Monte Carlo Method for the Estimates in a Model Calculation

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1. Introduction

Concerning the error propagation in a model calculation of cross sections, a group for discussing the Monte Carlo (MC) method was recently organized in the nuclear data community.[1] Even though there is a big, unresolved issue such that the covariance of model parameters are not well established, the MC method is regarded as a powerful tool in the evaluation of covariance of derived, *i.e.*, model-calculated, cross sections.

It is known that the most objective probability density function (pdf) of a quantity is the Gaussian if it can take a value in $[-\infty,+\infty]$ and only its mean and standard deviation are known. Being overwhelmed by this statement while neglecting the 'if' condition, very often it is assumed implicitly that a model-calculated quantity obeys the Gaussian distribution, too. However, it is recognized [Ref. 2 and its references] that such an assumption could cause a strange estimate as that in the so-called Peelle's Pertinent Puzzle (PPP). Then, a proper pdf, most likely non-Gaussian, for the derived quantity is requested for estimating the mean value and covariance of derived quantity.

The problem being addressed in this paper is as follows. We are given mean values and covariance of model parameters but the model is so complex that no analytical pdf for the derived quantity is available. Then, how do we construct the proper pdf or, rather directly, how do we get the estimates, *i.e.*, the mean value(s) and covariance, of the derived quantity? As an answer, the idea of MC estimation is presented below with a test application to the PPP.

2. Monte Carlo Estimation Algorithm

Suppose a model, $f(\mathbf{x})$, which is a function of m independent variables $\mathbf{x}$ (*i.e.*, model parameters) of which mean value vector is $\boldsymbol{\mu}$ and covariance matrix $\boldsymbol{\Sigma}$. Sampling N sets of $\mathbf{x}$ from a multivariate pdf, we have N values of f. The mean value of f and its variance V_f are computed simply as

$$\bar{f} = \sum_i^N f_i \Big/ N \,, \tag{1}$$

where $f_i = f(x_{1i}, x_{2i}, \ldots, x_{mi})$ calculated from the i-th set, and

$$V_f = \left(\sum_i^N f_i^2 \Big/ N\right) - \left(\sum_i^N f_i \Big/ N\right)^2 . \tag{2}$$

When we reasonably assume that the parameter vector $\mathbf{x}$ obeys the multivariate normal distribution

$$p(\mathbf{x}) = \frac{1}{(2\pi)^{\frac{m}{2}}\sqrt{|\boldsymbol{\Sigma}|}} \exp\left\{-\frac{1}{2}(\mathbf{x}-\boldsymbol{\mu})^t \boldsymbol{\Sigma}^{-1}(\mathbf{x}-\boldsymbol{\mu})\right\},$$

we can randomly sample $\mathbf{x}$ as follows.[3] At first, take m random samples, $r_1, r_2, \ldots, r_m$ from a normalized Gaussian $N(0,1)$ distribution. Then the random sample vector $\mathbf{x}$ is constructed from the vector $\mathbf{r}$ as

$$\mathbf{x} = \boldsymbol{\mu} + \mathbf{L}\,\mathbf{r}\,, \tag{3}$$

where $\mathbf{L}$ is the lower triangular matrix from the Cholesky decomposition of $\boldsymbol{\Sigma}$ such that $\boldsymbol{\Sigma} = \mathbf{L}\,\mathbf{L}^t$.

For other kinds of pdf's for the model parameters, a numerical method such as Gibbs sampling is available. When there is no information on the standard deviation of a parameter but the mean value, a uniform distribution is assumed as the pdf. However, it seems that a sampling method from a 'multivariate' (*i.e.* correlated) uniform distribution has not been established.

In case of a multi-dimensional derived quantity such as energy-dependent cross sections calculated by the optical model, the random sampling of the model parameters is same as the above while the scoring formulas are modified correspondingly. For example, the covariance between cross sections at E_j and E_k is computed as

$$Cov(\sigma_j, \sigma_k) = \left(\sum_i^N \sigma_{ij}\sigma_{ik} \Big/ N\right) - \left(\sum_i^N \sigma_{ij} \sum_i^N \sigma_{ik} \Big/ N^2\right) . \tag{4}$$

where $\sigma_{ij} = \sigma(E_j, x_{1i}, \ldots, x_{mi})$ is the cross section at E_j calculated with the i-th random sampled set of model parameters. Note that Eq. (4) is easily reduced to Eq. (2).

3. An Example: Pdf of a Function in Quotient Form

The PPP is an anomaly such that the estimate of a quantity, for which two correlated measurements are available, is below both values: The least-squares method estimate is 0.88±0.22 for the two measured data 1.0 and 1.5 with 10% statistical uncertainty each and 20% systematic uncertainty. Previous studies for resolving the puzzle will not be reviewed here, but a part of the puzzle is investigated below.

The problem simplified here is: what is the estimate of f,

$$f(a,c) = a/c?$$

The Bayesian method applied to the PPP[4] results in the posterior Gaussian pdf for a and c such that

$$p(a,c \mid a_0, \sigma_a, c_0, \sigma_c) \propto \exp\left\{-\frac{(a-a_0)^2}{2\sigma_a^2} - \frac{(c-c_0)^2}{2\sigma_c^2}\right\},$$

with values of $a_0 = 1.154 \pm 0.083$ and $c_0 = 1.0 \pm 0.2$.

With 10 million random pairs of a and c, the MC simulation resulted in a pdf of f that exactly overlaps the analytical pdf, which is found elsewhere.[5] Fig. 1 shows the pdf that is skewed towards a smaller x and is compared with the pdf causing the PPP, *i.e.* $N(0.88, 0.22^2)$.

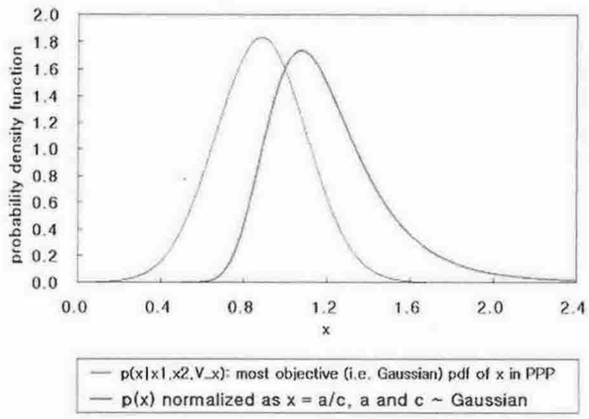

Fig. 1. Pdf's for the quantity under estimation in PPP

The estimate from the above pdf is compared in Table 1 with the estimates from some of resolutions for the PPP. The method utilizing the Box-Cox transformation is based on a recognition such that the measured data in PPP may not obey the Gaussian.[2] In addition to those in the table, there are four or more different solutions to PPP[4,6], but we are not going to review them all.

Table 1. Some of Solutions to Peelle's Pertinent Puzzle

Method	Estimate	Note
Least-Squares regression	0.882±0.218	original solution
Bayes' method	1.206±0.291	with $f = a/c$ model, estimated using MC
Law of error Propagation (first order)	1.154±0.245	with $f = a/c$ model
Using Box-Cox transformation	1.225±0.260	Ref. 2

It is stressed here that the pdf-weighted evaluation results in a significantly different estimate from that of the conventional, *i.e.*, the first order, law of error propagation, even with the same model ($f=a/c$). Recall that the 'estimate' includes not only the mean value but also the uncertainty (or covariance in multivariate cases). The MC method is used in such a numerical pdf-weighting, and it is a powerful tool for the mean value calculation as well as the assessment of the propagation of errors in model parameters to the error in the calculated mean value.

4. Summary and Concluding Remark

The points are summarized as follows:

- The pdf of a function of the model parameters that obey the Gaussian is not necessarily Gaussian,
- The estimation of the model-calculated values should be based on a proper (most likely non-Gaussian) pdf-weighting, and
- The MC method is a powerful tool for such a weighting computation.

These points may be neither new nor surprising, but often neglected in various fields. One of the examples is found in an evaluation of the U-235 fission cross sections. A recent evaluation[7] shows (preliminarily) 0.5% to 4% increases in the MeV region, and a part of such increases of up to 0.5% is achieved by eliminating the PPP effect in previous evaluation. Such elimination was achieved, in fact, not by the pdf-weighting. The important point here is that the new evaluation recognized a limited applicability of the conventional least-squares method that implicitly assumes the Gaussian distribution for the quantities under evaluation.

On the other hand, the method proposed would be applicable to a study on the source of a significant reduction of the uncertainties in the model-calculated cross sections.[5]

References

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