Modeling nuclear data relationships with Bayesian networks

ML coffee breakfast club
Collision experiments

Neutrons → Nucleus
Total cross section

interaction

no interaction
Velocity dependence of cross section

Total neutron-induced cross section of Au-197

1 barn = $10^{-28}$ m$^2$
Velocity dependence of cross section

Total neutron-induced cross section of Au-197

1 barn = $10^{-28}$ m$^2$
Different types of cross sections

- Elastic cross section
- Capture cross section
- (n,2n)
Relationship between cross section types

- **total xs**
  - elastic xs
  - non-elastic xs
    - residual production Lu(71,180)
    - residual production Hf(72,181)
      - (n,a)
      - (n,2n2p)
      - (n,nh)
      - (n,np)
      - (n,d)
      - proton production
      - neutron production
Network of functions

- non-elastic xs
  - residual production Lu(71,180)
    - (n,2n2p)
    - (n,nh)
    - proton production
  - residual production Hf(72,181)
    - (n,np)
    - neutron production
UQ of experimental data

Sample* (thickness, density, impurities)

detector

background noise

Experimental Data

*) Rights: Eckhard Pecher, http://creativecommons.org/licenses/by/2.5/
Scenarios in nuclear data evaluation

- Several nuclear physics models need to be consistently combined in an evaluation.
- Nuclear models may be combined with non-parametric statistical methods to improve the description of available experimental data.
- Sometimes we prefer to not use nuclear physics models and rely heavily on experimental data.
- We want to incorporate uncertainty information of experiments into the statistical analysis.
Bayesian inference

\[ \pi(\bar{p}_{\text{true}} | \bar{\sigma}_{\text{exp}}, M) \propto f(\bar{\sigma}_{\text{exp}} | \bar{p}_{\text{true}}, M) \pi(\bar{p}_{\text{true}} | M) \]

Monte Carlo

Optimization

GLS (sens. based)
An inspiration: composability of neural networks

Take simple building blocks (e.g., pooling layers, convolutional layers, etc.) and define their connection structure with a relatively simple language.

Can we do the same for Bayesian models?
Bayesian networks

\[ P(H_1, H_2, H_3) = P(H_1)P(H_2 \mid H_1)P(H_3 \mid H_1, H_2) \]

- Enable a more efficient way of storing information
- Enable a more efficient evaluation of the Bayesian update formula
- Preserve the identity of individual components
  (e.g., normalization errors and associated uncertainties)
Basic building block

\[ \vec{x} = \begin{pmatrix} x_1 \\ x_2 \\ \vdots \\ x_n \end{pmatrix} \]

(f may be non-linear)

\[ \vec{y} = f(\vec{x}) \]

(\(\vec{y} = \begin{pmatrix} y_1 \\ y_2 \\ \vdots \\ y_m \end{pmatrix}\))

(e.g., model predictions)

(e.g., convoluted model predictions)
Because of $\vec{y} = f(\vec{x})$ the distribution of $\vec{y}$ is not necessarily multivariate normal
Links between nodes

Log-normal distribution
(e.g., positive cross section)

\[ y_i = \exp(x_i) \]

Truncated normal distribution
(e.g., non-negative cross section)

\[ y_i = \max(0, x_i) \]

Linear interpolation
(e.g., model mesh to experimental mesh)

\[ y_j = \left( \frac{E_{i+1} - E_j'}{E_{i+1} - E_i} \right) x_i + \left( \frac{E_j' - E_i}{E_{i+1} - E_i} \right) x_{i+1} \]

if \( E_i \leq E < E_{i+1} \)

Convolution
(e.g., model mesh to experimental mesh with finite energy resolution)
Combination of nodes

For example:
Experimental measurement is the sum of convoluted model prediction and statistical error

\[ \vec{y} = f(\vec{x}) + g(\vec{z}) \]
Example of Iron-56 between 1 and 2 MeV

- Total (TOT)
- Elastic (EL)
- Inelastic (INL)
More fine-grained modeling
Coupling to experimental data
Final Bayesian network with many more regularizers

https://arxiv.org/abs/2110.10322
MAP estimates of average components

avg_EL + avg_INL = avg_TOT
MAP estimates of cross sections

EL + INL = TOT
Motivation for another use case of Bayesian networks

- High-quality evaluations take a lot of time
- Final evaluations are stored in nuclear data libraries (JEFF, JENDL, ENDF/B, CENDL, etc.)
- If problems with an evaluation in a nuclear data library are detected (e.g., discovered by new experimental data), it can take again a lot of time to update the evaluation

**Idea:** Employ Bayesian networks to *quickly and consistently* update evaluations in nuclear data libraries
Construction of Bayesian network, e.g. Ni-58
Prior assumptions

- ENDF/B-VIII.0 cross sections were used as prior mean values
- Prior uncertainty: 30% of prior cross section value
- **Introduction of prior for second derivative**
  - Prior values of 2\textsuperscript{nd} derivative taken from ENDF/B-VIII.0
  - Prior uncertainty: 30% of 2\textsuperscript{nd} derivative of prior values
Evaluation starting point

- The Ni cross section evaluations in ENDF/B-VIII.0 (MF3) were used as a starting point (i.e., as prior mean values)
- Not considering inelastic level scattering for the time being
- Limited energy range 1 to 20 MeV for this demonstration
  - All data are linear-linear interpolated
  - MT5 is absent in this energy range in all files and in the one where it is present has negligible cross section
- No energy mesh unification was done (for simplicity)
- In total 19704 mesh points (all isotopes and reaction channels)
- Reduced mesh size of elastic and total cross sections by averaging over 0.5 MeV bins (after reduction 3817 mesh points remaining)
Ni-58 evaluation
Ni-58 evaluation: (inl, el, tot)
Ni-60 evaluation
Ni-60 evaluation: (n, alpha)
Ni-60 evaluation: inl, el, tot

Ni-60

(n,n)

(n,n0)

(n,total)

cross section [mbarn]

energy [MeV]

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Ni-61 evaluation

Ni-61 cross sections as a function of energy [MeV].

- $(n,2n)$
- $(n,2p)$
- $(n,3n)$
- $(n,a)$
- $(n,d)$
- $(n,g)$
- $(n,n)$
- $(n,n\alpha)$
- $(n,nd)$
- $(n,\alpha\alpha)$
- $(n,\alpha\beta)$
- $(n,p)$
- $(n,pa)$
- $(n,t)$
- $(n,\alpha\beta)$

Cross sections are measured in mbarns.
Ni-61 evaluation: (n,p)
Ni-62 evaluation
Ni-62 evaluation: inl, el, tot

![Graphs showing cross section vs. energy for Ni-62 reactions](image_url)
Ni-64 evaluation

Ni-64

- (n,2n)
- (n,3n)
- (n,a)
- (n,d)
- (n,g)
- (n,n)
- (n,n0)
- (n,na)
- (n,nonel)
- (n,np)
- (n,p)
- (n,total)

Cross section [mbarn] vs. energy [MeV]
Connecting the individual Bayesian networks for consistent treatment of nat-Ni data

Ni-0: n,tot
Ni-0: n,n0
Ni-58: n,tot
Ni-58: n,n0
Ni-60: n,tot
Ni-60: n,n0
Evaluation of Ni-0 (coupled)
Evaluation of Ni-0 (coupled): inl, el, tot

Pay attention to how the discrepant data in (n,total) near 1 MeV affects the other isotopes!
Evaluation of Ni-58 (coupled)
Evaluation of Ni-58 (coupled): inl, el, tot
Evaluation of Ni-60 (coupled)
Evaluation of Ni-61 (coupled)
Evaluation of Ni-62 (coupled)
Evaluation of Ni-64 (coupled)
Ideas for discussion

• What is important to consider from the nuclear physics perspective? (e.g., constraints)

• Where do you anticipate difficulties in the application of Bayesian networks in the nuclear data context?

• Ideas for useful building blocks? (linked to experiments, nuclear models, constraints)

• Regarding making Bayesian network inference available as an online service or software package, any thoughts on APIs, frameworks, technology, design for a good user experience?