Covariance Analysis of Experimental Shape Data

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The analysis of shape data including normalization and the impact on prompt fission neutron spectrum measurements

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Why Shape Data are Different

The basic problem:

- Shape data (PFNS shape, probability distributions, relative measurements, etc.) are inherently different than absolute data (absolute cross sections, etc.)
- Primary difference is in the covariance treatment

Typical Experimentalist Treatment:

- I found a fully-correlated uncertainty source (beam flux, scaling factor)
  - I'm trying to report a shape result, so I can ignore it
- I found a partially correlated uncertainty source (most sources)
  - Keep it, or ignore part of it, or state that it's correlated, or something else...
  - How much do I keep? What is the covariance of the reduced uncertainty??
  - Give to evaluator and move on

A Normalization Procedure with Covariance Propagation Solves This Problem

The Basic Idea for the Covariance Math

Un-norm. Covariance → $$\text{cov}\left[p\right]_{ij} = \sigma_{ij}$$

Normalized Data → $$n_i = S\frac{p_i}{\sum_j p_j w_j} = S\,\frac{p_i}{A} \propto \frac{p_i}{A}$$

Sensitivity Matrix → $$\Delta_{ik} = \frac{\partial n_i}{\partial p_k} = \frac{\delta_{ik}}{A} - \frac{p_i}{A^2}w_k$$

Norm. Covariance → $$\text{cov}\left[n\right]_{ij} = \sum_k \sum_l \Delta_{ik}\sigma_{kl}\Delta_{jl} = \sum_k \sum_l \left(\frac{\delta_{ik}}{A} - \frac{p_i}{A^2}w_k\right)\left(\frac{\delta_{jl}}{A} - \frac{p_j}{A^2}w_l\right)\sigma_{kl}$$

Correlation Matrix → $$\text{cor}\left[n\right]_{ij} = \frac{\text{cov}\left[n\right]_{ij}}{\sqrt{\text{cov}\left[n\right]_{ii}\,\text{cov}\left[n\right]_{jj}}}$$

Expected: Fully-Correlated Uncertainties Drop Out

Consider a covariance source of the form: $\sigma_{ij} = f^2 p_i p_j$

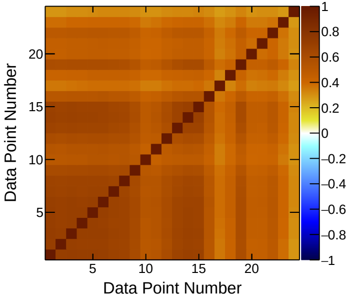
$$\text{cov}\left[n\right]_{ij} = \sum_k \sum_l \left(\frac{\delta_{ik}}{A} - \frac{p_i}{A^2} w_k \right) \left(\frac{\delta_{jl}}{A} - \frac{p_j}{A^2} w_l \right) f^2 p_k p_l.$$

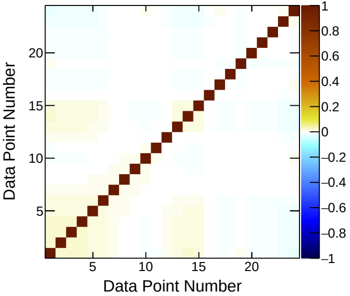
$$\begin{aligned}
\text{cov}\left[n\right]_{ij} &= \sum_k \sum_l \left(\frac{\delta_{ik}\delta_{jl}}{A^2} - \delta_{ik}\frac{p_j w_l}{A^3} - \delta_{jl}\frac{p_i w_k}{A^3} + \frac{p_i p_j w_k w_l}{A^4} \right) f^2 p_k p_l \\
&= \frac{f^2 p_i p_j}{A^2} \sum_k \sum_l \left(1 - \frac{p_l w_l}{A} - \frac{p_k w_k}{A} + \frac{p_k p_l w_k w_l}{A^2} \right), \\
&= \frac{f^2 p_i p_j}{A^2} \left(1 - \sum_l \frac{p_l w_l}{A} - \sum_k \frac{p_k w_k}{A} + \sum_k \frac{p_k w_k}{A} \sum_l \frac{p_l w_l}{A} \right),
\end{aligned}$$

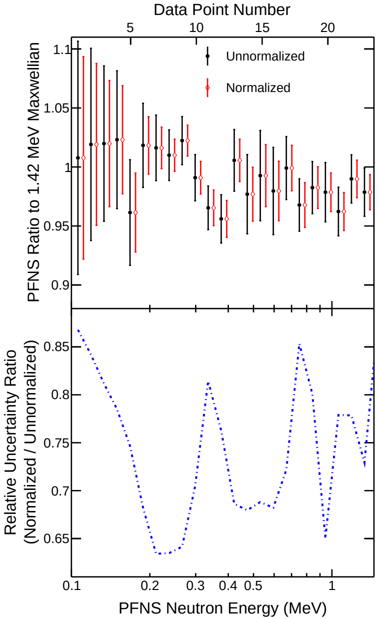
Each summation adds to unity, and so

$$\text{cov}\left[n\right]_{ij} = 0.$$

Expected: Fully-Correlated Uncertainties Drop Out







Maybe Unexpected: Redistribution of Covariances

Consider data set in which one data point, z, is known perfectly, so

$\sigma_{zz} = 0$ and $\sigma_{iz} = 0$ (no uncertainty, no correlations for point z)

but, $\sigma_{ij} \neq 0$ for all $i, j \neq z$

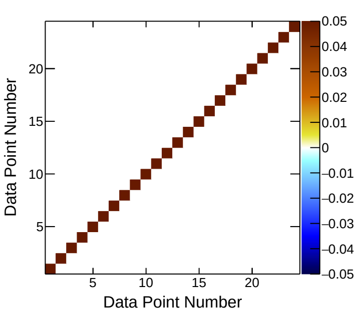
$$\text{cov}\left[n\right]_{iz} = \sum_{k\neq z}\sum_{l\neq z}\left(\frac{\delta_{ik}}{A} - \frac{p_i}{A^2}w_k\right)\left(-\frac{p_z}{A^2}w_l\right)\sigma_{kl},$$

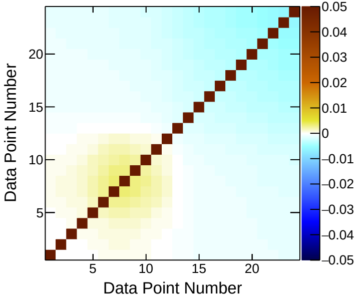
- This is generally non-zero, and therefore point z has nonzero variance and covariance with other points, i, j

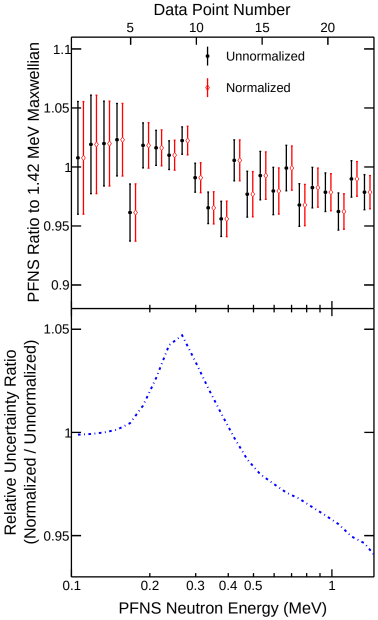
A well-measured data point gets a larger 1-D uncertainty assigned to it

- Odd to most experimentalists, but the *shape* is properly represented

Maybe Unexpected: Redistribution of Covariances



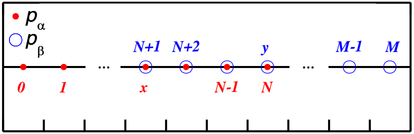




Necessary: Consistency When Combining Shapes

→ There are choices to make when combining shape data sets (relevant to reporting data from Chi-Nu PFNS results)

→ Only one single, correct shape exists for a set of data points



Independent Axis (Energy, time, etc.)

$$\rho = \left[\sum_{i=x}^{N} p_i w_i\right] \times \left[\sum_{j=N+1}^{y} p_j w_j\right]^{-1}.$$

$$u_i^{\beta\to\alpha} = \begin{cases} p_{\alpha i} & \text{if } 0 \le i \le N \\ \rho\, p_{\beta i} & \text{if } N < i \le M \end{cases}$$

$$u_i^{\alpha\to\beta} = \begin{cases} \rho^{-1} p_{\alpha i} & \text{if } 0 \le i \le N \\ p_{\beta i} & \text{if } N < i \le M \end{cases}$$

Necessary: Consistency When Combining Shapes

$$\text{cov}\left[u\right]_{ij}^{\beta\to\alpha} = \sum_k \sum_l \left(\delta_{ik}\rho^{\theta_\beta(i)} + p_i \frac{\partial \rho^{\theta_\beta(i)}}{\partial p_k}\right)\left(\delta_{jl}\rho^{\theta_\beta(j)} + p_j \frac{\partial \rho^{\theta_\beta(j)}}{\partial p_l}\right)\sigma_{kl}$$

$$\text{cov}\left[u\right]_{ij}^{\alpha\to\beta} = \sum_k \sum_l \left(\delta_{ik}\rho^{-\theta_\alpha(i)} + p_i \frac{\partial \rho^{-\theta_\alpha(i)}}{\partial p_k}\right)\left(\delta_{jl}\rho^{-\theta_\alpha(j)} + p_j \frac{\partial \rho^{-\theta_\alpha(j)}}{\partial p_l}\right)\sigma_{kl}$$

These covariances are not equal in general.

Normalize the combined data set to recover the single correct combined shape

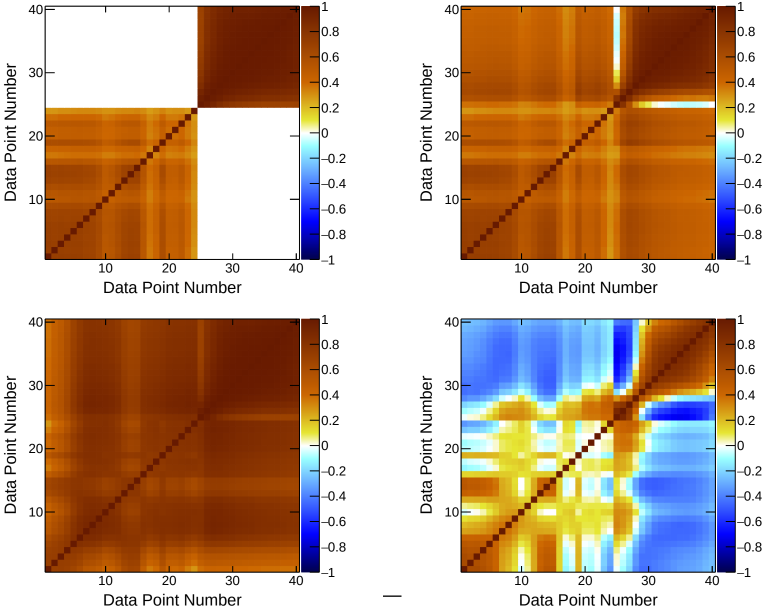
$$n_i^{\beta\to\alpha} = \begin{cases} p_i/A_T & \text{if } 0 \le i \le N \\ \rho\, p_i/A_T & \text{if } N < i \le M \end{cases} = \frac{\rho^{\theta_\beta(i)} p_i}{A_T}$$

$$\text{cov}\left[n\right]_{ij}^{\beta\to\alpha} = \sum_k \sum_l \Delta_{ik}^{\beta\to\alpha}\sigma_{kl}\Delta_{jl}^{\beta\to\alpha}$$

After some work, $\Delta_{ik}^{\alpha\to\beta} = \Delta_{ik}^{\beta\to\alpha}$

$$\Rightarrow \text{cov}\left[n\right]_{ij}^{\alpha\to\beta} = \text{cov}\left[n\right]_{ij}^{\beta\to\alpha}$$

Necessary: Consistency When Combining Shapes



Conclusions, Acknowledgements, References

- Normalization $\neq$ Scaling, even if scaling to have $A = 1$
- Covariance propagation of normalization of an unnormalized experimental data set yields the covariance matrix of the shape
- Normalization is a necessary part of experimental shape data analysis
  - Experimental shapes could be misrepresented in evaluations otherwise...

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