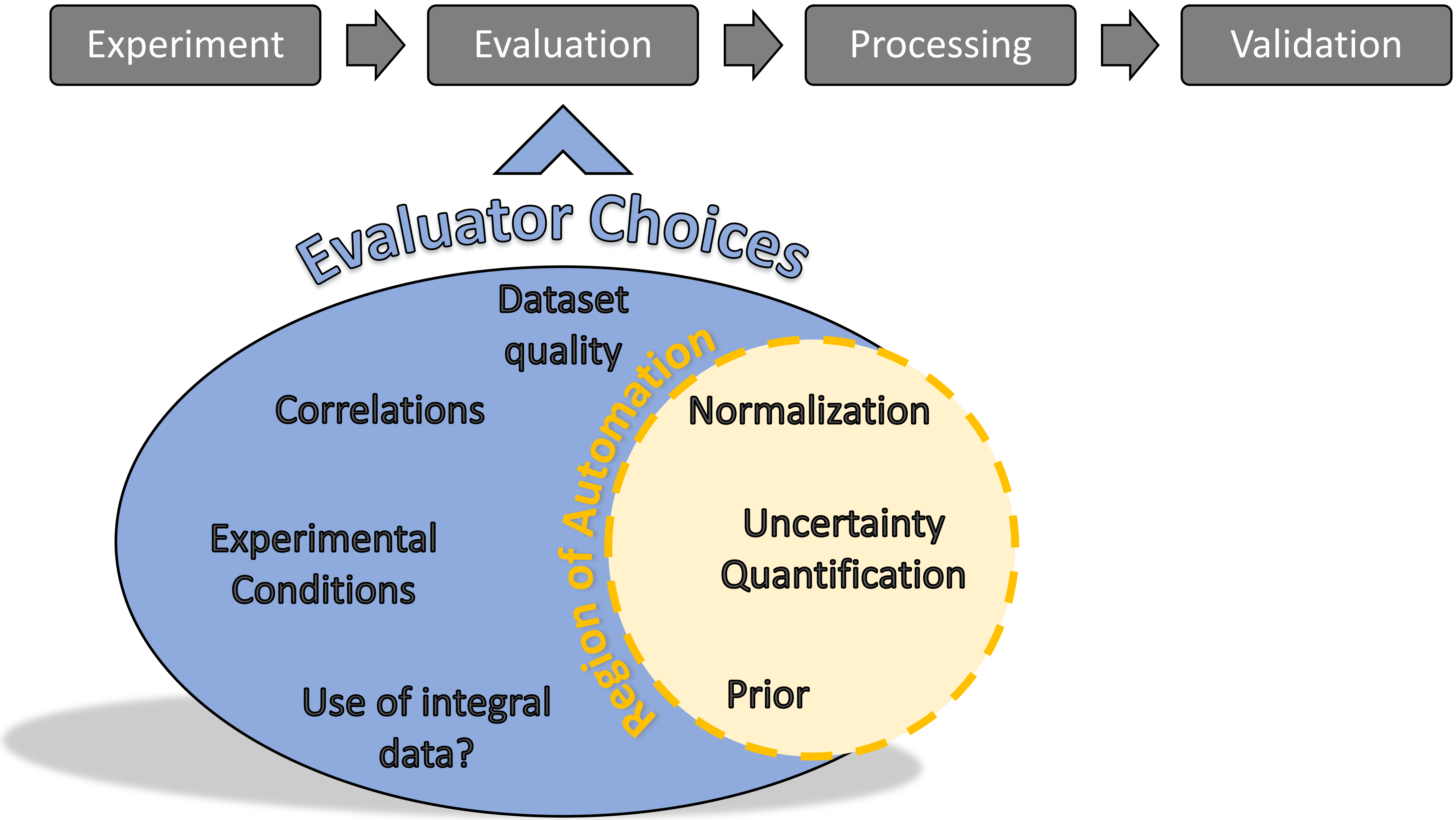




Leveraging AI/ML to benchmark region of automation



- Benchmarking the automation:
  1. Quantitative assessment at differential level
  2. Sensitivity to assumptions
     - Theoretical: parameter distributions
     - Experimental: unknown uncertainties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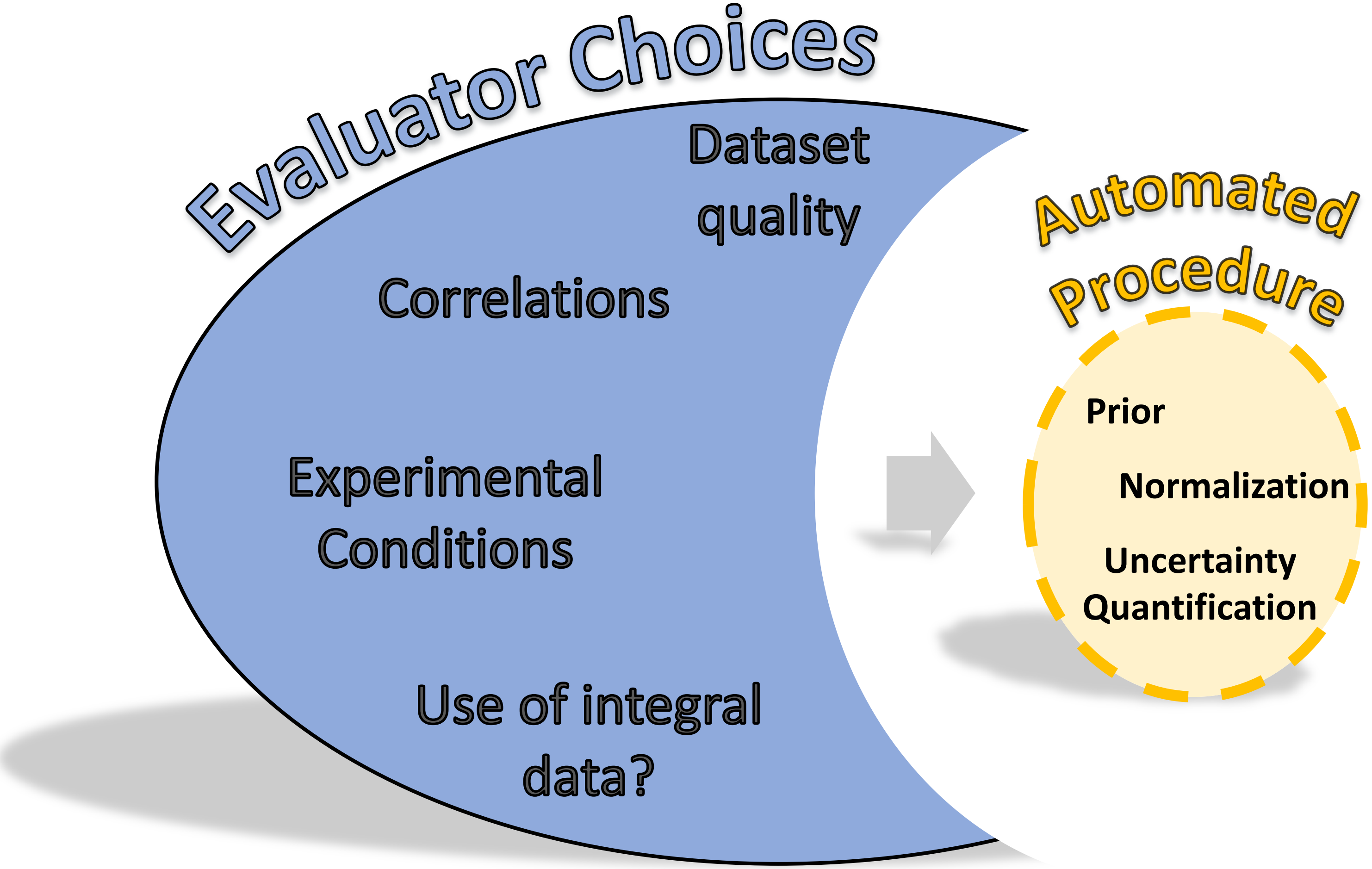
Region of Automation
Normalization
Uncertainty Quantification
Prior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