Bayesian Sparse Discrepancy Estimation Using the Horseshoe Prior Applied to Nuclear Data

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8/7/2024

Managed by Triad National Security, LLC for the U.S. Department of Energy's NNSA

AIACHNE is a multidisciplinary effort funded by the DOE Office of Science to use data-driven science to design experiments to improve nuclear data

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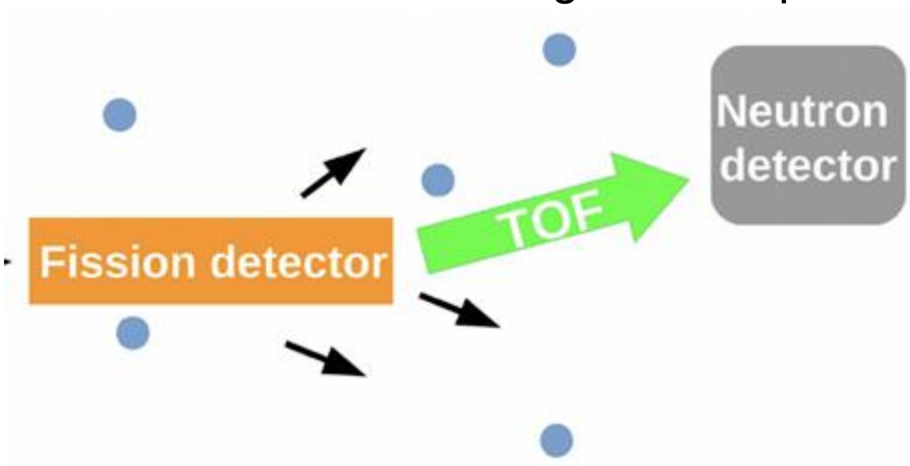
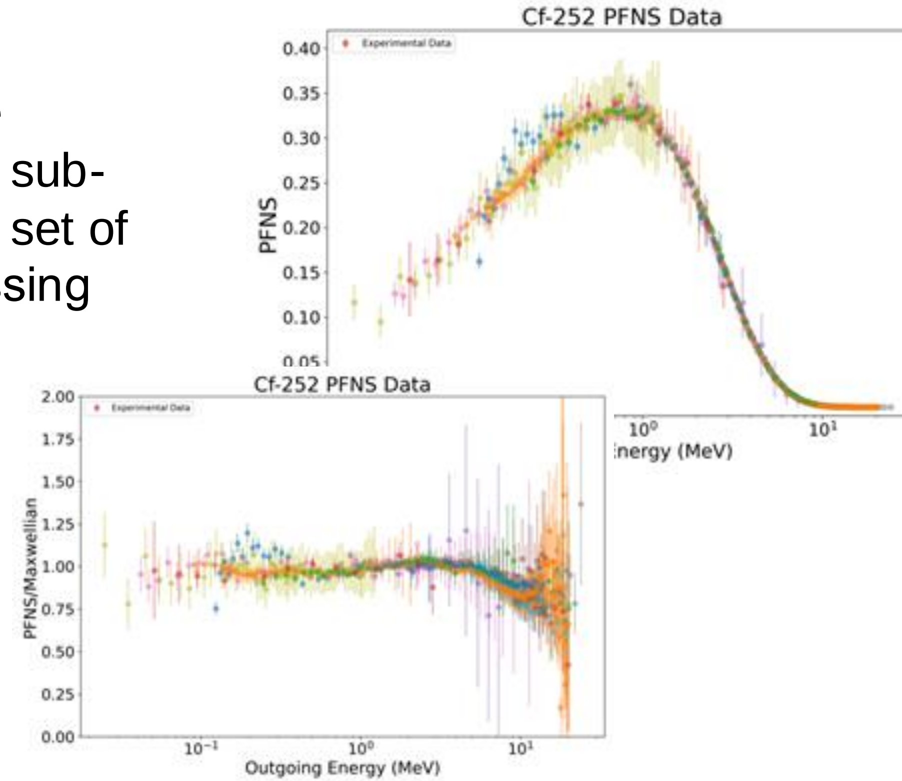
One central source of information for estimating nuclear data is through differential measurements

These experiments are composite measurements that depend on several sub-measurements characterized by a large set of "metadata" describing the data processing



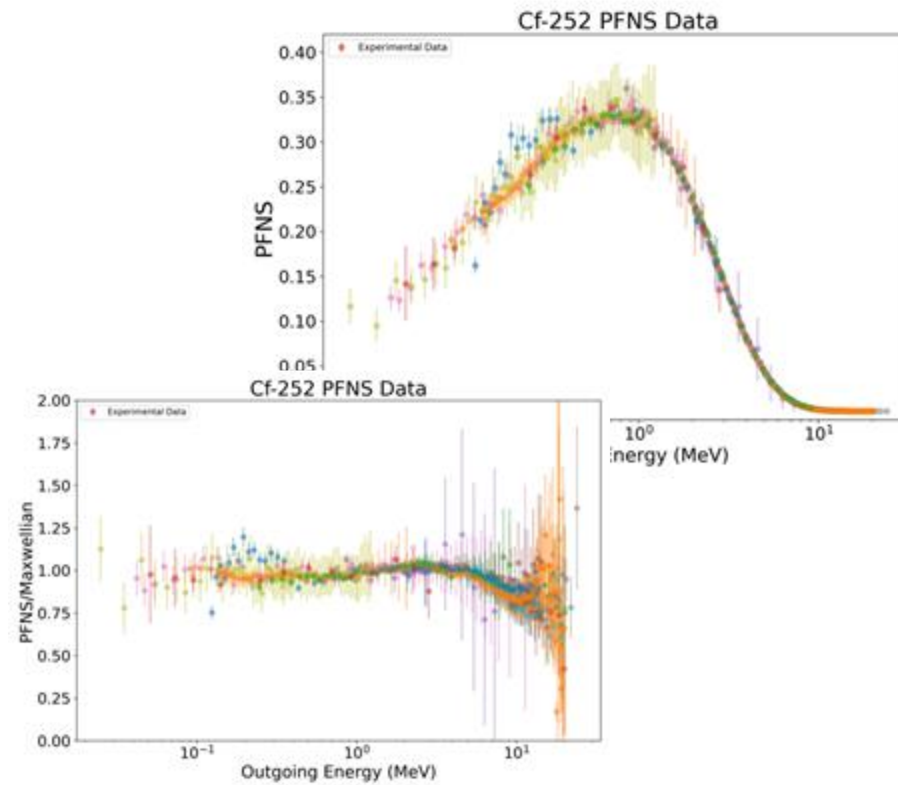


These experiments often disagree, beyond carefully quantified uncertainties. Understanding possible sources of experiment-to-experiment discrepancy is key to improving estimates and uncertainties

One way of estimating nuclear data is through direct, “differential” measurements

	Correction Features	Hardware Features	Method Features
0	ShadowBarBackground	FissionDetector1_raw	RandomCoincidence
1	BackgroundCorrected	FissionDetector1_caseA	BackgroundGeneral
2	RandomCoincidenceBackground	FissionDetector1_caseB	BackgroundAlpha
3	GammaBackground	FissionDetector1_caseC	GammaBackground
4	AlphaBackground	FissionParticleDetected	MSinSample
5	WrapAroundBackground	FissionFragmentDetectorEfficiency	MSinSurrounding
6	MultipleScatteringSampleBackingCorrected	FissionDetectorGas_raw	FissionDetectorEfficiencyMethod
7	MultipleScatteringSurroundingCorrected	FissionDetectorGas_caseA	FFAbsorptionAngularDistributionMethod
8	AttenuationSampleBackingCorrected	AngularAcceptanceofFFDetector	NeturonDetectorResponseMethod
9	AttenuationSurroundingCorrected	NeutronDetector_raw	NeturonDetectorEfficiencyMethod
10	FissionDetectionEfficiencyCorrected	NeutronDetector_caseA	DeadtimeDeterminationMethod
11	NeutronDetectionEfficiencyCorrected	AngularCoverageofNeutronDetector	
12	NeutronDetectionResponseCorrected	NeutronDetectorSizeCM	
13	SampleDecayCorrected	NeutronDetectorStructuralMaterialAu	
14	FissionFragmentAbsorptionInSampleCorrected	NeutronDetectorStructuralMaterialAl	
15	SignalPulsePileupCorrected		
16	DeadtimeCorrected		
17	AngularDistributionFissionFragmentsCorrected		
18	ImpuritiesCorrected		

This is a *filtered* list of feature categories!!!



These experiments often disagree, beyond carefully quantified uncertainties. Understanding possible sources of experiment-to-experiment discrepancy is key to improving estimates and uncertainties

AIACHNE is using a sparse Bayesian model to identify potential sources of bias in ^{252}Cf PFNS data

- The traditional approach to evaluation uses generalized least squares to evaluate values on fixed energy grid:

$$y = D\sigma + \varepsilon$$

$$\varepsilon \sim N\left(0, \mathrm{diag}(D\sigma u)^2\right)$$

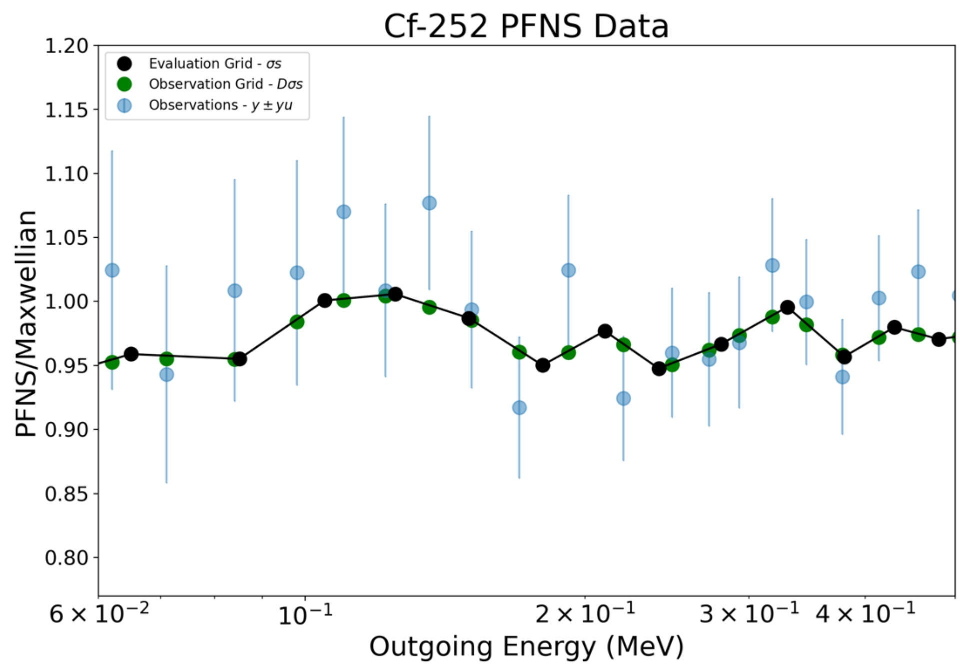
$y =$ data at arbitrary energies

$\sigma =$ Evaluated PFNS on fixed energy grid

$D =$ energy interpolation matrix

$D\sigma =$ interpolated PFNS

$u =$ 'known' relative std. dev. (error bars)

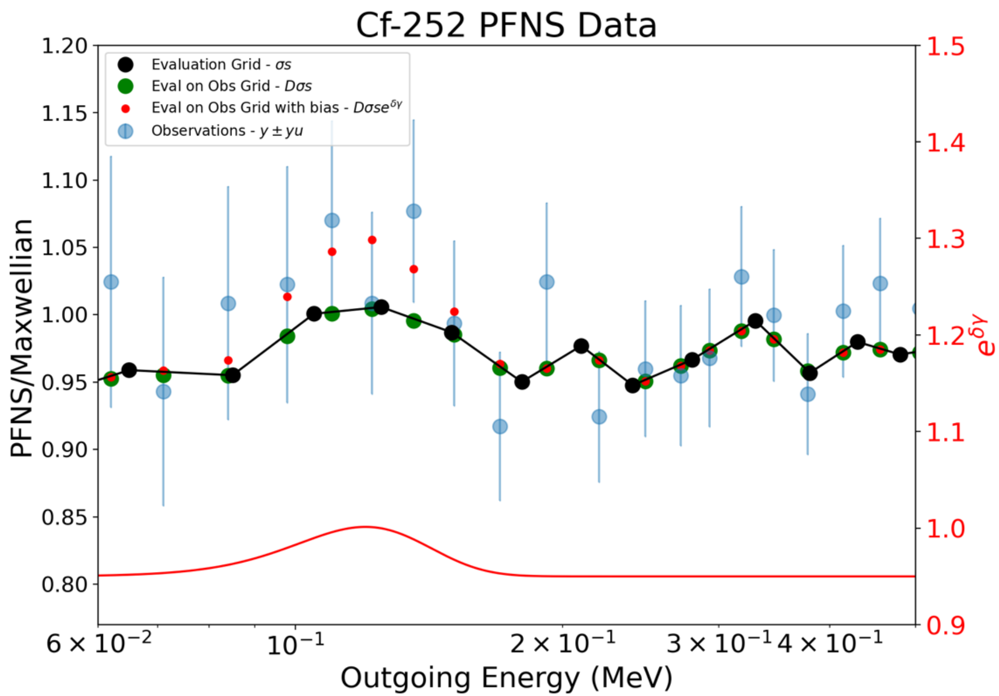


AIACHNE is using a sparse Bayesian model to identify potential sources of bias in ^{252}Cf PFNS data

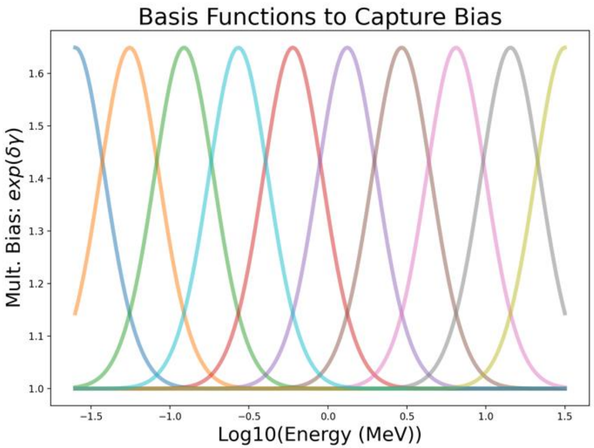
- We are extending this to include a feature/energy-dependent, multiplicative bias
  - Sparsity ensures there is no bias for most energies but the term is active when the data indicate the need

$$y = D\sigma \cdot e^{\delta} + \varepsilon$$

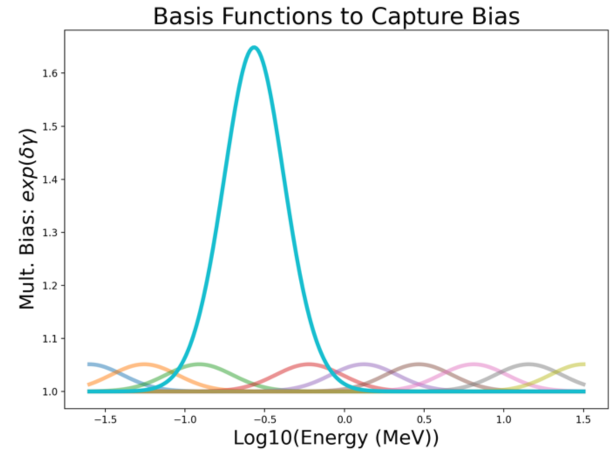
$\delta =$ $B\gamma =$ relative bias
$\mathbf{B} =$ bias basis matrix
$\gamma =$ bias coefficients
$\cdot =$ element-wise product

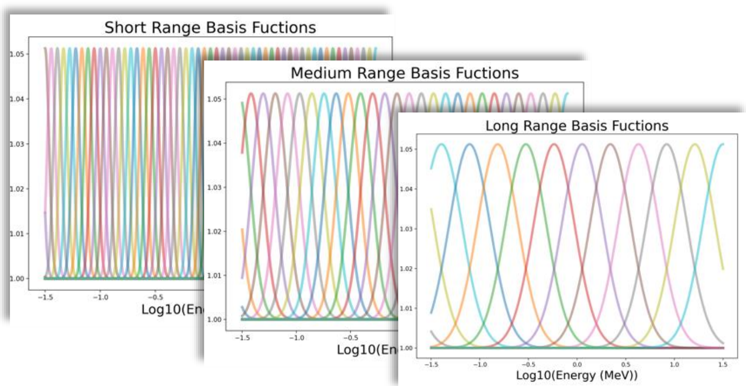


Rather than pre-select the width of the bases for the energy-dependent bias, we developed a sparse, multi-scale approach



We need to induce sparsity on γ



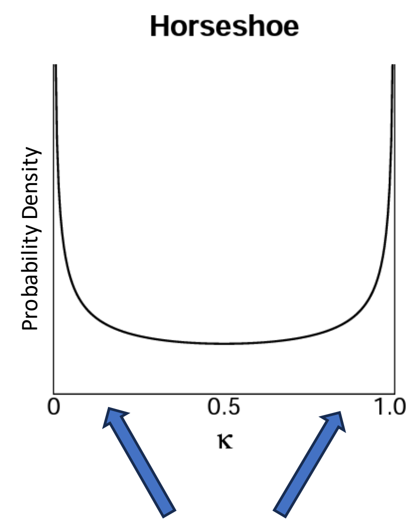


Sparsity-inducing Bayesian models provide sparse estimation with uncertainty

- The "horseshoe" prior proposed by Carvalho, et al. 2009 in AISTATS *encourages estimates to either be shrunk to 0 or completely dictated by the data.*
  - See the "horseshoe" shape in the lower right

$$\begin{aligned} \boldsymbol{\delta} &= \boldsymbol{B\gamma} = \textbf{relative bias} \\ \mathbf{B} &= \textbf{bias basis matrix} \\ \boldsymbol{\gamma} &\sim \boldsymbol{N}(\mathbf{0}, \boldsymbol{\lambda}_j^2 \boldsymbol{\tau}^2) \\ \boldsymbol{\lambda}_j &\sim \boldsymbol{C}^+(\mathbf{0}, \mathbf{1}) \\ \boldsymbol{\tau} &\sim \boldsymbol{N}^+(\mathbf{0}, \boldsymbol{\tau}_0) \end{aligned}$$

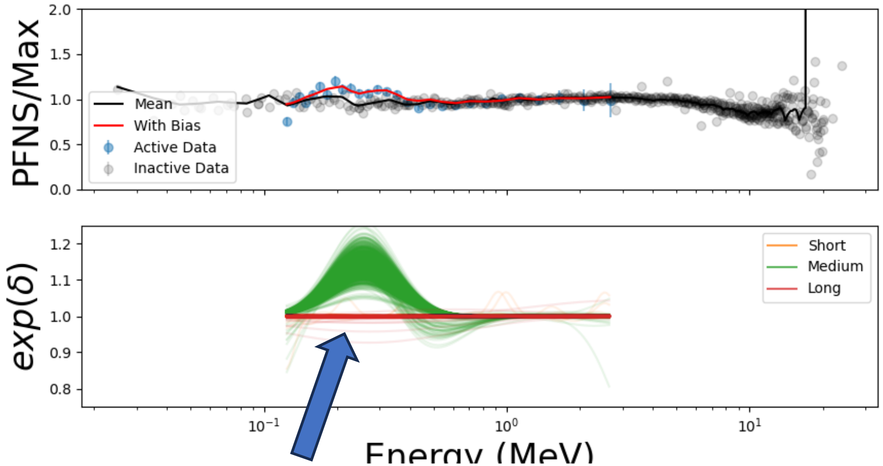
- $\boldsymbol{C}^+()$ is a Half-Cauchy distribution and $\boldsymbol{N}^+()$ is Half-Normal
- Sampling done in **Stan**
  - A python package for this model is in progress
- Bayesian sparse methods are slower than LASSO, but provide critical uncertainty information to improve scientific interpretation



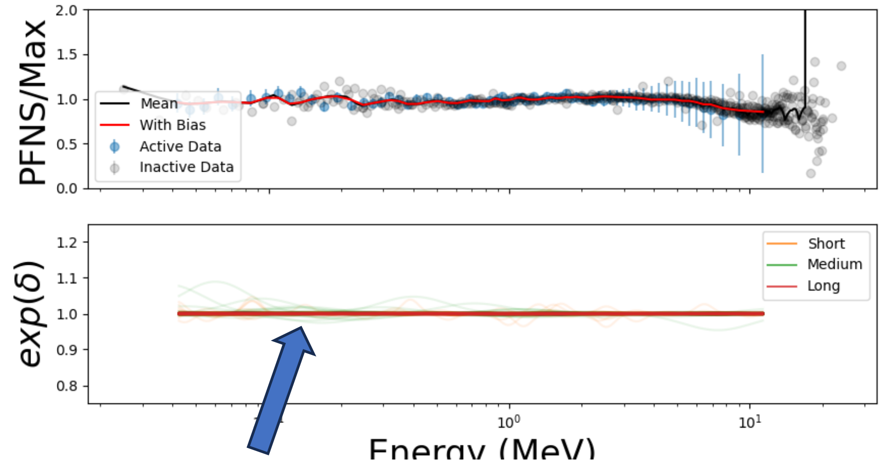
Model is weighted toward a spike at zero and spike at "no prior constraint"

The resulting model captures strongly suspected biases in the ^{252}Cf PFNS data

Neutron Detector – Li 6



Neutron Detector – Plastic Scintillator



Identified bias for experiments with a Li-6 Neutron Detector

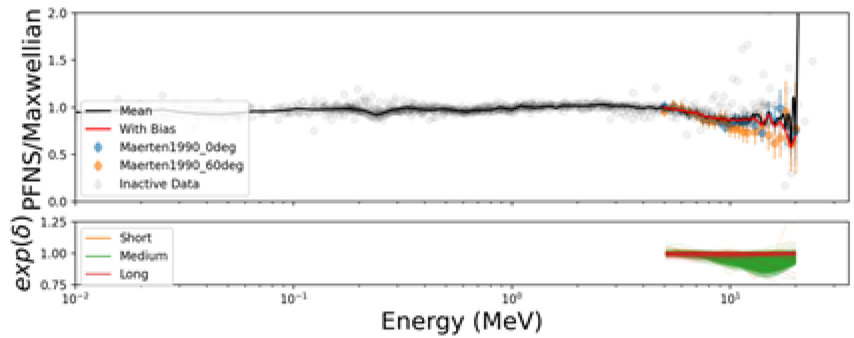
No bias identified for experiments with a plastic scintillator

High-E bias identified across several feature groups, less obvious but experimentally explainable.

Effect at high energies was attributed to many features. Detailed expert discussion and analysis of data pointed to fission detection (angular dependence of fission fragments).

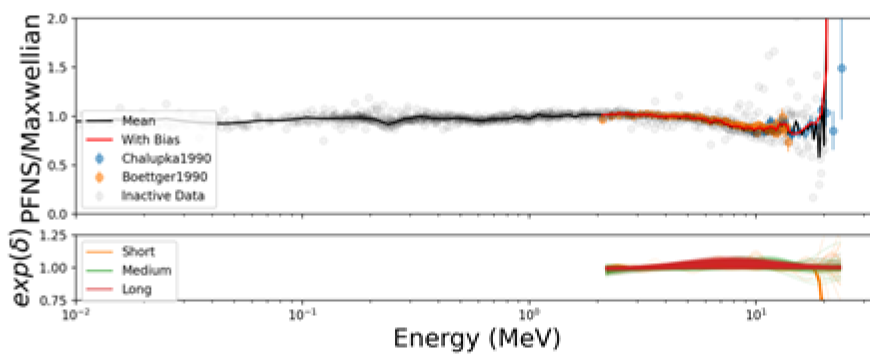
Effects suspected leading to bias might help us understand spread in experimental data for other reactions and isotopes.

Fission Detection Efficiency Correction Method: Calculated/Measured



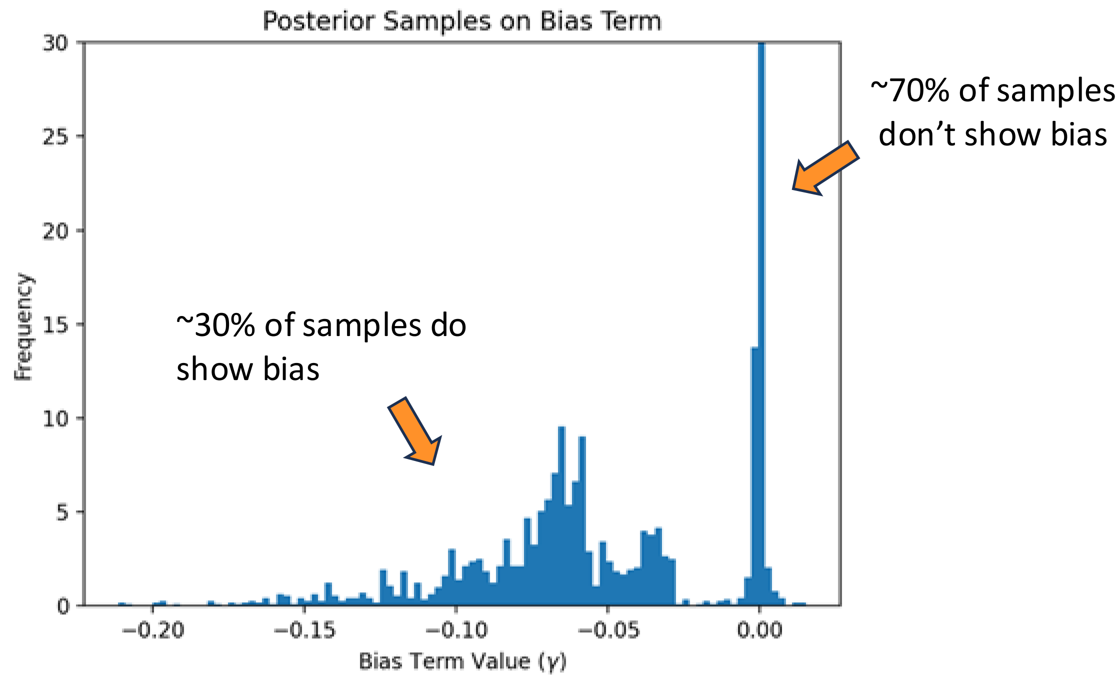
~30% of samples

Fission Detection Efficiency Correction Method: Calculated/Stapre



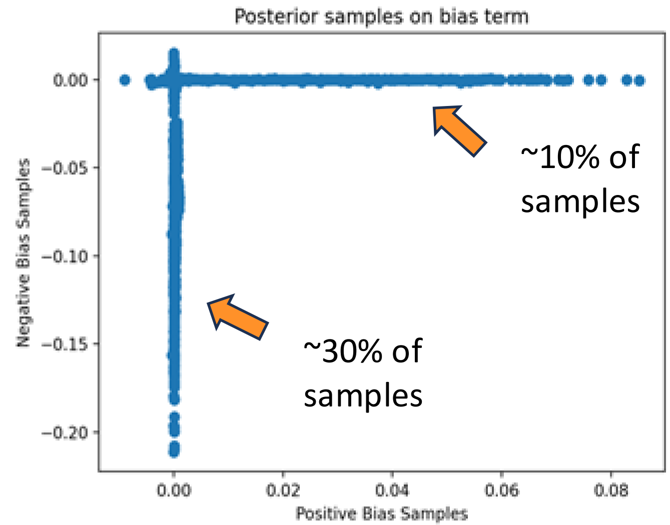
~10% of samples

Basis coefficients can be further used to estimate the evidence for a bias term existing for a feature in a particular energy range



Coefficient samples can also indicate when multiple explanations are consistent with the data

- For a given energy range, some experimental data were discrepant.
- The model can identify that either some data is biased high (positive values on the x-axis) or some data is biased low (negative values on y-axis).
  - Note that the model picks one of two explanations – it does not split the difference and say the middle is best.
  - The model also assigns probabilities to each explanation as seen on the right.
    - And the probability that there is no actual bias



In total, a bias seen in ~40% of samples

To summarize:

AIACHNE had developed a sparsity-inducing Bayesian model for capturing biases in experimental observations for nuclear data evaluation based on metadata features

- Leveraging sparse Bayesian methods to learn how experimental features are related to biased or discrepant data

- The methods we are developing provide power to discriminate across a large set of features while providing uncertainty in the estimated nuclear data values that incorporate the bias estimation

- We have obtained results applying the methods to ^{252}Cf data
  - These results have been used to guide to the experimental design efforts of AIACHNE and are applicable to a wide array of future problems in bias estimation and evaluation with discrepant experimental observations in nuclear data