

Differential Cross Sections and the Impact of Model Defects in Nuclear Data Evaluation

Georg Schnabel^{1,2,a} and Helmut Leeb^{1,b}

¹Atominstytut, TU Wien, Wiedner Hauptstrasse 8-10, 1040 Vienna, Austria

²CEA, Saclay, Irfu/SPhN, Gif-sur-Yvette, France

Abstract. A statistically consistent method for the inclusion of the so-called model defects into Bayesian evaluation methods based on extensive modeling is presented. The method uses Gaussian processes to define a-priori probability distributions for possible model defects. The inclusion is of particular importance for the proper evaluation of differential data, i.e. angle-differential cross sections and spectra of ejectiles. The method is successfully applied to a simple realistic example which clearly shows the impact of model defects in a simultaneous evaluation of angle-differential and angle-integrated cross sections.

1 Introduction

Nuclear data evaluation yields consistent sets of reaction data, comprising cross sections, spectra and production cross sections for a given group of isotopes. Recent demands triggered by the development of novel nuclear technologies and applications include the extension of the energy range as well as the inclusion of uncertainty information. Because of the scarcity of neutron-induced reaction data beyond 20 MeV, corresponding evaluations depend strongly on nuclear models. Nowadays it is well established that Bayesian statistics [1] is the proper mean for a consistent combination of experimental data with values obtained from nuclear model calculations. Corresponding evaluation procedures yield mean values of the observables and associated covariance matrices containing uncertainty information. However, the unreflected inclusion of results from model calculations into a Bayesian evaluation may lead to unrealistically small uncertainties. This effect is particularly striking in angle-differential cross sections, which are strongly correlated and additionally include phase information not available in angle-integrated data.

In this contribution we consider this problem in more detail. Especially, we show at a schematic example in section 2 that this finding may be the consequence of the assumption of perfect models, frequently used in nuclear data evaluation. In section 3 we present a novel evaluation concept which provides within Bayesian statistics a consistent treatment of model defects on the basis of Gaussian processes. The advantages of this extended procedure are demonstrated at an example simultaneously evaluating simple, but realistic sets of angle-differential and angle-integrated cross section data. The results of this first application are very promising and therefore concluding remarks and an outlook on the potential of the method are given in the final section 4.

^ae-mail: georg.schnabel@cea.fr

^bCorresponding author: e-mail: leeb@kph.tuwien.ac.at

2 Standard Bayesian Evaluation Procedure

In a standard evaluation process, it is usually assumed that the model $M(\mathbf{p})$ is perfect and describes the experimental values of the observables σ_{exp} within the experimental uncertainties ϵ_{exp} , i.e. $\sigma_{\text{exp}} = \sigma_{\text{mod}} + \epsilon_{\text{exp}}$. In most standard evaluation procedures [2], the combination of experimental and model values is governed by Bayes theorem [1],

$$\pi(\mathbf{p} | \sigma_{\text{exp}}) = \left[\int d^d p \ell(\sigma_{\text{exp}} | \mathbf{p}) \pi(\mathbf{p}) \right]^{-1} \ell(\sigma_{\text{exp}} | \mathbf{p}) \pi(\mathbf{p}). \quad (1)$$

Here, $\pi(\mathbf{p} | \sigma_{\text{exp}})$ is the a-posteriori distribution of the model parameters \mathbf{p} conditioned on the measured values σ_{exp} of the observables, $\ell(\sigma_{\text{exp}} | \mathbf{p})$ is the likelihood and $\pi(\mathbf{p})$ is the a-priori distribution which reflects the available *a-priori* knowledge. The integral in Eq. (1) acts as a normalization and is usually denoted as *evidence*. In the following discussion we substitute the parameter distributions $\pi(\mathbf{p})$, $\pi(\mathbf{p} | \sigma_{\text{exp}})$ by cross section distributions $\pi(\sigma)$, $\pi(\sigma | \sigma_{\text{exp}})$. For details on this approach see e.g. [2, p. 37]. Bayes theorem is applicable for arbitrary probability distributions, but for the sake of simplicity we restrict the present discussion to multivariate normal distributions,

$$\rho(\mathbf{t}) = \frac{1}{\sqrt{(2\pi)^d |\mathcal{V}|}} \exp \left[-\frac{1}{2} (\mathbf{t} - \langle \mathbf{t} \rangle)^T \mathcal{V}^{-1} (\mathbf{t} - \langle \mathbf{t} \rangle) \right], \quad (2)$$

where the mean value $\langle \mathbf{t} \rangle$ and the covariance matrix \mathcal{V} characterize the multivariate normal distribution denoted by $\mathcal{N}(\langle \mathbf{t} \rangle, \mathcal{V})$. Assuming a multivariate normal distribution for the experimental uncertainties with covariance matrix \mathcal{B} gives rise to the likelihood $\ell(\sigma_{\text{exp}} | \sigma) \sim \mathcal{N}(\sigma, \mathcal{B})$. Using the further assumption of a multivariate normal a-priori distribution $\mathcal{N}(\sigma_0, \mathcal{A}_0)$, Eq. (1) leads to a multivariate normal a-posteriori distribution $\pi(\sigma | \sigma_{\text{exp}}) \sim \mathcal{N}(\sigma_1, \mathcal{A}_1)$. The evaluated mean values and the covariance matrix are available in closed-form,

$$\sigma_1 = \sigma_0 + \mathcal{A}_0 \mathcal{S}^T (\mathcal{S} \mathcal{A}_0 \mathcal{S}^T + \mathcal{B})^{-1} (\sigma_{\text{exp}} - \mathcal{S} \sigma_0), \quad (3)$$

$$\mathcal{A}_1 = \mathcal{A}_0 - \mathcal{A}_0 \mathcal{S}^T (\mathcal{S} \mathcal{A}_0 \mathcal{S}^T + \mathcal{B})^{-1} \mathcal{S} \mathcal{A}_0, \quad (4)$$

where \mathcal{S} is the so-called sensitivity matrix providing the mapping from the angle/energy grid of the model vector σ to the grid of the experiment vector σ_{exp} . Especially, we set up \mathcal{S} in a way to implement bilinear interpolation for angle-differential and linear interpolation for angle-integrated cross sections.

In general, applications of the standard Bayesian evaluation procedures lead to reasonable mean values of the observables, while the uncertainties are frequently underestimated. In order to reveal the origin of this finding, we consider a schematic example of generated experimental data (Fig. 1a) and a linear model (Fig. 1b) as *a-priori* information. The result of the evaluation is displayed in Fig. 1c. The unrealistically small uncertainties associated with the evaluated observables are a direct consequence of the rigidity of the model. Moreover, in standard Bayesian evaluations the predictive power of the model has no influence on evaluated uncertainties – a questionable feature. The increase of the prior uncertainties, as frequently suggested, cannot cure the problem. The outcome of this schematic example indicates that one has to find either the *perfect model* or a proper method to account for model defects in the evaluation process.

3 Novel Evaluation Concept including Model Defects

In the past different approaches for the inclusion of model defects have been presented [3–6], but none of these is fully based on statistics and conserves sums. Therefore, we have formulated an extended

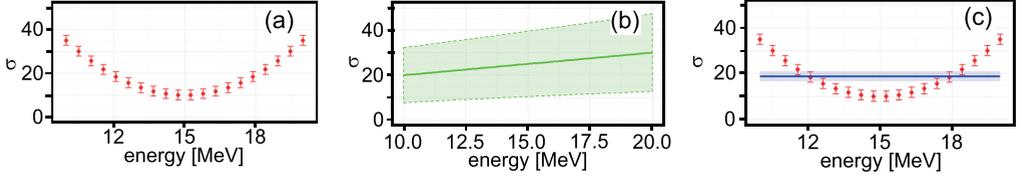


Figure 1. Evaluation based on schematic experimental data (red) and a model (blue), linear in the energy E . (a) generated experimental data set; (b) prior based on a linear model with given uncertainty; (c) Result of the standard Bayesian evaluation.

Bayesian evaluation procedure [2] assuming $\sigma_{\text{exp}} = \sigma_{\text{mod}} + \epsilon_{\text{mod}} + \epsilon_{\text{exp}}$. The inclusion of the model defects ϵ_{mod} requires an extension of Eq. (1),

$$\pi(\mathbf{p}, \epsilon_{\text{comb}} | \sigma_{\text{exp}}) = \hat{C} \ell(\sigma_{\text{exp}} | \mathbf{p}, \epsilon_{\text{mod}}) \pi(\mathbf{p}) \pi(\epsilon_{\text{comb}}) \quad (5)$$

with the extended evidence \hat{C} ,

$$\epsilon_{\text{comb}}^T = (\epsilon_{\text{pred}}^T, \epsilon_{\text{mod}}^T) \quad \text{and} \quad \pi(\epsilon_{\text{comb}}) \propto \exp\left(-\frac{1}{2} \epsilon_{\text{comb}}^T \mathcal{K}_0^{-1} \epsilon_{\text{comb}}\right). \quad (6)$$

The factorized form of the prior in Eq. (5) is due to the assumption of vanishing a-priori correlation between the model parameters \mathbf{p} and the model defects ϵ_{mod} . The covariance matrix \mathcal{K}_0 reflects the a-priori assumptions about possible model defects.

The determination of the model defect ϵ_{mod} is the key issue of the procedure because it is beyond the theory underlying the model. Usually, there is no knowledge about the specific functional form of ϵ_{mod} , but frequently we have an idea about the smoothness of the cross section curve and the overall quality of the model. Therefore, we adopted the concept of Gaussian processes [7, 8], which allows us to specify a probability distribution for the shape of an unknown function using the expected smoothness of the function and the expected magnitude of the function values. More specifically, a probability distribution $\rho(\cdot)$ on a function space \mathcal{F} corresponds to a Gaussian process if for any finite set of $\{\mathbf{x}_i\}_{i=1, \dots, N}$, $\forall \mathbf{x}_i \in \mathbb{R}^d$ the associated function values $\{f(\mathbf{x}_i)\}_{i=1, \dots, N}$ follow a multivariate normal distribution. A Gaussian process is completely characterized by a mean function $m(\mathbf{x})$ and a covariance function $k(\mathbf{x}, \mathbf{x}')$. The covariance function is used to construct the covariance matrix \mathcal{K}_0 introduced in Eq. (6).

We adopt the assumption $m(\mathbf{x}) \equiv 0$ meaning that the model prediction is a-priori regarded as the most likely guess to represent the true cross section. Further, we use for the evaluation of the angle-differential cross sections the covariance function

$$\tilde{k}(E, \theta; E', \theta') = \frac{d\sigma}{d\Omega}(E, \theta) \frac{d\sigma}{d\Omega}(E', \theta') \sum_{i=1,2} \alpha_i(\theta) \alpha_i(\theta') g(E - E', \theta - \theta'; \delta_i, \lambda_i, \eta_i) \quad (7)$$

with $\alpha_2(\theta) = 1 - \alpha_1(\theta)$,

$$g(E, \theta; \delta, \lambda, \eta) = \delta^2 \exp\left(-\frac{E^2}{2\lambda^2}\right) \exp\left(-\frac{\theta^2}{2\eta^2}\right) \quad \text{and} \quad \alpha_1(\theta) = \left[1 + \exp\left(\frac{a - \theta}{b}\right)\right]^{-1}. \quad (8)$$

This covariance function contains two components: one component for small angles and another one for big angles. Each component i is characterized by the magnitude of the model defect δ_i and the smoothness hyperparameters λ_i and η_i . The transition between the two angle domains is achieved via the function $\alpha(\theta)$ depending on the parameters a and b . The covariance function in Eq. (7) also

induces a covariance function for the model defects of the associated angle-integrated cross sections,

$$\tilde{k}(E, E') = (2\pi)^2 \int_0^\pi \int_0^\pi d\theta d\theta' \sin \theta \sin \theta' \tilde{k}(E, \theta; E', \theta'). \quad (9)$$

This relationship directly reflects the connection between angle-differential and associated angle-integrated cross sections.

If there is no idea about the values of the hyperparameters of the Gaussian process, one may determine these by maximizing the evidence \hat{C} . In general, this procedure leads to reasonable values for the hyperparameters (δ, λ, \dots) , but one must be aware that this method involves experimental values and is therefore not a completely independent *a-priori* information.

In principle, the extended Bayesian evaluation proceeds analogously to the standard procedure. Especially, one may use the linearized version for the Bayesian update (4). In addition to standard Bayesian evaluations, one also obtains mean values and covariance matrices for the model defects as well as cross correlations between observables and model defects.

The procedure outlined above can be applied simultaneously for angle-integrated and differential data. Especially for the evaluation of angle-differential cross sections, the inclusion of model defects is of great importance. Therefore, we present a test example of a simultaneous evaluation of a set of angle-differential cross sections at $E = 8.03$ MeV together with corresponding angle-integrated cross sections in the energy regime between 2 and 9 MeV. For the inclusion of model defects, we use the covariance functions (9) for angle-integrated cross sections and (7) for angle-differential cross sections. Assuming a model defect of $\delta_1 = 5\%$ in forward direction, we obtain the following values for the other hyperparameters by maximizing the evidence: $a = 23.014^\circ$, $b = 4.127^\circ$, $\lambda_1 = 1.121$ MeV, $\eta_1 = 60^\circ$, $\delta_2 = 0.69$, $\lambda_2 = 0.523$ MeV, $\eta_2 = 2.944^\circ$.

In Fig. 2 the evaluated differential cross sections at $E = 8.03$ MeV without and with model defects are shown. In both evaluations the experimental values of the differential cross sections are well reproduced. However, ignoring the model defects leads to an unrealistically small error band, while accounting for model defects leads to larger and more realistic uncertainties in the order of the experimental errors (see Fig. 3c). The method also yields the mean value of the model defect and its error band (Fig. 2c). Due to the conservation of sums, the inclusion of model deficiencies has also a direct impact on the evaluation of angle-integrated cross sections (Fig. 3). If model defects are ignored, the evaluated angle-integrated cross section deviates completely from the experimental value. Including model defects leads to a significantly better overlap between experimental and evaluated cross section. The remaining deviations reflect the fact that the values of the angle-integrated cross section are not compatible with available angle-differential data. Apart from mean values and associated uncertainties, the extended evaluation procedure yields also the complete set of covariance matrices.

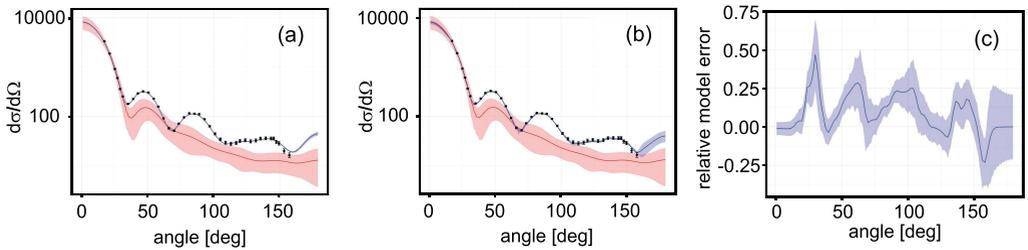


Figure 2. Evaluated (blue) and a-priori (red) angle-differential cross section data with the associated uncertainty band at $E = 8.03$ MeV. (a) Evaluation without model defects; (b) Evaluation accounting for model defects; (c) Mean value of the model defect and its uncertainty band.

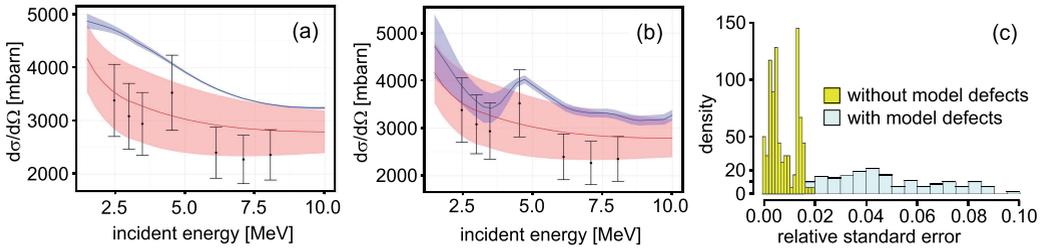


Figure 3. Evaluated (blue) and a-priori (red) angle-integrated cross section data with the associated uncertainty band. (a) Evaluation without model defects; (b) Evaluation accounting for model defects; (c) Histogram comparing the uncertainties without (yellow) and with (blue) model defects.

4 Conclusions and Outlook

We developed a statistically consistent procedure for the inclusion of model defects into nuclear data evaluations. The method is based on Gaussian processes, which allows to formulate the expected deviations from the nuclear model calculations in terms of reasonable assumptions for the covariance matrices. The method provides not only values for the evaluated observables and uncertainties, but also provides mean values and uncertainties of the model defects, which is an important information, especially for differential data. Applications of the method to evaluations of neutron-induced reaction data are currently in progress.

The presented method addresses the general problem of the assessment of the quality of models and is therefore not only of interest for nuclear data evaluation. Hence it has a high potential for applications in different fields of physics which strongly rely on modelling.

Acknowledgements

Work partly supported by the F4E Partnership Agreement grant F4E-FPA-168.02 and the associated KKKÖ project G. Schnabel of the Austrian Academy of Sciences as well as via the EURATOM project CHANDA. The views and opinions expressed herein do not reflect necessarily those of the European Commission.

References

- [1] T. Bayes, *An Essay towards Solving a Problem in the Doctrine of Chances*, Philosophical Transactions **53**, 370 (1763)
- [2] G. Schnabel, *Large Scale Bayesian Nuclear Data Evaluation with Consistent Model Defects*, PhD thesis, TU Wien (2015)
- [3] M.T. Pigni, H. Leeb, *Uncertainty estimates of evaluated ^{56}Fe cross sections based on extensive modelling at energies beyond 20 MeV* in: Proc. Int. Workshop on Nuclear Data for the Transmutation of Nuclear Waste (GSI Darmstadt, Darmstadt, 2003) PO21
- [4] H. Leeb, D. Neudecker, Th. Srdinko, Nucl. Data Sheets **109**, 2762 (2009)
- [5] A. Trkov *et al.*, Nucl. Instr. Meth. A **212**, 3098 (2011)
- [6] D. Neudecker, R. Capote, H. Leeb, Nucl. Instr. Meth. A **723**, 163 (2013)
- [7] D.G. Krige, J. Chemical, Metallurgical and Mining Society **52**, 119 (1951)
- [8] C.E. Rasmussen, Ch.K.I. Williams, *Gaussian Processes for Machine Learning* (MIT Press, Cambridge, 2006), ISBN: 0-262-18253-X 978-0-262-18253-9

