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Quality Quantification of Evaluated Cross Section Covariances

S. Varet,[1,*] P. Dossantos-Uzarralde,[2] and N. Vayatis[1]
[1] *ENS Cachan, 61 Avenue du Président Wilson, 94235 Cachan Cedex, France*
[2] *CEA/DAM/DIF, Bruyères-le-Châtel, 91297 Arpajon Cedex, France*
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Presently, several methods are used to estimate the covariance matrix of evaluated nuclear cross sections. Because the resulting covariance matrices can be different according to the method used and according to the assumptions of the method, we propose a general and objective approach to quantify the quality of the covariance estimation for evaluated cross sections. The first step consists in defining an objective criterion. The second step is computation of the criterion. In this paper the Kullback-Leibler distance is proposed for the quality quantification of a covariance matrix estimation and its inverse. It is based on the distance to the true covariance matrix. A method based on the bootstrap is presented for the estimation of this criterion, which can be applied with most methods for covariance matrix estimation and without the knowledge of the true covariance matrix. The full approach is illustrated on the ^{85}Rb nucleus evaluations and the results are then used for a discussion on scoring and Monte Carlo approaches for covariance matrix estimation of the cross section evaluations.

I. INTRODUCTION

An important component of nuclear cross section evaluations is the associated covariance matrix. Several methods (Bayesian [1], unified Monte Carlo (UMC) [2], backward-forward Monte Carlo (BFMC) [3], total Monte Carlo [4] and scoring [5] are some of them) have been proposed to estimate such matrices, producing many covariance matrix estimates (stored in databases such as ENDF/B-VII.1 [6] or TENDL [7]). For all these methods, the convergence rate of the estimated covariance is at least proportional to $1/\sqrt{n}$ (with n the sample size). However this convergence rate concerns each term of the covariance matrix and as a consequence, the convergence rate of the matrix estimation is slower. Thus, the theory does not allow discrimination of these different approaches. Moreover, for a given nucleus, according to the method and according to the assumptions, the covariance estimates can be different.

Therefore, a method to compare, in a quantitative way, the performance of different techniques in covariance estimation quality is important. For this purpose, a general and objective approach to quantify the quality of the covariance estimation of the evaluations is proposed. In this paper two versions of the Kullback-Leibler distance ([8], [9], [10]), based on the ratio between two Gaussian probability density functions with same mean, are proposed as distances between covariance matrices. Ideally, the quality of the covariance estimation would require computation of the Kullback-Leibler distance between the true covariance matrix and its estimation. Obviously, the true covariance matrix is unknown. To overcome this obstacle, this paper proposes a method based on the bootstrap, which is widely used resampling technique introduced by Efron [11] allowing for computation of statistics (the variance for example) of an estimator, whose convergence has been prooved in many settings ([12] and [13]). Thus, the Kullback-Leibler distance in combination with bootstrap allows the comparison of different covariance estimation method independently of the method used to obtain them and without any additional code runs.

In the next Section, the two versions of the Kullback-Leibler distance are defined. The bootstrap is described in Sect. III. The approach is illustrated on the ^{85}Rb nucleus evaluations and the obtained results are exploited for a discussion on the scoring and brute Monte Carlo methods in Sect. IV.

II. DISTANCE BETWEEN COVARIANCE MATRICES

In our context, the problem is to compare the true covariance matrix Σ, with its estimate $\widehat{\Sigma}$. The best choice of distance measure will depend on intended use of estimated covariance matrix. In order to be as general as possible, this paper focuses on a metric in the covariance matrix space. Because the estimation $\widehat{\Sigma}$ can be used in a generalized χ^2 distance, comparison of the true inverse

* Corresponding author: suzanne.varet@cmla.ens-cachan.fr

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covariance matrix Σ^{-1}, with its estimate $\widehat{\Sigma}^{-1}$ can also be important. The norm of the difference between the covariance matrix and its estimate could be used. One of the most famous matrix norms is the Frobenius norm. However, if the matrix coefficients are small, the norm of the difference can be small even if the matrices are very different. In order to avoid this problem, it is preferable to take a relative difference instead. However, the relative differencies can require other estimated quantities, such as the mean whose uncertainty can impact on the norm estimation. Therefore, another distance is proposed in this section: the Kullback-Leibler distance (also called the relative entropy) d_{KL}. It is defined on the basis of the distance between two probability density functions. More precisely,

$$d_{KL}(f,g) = \mathbb{E}_f\left(\log\left(\frac{f}{g}\right)\right), \tag{1}$$

where g and f are the two probability density functions to compare. This distance is not symmetric. Indeed, in most cases, $d_{KL}(f,g) \neq d_{KL}(g,f) = \mathbb{E}_g\left(\log\left(\frac{g}{f}\right)\right)$. Thus, in order to avoid confusion, the following versions

$$d_{KL1}(f,g) = d_{KL}(f,g) = \mathbb{E}_f\left(\log\left(\frac{f}{g}\right)\right), \tag{2}$$

$$d_{KL2}(g,f) = d_{KL}(g,f) = \mathbb{E}_g\left(\log\left(\frac{g}{f}\right)\right) \tag{3}$$

are used to clearly distinguish the two symmetric versions depending on the order of comparison. In the case of two Gaussian probability density functions $f = \mathcal{N}(\mu, \widehat{\Sigma})$ and $g = \mathcal{N}(\mu, \Sigma)$ with same mean μ, the previous formulas (Eqs. (2) and (3)) can be written as

$$d_{KL1}(\widehat{\Sigma}, \Sigma) = \mathrm{tr}(\widehat{\Sigma}\Sigma^{-1}) - \log(\det(\widehat{\Sigma}\Sigma^{-1})) - N, \tag{4}$$

$$d_{KL2}(\Sigma, \widehat{\Sigma}) = \mathrm{tr}(\widehat{\Sigma}^{-1}\Sigma) - \log(\det(\widehat{\Sigma}^{-1}\Sigma)) - N. \tag{5}$$

Thus, when $\widehat{\Sigma}$ is an estimation of Σ, the first version d_{KL1} is well adapted for covariance estimation assessment and the second version d_{KL2} is well adapted for assessment of its inverse. These two distances are positive, and when $\widehat{\Sigma} = \Sigma$ they are equal to zero. Obviously, the Kullback-Leibler distance can also be used to quantify the distance of some other covariance matrices (for example two estimations $\widehat{\Sigma}_1$ and $\widehat{\Sigma}_2$).

III. BOOTSTRAP ESTIMATION OF THE DISTANCE

As previously mentioned, the true covariance matrix Σ is unknown and therefore the computation of $d_{KL1}(\widehat{\Sigma}, \Sigma)$ and $d_{KL2}(\Sigma, \widehat{\Sigma})$ is not possible. Assuming that each evaluation is the realization of a N-dimensional centered Gaussian vector with covariance matrix Σ, it is known that the matrix $n\widehat{\Sigma}$ follows a Wishart law with mean Σ. The variance of $\widehat{\Sigma}$ can then be deduced from the the variance of the Wishart law. However, the Gaussian assumption is quite restrictive. The method proposed in this paper is based on a bootstrap approach and a plug-in estimator [11]. Indeed, this approach allows to overcome the fact that the true covariance matrix is unknown without assumptions on the distribution of the evaluations. In our study, n evaluations $(f_1^{\mathrm{eval}}, \ldots, f_n^{\mathrm{eval}})$ of the cross section, considered as n random vectors $(X_1, \ldots, X_n)$ following an unknown law of probability, F, are observed. The quantity of interest is a functional T of this law and, in our case, corresponds to the covariance matrix $T(F) = \Sigma$. From this observed sample, the law F can be approximated by $\hat{F}$ and then the functional $T(F) = \Sigma$ can be approximated by $T(\hat{F}) = \widehat{\Sigma}$, called the plugin estimator because the law F has been plugged in by $\hat{F}$. The bootstrap strategy consists in creating a new n-sample $(X_1^*, \ldots, X_n^*)$, called a bootstrap sample, according to the $\hat{F}$ law. From this bootstrap sample it is possible to compute an estimate $\widehat{\Sigma}^*$ of $\widehat{\Sigma}$ in the same way as $\widehat{\Sigma}$ from $(X_1, \ldots, X_n)$. In repeating this resampling B times, B bootstrap matrices are obtained and it is then possible to compute statistics on $\widehat{\Sigma}$, such as its mean, variance, bias and so on. In our case, the statistics of interest are the two versions of the Kullback-Leibler distance (Eqs. (4) and (5)). They are estimated, respectively, by

$$\widehat{d_{KL1}}(\widehat{\Sigma}, \Sigma) = \frac{1}{B}\sum_{b=1}^{B} d_{KL1}(\widehat{\Sigma}^{*b}, \widehat{\Sigma}) \tag{6}$$

and

$$\widehat{d_{KL2}}(\Sigma, \widehat{\Sigma}) = \frac{1}{B}\sum_{b=1}^{B} d_{KL2}(\widehat{\Sigma}, \widehat{\Sigma}^{*b}). \tag{7}$$

This strategy is justified by a general result from Bickel and Freedman [12]. Indeed they have shown that if $\sqrt{n}(T(\hat{F}) - T(F))$ converges in law to a law P then $\sqrt{n}(T(\hat{F}^*) - T(\hat{F}))$ converges in law to the same law. And in the particular case of the covariance matrix, Beran and Strivastava [13] have shown that, if $\hat{F}$ is the empirical cumulative distribution function, then $\sqrt{n}(\widehat{\Sigma} - \Sigma)$ converges in law to a centered Gaussian law and $\sqrt{n}(\widehat{\Sigma}^* - \widehat{\Sigma})$ converges in law to the same law.

IV. APPLICATION

In order to ensure the bootstrap allows a numerical comparison of the covariance estimation obtained with different methods, two methods have been used: the scoring and the brute Monte Carlo; and, concerning the comparison of the different assumptions, three assumptions have been used for the scoring approach.