Adaptive Monte Carlo for Nuclear Data Evaluation

Georg Schnabel
Outline

Nuclear data evaluation

Pros & cons of existing evaluation methods

Adaptive Monte Carlo method

General procedure to fit complex non-linear models to data providing detailed uncertainty information of parameters
Application chain

Models

- TALYS
- INCL

Experiments

Simulation

- MCNP, GEANT4, ...

Evaluation method

- Linearized method
- Monte Carlo method

Simulation

- Perturbation Theory
- Total Monte Carlo

Element Production

- El. Prod. #1
- El. Prod. #2
- ...

Production + Cov

Database (DB)

- EXFOR

Production + Cov

Production + Cov
Linearized method

\[ \tilde{\rho}_1 = \tilde{\rho}_0 + A_0 S^T (S A_0 S^T + B)^{-1} (\tilde{\sigma}_{\text{exp}} - M_{\text{Lin}}(\tilde{\rho}_0)) \]

\[ A_1 = A_0 - A_0 S^T (S A_0 S^T + B)^{-1} S A_0 \]
Iterative linearized method

Starting at best prior estimate $p_0$

Starting somewhere else
Comparison of results

Note:
Not happy with any of the results? In Bayesian statistics, you get what you assume.

What about giving up the assumption of a perfect model?
Monte Carlo method

Ideally, draw samples $p_1, p_2, \ldots$ from posterior

$$\pi(p | \bar{\sigma}_{\text{exp}}) \propto \mathcal{N}(\bar{\sigma}_{\text{exp}} | \mathcal{M}(p), B) \times \mathcal{N}(p | \bar{p}_0, A_0)$$

Not possible, use another distribution, e.g.

$$\tau(p) = \mathcal{N}(p | \bar{p}_0, A_0)$$

Calculate weights for the results $p_i$ afterwards

$$\omega_i = \frac{\pi(p_i | \bar{\sigma}_{\text{exp}})}{\tau(p_i)}$$

Calculate mean, etc.

$$\bar{\sigma}_{\text{eval}} = \frac{\sum_{i=1}^{N} \omega_i \mathcal{M}(p_i)}{\sum_{i=1}^{N} \omega_i}$$
Monte Carlo in practice

Effective Sample Size

\[ N_{\text{eff}} = \frac{\left( \sum_{i=1}^{N} \omega_i \right)^2}{\sum_{i=1}^{N} \omega_i^2} \]

\[ N = 500 \text{ but } N_{\text{eff}} = 1 \]
Best of both worlds

Linearized method
  **fast** computation
  inaccurate results

Monte Carlo method
  **accurate** results
  slow computation

Adaptive Monte Carlo
  **fast** computation
  **accurate** results
Adaptive Monte Carlo

If effective sample size too low:

\[ N_{\text{eff}} = \left( \frac{\sum_{i=1}^{N} \omega_i}{\sum_{i=1}^{N} \omega_i^2} \right)^2 \]

then select the \( K \) parameter configurations \( p_k \) with highest weights \( w_k \) and for each of them construct a

**linearized nuclear model**

\[ M_{\text{Lin}}^{k}(\bar{p}) = M(\bar{p}_k) + S_k(\bar{p} - \bar{p}_k) \]

and apply

**linearized evaluation method**

\[
\begin{align*}
\bar{p}_{ev,k} &= \bar{p}_0 + A_0 S_k^T (S_k A_0 S_k^T + B)^{-1} (\tilde{\sigma}_{\exp} - M_{\text{Lin}}^{k}(\bar{p}_0)) \\
A_{ev,k} &= A_0 - A_0 S_k^T (S_k A_0 S_k^T + B)^{-1} S_k A_0
\end{align*}
\]

to improve sampling distribution

\[ \tau_{s+1}(\bar{p}) = \tau_s(\bar{p}) + \sum_{k=1}^{K} \beta_k N(\bar{p} | \bar{p}_{ev,k}, A_{ev,k}) \]
Adaptive Monte Carlo

Draw first sample

Learning step
1) Select points with largest weights

N_{\text{eff}} \text{ too low}

Draw second sample

2) Apply linearized method for these points

Draw third sample

\[ \tau_{s+1}(\vec{p}) = \tau_s(\vec{p}) + \sum_{k=1}^{K} \beta_k N(\vec{p} | \vec{p}_{ev,k}, \mathbf{A}_{ev,k}) \]
Evolution of sampling
Comparison of distributions

sampling distribution

posterior distribution
Summary

Adaptive Monte Carlo scheme*
- faster than usual Monte Carlo Methods
- more accurate than Linearized Methods

General purpose optimization algorithm
- exploits parallel computation
- provides detailed uncertainty information

* can be adapted to work with non-Gaussian parameter distributions or non-Gaussian uncertainties in experiments
Outlook

- Non-parametric optimization and uncertainty quantification of INCL cross sections
- Make treatment of model defects feasible in Monte Carlo evaluation methods
- Speed up Total Monte Carlo approach
- Constrain nuclear model parameters by both differential and integral data
- Optimize geometry with respect to integral observables
- Generate R-matrix fits
- ...

Thank you!

project CHANDA
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Georg Schnabel
georg.schnabel@cea.fr