A new module for large scale Bayesian nuclear data evaluation

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Motivation

- Bayesian statistics offers a framework to combine model data and experimental data in a statistically consistent way
- Successfully applied to integral cross sections
- Extension to differential data desirable to make best use of available data
- Huge amounts of data have to be processed ➔ How to do it?
Flow Chart of Nuclear Data Evaluation

PRIOR GENERATION
via Monte Carlo from Nuclear Models
  e.g. TALYS, ...

EXPERIMENTAL DATA
mean values and construction of covariance matrices of experiments

BAYESIAN UPDATE
PROCEDURE
large scale linearized version

FILE GENERATION
VALIDATION and BENCHMARKING
The statistical basis

Prior:

\[ \rho_{\text{prior}} (\vec{\sigma}_{\text{true}}) = C_1 \exp \left[ (\vec{\sigma}_{\text{true}} - \vec{\sigma}_{\text{mod}})^T A^{-1} (\vec{\sigma}_{\text{true}} - \vec{\sigma}_{\text{mod}}) \right] \]

Likelihood:

\[ \rho_{\text{like}} (\vec{\sigma}_{\text{true}}) = C_2 \exp \left[ (S\vec{\sigma}_{\text{true}} - \vec{\sigma}_{\text{exp}})^T B^{-1} (S\vec{\sigma}_{\text{true}} - \vec{\sigma}_{\text{exp}}) \right] \]

Posterior:

\[ \rho_{\text{post}} (\vec{\sigma}_{\text{true}}) = C_3 \rho_{\text{prior}} (\vec{\sigma}_{\text{true}}) \rho_{\text{like}} (\vec{\sigma}_{\text{true}}) \]
**Update Procedure**

**UPDATE PROCEDURE**

mean values:  
\[ \bar{\sigma}'_{\text{mod}} = \bar{\sigma}_{\text{mod}} + AS^T (SAS^T + B)^{-1} (\bar{\sigma}_{\text{exp}} - S\bar{\sigma}_{\text{mod}}) \]

covariance matrix:  
\[ A' = A - AS^T (SAS^T + B)^{-1} SA \]

**aposterior probability density distribution**  
\[ \rho_{\text{post}} (\bar{\sigma}_{\text{true}}) = C_1 \exp \left[ \left( \bar{\sigma}_{\text{true}} - \bar{\sigma}'_{\text{mod}} \right)^T (A')^{-1} (\bar{\sigma}_{\text{true}} - \bar{\sigma}'_{\text{mod}}) \right] \]
Prior construction (TALYS)

Best calculation
parameters for OMP: global parameterisation [Koning and Delaroche]

Prior covariance
uniform sampling of OMP and level density params around best parameter set

\[
A = \frac{1}{n-1} \sum_{k=1}^{n} (\sigma_k - \sigma_{\text{mod}}) (\sigma_k - \sigma_{\text{mod}})^T
\]

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(In-)Feasibility

- Possible hundreds of reactions at high energies, for each up to seven distinct inclusive particle spectra (g,n,p,d,t,h,a), about 100 incoming energies and 100 outgoing energies \(\rightarrow 100 \times 100 \times 100 \times 7 \sim 10^7\) quantities

- Prior covariance matrix: \(10^7 \times 10^7 = 10^{14} \sim 800\) terabyte

- **BUT:** Constructed from \(10^3\) samples: \(10^3 \times 10^7 = 10^{10}\) \~ 80 gigabytes \(\rightarrow\) **Redundancy?**
Pseudo projection

\[ x' = x + A S T (S A S^T + B)^{-1}(\sigma - S x) \]

\[ A = \frac{1}{N-1} \sum_{i=1}^{N} \mathcal{J}_i \mathcal{J}_i^T \]

\[ \omega_i = \mathcal{J}_i^T S^T (S A S^T + B)^{-1}(\sigma - S x) \frac{1}{N-1} \]

\[ x' = x + \sum_{i=1}^{N} \omega_i \mathcal{J}_i \]
Pseudo projection

\[ x' = x + A S^T (S A S^T + B)^{-1} (\sigma - S x) \]

\[ A = \frac{1}{N-1} \sum_{i=1}^{N} \tilde{J}_i \tilde{J}_i^T \]

\[ \omega_i = \tilde{J}_i^T S^T (S A S^T + B)^{-1} (\sigma - S x) \frac{1}{N-1} \]

\[ x' = x + \sum_{i=1}^{N} \omega_i \tilde{J}_i \]
Sum rules

\[ \omega_1 \begin{pmatrix} a_1 \\ b_1 \\ c_1 \end{pmatrix} + \omega_2 \begin{pmatrix} a_2 \\ b_2 \\ c_2 \end{pmatrix} = \begin{pmatrix} \omega_1 a_1 + \omega_2 a_2 \\ \omega_1 b_1 + \omega_2 b_2 \\ \omega_1 c_1 + \omega_2 c_2 \end{pmatrix} \]

\[ \sigma(E) = \int \frac{d\sigma(\theta;E)}{d\Omega} d\Omega = c_1 \frac{d\sigma(\theta_1;E)}{d\Omega} + c_2 \frac{d\sigma(\theta_2;E)}{d\Omega} + \ldots \]
Sensitivity matrix

\[ \omega_i = \mathcal{J}_i^T S^T (S A S^T + B)^{-1} (\sigma - S x) \frac{1}{N-1} \]

Options for \( S \) matrix: (bi)linear interpolation, splines, Fourier series, ...

Size of \( S \) matrix e.g. \( 10^7 \times 10^3 = 80 \) gigabytes

\( \rightarrow \) sparse matrix

\( \rightarrow \) linear / bilinear interpolation
Energy grid and interpolation scheme

\[ \tilde{\sigma}_{\text{expgrid}} = S \tilde{\sigma}_{\text{modgrid}} \]

model grid

\[ E_{\text{mod},1}, E_{\text{mod},2}, E_{\text{mod},3}, \ldots \]

experiment grid

\[ E_{\text{exp},1}, E_{\text{exp},2}, E_{\text{exp},3}, \ldots \]

\[ S = \begin{pmatrix} 0 & 0 & 0 & 0 & x & x & 0 & 0 & \ldots & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & x & x & \ldots & 0 \\ x & x & x & x & 0 & 0 & 0 & 0 & \ldots & 0 \end{pmatrix} \]

maximal 4*M model points involved, M is the number of exp. Data

model grid sorted: computational complexity 4*M*log2(N)

M ... number of exp. points; N ... number of model points

example: M = 5000, N=10^7 \rightarrow 4*5000*\log2(10^7) \sim 5*10^5
• Infeasible to calculate it completely (800 terabytes...). No processing/simulation code could handle that anyway

• Calculating pieces of it (e.g. all integral CS, one particular spectrum) can be performed quickly (database-like query)

• TMC approach: sampling from the posterior maybe possible (Gram-Schmidt orthogonalization of subspace)
Exact vs. Approximate
Model deficiencies

Sampled cross section curves for the (n,g) channel

neutron production spectra

\[ \text{cross section [mb]} \]

incident energy [MeV]

\[ 0.01 \quad 0.10 \quad 1.00 \quad 10.00 \]

\[ 1e+03 \quad 1e+01 \quad 1e-01 \]

\[ \text{neutron emission energy [MeV]} \]

\[ 2 \quad 4 \quad 6 \quad 8 \]

\[ 1000 \quad 100 \quad 10 \]

\[ E_{\text{inc}} [\text{MeV}] \]

- 6.7
- 7.45
- 7.94

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Conclusion

• Linearized (=Gaussian pdfs) Bayesian update extended to differential cross sections

• Dozens of millions of observables can be tackled on a personal computer, speed determining factor is the burst read time of the harddisk

• Model defects may have a significant impact on the evaluation (leverage effects)

• If not already for the integral CS, the consideration of model defects seems to be a necessity to efficiently include differential information into the Bayesian evaluation → Further investigation required
THANK YOU FOR YOUR ATTENTION
Surrogate Model

Prior generation:
provides **mean values** and **prior covariance matrices** on a chosen energy mesh

Representation in the update procedure:
representation of cross sections, spectra, etc. via an interpolation scheme

**Spline:** advantage - linear mapping, continuous and smooth
drawback – oscillatory, negative cross sections may occur

**Linear interpolation:**
advantage – monotonicity, simple, sum rules conserved at interpolation points
drawback – non continuous, more mesh points required

\[ \sigma < 0 \text{ may occur for splines} \]

This simple representation contains important features of the original nuclear model calculation via the prior covariance matrix \( A \)