Recommendations and Case Studies on Peelle's Pertinent Puzzle

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Based on paper at
Phys. Rev. D 113, 012011

Introduction to Peelle's Pertinent Puzzle (PPP)

- PPP is the degradation/failure of a model fit to data resulting from an improper treatment in the data, model, or their comparison

- Most obvious symptom is a massive deficit in post-fit model normalization

- However, we also consider the potential for fit degradations outside of normalization

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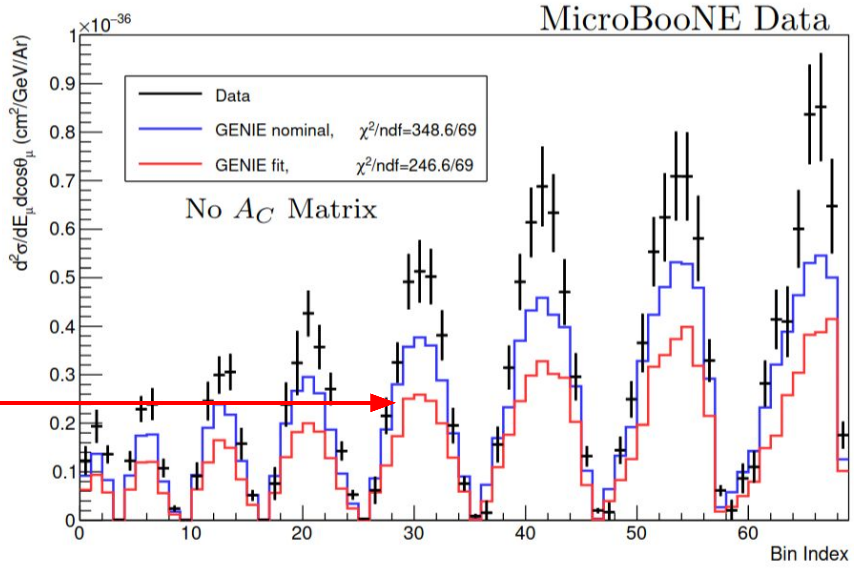
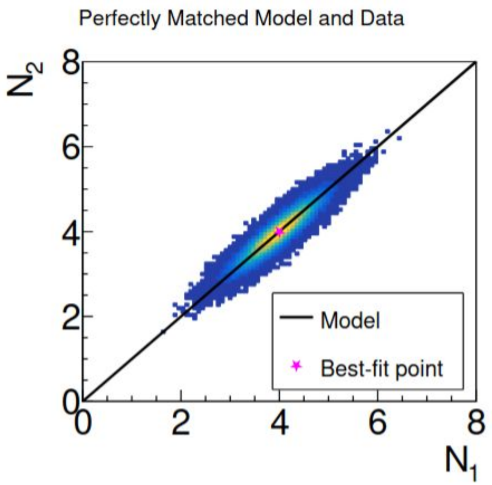


What Causes PPP?

- Strong correlations between measurement bins are a requirement
  - Physics data often is highly correlated! Think of flux normalization uncertainty

- However, successful fits to correlated measurements are possible
  - There's another feature driving PPP



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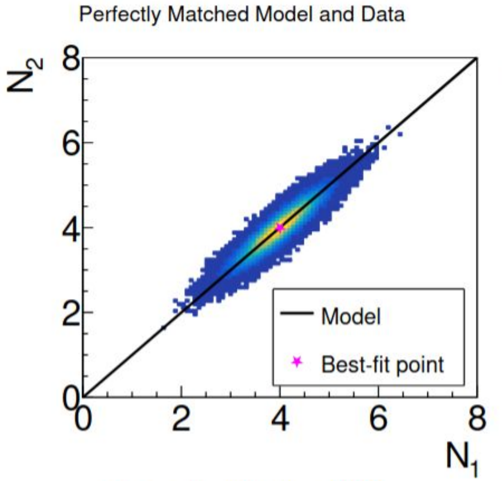
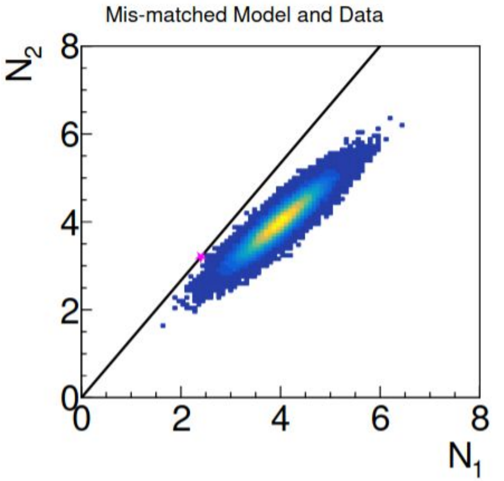
  - There's another feature driving PPP
- Mismatch between data and model causes tension in χ^2 that drives PPP
  - Large normalization uncertainty makes it preferable to address shape difference indirectly by reducing normalization
  - As norm -> 0, shape differences also go to 0





Simple Example of PPP

- Imagine taking two measurements of the same object with the same thermometer and getting values of y_1, y_2 = 90, 100

- Model the uncertainty as 2% uncorrelated plus 10% correlated (normalization):

$$\text{Covariance } C = \underbrace{\begin{pmatrix} 1.8^2 & 0 \\ 0 & 2^2 \end{pmatrix}}_{\text{Uncorrelated}} + \underbrace{\begin{pmatrix} 9^2 & 9\cdot 10 \\ 9\cdot 10 & 10^2 \end{pmatrix}}_{\text{Normalization}} = \underbrace{\begin{pmatrix} 84.2 & 90 \\ 90 & 104 \end{pmatrix}}_{\text{Total}}$$

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- Answer: 83
  - Yes, that's right. A value outside the [90, 100] bounds of the two measurements!

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- What is the best-fit temperature from these two measurements?

- Answer: 83
  - Yes, that's right. A value outside the [90, 100] bounds of the two measurements!
  - High correlation of ϱ~0.96 means it's highly penalized for Δy_1, Δy_2 to differ significantly. Instead, it's preferred to find a lower value outside [90,100] so that $\Delta y1 \cong \Delta y2$

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- What went wrong?
  - Premise is flawed. These uncertainties do not reflect the actual variation in the data.
  - Likely that 2% uncorrelated uncertainty is wrong (and perhaps also the 10% normalization)
  - In other words, there was a mismatch between the data and the model

Small Author Paper Investigating Causes of PPP

- Identified improper treatments that can drive PPP
  - Limited model that lacks flexibility to describe data
  - Improper treatment of flux uncertainties through use of real-flux-averaged measurement
  - Omission of regularization matrix in data-model comparison

- Recommended best-practices to avoid PPP

- Discussed mitigation strategies when PPP cannot be avoided

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Improving neutrino-nuclei interaction models: Recommendations and case studies on Peelle's Pertinent Puzzle

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Conditional Constraint Fitting

- Standard fit procedure requires varying model parameters and resimulating prediction, try to minimize χ^2
  - Struggles to find global minimum for large number of fit parameters
  - Forces fits to limit number of free parameters -> artificially reduce model flexibility

- Alternate approach: construct covariance matrix between model parameters and measurement space
  - Update model prediction using Bayes' theorem and data measurement
  - No issue with fit minimization -> can simultaneously fit any number of parameters
  - Yields an approximate solution that can be fed into a fitter to easily converge to global minimum

$$\text{Covariance matrix } \Sigma = \begin{matrix} \Sigma^{XX} & \Sigma^{XY} \\ \Sigma^{YX} & \Sigma^{YY} \end{matrix}$$

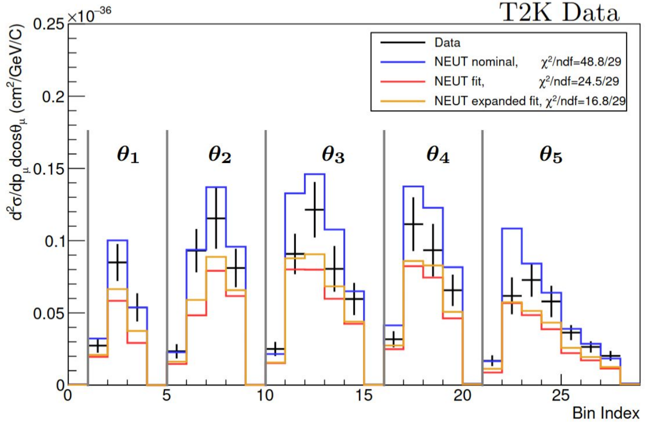
X: measurement space
Y: parameter space

$$\mu^{X,\text{constrained}} = \mu^{X} + \Sigma^{XX} \cdot (\Sigma^{YY})^{-1} \cdot (n^{Y} - \mu^{Y})$$
$$\Sigma^{XX,\text{constrained}} = \Sigma^{XX} - \Sigma^{XY} \cdot (\Sigma^{YY})^{-1} \cdot \Sigma^{YX}$$

n: measurement
μ: prediction

Data-Model Inconsistencies from Model Limitations

- ν_μ CC0π $d^2\sigma/dP_\mu d\cos\theta_\mu$ measurement from T2K: Phys. Rev. D 101.112004
- Fit with versions of NEUT 5.8.0
  - First use version with spectral function
- NEUT base model is unable to describe data within uncertainties
  - When fit with 6 free parameters a PPP issue is seen
  - When the fit is expanded to 9 free parameters there is still a PPP issue but it is smaller



M_AQE
Optical Potential
High-Q^2 Norm
2p2h Norm
M_ARes
C_5^A (Resonance production)

Six NEUT free parameters

Ad-hoc High-Q^2 Norm 2
Ad-hoc High-Q^2 Norm 3
Low Q^2 Pauli Blocking parameter

Three new parameters

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- NEUT base model is unable to describe data within uncertainties
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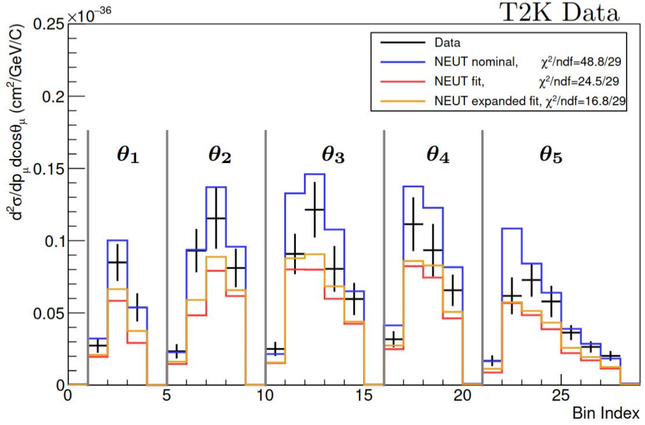
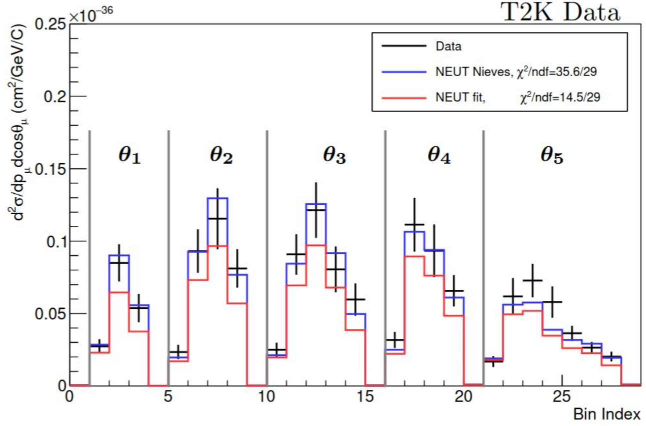
- NEUT with Nieves 1p1h obtains better pre-fit chi2
  - Even less PPP issue
  - Suggests insufficient model is driving PPP





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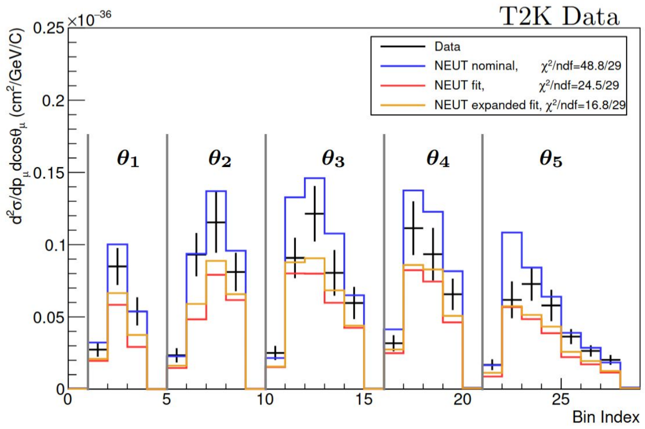
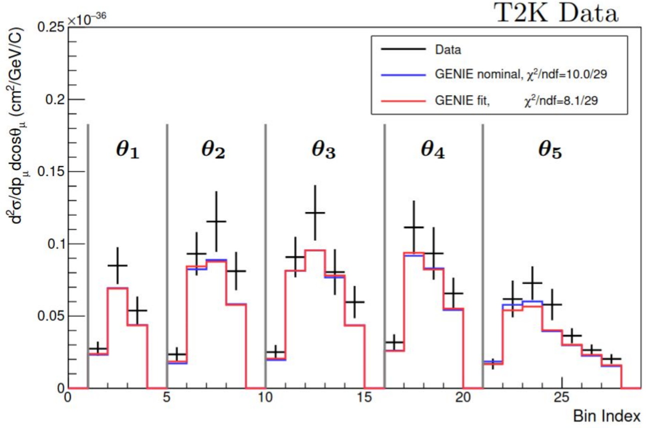
- GENIE can describe the data within uncertainties.
  - Genie v3.0.6 G18_10a_02_11a (uBooNE tune)
  - When fit with 4 parameters no PPP issue is seen
  - Suggests model differences responsible for NEUT PPP





Data-Model Inconsistencies from Real vs. Nominal Neutrino Flux Discrepancy

- Cross sections are averaged over a neutrino flux distribution
    - Can average over the real flux observed by the experiment
    - Can also average over the predicted (nominal) flux
    - Real-flux-averaged is less model dependent but comparisons with model predictions still rely on nominal flux prediction
    - Real-flux struggles to account for flux correlations between meas and pred

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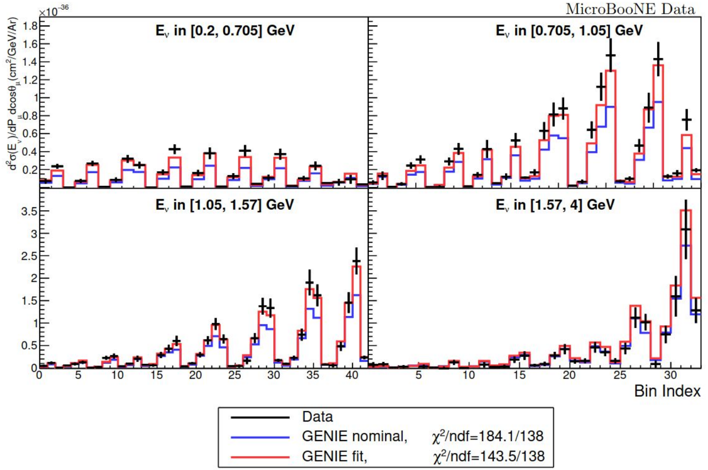
- ν_μ CC Inclusive $d^2\sigma(E_\nu)/dP_\mu d\cos\theta_\mu$ measurement from MicroBooNE
  - [PLB Volume 870, 139939]

- Fit with GENIE v3 (uBooNE tune), varying all 55 model parameters



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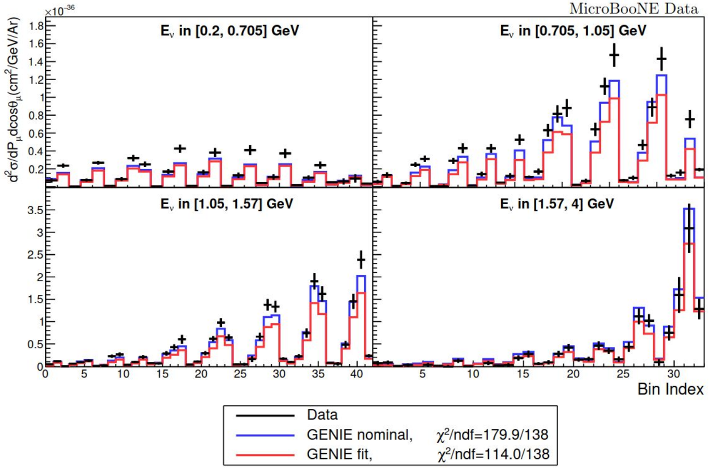
- Flux mismodeling induced by generating model prediction from alternate flux
  - Mimics situation of real-flux measurement compared to model with incorrect nominal flux
  - Principal component of flux cov varied at 2σ
  - Flux shape uncertainties removed

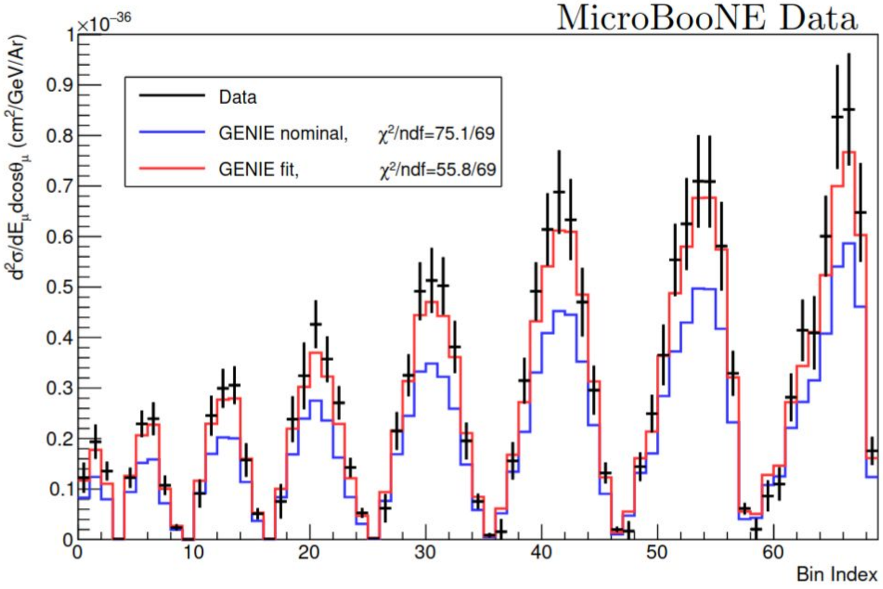
- PPP observed in fit with alternate flux model



Incorrect Flux Treatment

Data-Models Inconsistencies from Regularization in Data Unfolding

- ν_μ CC Inclusive $d^2\sigma/dP_\mu d\cos\theta_\mu$ measurement from MicroBooNE
  - [Phys. Rev. Lett. 133.041801]
- Unfolded with WienerSVD
  - Regularization smears result, captured in "A_C" matrix
- Fit with GENIE v3 (uBooNE tune), varying all 55 model parameters
- When model is also smeared by A_C matrix, proper comparison yields successful fit



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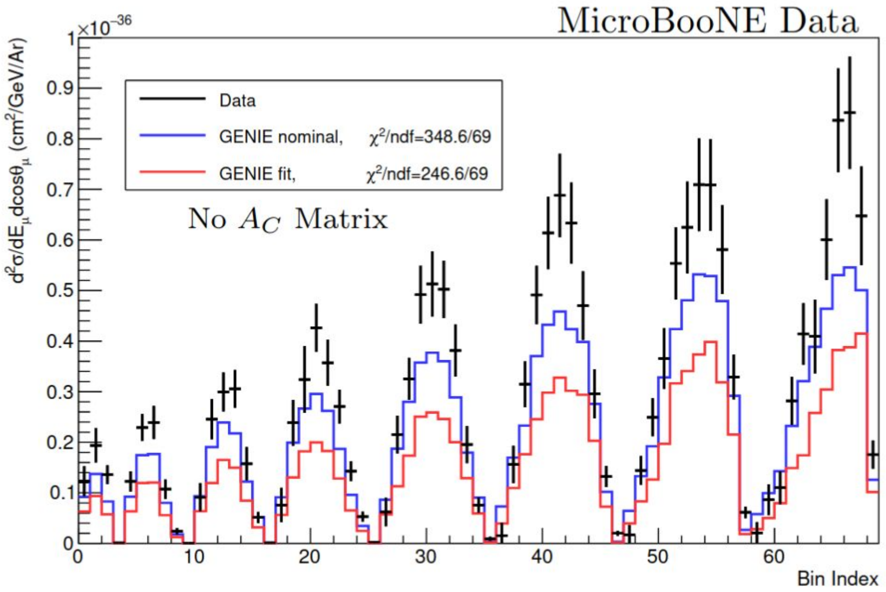
- When A_C matrix is omitted in comparison with model, improper comparison yields PPP issue

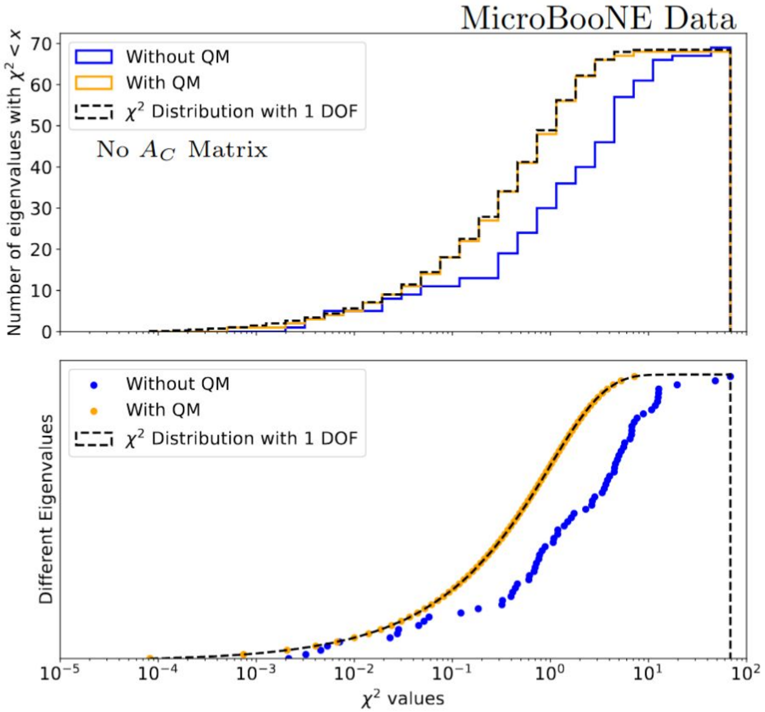


PPP Mitigation Strategies

- Remove data correlations
  - Throws away a lot of useful information
- Separate normalization and shape covariance
  - Imperfect decomposition into norm, norm+shape, and shape components
  - What PPP issue occurs in non-norm degree of freedom (DoF)?
- Enlarge uncertainties until model can describe data
  - Conservative approach of adding uncertainty
  - Can address data-model mismatch in any DoF(s)
  - Generalizes to simultaneous fit to multiple data sets

Uncertainty Enlargement with Quantile Mapping

- If model can explain data within uncertainties, then data-model disagreement in each bin should sample from χ^2 distribution with 1 DoF
    - Assumes uncorrelated bins -> first transform to basis with diagonal covariance



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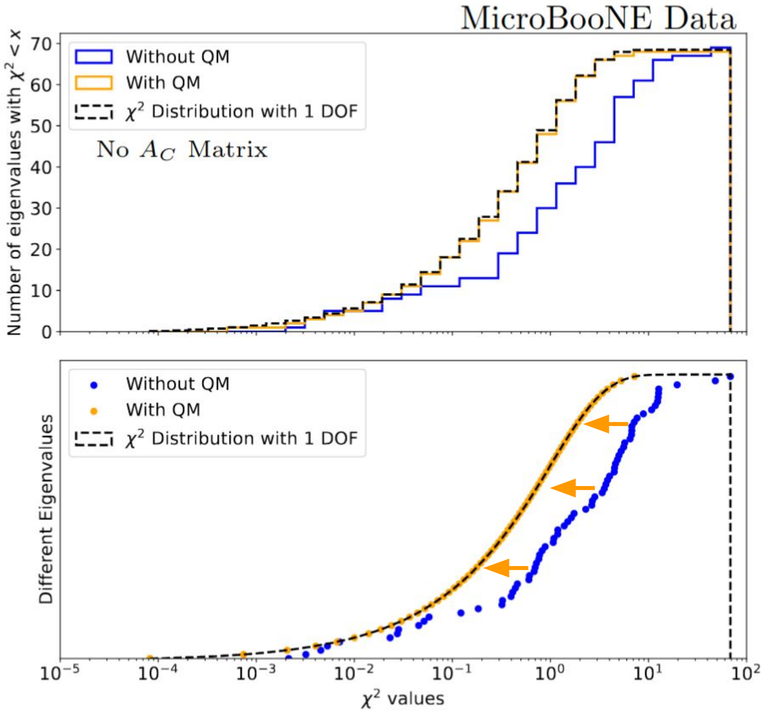
  - Reduces each χ^2_i value

- Transform back to measurement space with new covariance
  - DoF with extreme tension are relaxed



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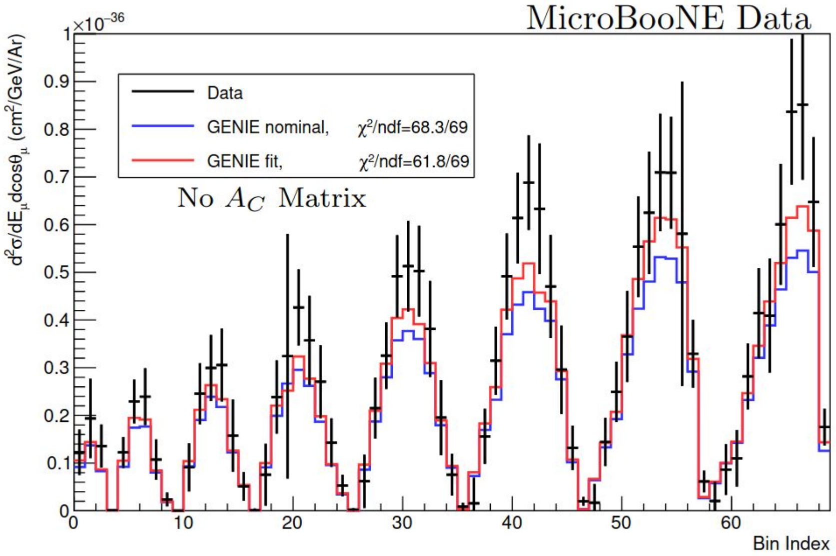

Summary

- PPP is driven by improper treatments in data, model, or both
  - Model limitations such as few free parameters in fit or poor base model
  - Poor nominal flux model, improper correlation treatment in real-flux comparison
  - Use of regularization in unfolding without providing A_C matrix or similar
- Recommend to avoid known improper treatments
  - Further recommend to test fits to data for PPP before publishing
  - Covariance matrix fitting eliminates need to limit model parameters
- When PPP is observed in fitting exercises, mitigate carefully
  - Uncertainty enlargement is a conservative and generalizable approach
  - Quantile mapping provides mechanism for deciding how to enlarge unc

Backup

Simple Example of PPP (General Solution)

- Imagine taking two measurements with the same thermometer and getting values of y_1, y_2 = 90, 100

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$$C^{-1} = \frac{1}{657}\begin{pmatrix} 104 & -90 \\ -90 & 84.2 \end{pmatrix}$$

- $\lambda = \sum^N_{i=1} w_i\cdot y_i$

- $w_i = (\sum^N_{j=1} C^{-1}_{ij}) / (\sum^N_{k=1}\sum^N_{l=1} C^{-1}_{kl})$

=>

$\lambda = w\cdot y_1 + (1-w)\cdot y_2$

$w = (C^{-1}_{11}+C^{-1}_{12}) / (C^{-1}_{11}+C^{-1}_{12}+C^{-1}_{21}+C^{-1}_{22})$

Model	$\sigma(10^{-38}\mathrm{cm}^2/C)$
T2K Measurement	5.64 ± 0.72
NEUT nominal	6.27
NEUT fit	3.54
NEUT expanded fit	4.13
NEUT Nieves	5.73
NEUT Nieves fit	4.21
GENIE nominal	3.00
GENIE fit	3.02