Peelle's Pertinent Puzzle and D'Agostini Bias — *Estimating the Mean with Relative Systematic Uncertainty*

Speaker: Mike Grosskopf

Co-authors:

Scott Vander Wiel

Denise Neudecker

Peelle's Pertinent Puzzle (PPP)

- In 1987 at Oak Ridge National Lab, R.W. Peelle described having two observations to estimate a shared mean:

$$y_1 = 1.0 \pm 10\% \qquad y_2 = 1.5 \pm 10\%$$

and 20% fully correlated uncertainty

- Uncertainties
  - "Fully correlated" means multiplicatively up or down together.
  - Three uncertainties are taken to be independent.
  - Relative uncertainties are assumed to be "1 sigma" values
- Peelle was a physicist doing nuclear data evaluation and he worked out the generalized least squares (GLS) estimate of the mean, as is standard in the field

Peelle's Pertinent Puzzle (PPP)

- Generalized least squares as per Peelle:

$$\boldsymbol{y} = (1.0, 1.5)^T$$

$$\Sigma = 0.1^2 \cdot \mathrm{diag}(\boldsymbol{y}^2) \; + \; 0.2^2 \cdot \boldsymbol{y}\boldsymbol{y}^{\mathrm{T}}$$

$$\hat{\mu} = (\mathbf{1}^T \Sigma^{-1} \mathbf{1})^{-1} \mathbf{1}^T \Sigma^{-1} \boldsymbol{y}$$

$$\hat{\sigma}^2 = (\mathbf{1}^T \Sigma^{-1} \mathbf{1})^{-1}$$

- And the answer is …

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- And the answer is …

$$\hat{\mu} = 0.88 \pm 0.25$$

below **both** observations!

- Terminology: *Data Weighted – Generalized Least Squares (**DW-GLS**)* refers to GLS with $\boldsymbol{y}$ in the assumed covariance matrix
  - Many scientists don't consider having $\boldsymbol{y}$ in its own covariance as odd

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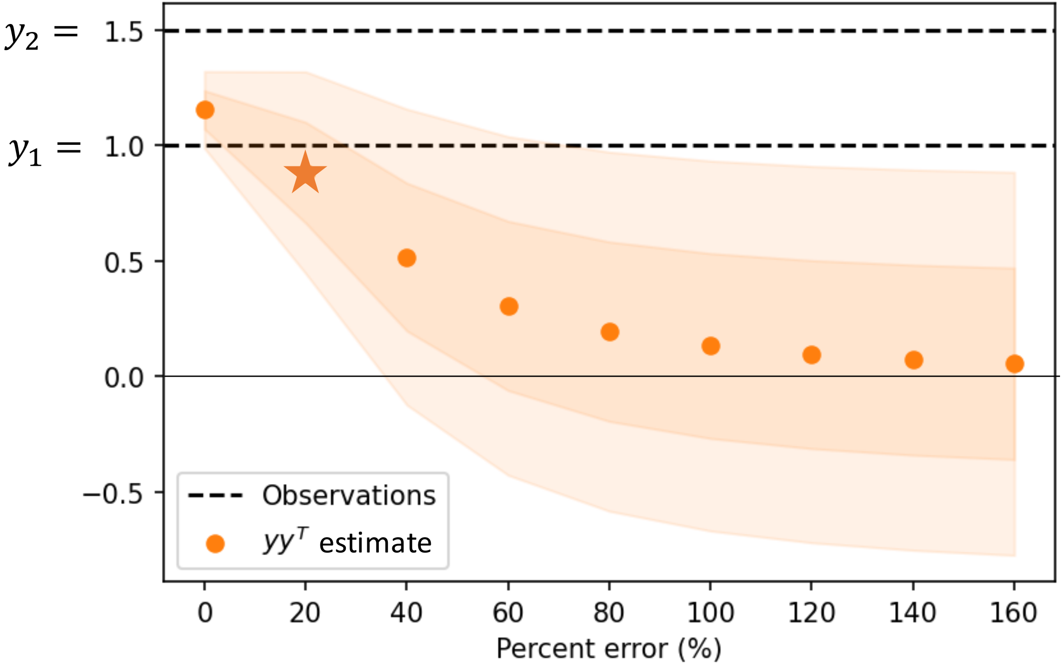
As fully-correlated error increases we expect

- *proportional* increase in uncertainty,
- *and not* additional bias…



… but neither holds with DW-GLS

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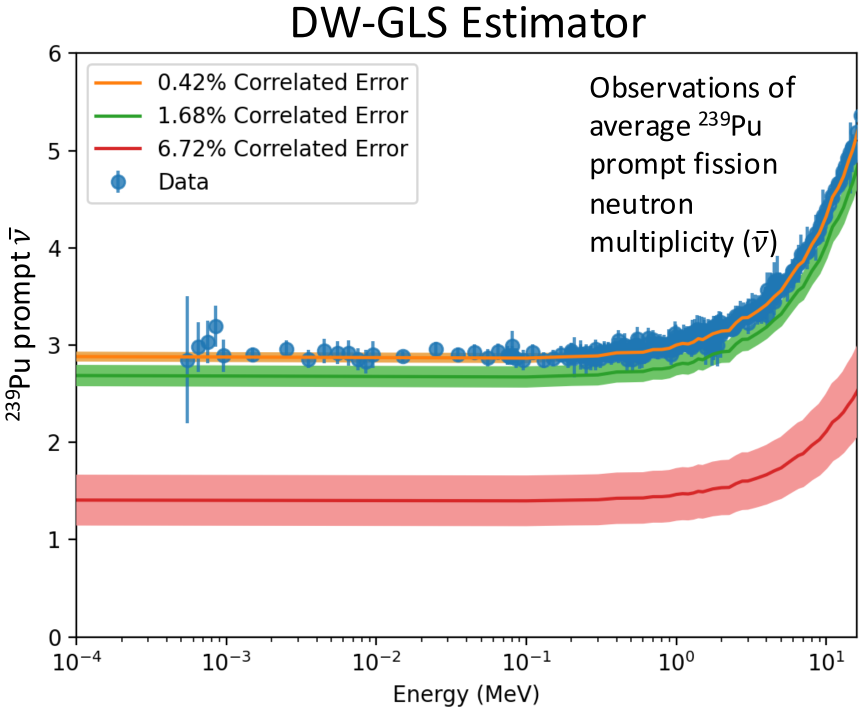
This problem exists more widely when using generalized least squares for nuclear data evaluation



Fitted curves (prior not shown)

- **Nominal case** has 0.42% fully-correlated error and looks OK but
  - fitted is 0.7% below data
  - 73% of residuals are positive
- Increasing the fully-correlated error by **4x** and **16x** reveals dramatic bias

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(Data from Marini et al., Phys Letters B, 835, 2022,137513)

High-Energy Physicists know this as *D'Agostini Bias*

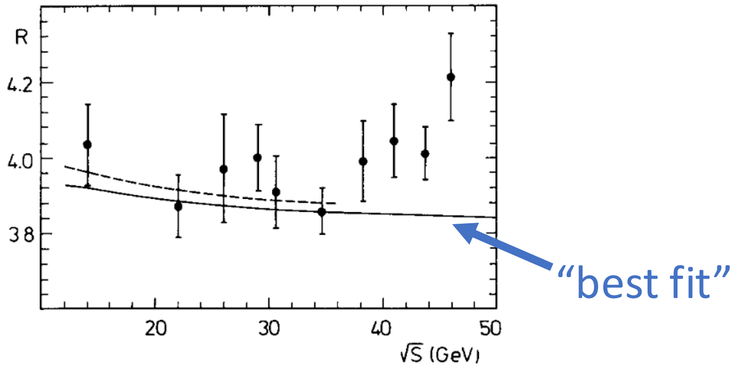

Fig. 2. R measurements from PETRA and PEP experiments with the best fits of QED + QCD to all the data (full line) and only below 36 GeV (dashed line). All data points are correlated (see text).

Example of a recent non-explanation

“The best-fit undershoots the data, essentially because with multiplicative uncertainties a lower prediction has a smaller uncertainty [D’Agostini, 1994].”

D'Agostini, Giulio. "On the use of the covariance matrix to fit correlated data." *Nuclear Instruments and Methods in Physics Research Section A: Accelerators, Spectrometers, Detectors and Associated Equipment* 346.1-2 (**1994**): 306-311.

Ball, Richard D., et al. "Precision determination of the strong coupling constant within a global PDF analysis: NNPDF Collaboration." *The European Physical Journal* C 78 (**2018**): 1-16.

What is going on in PPP?

- **Is this not a problem at all?**
  - Two observations with correlated errors aren't at all unlikely to fall on the same side of the mean
    - Why biased low rather than high? Symmetry would seem to make a case for no preference in either direction
    - Why so far outside the data? **The estimate makes one observation a 3σ outlier**

- Is this a problem with the GLS estimator for relative, correlated errors?

- Is this a fluke of the two-observation problem?

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What is going on here?

- Is this not a problem at all?
  - Two observations with correlated errors aren't at all unlikely to fall on the same side of the mean
- **Is this a problem with the GLS estimator for relative, correlated errors?**
  - Let's explore a couple other estimators:
    - Maximum likelihood estimator: $\boldsymbol{y} \sim \mathrm{MVN}(\boldsymbol{\mu}, \mathrm{diag}(0.1^2\boldsymbol{\mu}^2) + 0.2^2\boldsymbol{\mu}\boldsymbol{\mu}^\mathrm{T})$
    - Iteratively re-weighted least squares: Do GLS, but iterate from initial $\hat{\boldsymbol{\mu}} = \boldsymbol{y}$ using $\Sigma = \mathrm{diag}(0.1^2\, \hat{\boldsymbol{\mu}}^2) + 0.2^2\, \hat{\boldsymbol{\mu}}\hat{\boldsymbol{\mu}}^\mathrm{T}$
- Is this a fluke of the two-observation problem?

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What is going on here?

Recall
$y_1 = 1.0 \pm 10\%$
$y_2 = 1.5 \pm 10\%$

- Is this not a problem at all?
  - Two observations with correlated errors aren't at all unlikely to fall on the same side of the mean
- **Is this a problem with the GLS estimator for relative, correlated errors?**
  - Let's explore a couple other estimators:
    - Maximum likelihood estimator: $\hat{\mu}_{MLE} = 1.531$
    - Iteratively re-weighted least squares: $\hat{\mu}_{IRLS} = 1.25$
- Is this a fluke of the two-observation problem?

MLE is **above** both observations!

Observations just touch at $\pm 2\sigma$

MLE links the mean to this spread.

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What is going on here?

- Is this not a problem at all?
  - Two observations with correlated errors aren't at all unlikely to fall on the same side of the mean
- Is this a problem with the GLS estimator for relative, correlated errors?
- **Is this a fluke of the two-observation problem?**
  - Simulate 500 samples, each with
    - *n*=100 observations
    - mean=1.25
    - SDs: 10% independent + 20% fully-correlated

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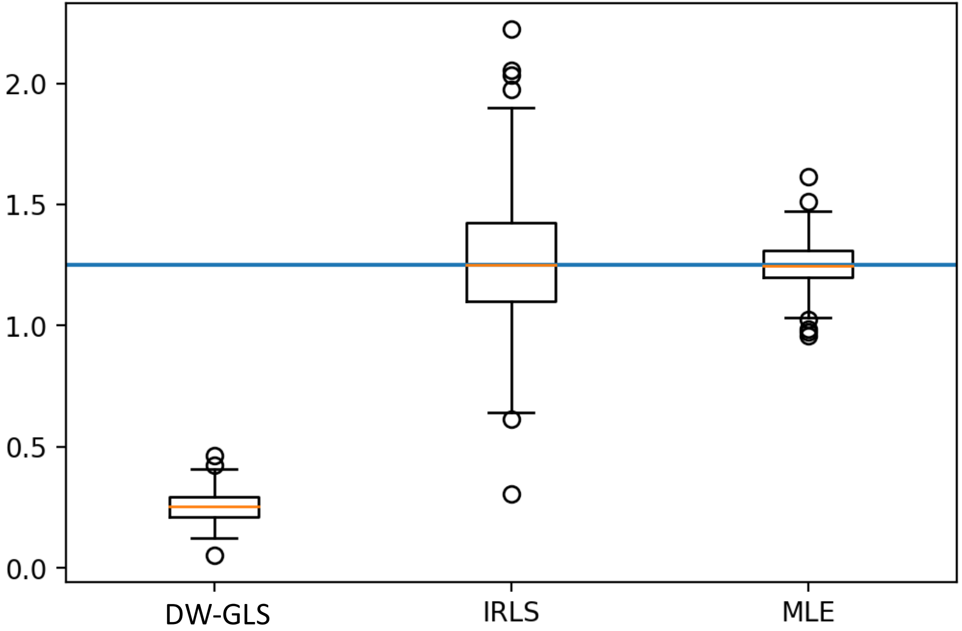
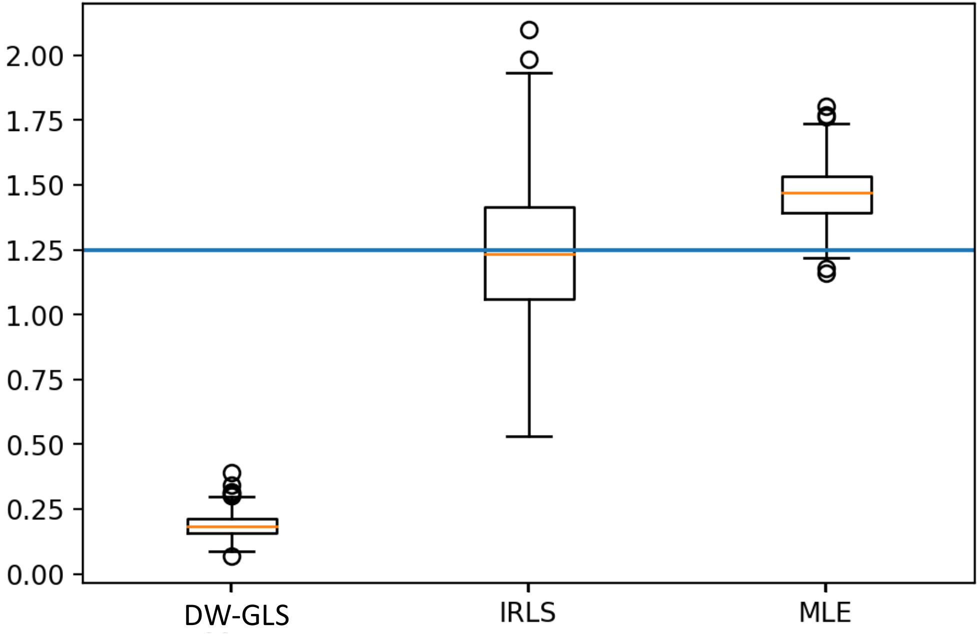
Estimates of the mean parameter from 500 simulated samples



Now the MLE looks great!

Why does the MLE look great now?

Estimates of the mean parameter with data generated with 12% independent error when 10% is assumed



The MLE no longer looks so great

The MLE is sensitive to mis-specified uncertainty!

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Conclusions so far:

- DW-GLS (i.e., using $\sigma^2 \boldsymbol{y}\boldsymbol{y}^{\mathrm{T}}$ in the covariance) biases estimates toward zero
  - large $\sigma \Longrightarrow$ bad bias.

- The MLE (and Bayes) is efficient but sensitive to mis-specified uncertainties

- IRLS is unbiased and robust to mis-specified uncertainties

PPP / D'Agostini Bias features in many papers over 30 years

In fact, IRLS has been reinvented to fix the bias

- but it is not recognized as fully legit

E.g., from Capote, *et al.* (2009)

An empirical "fix" compensates for PPP in a practical way as suggested by Chiba and Smith (1991).

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Why does DW-GLS behave so badly?

Insight from a regression problem

Regress $\mathbf{y}$ on two predictors

$$\mathbf{y} = \alpha\mathbf{1} + \beta\boldsymbol{x} + \gamma\boldsymbol{z} + \boldsymbol{\epsilon}$$

Suppose we care about α, β, but γ is just a nuisance with priors

$$\gamma \sim \mathrm{N}\left(0, \sigma_\gamma^2\right), \qquad \boldsymbol{\epsilon} \sim \mathrm{N}(\mathbf{0}, \sigma_\epsilon^2 \boldsymbol{I})$$

Integrating over γ:

$$\mathbf{y} = \alpha\mathbf{1} + \beta\boldsymbol{x} + \boldsymbol{e}$$
$$\boldsymbol{e} \sim \mathrm{N}\left(\mathbf{0},\ \sigma_\epsilon^2 \boldsymbol{I} + \sigma_\gamma^2 \boldsymbol{z}\boldsymbol{z}^{\boldsymbol{T}}\right)$$

I.e., one-predictor but correlated errors

Application to DW-GLS

DW-GLS uses

$$\Sigma = 0.1^2 \cdot \mathrm{diag}(\boldsymbol{y}^2) + 0.2^2 \cdot \boldsymbol{y}\boldsymbol{y}^{\mathrm{T}}$$

and the $\boldsymbol{y}\boldsymbol{y}^{\mathrm{T}}$ is like regressing $\boldsymbol{y}$ on itself!

With $\boldsymbol{z} = \boldsymbol{y}$, the covariance absorbs the signal and

$$\left(\hat{\alpha}\ \hat{\beta}\right) \to (0,0) \quad \text{as} \quad \sigma_\lambda \to \infty$$

Larger correlated error ⇒ more over-fitting

That is, DW-GLS with a fully correlated term $\boldsymbol{y}\boldsymbol{y}^{\mathrm{T}}$ is inherently biased toward zero.

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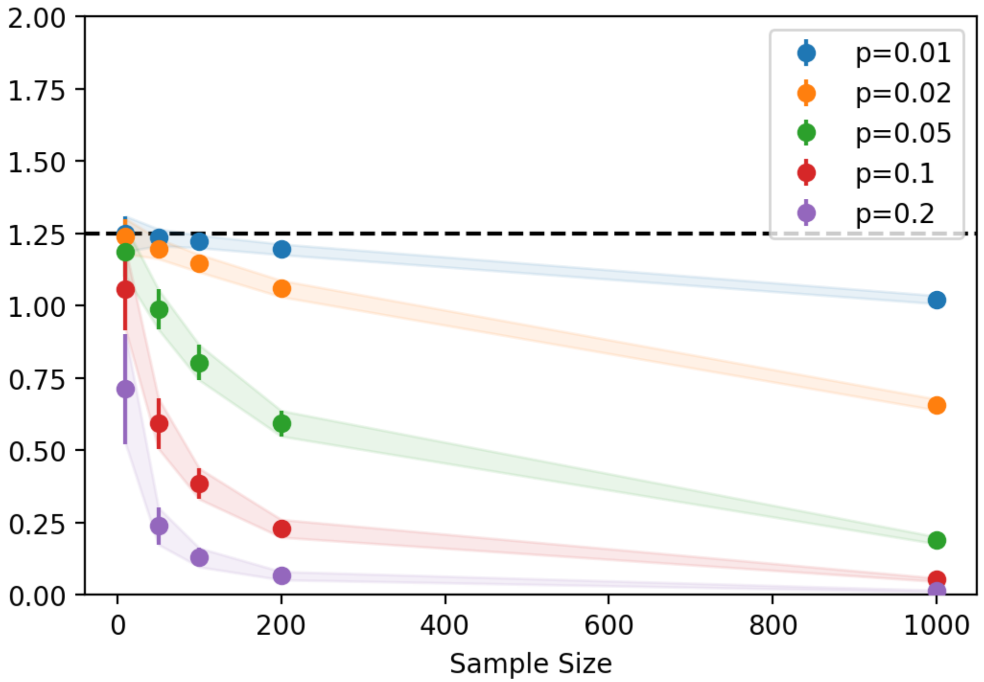
Coming back to DW-GLS, is it at least OK for small correlated uncertainty?

No

- It is not consistent.
- Adding more data drives the estimate to 0 for *any* relative correlated uncertainty, *p>0*



Conclusions

Advice for analysts

- **DO NOT** represent fully-correlated relative uncertainty as $p^2 \boldsymbol{y}\boldsymbol{y}^{\mathrm{T}}$
  - equivalent to adding $\boldsymbol{y}$ as a predictor for $\boldsymbol{y}$ itself
  - this drives the signal of interest to zero
  - Results in bad mean AND bad uncertainty
- **DO** represent the uncertainty as $p^2\, \widehat{\boldsymbol{\mu}}\, \widehat{\boldsymbol{\mu}}^{\boldsymbol{T}}$ and use IRLS
  - this is robust to mis-specified p
  - also robust to mis-specified independent error
- **DO** carefully consider how relative error can allow noise to influence the mean estimates with MLE and Bayesian inference

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