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Nuclear data adjustment using Bayesian inference, diagnostics for model fit and influence
Nuclear data adjustment and Transposition

- **Nuclear data evaluation**: neutron induced reactions, theoretical models.
- Model *parameters* are predicted theoretically and are **uncertain** — Uncertainty in ND

- Best set of *parameters*: comparing theory to experiments.
  - Adjusted set of parameters
  - Improved nuclear data
  - Adjusted (reduced) nuclear data uncertainties
  - Improved covariance matrices
  - Transposition

Nuclear data and Covariances
CEA-COMAC files *(prior)*

Integral experiments
(JEZEBEL, FLATTOP.....)
[K_{eff} (C/E): uncertainty, sensitivity]

Nuclear data and Covariances
CEA-COMAC files *(posterior)*

ASTRID (Concept Reactor)
[K_{eff}: uncertainty, sensitivity]
What we are looking for:

- Is the adjustment reliable?
  - How good is the adjusted data?
  - How many integral experiments are sufficient to adjust the nuclear data?
  - How many experiments are enough to represent a concept reactor?
  - How is an individual experiment (or ND) impacting the posterior?

- Ways to convince:
  - Recipes to convince people about the methods:
    - Indicators for robustness of the method.
    - Validation domain and demonstrations to show that we are mastering the impact of inputs.
    - Model selection criterion

What we have:
1. Nuclear data
2. Integral experiments
3. Adjustment method (Bayesian inference)
4. Transposition: to interpolate the effect of ND uncertainties on concept reactor
Approach: Bayesian inference

- $y = \{y_1, y_2, \ldots, y_N\}$: experimentally measured values
- $x$: parameters defining a model (M) to simulate $y$
- $t$: calculated values using model to compare with $y$
- Conditional probability for the analysis of a new data set $y$

\[
p(x|M, y, U) = \frac{p(x|M, U) \cdot p(y|x, M, U)}{\int dx \cdot p(x|M, U) \cdot p(y|x, M, U)}
\]

$\text{From theory}$

$\text{PDF of observed data set knowing } x$

$posterior [p(x|y, U)] = prior [p(x|U)] \cdot \text{likelihood } [p(y|x, U)]$
Bayesian inference

- Assimilate measurements information to adjust, update or reduce uncertainties

\[ \text{posterior } [p(x|y, U)] \propto e^{-(1/2)((x-x_m)^T M_x^{-1}(x-x_m) + (y-t)^T M_y^{-1}(y-t))} \]

- The minimization of the following cost function:

\[ \chi^2_{GLS} = (x - x_m)^T M_x^{-1}(x - x_m) + (y - t)^T M_y^{-1}(y - t) \]

- Alternatively, BMC method can be also used.

* C. De Saint Jean et al., Evaluation of Neutron-induced Cross Sections and their Related Covariances with Physical Constraints, Nuclear Data Sheets, 2018.
Use of Integral experiments

State update

\[ \sigma - \sigma_0 = M_\sigma . S^T (M_E + S . M_\sigma . S^T)^{-1} . (E - C(\sigma_0)) \]

Cov. update

\[ \tilde{M}_\sigma = M_\sigma - M_\sigma . S^T (M_E + S . M_\sigma . S^T)^{-1} . S . M_\sigma \]

\( \sigma = \) Vector of nuclear data (cross sections, spectra...)
\( N_\sigma = \) # isotopes X # reactions X # energy groups

\( M_\sigma : \) Prior cov. For ND
\( M_E : \) Cov. for E
\( \sigma_0 : \) Prior information
\( S: \) sensitivity of int exp \{E\} for p wrt ND
Test case:

Pu239 Fission and Capture in 33 energy groups

Prior nuclear data: CEA-COMAC-V1 file (Corr. matrix)

Pu239 Fission correlation

Pu239 Capture correlation

Integral experiment: JEZEBEL
Fitted parameters:
Case. Pu239 (Cap, Dis, Elas, Fiss, Inel, Nu, NXN )
Uncertainty reduction in Pu239_Cap

Trends for Pu239 CAPTURE (% differences in ND)

Uncertainties Before and After Adjustment

Standard deviation [%] for Pu239 Capture: before and after adjustment
Issues:

- Which data or model parameters have the largest impact on fit.
  - If you construct a model with fewer parameters / less data, which model can be considered the best model.

- Fitting test
  - Chi square test
    - Effective degree of freedom
  - Cook’s distance: which ingredient is affecting the fit.
    - Nuclear data (isotope, reactions….)
    - Experiment
  - Other test for selecting best model
    - AIC, BIC, DIC, WAIC, Leave-one-out
Cook’s distance

Shows the influence of a data point in least square regression analysis

• In a regression fit, if the square error is:

\[ e'e = (Y-X\beta)'(Y-X\beta) \]

• The mean square error: 

\[ s^2 = e'e/(n-p) \]

Where

- \( n \): number of observation,
- \( P \): number of fitted parameters

• The Cook’s distance for the observation \( i \)

\[ D_i = \sum_{j=1}^{N} \frac{(f(x_j) - f(x_j)_i)^2}{ps^2} \]

Where \( f(x_j)_i \) is the fitted response when the \( i^{th} \) observation is excluded.
Example

<table>
<thead>
<tr>
<th>X1</th>
<th>X2</th>
<th>Y</th>
</tr>
</thead>
<tbody>
<tr>
<td>68</td>
<td>60</td>
<td>75</td>
</tr>
<tr>
<td>49</td>
<td>94</td>
<td>63</td>
</tr>
<tr>
<td>60</td>
<td>91</td>
<td>57</td>
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<tr>
<td>68</td>
<td>81</td>
<td>88</td>
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<td>97</td>
<td>80</td>
<td>88</td>
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<tr>
<td>82</td>
<td>92</td>
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<td>59</td>
<td>74</td>
<td>82</td>
</tr>
<tr>
<td>50</td>
<td>89</td>
<td>73</td>
</tr>
<tr>
<td>73</td>
<td>96</td>
<td>90</td>
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<td>39</td>
<td>87</td>
<td>62</td>
</tr>
<tr>
<td>71</td>
<td>86</td>
<td>70</td>
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<tr>
<td>95</td>
<td>94</td>
<td>96</td>
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<tr>
<td>61</td>
<td>94</td>
<td>76</td>
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<td>72</td>
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<td>87</td>
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<td>85</td>
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<tr>
<td>40</td>
<td>50</td>
<td>40</td>
</tr>
<tr>
<td>66</td>
<td>92</td>
<td>74</td>
</tr>
<tr>
<td>58</td>
<td>82</td>
<td>70</td>
</tr>
<tr>
<td>58</td>
<td>94</td>
<td>75</td>
</tr>
<tr>
<td>77</td>
<td>78</td>
<td>72</td>
</tr>
</tbody>
</table>
Cooks distance

- Proceeding WONDER 2018

Issues:
- Large data size of corr. Matrix leads to determinant of corr. very small, order of $10^{-100}$.
- Issues like inversion of prior corr matrices lead to some unexpected results.
- No concrete solution for this issue.

Figure: Cooks distance for Pu239 reaction
(Covariance is based on variance matrix)
Prior nuclear data and numerical issues

For Pu239 Elastic 33 energy groups:

\[ \text{Det (Corr)} = 6.23^{-80} \]

\[ \text{Det(inv(Corr))} = 1.61^{79} \]

For first 10 energy groups:

\[ \text{Det (Corr)} = 1.50^{-24} \]

\[ \text{Det(inv(Corr))} = 6.68^{23} \]

Complexity increases when several reactions are used simultaneously

Dimension of corr matrix = #isotopes # reactions # energy groups
Other tests

- Influence of different integral experiments

- Issues
  - Fitting test: Chi Square\_opt/p_D \neq 1.
  - Effective degrees of freedom (p_D)

- Other statistical tests for model selection
  - Overfitting
  - Akaike information criteria (AIC)
  - Bayesian information criteria (BIC)
  - Deviance information criteria (DIC)
Model selection
Model complexity and Fit (D. J. Spiegelhalter)

Information theory
Kullback-Leiber (KL) distance = $E[\log\{p^T(Y)\}/p(Y|x^T)]$

Good model assumption: Bayesian analysis relies on $p(Y|x^T)$ being a reasonable approximation to $p^T(Y)$

Criterion for model selection: AIC, BIC, DIC

{Model complexity + fit}
Diagnostics for fit and influence

• Bayesian criteria for model comparison:

• Akaike Information Criteria (AIC)
  \[ \text{AIC} = 2n_{\text{data}} - 2\ln(L) \]

• Bayesian Information Criteria (BIC)
  \[ \text{BIC} = \ln(k)n_{\text{data}} - 2\ln(L) \]

• Deviance information criteria
  \[ \text{DIC} = -2\ln(L) + 2p_D \]

**Effective degrees of freedom**
\[ p_D = n_{\text{data}} - \text{tr}(M_{\text{prior}}^{-1}M_{\text{post}}) \]

- \( L \) = likelihood
- \( k \) = no. of experiments
- \( n_{\text{data}} \) = no. of model param
- \( p_D \) = measure of complexity

Smallest AIC/BIC/DIC → best model
**Case 1: Nuclear data**

Pu239(cap, dis, Elas, Fiss, InElas, Nu, nXn)

<table>
<thead>
<tr>
<th>Removed data Remaining data</th>
<th>Cap All-Cal</th>
<th>Dis All-Dis</th>
<th>Elas All-Elas</th>
<th>Fiss All-Fiss</th>
<th>InElas All-InEl</th>
<th>Nu All-Nu</th>
<th>nXn All-nxn</th>
</tr>
</thead>
<tbody>
<tr>
<td>Cook(x10^{-3})</td>
<td>1.30</td>
<td>0.001</td>
<td>0.11</td>
<td>0.34</td>
<td>2.42</td>
<td>0.001</td>
<td>0.37</td>
</tr>
<tr>
<td>AIC(x10^{2})</td>
<td>3.68</td>
<td>3.68</td>
<td>3.68</td>
<td>3.68</td>
<td>4.02</td>
<td>3.02</td>
<td>4.28</td>
</tr>
<tr>
<td>BIC(x10^{-5})</td>
<td>0.0060</td>
<td>0.0056</td>
<td>0.0054</td>
<td>0.5197</td>
<td>0.0050</td>
<td>0.0057</td>
<td>0.0053</td>
</tr>
<tr>
<td>DIC</td>
<td>1.82</td>
<td>1.80</td>
<td>1.89</td>
<td>1.44</td>
<td>1.83</td>
<td>1.71</td>
<td>1.72</td>
</tr>
<tr>
<td>Eff. Degree of Freedom</td>
<td>0.91</td>
<td>0.90</td>
<td>0.94</td>
<td>0.72</td>
<td>0.92</td>
<td>0.86</td>
<td>0.86</td>
</tr>
</tbody>
</table>

- These criteria are valid for \( k \gggg n \), here \( k = \text{no. of experiments} = 1 \)

Not conclusive!
Case 2: Nuclear data
Pu239 (fission\_g3, fission\_g4, fission\_g5)

<table>
<thead>
<tr>
<th>Removed param Remaining param</th>
<th>Fiss_g3 (g4,g5)</th>
<th>Fiss_g4 (g3,g5)</th>
<th>Fiss_g5 (g3, g4)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Cook</td>
<td>5.32</td>
<td>5.66</td>
<td>1.45</td>
</tr>
<tr>
<td>AIC</td>
<td>4.02</td>
<td>4.04</td>
<td>4.04</td>
</tr>
<tr>
<td>BIC</td>
<td>0.02</td>
<td>0.04</td>
<td>0.04</td>
</tr>
<tr>
<td>DIC</td>
<td>1.52</td>
<td>1.36</td>
<td>1.35</td>
</tr>
<tr>
<td>Eff. Degree of Freedom</td>
<td>0.75</td>
<td>0.66</td>
<td>0.65</td>
</tr>
</tbody>
</table>

Not conclusive!
Case 3: Resonance parameters Gd155

Reactions = "ELASTIC_SCATTERING RADIATIVE_CAPTURE"

- \([/Theory/ResonanceParameters_1/] : \text{GammaG1, GammaN1}\)
- \([/Theory/ResonanceParameters_2/] : \text{GammaG2, GammaN2}\)

### Removed vs. Remaining Parameters

<table>
<thead>
<tr>
<th>Removed param:</th>
<th>G1 (N1, G2, N2)</th>
<th>N1 (G1, G2, N2)</th>
<th>G2 (G1, N1, N2)</th>
<th>N2 (G1, N1, G2)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Cook (x10^3)</td>
<td>4.63</td>
<td>0.53</td>
<td>5.49</td>
<td>0.29</td>
</tr>
<tr>
<td>AIC (x10^4)</td>
<td>9.16</td>
<td>8.21</td>
<td>9.30</td>
<td>8.17</td>
</tr>
<tr>
<td>BIC (x10^4)</td>
<td>9.17</td>
<td>8.21</td>
<td>9.30</td>
<td>8.17</td>
</tr>
<tr>
<td>DIC (x10^4)</td>
<td>9.16</td>
<td>8.21</td>
<td>9.30</td>
<td>8.17</td>
</tr>
<tr>
<td>Eff. Degree of Freedom</td>
<td>2.70</td>
<td>2.76</td>
<td>2.82</td>
<td>2.94</td>
</tr>
</tbody>
</table>

- The largest Cooks distance in G2 suggests that it’s a very important parameter for fit.
- AIC, BIC and DIC also suggest that if G2 is removed from the fit, the model is rejected.
- N2 is not an important parameter in the fit.
- Model with G1, N1, G2 is the best model out of given 4 options.

⇒ All approaches (AIC, BIC, DIC and cooks distance) give the same conclusion.
Conclusions

- Test for data adjustment is being studied using Cook’s distance, AIC, BIC, and DIC criteria.
  - Effective degree of freedom is also estimated.
  - Effect of Gd155 resonance parameters is estimated.
  - Effect of Pu239 nuclear reactions is estimated.
  - Results are comparable when estimators are used for model parameters (Case 3).
  - Cases where nuclear data is adjusted (Cases 1, 2) are not straightforward.
- Automated matlab code outside CONRAD is compared and validated with the one developed inside CONRAD.
  - Accuracy of the nuclear data written to files can lead to very different results.
- More investigation is needed.