Bayesian Monte-Carlo Evaluation Framework for Imperfect Data

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Assumptions or approximations used with Bayes' Theorem

1. The *model and* the prior PDF of *data* are assumed to be *perfect*
2. The model is approximated by its 1st order (*linear*) expansion
3. Prior and posterior PDFs are approximated by *normal* PDFs.

- We recognize that 1. is equivalent to constraining the *posterior* expectation values of δ, and of its covariance matrix, to 0:

$$\langle\delta\rangle' = 0 \qquad \boldsymbol{\Delta}' \equiv \langle(\delta - \langle\delta\rangle')(\delta - \langle\delta\rangle')^\intercal\rangle' = \mathbb{0} \qquad \delta \equiv \delta(z, T(P)) \equiv T(P) - D \qquad z \equiv \begin{pmatrix} P \\ D \end{pmatrix}$$

- We remove 1. by letting evaluator choose values of $\langle\delta\rangle'$ and $\boldsymbol{\Delta}'$
- 2. and 3. can be removed by Metropolis-Hastings Monte Carlo

Overview of approximations used by ORNL codes

Code name	<delta>'	Delta'	Prior/Post PDF	Cost Function	Minimization
SAMMY	0	0	Normal/Normal	$\chi^2(z=(P,T(P)),\langle z\rangle,\boldsymbol{C})$	Linear, iterative
TSURFER	0	0	Normal/Normal	$-\|\|-$	Linear, 1 step
BMC	Any	Any	Any/any	$X^2(z,\langle z\rangle,\boldsymbol{C},T(P),\lambda,\boldsymbol{\Lambda})$	MHMC

- Bayes' theorem with arbitrary constraints:

$$\boldsymbol{\Lambda}=\boldsymbol{\Lambda}(\langle\delta\rangle',\boldsymbol{\Delta}',\langle z\rangle,\boldsymbol{C})$$
$$\lambda=\lambda(\langle\delta\rangle',\boldsymbol{\Delta}',\langle z\rangle,\boldsymbol{C})$$

$$p'(z|\beta\gamma)=p'(z|\gamma\beta)=N'\mathcal{L}(\beta|z\gamma)\times p(z|\gamma)$$

$$\mathcal{L}(\beta|z,\gamma)\leftarrow\mathcal{L}(\langle\delta\rangle',\boldsymbol{\Delta}'|z,\gamma)=e^{-\frac{1}{2}(\delta-\lambda)^{\intercal}\boldsymbol{\Lambda}^{-1}(\delta-\lambda)}$$

$$\begin{aligned}\beta &\leftarrow \{\text{any constraints on } \textit{posteriors} \text{ imposed by } \textit{evaluator}\},\\ \gamma &\leftarrow \{\text{any parameters needed to define the prior PDF, } p(z|\gamma)\}\end{aligned}$$

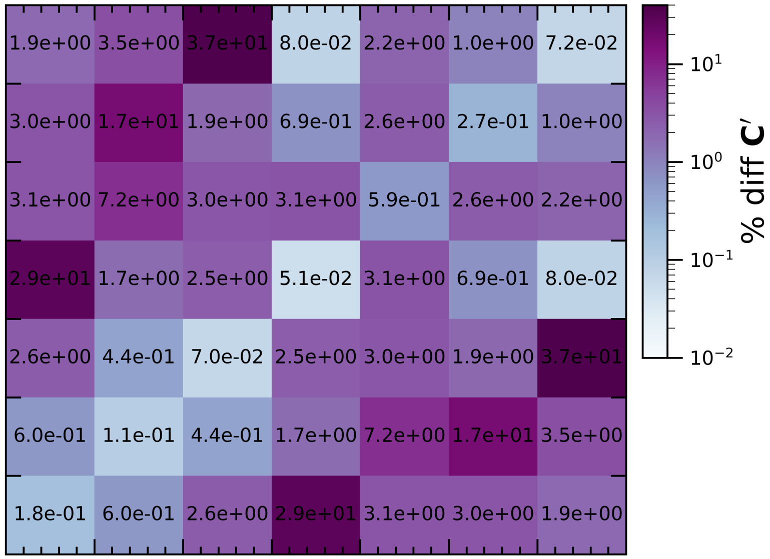
- GLS is recovered, i.e., $X^2\rightarrow\chi^2$, for $(\Lambda=\lambda=0)\leftarrow(\Delta'=\langle\delta\rangle'=0)$.

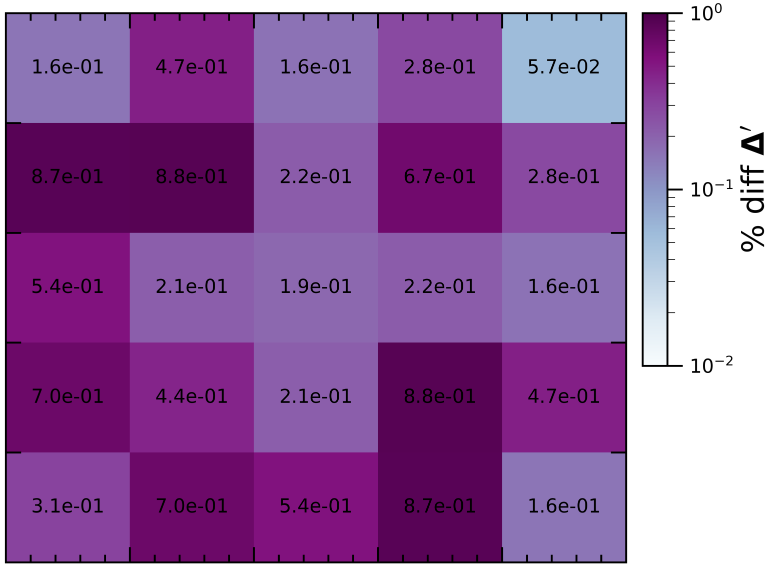
Metropolis Hastings Monte Carlo (MHMC) Algorithm

$N \leftarrow$ iterations ▹ necessary number of iterations for convergence
$i \leftarrow 0$
$z_0 \leftarrow$ arbitrary values ▹ z_i can be of arbitrary dimension
while $i < (N + 1)$ **do**
    Generate random candidate sample z' from $g(z'|z_i)$
    $A = \min\left(1, \frac{p(z')}{p(z_i)} \frac{g(z_i|z')}{g(z'|z_i)}\right)$
    Generate random value of u from uniform distribution between $(0, 1)$
    if $u < A$ **then**
        $z_{i+1} \leftarrow z'$
    else
        $z_{i+1} \leftarrow z_i$
    $i \leftarrow i + 1$

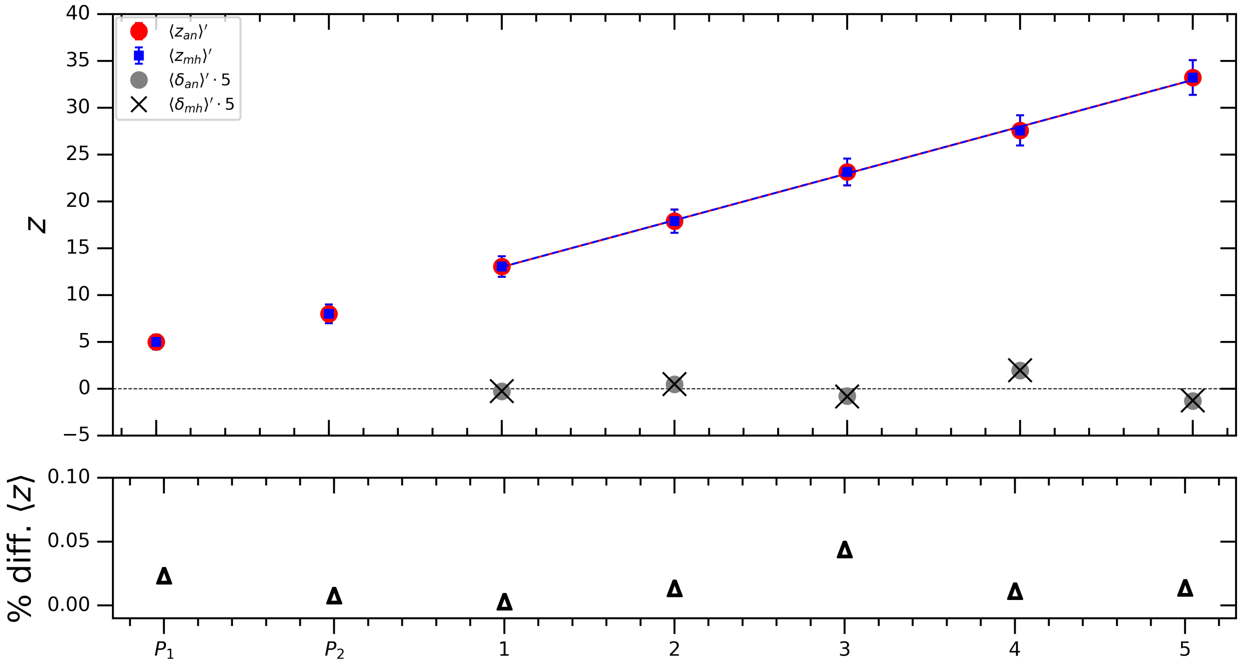
Analytical solutions: Linear models

- The upper plot shows the perfect (within statistical uncertainty) agreement between the analytical and MHMC values for $\langle z \rangle'$ and $\langle \delta \rangle'$
- The lower plot shows that the difference between the analytical and MHMC $\langle z \rangle'$ is not $> \ 0.06\%$ for any element of z





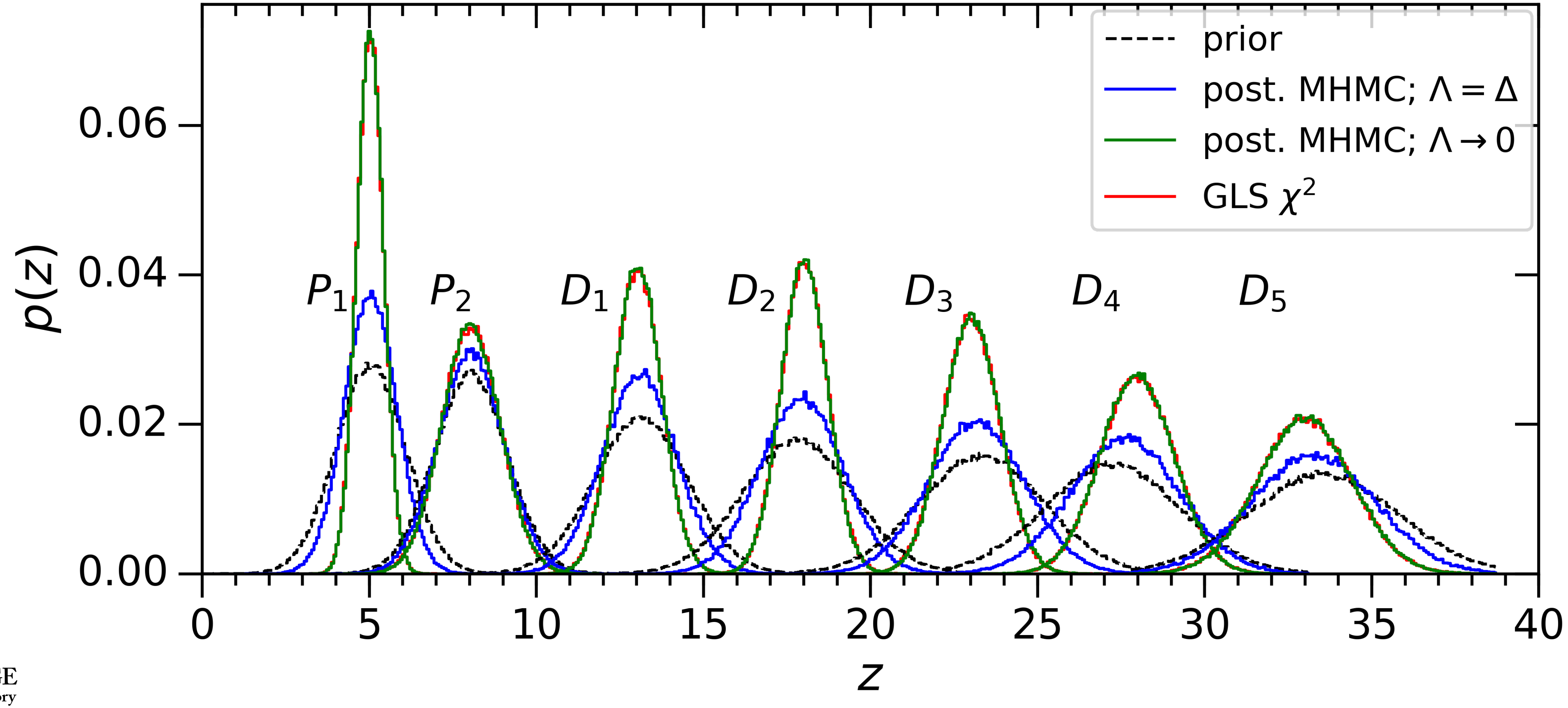
- Diagonal of $\boldsymbol{C}'$ matches analytical to within $< \ 0.6\%$, off-diagonal requires more iterations
- $\boldsymbol{\Delta}'$ matches well throughout



$$\boxed{T(P) = P_1 x + P_2}$$

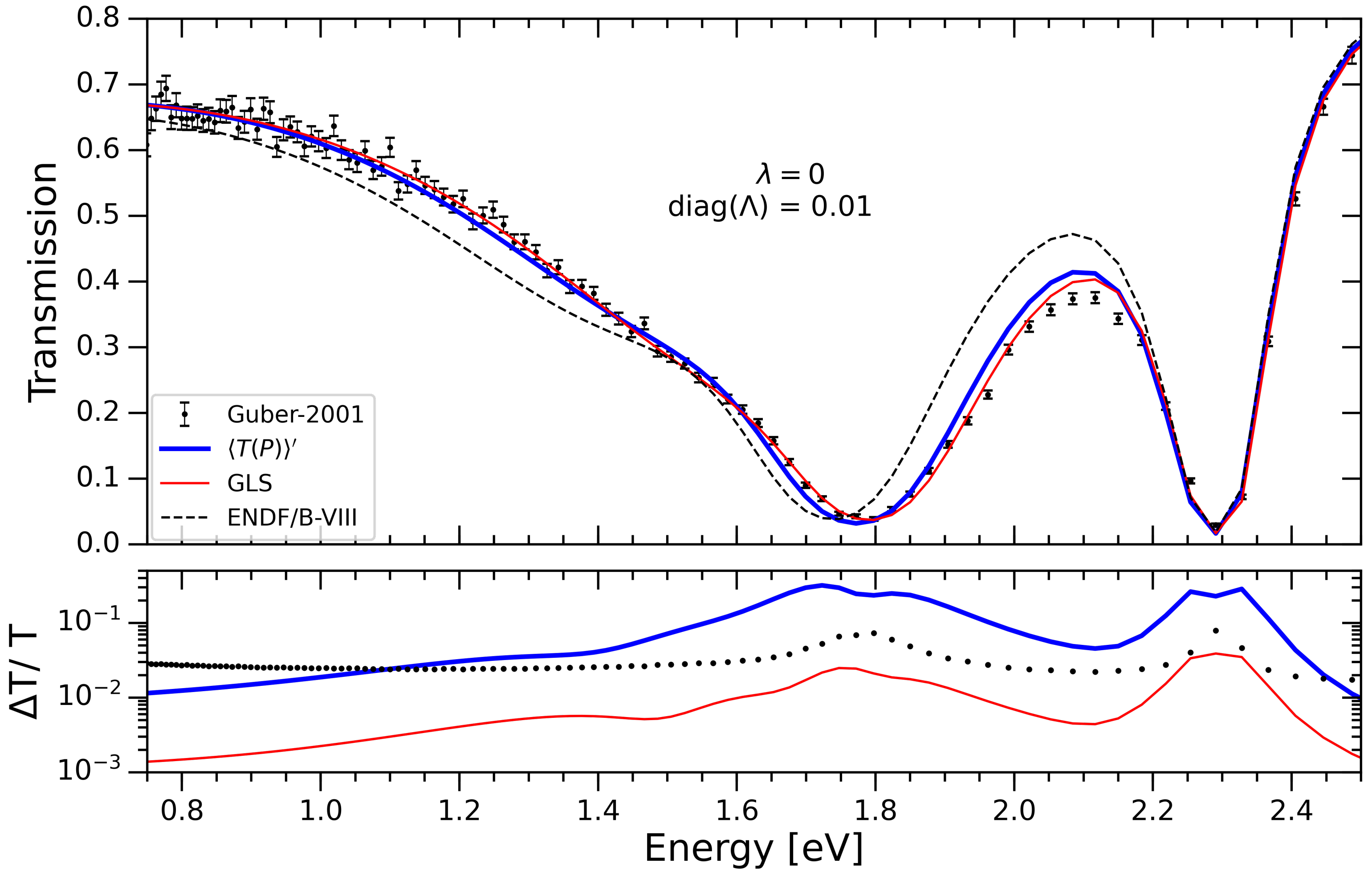
Comparison to GLS

- Case $\Lambda = \Delta$: solves for $\mathbf{\Delta}' = \mathbf{\Delta}/2$ **and** $\langle \boldsymbol{\delta} \rangle' = \langle \boldsymbol{\delta} \rangle/2$ by using $\Lambda = \Delta$ and $\lambda = 0$
- Case $\Lambda \to 0$: solves for $\mathbf{\Delta}' = \mathbf{0}$ **and** $\langle \boldsymbol{\delta} \rangle' = \mathbf{0}$ by using $\Lambda \to 0$ and $\lambda \to 0$ (matches GLS)
- Demonstrates the effect of the GLS assumption: $\langle \delta \rangle' = 0, \Delta' = 0$

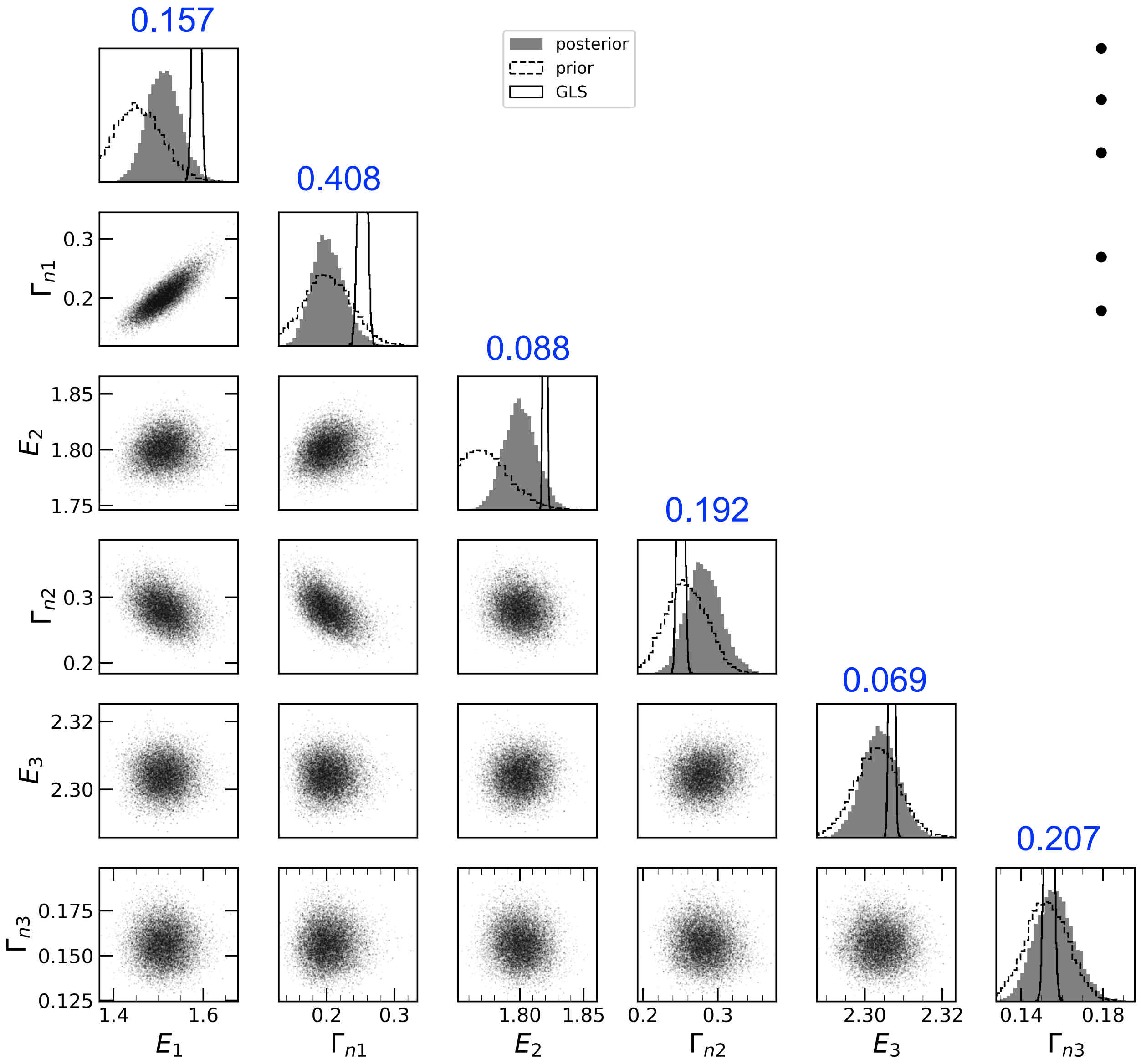


Application to RRR evaluation: U-233

- Fit 3 resonances allowing the energy eigenvalues and neutron widths to vary
- The explicit application of $\delta! = 0$ gives the evaluator control over model/data defects (background, normalization, etc.)
- Uncertainty on model now envelopes the data

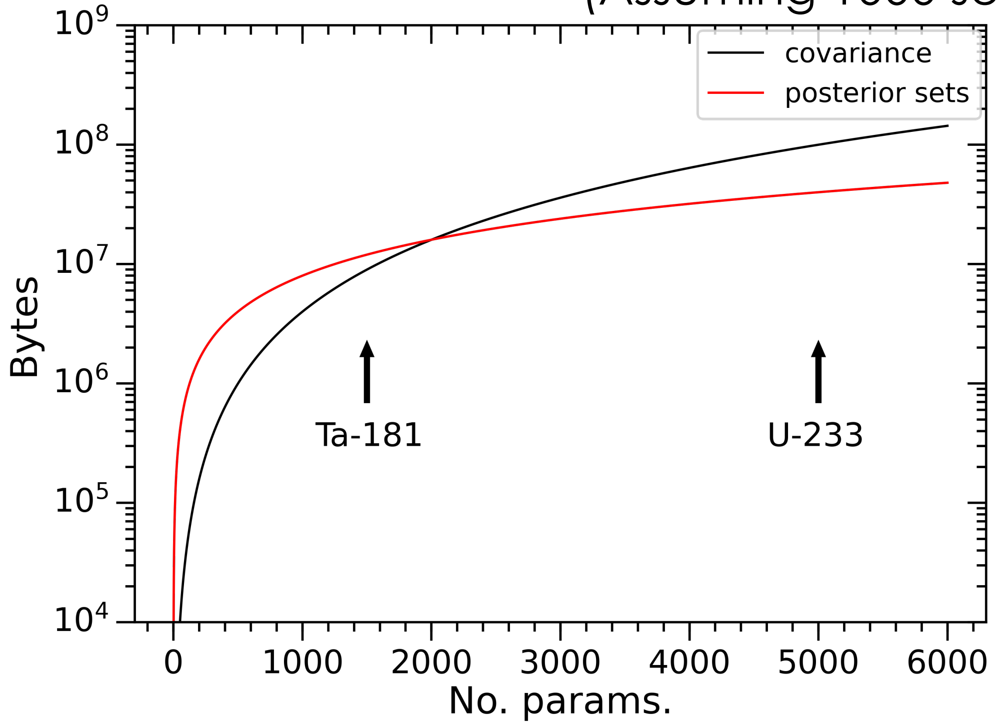


Uncertainty analysis: covariance and beyond



- 6 resonance parameters
- ~30,000 posterior sets make up PDF
- Posterior PDFs compared to GLS (black) and prior (black-dashed) PDFs
- Instead of storing covariance, store posterior sets
- All PDFs are positively skewn (blue)

(Assuming 1000 sets)



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Considerations

- BMC evaluation is a tool to address:
  - **Imperfect data & models**
  - **non-linear models,**
  - **non-normal PDFs**
- fitAPI implementation validated with analytical solutions for linear models
- New posterior PDFs *may need new storage formats* to allow storage of non-normal PDFs
  - Storing posterior sets allows for: variance, covariance, skewness, etc.

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