Nuclear data evaluation with Bayesian networks

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Short bio

- Studied physics at TU Vienna
- PhD in nuclear data evaluation 2015
- Postdoc at CEA Saclay (2015-2018) and Uppsala University (2018-2019)
- Since 2020 nuclear physicist in Nuclear Data Section at IAEA dealing with nuclear data library projects and code development
Probabilities of various nuclear interactions involving the atomic nuclei, e.g., cross sections.

Relevant for:

- Reactor physics
- Radiation dosimetry
- Radiation protection
- Radioactive waste management
- Astrophysics
- Nuclear medicine
- Fusion research
- …
Nuclear data evaluation

Models

- TALYS
- INCL
- EMPIRE

Experiments

- Probability
- EXFOR

Evaluation method

- Linearized method
- Monte Carlo method

Simulation

- MCNP, OpenMC, Geant4, etc.

Evaluation method

- ENDF + Cov
- ENDF #1
- ENDF #2
- ...
Nuclear data evaluation

Models
- TALYS
- INCL
- EMPIRE

Experiments
- EXFOR

Evaluation method
- Linearized method
- Monte Carlo method

Simulation
- MCNP, OpenMC, Geant4, etc.

Production
- El. Prod. #1
- El. Prod. #2
- ...
Another perspective on the nuclear data evaluation process

Keywords: meta-analysis, sensor fusion, digital twins
“Truth” - System of reactions

- Total xs
  - Elastic xs
    - Residual production Lu(71,180)
      - (n,a)
      - (n,2n2p)
    - (n,nh)
    - (n,np)
  - Non-elastic xs
    - Residual production Hf(72,181)
      - (n,d)

- Proton production
- Neutron production
“Truth” - System of reactions

non-elastic xs

residual production
Lu(71,180)

residual production
Hf(72,181)

(n,2n2p)  (n,nh)  (n,np)

proton production  neutron production
Experimental data

Sample* (thickness, density, impurities)

detector

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background noise
Bayesian statistics …
  … allows inference in sophisticated probabilistic models
  … inference is a computational challenge (e.g., MCMC)

Neural networks …
  … scale to huge datasets
  … are not that easily amenable to UQ
  … are composed of simple building blocks
Best of both worlds*

Bayesian networks …  
... use Bayesian inference  
... build models by composing simple building blocks  
... similar to how it is done for neural networks

Judea Pearl**

* at least for nuclear data evaluation

** Better Than Bacon – Judea Pearl at NIPS 2013
Basic building block

\[ \tilde{y}_J = \tilde{y}_{\text{ref},J} + T (\tilde{y}_I - \tilde{y}_{\text{ref},I}) + (\tilde{\tau} - \tilde{\tau}_{\text{ref}}) \]

\[ \tilde{y}_I \sim \mathcal{N}(\tilde{u}_I, \mathbf{U}_{I,I}) \]

\[ \tilde{\tau} \sim \mathcal{N}(\tilde{u}_J, \mathbf{U}_{J,J}) \]
Versatile building block

\[ \vec{y}_J = \vec{y}_{\text{ref}, J} + \mathbf{T} (\vec{y}_I - \vec{y}_{\text{ref}, I}) + (\vec{t} - \vec{t}_{\text{ref}}) \]

Fourier

Convolution

Linearized nuclear model

\[ \vec{y}_I \sim \mathcal{N}(\vec{u}_I, \mathbf{U}_{II}) \]

\[ \vec{t} \sim \mathcal{N}(\vec{u}_J, \mathbf{U}_{JJ}) \]
Bayesian inference

Posterior

\[ \tilde{y}_I \sim \mathcal{N}(\bar{u}_I', U_{I,I}') \]

Analytic update equations

\[ \bar{u}_I' = \bar{y}_{\text{ref},I} + U_{I,I}' \left( S_{J,I}^{T} U_{J,J}^{-1} (\bar{r} - \bar{y}_{\text{ref},J}) + U_{I,I}^{-1} (\bar{u}_I - \bar{y}_{\text{ref},I}) \right) \]

\[ U_{I,I}' = \left( S_{J,I}^{T} U_{J,J}^{-1} S_{J,I} + U_{I,I}^{-1} \right)^{-1} \]
Bayesian inference

Analytic update equations
(aka Generalized Least Squares (GLS))

\[
\begin{align*}
\vec{u}_I' &= \vec{y}_{\text{ref},I} + \mathbf{U}_{I,I}' \left( \mathbf{S}_{J,I}^T \mathbf{U}_{J,J}^{-1} (\vec{r} - \vec{y}_{\text{ref},J}) \right. \\
& \quad \left. + \mathbf{U}_{I,I}^{-1} (\vec{u}_I - \vec{y}_{\text{ref},I}) \right) \\
\mathbf{U}_{I,I}' &= \left( \mathbf{S}_{J,I}^T \mathbf{U}_{J,J}^{-1} \mathbf{S}_{J,I} + \mathbf{U}_{I,I}^{-1} \right) 
\end{align*}
\]

\[
\vec{y}_I \sim \mathcal{N}(\vec{u}_I', \mathbf{U}_{I,I}')
\]
Composability – nested relationships

apply chain rule to get a compound Jacobian matrix

\[ S = \begin{pmatrix} 1 & 0 & J_{pos}J_{mod} & J_{norm} \\ 0 & 1 & J_{mod} & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix} \]

can be done automatically: “automatic differentiation”
Framework flexible enough?

- Multivariate normal distribution
  - Negative values are regarded possible
  - Tails not heavy enough? Too symmetric?
- Linearity assumption
  - Nuclear physics models are non-linear
  - Many non-linear interactions between variables

Not flexible enough (yet)
Non-linear relationships

- Permit non-linear relationships between nodes
- Embed GLS method in an iterative scheme* to obtain Maximum A Posteriori (MAP) estimate:

\[
U'_{I,I} = \left( S_{I,I}^T U_{I,I}^{-1} S_{I,I} + U_{I,I}^{-1} \right)^{-1} \quad \Rightarrow \quad U'_{I,I} = \left( S_{A,I}^T U^{-1} S_{A,I} + \lambda D \right)^{-1}
\]

* aka (modified) Levenberg-Marquardt algorithm
Non-linear relationships

- Permit non-linear relationships between nodes
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\[ U'_{I,I} = \left( S_{J,I}^{T} U_{J,J}^{-1} S_{J,I} + U_{I,I}^{-1} \right)^{-1} \quad \rightarrow \quad U'_{I,I} = \left( S_{A,I}^{T} U^{-1} S_{A,I} + (\lambda D)^{-1} \right) \]

Enhanced modeling possibilities:

- Other distribution functions, e.g., log-normal distribution, via non-linear transformation
- Integration of more realistic relationships, e.g., non-linear physics model

* aka (modified) Levenberg-Marquardt algorithm
Nuclear data evaluation example
Summary

- Bayesian inference + network = Bayesian network
- Composability can be a great accelerator in the design of probabilistic models
- Simple distribution assumption (MVN) in combination with non-linear relationships yields a flexible yet tractable inference framework
- In the nuclear data evaluation context, we mostly deal with a system of functions linked by linear and non-linear relationships
- The future: link functions may be given by neural networks trained on lots of data if available
- Mathematical details and description of Bayesian network examples here:

  G. Schnabel, R. Capote, A.J. Koning, D.A. Brown, “Nuclear data evaluation with Bayesian networks”, arXiv:2110.10322