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Interfacing TALYS with a Bayesian treatment of model defects and inconsistent data

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Human vs and Machine

- Expert knowledge is indispensable
- Automated procedures provide reference evaluations
- Nowadays humans are still pushing the buttons but the effected operations are more abstract and complex
Generalized Least Squares (GLS)

Experiments
\( \tilde{\sigma}_{\text{exp}}, C_{\text{exp}} \)

Model
\( \tilde{\rho}_0, P \)

GLS

\( \tilde{\rho}_{\text{upd}}, P_{\text{upd}} \)

We work in the parameter domain

\[
\tilde{\sigma}_{\text{mod}} = f(\tilde{\rho}) \\
S = \frac{\partial}{\partial \tilde{\rho}} f(\tilde{\rho})
\]
Recent developments

Experiments

\[ \tilde{\sigma}_{\text{exp}}, C_{\text{exp}} \]

rule-based covariances

uncertainty correction (MLO)

Model

Levenberg-Marquardt algorithm

\[ \tilde{p}_0, P \]

Gaussian processes for energy-dependent parameters

GNLLS

\[ \tilde{p}_{\text{upd}}, P_{\text{upd}} \]

No toy model \(^{56}\text{Fe}\): We go big!
925 TALYS parameters considered
144 TALYS parameters adjusted
4322 experimental data points
Preprocessing steps

Experiments

\[ \tilde{\sigma}_{\text{exp}}, C_{\text{exp}} \]

- rule-based covariances
- uncertainty correction (MLO)

Model

- TALYS
- \( \tilde{p}_0, P \)

Levenberg-Marquardt algorithm

GNLLS

\[ \tilde{p}_{\text{upd}}, P_{\text{upd}} \]

Gaussian processes for energy-dependent parameters

No toy model (\(^{56}\text{Fe})\): We go big!
925 TALYS parameters considered
144 TALYS parameters adjusted
4322 experimental data points
Preprocessing steps

- Construction of experimental covariance matrix $C_{\text{exp}}$
  - Rule-based extraction of uncertainties from EXFOR
  - Extra systematic uncertainty if necessary (MLO approach)

- Construction of parameter covariance matrix $P_0$
  - 10% uncertainty for non-energy dependent parameters
  - Gaussian processes for energy-dependent parameters

MLO applied to integral benchmark experiments:
Presentation of Henrik Sjöstrand on Wednesday
Examples: uncertainty correction

Systematic extra uncertainty

(references to data upon request)
Energy-dependent parameters

- The adjustment of parameter functions in a model is a powerful capability (e.g., DFT)
- We use Gaussian processes as prior knowledge on energy-dependent TALYS parameters
- The idea: Inject more flexibility into model to simulate the treatment of model defects

What is a Gaussian process?

- A random function (e.g., stock price)
- Properties of possible realizations defined by a covariance function and its parameters:

\[
\text{cov} [f(E), f(E')] = \delta^2 \exp \left[ -\frac{1}{2} \left( \frac{E - E'}{\lambda} \right)^2 \right]
\]

Sample of functions (\(\delta=\lambda=1\))

Constraining with observations
Good news about GPs

- No sampling (BMC-like procedure) necessary to constrain with observations
- A GP can be updated by using the GLS formulas

Sample of functions ($\delta=\lambda=1$)

Posterior uncertainty band (GLS)
How to do in practice?

1) Preprocessing: Apply MLO to tune hyperparameters (amplitudes $\delta$ and length-scales $\lambda$) of cov functions

2) Apply the Levenberg-Marquardt algorithm to solve the non-linear GLS problem

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<th>index</th>
<th>parameter</th>
<th>$\bar{\rho}_0$</th>
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<td>wso2adjust t</td>
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</tbody>
</table>
LM algorithm: iterative algorithm to solve the non-linear GLS problem

Red
Real improvement checked by running TALYS

Green
Current approximation

Blue
Improvement expected due to linear approximation of TALYS

Levenberg-Marquardt (LM) algorithm
Levenberg-Marquardt in action

**iteration: 1**

**Green:**
current approximation

**Blue**
Expected improvement

**Red**
Real improvement
after the correction of experimental data using MLO, the adjustment of GPs hyperparameters associated with energy-dependent parameters using MLO, and solving the non-linear GLS problem with the LM algorithm

Observations
1) The procedure provides reasonable fits
2) Uncertainties are too low in domains of lots of experimental data
   => We need also model defects on the observable side
Final result

Posterior of angle-integrated cross sections

(26-FE-56(N,2N)26-FE-55,,SIG)

(26-FE-56(N,A)24-CR-53,,SIG)

(26-FE-56(N,D)25-MN-55,,SIG)

(26-FE-56(N,EL)26-FE-56,,SIG)

(26-FE-56(N,INL)26-FE-56,,SIG)

(26-FE-56(N,N+P)25-MN-55,,SIG)

(26-FE-56(N,P)25-MN-56,,SIG)

(26-FE-56(N,T)25-MN-54,,SIG)

(26-FE-56(N,TOT) SIG)

(references to data upon request)
Final result

Parameter posterior + uncertainty band
(selection of parameters)
A. Koning, D. Rochman, J.-Ch. Sublet et al, TENDL: Complete Nuclear Data Library for Innovative Nuclear Science and Technology, Nuclear Data Sheets, 155, 2019

\( \{ \vec{p}_i \} \) \( i=1..N \) \( \rightarrow \) runs

\( \{ \vec{\sigma}_i \} \) \( i=1..N \) \( \rightarrow \) passes

TASMAN \( \rightarrow \) Pooled Results \( \rightarrow \) TEFAL \( \rightarrow \) ENDF file

\( \vec{p}_i \ldots \text{parameter set for } i\text{-th TALYS run} \)

\( \vec{\sigma}_i \ldots \text{predictions of } i\text{-th TALYS run} \)
Interfacing evaluation code with T6

Varied parameters from posterior

TASMAN’
(extension: read external variations)

TALYS

Pooled Results

TEFAL

creates

ENDF file

\{\vec{p}_i\}_{i=1..N}

\{\vec{\sigma}_i\}_{i=1..N}

\vec{p}_i \ldots \text{parameter set for } i\text{-th TALYS run}

\vec{\sigma}_i \ldots \text{predictions of } i\text{-th TALYS run}

A. Koning, D. Rochman, J.-Ch. Sublet et al, TENDL: Complete Nuclear Data Library for Innovative Nuclear Science and Technology, Nuclear Data Sheets, 155, 2019
Open Science, reproducibility, etc.

- All codes can be found on [https://github.com/gschnabel](https://github.com/gschnabel)
- Docker container with complete evaluation pipeline in preparation and will be published within the next weeks
• Exemplary evaluation of neutron-induced cross sections of $^{56}$Fe with several innovations in methodology
• Created and delivered a complete ENDF-file by interfacing our evaluation code with T6
• Necessary development: Combining these developments with the treatment of model defects on observable side (developed at TU Vienna)
Introduction of extra uncertainty

- Use a smooth spline-like function as “model”
- Maximize the probability for the data (MLO)

\[ \rho(\tilde{\sigma}_{\text{exp}}) = \mathcal{N}(\tilde{\sigma}_{\text{exp}} \mid \tilde{\sigma}, M) \]

\[ M = SAS^T + C_{\text{exp}} \]

- Prior covariance matrix A designed to represent a spline-like function
- Mapping matrix S interpolates linearly from “model” grid to experimental grid
- The experimental covariance matrix \( C_{\text{exp}} \) is composed of EXFOR components and systematic extra uncertainties