Treating inconsistent data in integral adjustment using Marginal Likelihood Optimization.

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Inconsistent data

IEU-Met-Fast and HEU-Met-Fast\(^1\)
1000 TENDL2014 files

\(^1\)Curtesy of Steven Van Der Marck
Inconsistent data - causes

• Model defects
  – e.g., ND uncertainties or correlation not taking into account (lack of nuisance parameters).
  – models inability to reproduce the true ND.
• Unaccounted experimental uncertainties or correlations.
• Underestimated statistical uncertainties.
• Isotopes not taken into account.

\[
\sigma_{B,J}^2 = \sigma_{rep}^2 + \sigma_{stat}^2 + \sigma_{defects}^2 + \sigma_{other}^2 + \sum_{\text{overall } p \text{ where } p \neq J} \sigma_{ND,p}^2
\]
Previous attempts to address inconsistent integral experiments

Adjustment Margin (AM)

$$\frac{\Delta C}{C} + \frac{\Delta E}{E} - \left| \frac{C - E}{E} \right| = AM < 0$$

$\Delta \chi^2$ filtering

$$\chi^2 = (E - C(\sigma))^T (M_C + M_E)^{-1} (E - C(\sigma))$$

Includes correlations

$$\chi^2 - \chi^2_{\neq i} = \Delta \chi^2 > Th$$

$$Th = 1.2 \text{ (Scale)}$$

Credit to Daniel Siefman
Possible issues

**AM**

1) does not take into account correlations.

2) is binary.

**Δχ² filtering**

1) is binary.

2) The choice of 1.2 is rather arbitrary? It should depend on the number of experiments. (Can be resolved)
Before and after calibration

IEU-Met-Fast and HEU-Met-Fast

1000 TENDL2014 files

AM would not reject any of the experiments.
Treating inconsistent data using Marginal Likelihood Optimization (MLO)

$L = f$ (Extra uncertainty)

R033 – G. Schnabel, Interfacing TALYS with A Bayesian Treatment of Inconsistent Data and Model Defects, ND2019
MLO for integral data and BMC

- We add an extra uncertainty to each experiment.

\[
\sigma_{B,J}^2 = \sigma_{rep}^2 + \sigma_{stat}^2 + \sigma_{defects}^2 + \sigma_{other}^2 + \sum_{\text{overall p where } p \neq J} \sigma_{ND,p}^2
\]

\[
\sigma_{B,l,J}^2 = \sigma_{rep}^2 + \sigma_{stat}^2 + \sigma_{extra,l}^2
\]

- \(\sigma_{\text{extra}}\) found by maximizing \(L\):

\[
L = \frac{1}{\sqrt{2\pi n \left| \text{cov}_{\text{rep,stat,extra}} \right|}} \sum_i e^{-\frac{\chi_i}{2}}
\]

\(n = \text{number of experiments}\)

1 Here MC and integral information. Compare with
1G. Schnabel, Fitting and analysis technique for inconsistent data, MC2017
Adding a prior

\[ \text{prior}(\sigma_{\text{extra}}) = e^{-\beta \sigma_{\text{extra}}^2} \quad \text{or,} \]

\[ \text{prior}(\sigma_{\text{extra}}) = e^{-\beta \sigma_{\text{extra}}} \]

\[ L = \frac{1}{\sqrt{2\pi n} |\text{cov}_{\text{rep,stat,extra}}|} \sum_i e^{-\beta \sum_{\text{extra}}^2} \frac{-\chi_i}{2} \]

To favor small extra uncertainties. Includes more of expert judgement.

\[ \beta \text{is chosen by expert judgement} \quad \text{or in a data-driven approach}^{1}. \]

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\(^1\)G. Schnabel, *Fitting and analysis technique for inconsistent data*, MC2017
MLO for BMC / GLS

\[ L_{\text{BMC}} = \frac{1}{\sqrt{2\pi n} \left| \text{cov}_{\text{rep}} + \text{cov}_{\text{extra}} \right|} e^{-\beta \sum \sigma^2_{\text{extra}}} \sum e^{\frac{\chi_i}{2}} \]

\[ L_{\text{GLS}} = \frac{1}{\sqrt{2\pi n} \left| S A_0 S^T + \text{cov}_{\text{rep}} + \text{cov}_{\text{extra}} \right|} e^{-\beta \sum \sigma^2_{\text{extra}}} e^{\frac{\chi^2}{2}} \]

\( A_0 = \text{prior covariance} \)

\( n = \text{number of experiments} \)
Synthetic data study MLO - GLS

- Characterize MLO’s performance,
  - GLS
  - No prior on the extra uncertainty
- Take hypothetical integral parameters (IPs)
- Have calculated values (C) and experimental (E), which have covariance matrices $M_E$ and $M_C$
- Manipulate the reported uncertainty in $M_E$ to see if MLO can account for it
  - Under-reported: $M_{E}^{\text{fake}} = M_{E} * 0.1$
  - Give $M_{E}^{\text{fake}}$ to MLO, and see if it reproduces $M_{E}$
Under-estimated E Uncertainty

- Chi2 plotted with sample mean, std from chi2 distribution

\[(C - E)^T (M_E^{fake} + M_C) \chi^2 \text{ per DOF with MLO}

\[(C - E)^T (M_E^{fake} + M_C)^{-1} (C - E) \chi^2 \text{ per DOF no MLO}
Under-estimated E Uncertainty

- Averaged across all IPs

\[
\sqrt{\delta_{Efake}^2 + \delta_C^2 + \delta_{MLO}^2} \div \sqrt{\delta_E^2 + \delta_C^2}
\]
MLO Applied to SG33 Benchmark

- Apply MLO to controlled set of benchmarks using GLS version of the formula
  - No prior on extra uncertainty and no experimental correlations between the IP.
- Conceptually easy case: one inconsistent IP
- Perhaps not ideal case:
  - Prior chi2 is already too small, likely overconsistent, (data already tuned to these experiments?)
- Using MLO here to only identify inconsistent IP
- 33 group ENDF/B-VII.0 and COMMARA- 2.0.
- B-10, O-16, Na-23, Fe-56, Cr-52, Ni-58, U-235/238, Pu-239/240/241
MLO Effects on SG33 Benchmark

Without MLO

With MLO

- JEZEBEL Pu-239 $k_{eff}$
- JEZEBEL Pu-239 F28/F25
- JEZEBEL Pu-239 F49/F25
- JEZEBEL Pu-239 F37/F25
- JEZEBEL Pu-240 $k_{eff}$
- FLATTOP $k_{eff}$
- FLATTOP F28/F25
- FLATTOP F37/F25
- ZPR6-7 $k_{eff}$
- ZPR6-7 F28/F25
- ZPR6-7 F49/F25
- ZPR6-7 C28/F25
- ZPR6-7 Pu-240 $k_{eff}$
- ZPPR-9 $k_{eff}$
- ZPPR-9 F28/F25
- ZPPR-9 F49/F25
- ZPPR-9 C28/F25
- ZPPR-9 Step 3
- JOYO $k_{eff}$

- C
- E std
- ND std

- E+MLO std
- C std

C/E - 1 (%)
Posterior Nuclear Data Adjustments

Pu-239 (n, inelastic)

Rel. Adj. (%) vs. Energy (MeV)

Rel. Std. (%) vs. Energy (MeV)

with MLO
without MLO
Prior
Posterior Nuclear Data Adjustments

Pu-239 (n, capture)

- Relative Adjustment (%)

- Energy (MeV)

- Lines:
  - Blue: with MLO
  - Orange Dash: without MLO
  - Black Dash: Prior

- Y-axis:
  - Values range from 0 to 4.5

- X-axis:
  - Energy range from $10^{-4}$ to $10^1$ MeV
Posterior Nuclear Data Adjustments

Correlations were also changed.
BMC case

IEU-Met-Fast and HEU-Met-Fast\(^1\)
1000 TENDL2014 files

- Red dots: Before calibration + U5U8 unc.
- Blue dots: After calibration + U5U8 unc.
- Orange line: Benchmark uncertainty
Benchmark errors are correlated: Adding a correlation term

- Correlations: $\sigma_E$, $\sigma_{\text{defect}}$, $\sigma_{\text{other isotopes}}$
- A fully correlated uncertainty is added to all experiments.

$$\sigma_{B,l}^2 = \sigma_{E,l}^2 + \sigma_{\text{stat},l}^2 + \sigma_{\text{extra},l}^2 + \sigma_{\text{extra all}}^2$$

$$\max(L) \rightarrow \sigma_{\text{extra},l}^2 + \sigma_{\text{extra all}}^2$$
Results – with correlation

<table>
<thead>
<tr>
<th>Benchmark uncertainties [PCM]</th>
<th>HMF1_1</th>
<th>HMF8</th>
<th>IMF2</th>
<th>IMF3_2</th>
<th>IMF7_4</th>
<th>Fully correlated</th>
</tr>
</thead>
<tbody>
<tr>
<td>No ML: Reported uncertainties</td>
<td>100</td>
<td>160</td>
<td>300</td>
<td>170</td>
<td>80</td>
<td>0</td>
</tr>
<tr>
<td>Uptated uncertainties</td>
<td>153</td>
<td>204</td>
<td>300</td>
<td>580</td>
<td>390</td>
<td>0</td>
</tr>
<tr>
<td>With correlation</td>
<td>267</td>
<td>329</td>
<td>333</td>
<td>591</td>
<td>409</td>
<td><strong>257</strong></td>
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## Results with an added prior

### Benchmark uncertainties [PCM]

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<td>409</td>
<td>257</td>
</tr>
<tr>
<td>With prior</td>
<td>232</td>
<td>263</td>
<td>366</td>
<td>468</td>
<td>228</td>
<td>209</td>
</tr>
</tbody>
</table>

### Posterior

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<th>HMF1_1</th>
<th>HMF8</th>
<th>IMF2</th>
<th>IMF3_2</th>
<th>IMF7_4</th>
<th>Chi2</th>
<th>p_value</th>
</tr>
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<tbody>
<tr>
<td>No ML</td>
<td>69</td>
<td>28</td>
<td>103</td>
<td>52</td>
<td>34</td>
<td>2,1</td>
<td>6%</td>
</tr>
<tr>
<td>Uptated uncertainties</td>
<td>139</td>
<td>131</td>
<td>234</td>
<td>183</td>
<td>273</td>
<td>0,38</td>
<td>86%</td>
</tr>
<tr>
<td>With correlation</td>
<td>264</td>
<td>254</td>
<td>313</td>
<td>290</td>
<td>351</td>
<td>0,4</td>
<td>84%</td>
</tr>
<tr>
<td>With Prior</td>
<td>253</td>
<td>214</td>
<td>288</td>
<td>256</td>
<td>265</td>
<td>0,58</td>
<td>72%</td>
</tr>
</tbody>
</table>
A larger data set / BMC – No MLO

8500 TENDL files, MCNP6, PU9, U8 and U5
If allowed, the **MLO reduces the uncertainties** for most of the experiments, indicating that some tuning to these experiments have already been done.
Conclusion

• We need to find and treat unrecognized systematic uncertainties (USU).
• Marginal Likelihood Optimization (MLO) can be an effective tool for this.
• Treating USU reduces the risk of overfitting to the integral data.

• MLO is our preferred method
  ❖ Includes correlations
  ❖ Can introduce correlations
  ❖ Transparent
  ❖ Not binary
  ❖ Statistical well-founded
  ❖ Can be combined with expert judgment.
  ❖ Works with both GLS and BMC adjustment.
Next step: include the full likelihood functions.

- All values of the likelihood functions are possible, hence should be taken into account.
  - affects the best-estimate and normally increase the uncertainty → decrease the adjustment.
- Can be achieved by, e.g., sampling.
- Performed for differential data (reported in SG 44)
THANK YOU FOR YOUR ATTENTION!
References


4. C. De Saint Jean et al., Evaluation of Cross Section Uncertainties Using Physical Constraints: Focus on Integral Experiments, Nuclear Data Sheets, Volume 123, Pages 178-184

5. G. Schnabel, Fitting and analysis technique for inconsistent data, MC2017

6. G. Schnabel, Interfacing TALYS with a Bayesian Treatment of Inconsistent Data and Model Defects, ND2019