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A New Module for Large Scale Bayesian Evaluation in the Fast Neutron Energy Region

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We present an improved update scheme for the Linearized Bayesian Update procedure (LBUP). The revised procedure extends the application of the LBUP to a large number of observables. The consistent update of dozens of millions of observables becomes manageable by circumventing the costly calculation of the prior covariance matrix. Nuclear data evaluations based on the revised scheme may exhaustively enclose all differential and angle-integrated channels, treating all correlations between them exactly in the update procedure.

I. INTRODUCTION

Modern nuclear data evaluation requires the consideration of an extended energy range (incident energies up to at least 150 MeV) and the provision of uncertainties. Hence, such evaluations must rely on both experimental data and results of model calculations to make predictions for physical observables, e.g. cross sections, and to assess their uncertainties. The latter are usually given in terms of covariance matrices of cross section uncertainties. The result of such an evaluation process is cast into an *evaluated nuclear data file* using the ENDF-format [1]. In a processed form this ENDF-file is an indispensable requisite for applications that require neutron transport and/or activation calculations. The reliability of these calculations is strongly dependent on the quality of the nuclear data files used.

The selection and uncertainty assessment of experimental data as well as the choice of nuclear models represent the first step of any evaluation. The latter together with mathematical constraints describe an *apriori* knowledge which should be combined with the experimental data to reflect our best knowledge of the observables. The evaluation process is straightforward if sufficient experimental data are available in the whole energy range of the evaluation [2, 3]. In this case, the *apriori* knowledge plays a minor role. However, at energies above 20 MeV experimental data are scarce, and consequently current nuclear data evaluations up to 200 MeV rely on nuclear models and thus on *apriori* knowledge. At present there is an ongoing discussion about the most appropriate evaluation procedure. Several methods for nuclear data evaluation were proposed by different groups, e.g. [4–11]. Among these, the methods based on Bayesian statistics, e.g. [5, 6, 9–11], are most appealing and have been successfully applied for nuclear data evaluation in the past.

Bayesian statistics is mathematically well founded and its application can be regarded as automated logical reasoning based on incomplete or vague information [12]. It provides a consistent and well-defined procedure to combine experimental data and *apriori* knowledge. Hence it is widely accepted to provide a well suited framework for nuclear data evaluation.

With increasing incident energy the number of energetically open channels is increasing, and consequently the number of observables included in the evaluation process gets significantly larger. In principle, an extended energy range will not lead to difficulties as long as the evaluation is limited to the nuclear model space, i.e. the search for the set of best model parameters which provide a fair description of the experimental data. In this case, the number of model parameters to be estimated will be the same or only moderately growing with increased incident energy. However, in actual evaluations within the Linearized Bayesian Update Procedure [11], one is interested in flexibilities beyond the strict model space. Hence, one performs the evaluation relying on a surrogate model where the observables at given mesh points serve as parameters of the model. Thus, one is faced with a large number of parameters which must be handled in an evaluation process.

In this contribution we consider the *Linearized Bayesian Update Procedure* (see e.g. [11]) which assumes Gaussian distributions for both the prior distribution of the observables, i.e. cross sections, and the likelihood function of the experimental data. We develop a new numerically efficient update procedure of the mean values of the observables without explicitly calculating the prior covariance matrix. The novel procedure allows an exact treatment of a huge number of observables within

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the Linearized Bayesian Update Procedure. Thus, we can implicitly deal with prior covariance matrices of dimension $10^7 \times 10^7$ or higher on a modern personal computer. The millions of quantities a nuclear model code may produce, i.e. angle-integrated cross sections, angle-differential cross sections and spectra, can be consistently updated in one step.

After this introduction, we briefly recall the basics of Bayesian statistics in Sect. II, in order to provide the most important relationships. In Sect. III we reformulate the Linearized Bayesian Update Procedure to make its application feasible for a large number of observables. A summary and outlook is given in Sect. IV.

II. STATISTICAL BASIS

The cornerstone of Bayesian statistics is Bayes theorem

$$P(x|y) \propto P(y|x)\, P(x) \tag{1}$$

with the vector of model parameters x and the experimental data y. The posterior probability density function (pdf) $P(x|y)$ gives the probability density of a parameter set x under the condition that the given data y have been measured. The posterior pdf is – apart from a normalization constant – the product of the likelihood $P(y|x)$ and the prior pdf $P(x)$. Similarly, the likelihood gives the probability density that a certain set of experimental data is obtained under the condition that the set of model parameters x is true. The prior pdf gives the *apriori* probability density for a certain set of model parameters x if no data are measured.

In the Linearized Bayesian Update Procedure (LBUP) Gaussian probability distributions are assumed for both the prior pdf and the likelihood. Thus, the prior pdf takes the form

$$P(x) \propto \exp\left(-\frac{1}{2}(x-\overline{x})^T A^{-1}(x-\overline{x}\right), \tag{2}$$

where $\overline{x}$ is the *apriori* expectation vector for the observables and A the associated covariance matrix. The prior expectation vector $\overline{x}$ may contain angle-integrated cross sections, angle-differential cross sections and spectra. As briefly outlined in the introduction (section I), we use a surrogate model and for the benefit of flexibility we do not work on the level of nuclear models. Thus, the "model parameters" are the physical observables, and not optical model or level density model parameters. However, from the statistical point of view, other observables than the aforementioned could also be included as long as they are continuous quantities. This prior pdf gives the probability density that a certain vector x represents the true values of the observables under the assumption of a valid model. The normalization constant of the Gaussian distribution is not relevant for further discussion.

The prior expectation vector $\overline{x}$ and the prior covariance matrix A are constructed from the results of model calculations where model parameters have been sampled according to a given distribution. The choice of the boundaries for the model parameters and from which distribution they are sampled depends on the specific nuclear model as well as the nuclear system considered. The further considerations are independent of the specific choice.

Let's assume that the model calculations are already available and the resulting observables of the i^{th} model calculation are collected in a column vector x_i. Using these sample vectors x_i, the prior expectation $\overline{x}$ and covariance matrix A can be calculated by

$$\overline{x} = \frac{1}{n}\sum_{i=1}^{n} x_i\,, \tag{3}$$

$$A = \frac{1}{n-1}\sum_{i=1}^{n}(x_i-\overline{x})(x_i-\overline{x})^T\,. \tag{4}$$

For the likelihood containing the experimental information, we also assume a Gaussian density distribution,

$$P(y|x) \propto \exp\left(-\frac{1}{2}(y-Sx)^T B^{-1}(y-Sx)\right). \tag{5}$$

It expresses the probability density of the measured data vector y if x contains the true values of the observables. Here, B is the covariance matrix for the uncertainties of the experiments. Because the observables within the vector x are given on predefined energy and angle grids, the information in x has to be transferred to the energies and angles of the experimental data. This transfer is accomplished by the *sensitivity matrix* S which can exactly account for all kinds of linear mapping schemes, such as linear interpolation, spline interpolation or Fourier series. We used linear interpolations for angle-integrated and bilinear interpolation for differential data. Reasons for this choice are given in the next section.

The posterior pdf, i.e. the new state of knowledge, is apart from a normalization constant the product of prior pdf and likelihood, see Eqs. (2) and (5). Because both prior pdf and likelihood are Gaussian, the posterior pdf is also a Gaussian distribution function and the following standard matrix formulas (e.g. [13, 14]) can be used to calculate its mean vector $\overline{x}'$ and covariance matrix A',

$$\overline{x}' = \overline{x} + AS^T(SAS^T+B)^{-1}(y-S\overline{x})\,, \tag{6}$$

$$A' = A - AS^T(SAS^T+B)^{-1}SA\,. \tag{7}$$

These update formulas are convenient for numerical calculations because the required inversion is performed on the experimental grid, which is usually of much lower dimension than the model grid. Mathematically equivalent alternative update formulas exist which involve an inversion on the model grid.

If for consistency, all angular differential, spectral and angle-integrated data are included in the model vector $\overline{x}$, the associated prior covariance matrix A could become