This is the accepted version of a paper presented at 2019 International Conference on Nuclear Data for Science and Technology.

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Integral adjustment of nuclear data libraries Finding unrecognized systematic uncertainties and correlations
In:

N.B. When citing this work, cite the original published paper.

Permanent link to this version:
http://urn.kb.se/resolve?urn=urn:nbn:se:uu:diva-396767
MC Integral adjustment

Random nuclear data from the 1st step is used as the prior for the 2nd step.

Physical models parameters: TALYS based system (T6)

1st level of constraint: Differential data

A large set of acceptable ND libraries

2nd level of constraint: Integral benchmarks

Assign weights to random files

Simulations: MCNP etc.

Applications: Criticality, burnup, Fuel cycle etc.

\[ W_i \propto e^{-\frac{\chi^2_i}{2}} \]

Prior \( k_{\text{eff}} \) distribution

Posterior

Figure adapted from artwork by E. Alhassan
Important to also include the calculation uncertainty

\[ \chi^2_{i,J} = \sum_B \frac{(C_{B,i} - E_B)^2}{\sigma_{B,J}^2} \], \( i = \text{random file}, J = \text{isotopes}, B = \text{benchmark} \)

\[ w_i \propto e^{-\chi_i^2/2} \]

- C/E\( \neq 1 \) can be due to \( \sigma_E, \sigma_{\text{stat}}, \) error in the isotopes that we are adjusting, errors in other isotopes, or other errors not accounted for.

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

- Random files for major isotopes are varied simultaneously.
  - Investigated for U8 and U5.
  - 5 criticality experiments from ICSBEP: IEU-Met-Fast and HEU-Met-Fast
  - $k_{\text{eff},i} = f(U_{8i}, U_{5i})$
    i=randomfile number

- MCNP6, TENDL2014

Intrinsically the uncertainty of U8 and U5 are taking into account simultaneously

\[
\begin{align*}
  w_i &= e^{-\frac{\chi_i^2}{2}} \\
  \chi_i^2 &= (C - E)^T \text{COV}_{B,J}^{-1} (C - E) \\
  \text{COV}_{B,J} &= \text{COV}_E + \text{COV}_{\text{stat}}
\end{align*}
\]
Before and after calibration

IEU-Met-Fast and HEU-Met-Fast\textsuperscript{1}

1000 TENDL2014 files

\textsuperscript{1}Courtesy of Steven Van Der Marck
Difficult to fit
- prior correlations

ND (U5U8) prior correlations

- IMF7_4
- IMF3_2
- IMF2
- HMF8
- HMF1_1

HMF1_1  HMF8  IMF2  IMF3_2  IMF7_4

0.0  0.2  0.4  0.6  0.8  1.0
Difficult to fit
- inconsistent data

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

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

\[
\chi_i^2 - \chi_{\neq i}^2 = \Delta \chi^2 > Th
\]

\(Th = 1.2\) (Scale)
Possible issues

**AM**
1) it does not take into account correlations.

2) it might reject experiments when it is actually the model that is wrong.

3) It is binary.

**$\Delta \chi^2$ filtering**
1) It is binary.

2) The choice of 1.2 is rather arbitrary? It should depend on the number of experiments.
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)

\[ L = f(\text{Extra uncertainty}) \]

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

• We add an extra uncertainty to each experiment.

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

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

• \( \sigma_{extra} \) found by maximizing\(^1\) L:

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

\( n \) = number of experiments

\(^1\) Here MC and integral information. Compare with
\(^{\text{G.Schnabel, Fitting and analysis technique for inconsistent data,MC2017}}\)
Results

<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>
</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>
</tr>
<tr>
<td>Uptated uncertainties</td>
<td>153</td>
<td>204</td>
<td>300</td>
<td>580</td>
<td>390</td>
</tr>
</tbody>
</table>
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.

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

$$L = \frac{1}{\sqrt{2\pi n|\text{cov}_{\text{exp,stat,extra}}|}} \sum_l e^{-\frac{x_l^2}{2}}$$

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

Benchmark uncertainties [PCM]

<table>
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<tr>
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<th>HMF1_1</th>
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<td>0</td>
</tr>
<tr>
<td>Updated uncertainties</td>
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<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>257</td>
</tr>
</tbody>
</table>
Adding a prior

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

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

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

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

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

\[ ^1 \text{G.Schnabel, Fitting and analysis technique for inconsistent data,MC2017} \]
# Results with an added prior

## Benchmark uncertainties [PCM]

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<tr>
<td>With prior</td>
<td>232</td>
<td>263</td>
<td>366</td>
<td>468</td>
<td>228</td>
<td>209</td>
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## 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>
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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>

![Graph showing changes in uncertainties before and after calibration and with benchmark uncertainties](image-url)
Posterior correlations

ND (U5U8) prior correlations

ND (U5U8) posterior correlations
A larger data set – 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

• You need to find and treat unrecognized systematic uncertainties.

• Marginal Likelihood Optimization (MLO) can be an effective tool for this.

• MLO is our preferred method
  ✓ Includes correlations
  ✓ Can introduce correlations
  ✓ Transparent
  ✓ Not binary
  ✓ Statistical well-founded
  ✓ Can be combined with expert judgment.
THANK YOU FOR YOUR ATTENTION!

Advertisement, postdoc-position at Uppsala university,
https://tinyurl.com/UU-ND2019
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
Cross-isotope correlations

D. Rochman: Nuclear data correlation between different isotopes via integral information
The posterior is constrained by both the differential and integral data.

Physical models parameters: TALYS based system (T6)

1st level of constraint: **Differential data**
- A large set of acceptable ND libraries
- Simulations: mcnp etc.

2nd level of constraint: **Integral benchmarks**
- Assign weights to random files
- Weighted random files
- Simulations: MCNP
- Validation with a set of benchmarks

Applications: Criticality, burnup, Fuel cycle etc.

$\omega_i = e^{\frac{-\chi_i^2}{2}}$

Rather complete on uncertainties, correlations and higher moments. Improvements possible.
\[
\log L = c - 0.5 \left| \text{cov}_{\text{exp}} + \text{cov}_{\text{extra}} \right| + \ln \left( \sum e^{-\frac{\chi^2}{2}} \right)
\]

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<th>Chi2_post(exp)</th>
<th>Chi2_prior(tot)</th>
<th>Chi2_post(tot)</th>
<th>p_value-post</th>
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<td>2.3</td>
<td>1.81</td>
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Adressing inconsistencies...
Previous attempts to address inconsistent integral experiments

Adjustment Margin (AM)

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

\[ \Delta \chi^2 \text{ filtering} \]

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

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

\[ Th = 1.2 \text{ (Scale)} \]

\[ Th = 1 + \alpha \sqrt{2n / n} \text{ (We suggest)} \]

\( \alpha = \) multiples of standard deviations to accept

\( n = \) number of experiments

Credit to Daniel Siefman

Includes correlations