Generalized Bayesian Framework for Evaluation of Integral Benchmark Experiments[1]

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INTRODUCTION

A recently published generalized Bayesian optimization framework [1] has provided a way to retract any or all of the three common assumptions underlying the conventional Generalized Linear Least Squares (GLLS) optimization method based on the concepts introduced in Ref. [2]. These assumptions are:

1. **Perfection**: The model used for data evaluation and the prior probability distribution function (PDF) of generalized[*] data are *perfect*.

2. **Normality**: The prior and posterior PDF are *normal*.

3. **Linearity**: The model is *linear*.

In this work we outline how the framework in [1] could be directly adopted for improved evaluation of nuclear criticality integral benchmark experiments (IBEs) by:

1. Removing the first assumption alone by utilizing the concept of *imperfections* introduced in [1] to enable evaluation in the presence of discrepancies between the data and model or of missing covariance information by a GLLS method that will be seen as a generalization of the conventional GLLS method employed by the TSURFER code, and by

2. Removing the remaining two assumptions by implementing a Markov Chain Monte Carlo method for computation of the posterior PDF in the SAMPLER code,

where TSURFER[3, 4] and SAMPLER[5, 6] are the uncertainty quantification (UQ) codes for IBEs in the SCALE code system [7] based on the GLLS and the stochastic method, respectively. The graphic in Figure 1 categorizes the methods discussed in terms of the assumptions that they employ to determine posterior PDFs.

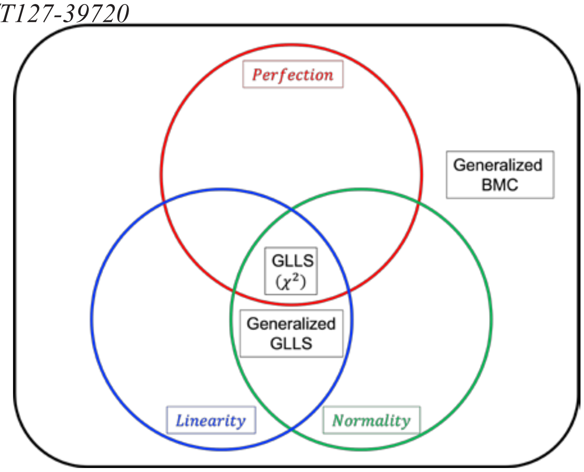

Fig. 1. A schematic representation of the three assumptions commonly employed in Bayesian evaluation methods. The generalized Bayesian evaluation framework enables removal of any one, two, or all, of the assumptions, depending on the nature of data and models being evaluated. An enforced assumption is represented by the interior of its respective circle, and its removal by the exterior. The methods or codes used have been indicated for those most relevant for IBEs.

GENERALIZED GLLS FORMALISM FOR IBES

For simplicity, the formalism derived in [1] is translated into a notation used in documentation of the TSURFER code [7]. This translation becomes particularly simple when the uncertainties and sensitivities are expressed in *absolute* terms, given by Eqs. (6.6.20-26) of [7], rather then in relative terms, given by Eqs. (6.6.14-19) of [7], where the former quantities are distinguished from the latter by a tilde symbol. Then the generalization of the TSURFER formalism enabled by [1] amounts to the removal of the first assumption while maintaining the remaining two. Formally, this amounts to relaxation of the strict constraints imposed by the TSURFER implementation of the χ^2 minimization method. These constraints are imposed on the *posterior*[†] expectation values of deviations between the calculated responses of IBEs, $\mathbf{k}'(\alpha')$[‡], and the IBEs measurements, $\mathbf{m}'$. The strict conventional choice of constraints (that enforces the assumption of perfect data and model) on the posterior expectation values of the deviations and their covariance matrix is

$$\tilde{\mathbf{d}}' \equiv \mathbf{k}'(\alpha') - \mathbf{m}' = \mathbf{0} \quad (1)$$

$$\tilde{\mathbf{C}}_{\mathbf{d}'\mathbf{d}'} = \mathbf{0}. \quad (2)$$

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[*]*Generalized* data is a union of model parameters and measured data; in the context of IBEs, the model is a neutron transport simulation, the model parameters are nuclear data cross sections, geometry or the isotopic composition of an IBE, and the measured data generally includes neutron multiplication numbers.

[†]Posterior expectation values are denoted by the prime symbol.

[‡]The posterior expectation value of cross sections, α', is conventionally referred to as the "adjusted" expectation value in the TSURFER nomenclature.

Evaluators may choose nonzero values for these constraints to convey their expert judgment of imperfections inherent to an evaluation. Setting a nonzero constraint on $\tilde{\mathbf{d}}'$ is expected to be useful to accommodate finite average deviations among the data or model calculations. Setting a nonzero constraint on matrix elements of $\tilde{\mathbf{C}}'_{\mathbf{dd}}$ is expected to be useful to accommodate statistical fluctuations of the same discrepancies around their mean values. The full power of the generalized method could be utilized by judiciously selecting both sets of values. This method, in contrast to the entrenched method of adjusting the posterior expectation values and covariances before or after application of Bayes' theorem, remains completely consistent with Bayes' theorem because the imperfections have now been made an integral part of the Bayesian evaluation.

An IBE evaluator could impose judiciously selected nonzero constraints on posterior expectation values of deviations as a way to estimate the effect of any large *discrepancies* between an IBE simulation and measurement. Similarly, nonzero values for the constraints on the corresponding covariance matrix could be used to mitigate the unreasonably small posterior uncertainties caused by unaccounted covariance among IBE data.

The formal solution of the generalized GLLS becomes particularly simple to state in a generalized data notation, that, in the TSURFER notation for IBEs, may be defined as

$$\mathbf{z} \equiv \begin{pmatrix} \boldsymbol{\alpha} \\ \mathbf{m} \end{pmatrix}, \tag{3}$$

whose covariance matrix, $\tilde{\mathbf{C}}_{\mathbf{zz}}$, is a 2×2 block matrix,

$$\tilde{\mathbf{C}}_{\mathbf{zz}} = \begin{pmatrix} \tilde{\mathbf{C}}_{\alpha\alpha} & \tilde{\mathbf{C}}_{\alpha\mathbf{m}} \\ \tilde{\mathbf{C}}_{\mathbf{m}\alpha} & \tilde{\mathbf{C}}_{\mathbf{mm}} \end{pmatrix}. \tag{4}$$

A generalized sensitivity matrix in the context of IBEs is

$$\tilde{\mathcal{S}} \equiv \nabla_{\mathbf{z}} \tilde{\mathbf{d}}^{\intercal} = \begin{pmatrix} \nabla_\alpha \\ \nabla_{\mathbf{m}} \end{pmatrix} (\mathbf{k}(\boldsymbol{\alpha}) - \mathbf{m})^{\intercal} = \begin{pmatrix} \nabla_\alpha \mathbf{k}(\boldsymbol{\alpha})^{\intercal} \\ -\nabla_{\mathbf{m}} \mathbf{m}^{\intercal} \end{pmatrix} = \begin{pmatrix} \tilde{\mathbf{S}}^{\intercal}_{\mathbf{k}\alpha} \\ -\mathbb{1} \end{pmatrix}, \tag{5}$$

where $\tilde{\mathbf{S}}_{\mathbf{k}\alpha}$ is the sensitivity matrix given in TSURFER notation, and where the tilde symbols indicates that all quantities are given in absolute rather than relative terms.

The notation defined above enables a compact generalization of the expression for the posterior covariance matrix,

$$\tilde{\mathbf{C}}^{-1}_{\mathbf{z}'\mathbf{z}'} = \tilde{\mathcal{S}}[\tilde{\mathbf{C}}^{-1}_{\mathbf{d}'\mathbf{d}'} - \tilde{\mathbf{C}}^{-1}_{\mathbf{dd}}]\tilde{\mathcal{S}}^{\intercal} + \tilde{\mathbf{C}}^{-1}_{\mathbf{zz}}. \tag{6}$$

and the posterior expectation values of generalized data,

$$\mathbf{z}' = \mathbf{z} + \tilde{\mathbf{C}}_{\mathbf{zz}} \tilde{\mathcal{S}} \tilde{\mathbf{C}}^{-1}_{\mathbf{dd}} (\tilde{\mathbf{d}}' - \tilde{\mathbf{d}}). \tag{7}$$

The details of the derivation are relegated to the Appendix.

GENERALIZED BAYESIAN MC FOR IBE'S

In this section we outline the most general form of the Bayesian framework in which all three assumptions enumerated in the Introduction are removed. Unlike for normal PDFs and linear models of the previous section, the prior and posterior expectation values of any quantity must now be explicitly denoted using angular brackets. For example, $\langle \mathbf{z} \rangle$ and $\langle \mathbf{z} \rangle'$ represent the prior and posterior expectation values of generalized data, respectively, and are to be computed as expectation values using the respective prior and posterior PDF. A generalized Bayesian posterior PDF found in [1] is translated into the TSURFER notation as

$$\begin{aligned} p'(\mathbf{z}|\langle\tilde{\mathbf{d}}\rangle', \tilde{\mathbf{C}}_{\mathbf{d}'\mathbf{d}'}, \langle\mathbf{z}\rangle, \tilde{\mathbf{C}}_{\mathbf{zz}}) \quad \propto \quad & \mathcal{L}(\langle\tilde{\mathbf{d}}\rangle', \tilde{\mathbf{C}}_{\mathbf{d}'\mathbf{d}'}|\mathbf{z}, \langle\mathbf{z}\rangle, \tilde{\mathbf{C}}_{\mathbf{zz}}) \\ & \times \; p(\mathbf{z}|\langle\mathbf{z}\rangle, \tilde{\mathbf{C}}_{\mathbf{zz}}), \end{aligned} \tag{8}$$

where the likelihood function is found to be of exponential form [8], namely,

$$\mathcal{L}(\langle\tilde{\mathbf{d}}\rangle', \tilde{\mathbf{C}}_{\mathbf{d}'\mathbf{d}'}|\mathbf{z}, \langle\mathbf{z}\rangle, \tilde{\mathbf{C}}_{\mathbf{zz}}) = e^{-\frac{1}{2}(\tilde{\mathbf{d}}-\boldsymbol{\lambda})^{\intercal}\boldsymbol{\Lambda}^{-1}(\tilde{\mathbf{d}}-\boldsymbol{\lambda})}, \tag{9}$$

and where $p(\mathbf{z}|\langle\mathbf{z}\rangle, \tilde{\mathbf{C}}_{\mathbf{zz}})$ is a prior PDF of generalized data. The prior PDF, in practice, is approximated by a normal PDF defined by prior expectation values, $\langle\mathbf{z}\rangle$, and the prior covariance matrix, $\tilde{\mathbf{C}}_{\mathbf{zz}}$, as

$$p(\mathbf{z}|\langle\mathbf{z}\rangle, \tilde{\mathbf{C}}_{\mathbf{zz}}) = e^{-\frac{1}{2}(\mathbf{z}-\langle\mathbf{z}\rangle)^{\intercal}\tilde{\mathbf{C}}^{-1}_{\mathbf{zz}}(\mathbf{z}-\langle\mathbf{z}\rangle)}. \tag{10}$$

An iterative algorithm for computing $\boldsymbol{\lambda}$ and $\boldsymbol{\Lambda}$ given the constraints imposed on posterior expectation values, $\langle\tilde{\mathbf{d}}\rangle'$ and $\tilde{\mathbf{C}}_{\mathbf{d}'\mathbf{d}'}$, has been derived in [1]. With the values of $\boldsymbol{\lambda}$ and $\boldsymbol{\Lambda}$ thus determined, the posterior PDF above could be computed using a Markov Chain Monte Carlo (MC) method, *e.g.*, a well known Metropolis-Hastings MC (MHMC) algorithm [9, 10]. This form of the posterior PDF of generalized data turns out to be more efficient for MHMC computation than the conventional posterior PDF of model parameters given by Eq. (19) because the extremely small probabilities computed by the latter make the MHMC acceptance rate too low to yield the posterior PDF when using the prior PDF of model parameters for random sampling. In contrast, using the prior PDF of generalized data in Eq. (10) for sampling is guaranteed to yield probabilities optimal for MHMC thanks to the central limit theorem. The superiority of the posterior PDF in Eq. (8) was demonstrated in [1] by using it to compute the conventional posterior PDF in Eq. (19) with the MHMC method by iteratively halving $\boldsymbol{\Lambda}$ until the Eq. (19) was reached; a feat that could not be achieved by sampling Eq. (19) outright.

Since the posterior PDF is known to be not normal for nonlinear models, the posterior PDF should be computed by the MHMC method. A comparison to the solution computed by the TSURFER code would then reveal the effect of approximating the posterior PDF by a normal one. The SAMPLER code provides a good foundation for implementing the MHMC method and thus removing all three of the assumptions (listed in the Introduction; see Figure 1) that underlie the GLLS method.

An abbreviated description of the MHMC method implemented in Ref. [1] will make the connection to use in SAMPLER more clear; Algorithm 1 describes the computational instructions. It should be noted that the probability distribution $g(z'|z_i)$ is arbitrarily chosen in the general MHMC algorithm, but in the implementation given in [1] it is a distribution closely resembling the prior PDF. Sampler (as a simplified description) is already carrying out the bulk of these instructions: it iterates for a finite number of iterations N, it draws samples from the prior PDF (analogous to line 5), and

Algorithm 1 Metropolis–Hastings Algorithm

```
1:  N ← iterations
2:  i ← 0
3:  z_0 ← arbitrary values          ▷ z_i is of arbitrary dimension
4:  while i < (N + 1) do
5:      Draw random z' from g(z'|z_i)
6:      p(z') = e^{-1/2 X^2(z')}
7:      A = min(1, [p(z')/p(z_i)] [g(z_i|z')/g(z'|z_i)])
8:      Draw random u from uniform distribution U(0, 1)
9:      if u < A then
10:         z_{i+1} ← z'
11:     else
12:         z_{i+1} ← z_i
13:     i ← i + 1
```

it calculates the theoretical model needed to compute $p(z')$ (necessary for line 6). To implement Generalized Bayesian MC (BMC) in Sampler, the only changes required would be to: provide new input instructions to specify $\langle\tilde{\mathbf{d}}\rangle'$ and $\tilde{\mathbf{C}}_{\mathbf{d}'\mathbf{d}'}$, compute the cost function $X^2(z')$ (see Appendix, Eq. 12) and posterior probability $p(z')$, and store the posterior values of z_i that make up the full posterior PDF.

In terms of the three assumptions shown in Fig. 1, the BMC method would remove the assumptions of PDF normality and model linearity by directly sampling the prior PDF and building a posterior PDF by iteratively applying a cost function in a Markov-Chain MC algorithm. To remove the assumption of perfection in the model and prior, the new cost function $X^2(z)$ is applied.

CONCLUSIONS

A suggested adoption of the generalized Bayesian framework developed in [1] and the advantages it may offer for evaluation and uncertainty quantification of integral benchmark experiments (IBEs) were explored by formally translating the general formalism of [1] into a specialized mathematical notation used by the IBE evaluation community. It is hoped that a familiar notation would make apparent the potential of the generalized formalism to improve the extant IBE evaluation methods.

In particular, a generalization of the GLLS formalism implemented in the TSURFER code for analysis of IBEs was expressed in a compact but powerful form using a generalized data notation. Finally, the generalized formalism was shown to be relevant to the stochastic sampling code SAMPLER that already provides a sound foundation for developing the most general form of the Bayesian framework developed in [1]. Although the original motivation for developing the Bayesian framework [1] was to address issues[§] affecting the nuclear data evaluation field [11], this framework is sufficiently general to address the same issues in the field of IBE evaluations. The framework's flexibility stems from recognizing the three generic assumptions[¶] commonly made in any Bayesian data evaluation, regardless of the nature of the data or the model used for evaluation, namely: 1) the perfection (of data and model), 2) normal form of PDFs, and 3) linear models. The general Bayesian framework of [1] provides a way to undo any or all of the three assumptions. In particular, the assumption of perfection alone was rolled back to generalize the GLLS formalism of the TSURFER code, and all three assumptions were undone for the Bayesian MHMC suggested for the SAMPLER code.

By removing assumptions traditionally used in Bayesian analysis of nuclear data more realistic posterior PDFs of nuclear data can be calculated. Simply by defining a new cost function, we can remove the inherent assumption in traditional GLLS that prior model and data PDFs are perfect. Further, we can remove the other inherent assumptions in GLLS of linearity and normality by employing MC algorithms. We can also selectively choose some of these assumptions based on validity, which can be determined by comparison to optimization with the full Bayesian Monte Carlo method, which removes all three of the assumptions made by GLLS. With more realistic distributions of nuclear data we can better estimate uncertainty in the behavior of systems of nuclear criticality.

APPENDIX: GENERALIZED COST FUNCTION

The exponents of the likelihood function in Eq. (9) and the prior (normal) PDF in Eq. (10) are combined to render the posterior PDF given by Eq. (8) as

$$p'(\mathbf{z}|\langle\tilde{\mathbf{d}}\rangle', \tilde{\mathbf{C}}_{\mathbf{d}'\mathbf{d}'}, \langle\mathbf{z}\rangle, \tilde{\mathbf{C}}_{\mathbf{zz}}) \propto e^{-\frac{1}{2}X^2(\mathbf{z})} \qquad (11)$$

where $X^2(\mathbf{z})$ is a generalized data cost function,

$$X^2(\mathbf{z}) \equiv (\tilde{\mathbf{d}} - \lambda)^\intercal \mathbf{\Lambda}^{-1}(\tilde{\mathbf{d}} - \lambda) + (\mathbf{z} - \langle\mathbf{z}\rangle)^\intercal \tilde{\mathbf{C}}_{\mathbf{zz}}^{-1}(\mathbf{z} - \langle\mathbf{z}\rangle), \qquad (12)$$

and where λ and $\mathbf{\Lambda}$ are the Lagrange multipliers that are determined from the constraints imposed on the posterior expectation values $\langle\tilde{\mathbf{d}}\rangle'$ and $\tilde{\mathbf{C}}_{\mathbf{d}'\mathbf{d}'}$ computed by the posterior PDF in Eq. (11). For normal PDFs and linear models they are:

$$\mathbf{\Lambda}^{-1} = \tilde{\mathbf{C}}_{\mathbf{d}'\mathbf{d}'}^{-1} - \tilde{\mathbf{C}}_{\mathbf{dd}}^{-1}, \qquad (13)$$

$$\mathbf{\Lambda}^{-1}\lambda = \tilde{\mathbf{C}}_{\mathbf{d}'\mathbf{d}'}^{-1}\langle\tilde{\mathbf{d}}\rangle' - \tilde{\mathbf{C}}_{\mathbf{dd}}^{-1}\langle\tilde{\mathbf{d}}\rangle. \qquad (14)$$

The cost function in Eq. (12) for normal PDFs can be expanded around its minimum as:

$$X^2(\mathbf{z}) = X^2(\langle\mathbf{z}\rangle') + (\mathbf{z} - \langle\mathbf{z}\rangle')^\intercal \tilde{\mathbf{C}}_{\mathbf{z}'\mathbf{z}'}^{-1}(\mathbf{z} - \langle\mathbf{z}\rangle') \qquad (15)$$

where

$$X^2(\langle\mathbf{z}\rangle') = (\langle\tilde{\mathbf{d}}\rangle - \langle\tilde{\mathbf{d}}\rangle')^\intercal \frac{1}{\tilde{\mathbf{C}}_{\mathbf{dd}} - \tilde{\mathbf{C}}_{\mathbf{d}'\mathbf{d}'}}(\langle\tilde{\mathbf{d}}\rangle - \langle\tilde{\mathbf{d}}\rangle') \qquad (16)$$

is the value of the cost function at its minimum[‖],

$$\tilde{\mathbf{C}}_{\mathbf{z}'\mathbf{z}'}^{-1} = \tilde{\mathcal{S}}\mathbf{\Lambda}^{-1}\tilde{\mathcal{S}}^\intercal + \tilde{\mathbf{C}}_{\mathbf{zz}}^{-1} \qquad (17)$$

[§]For example, discrepant data sets or models and the absence of data covariance information leading to unrealistically small evaluated uncertainties.

[¶]Any assumptions that may not be met would lead to potentially unrecognized errors.

[‖]This expression may be seen as a generalization of the minimum value of the conventional cost function that is recovered by setting $\langle\mathbf{d}\rangle' = 0$ and $\tilde{\mathbf{C}}_{\mathbf{d}'\mathbf{d}'} = \mathbb{0}$; for example, see Eq. (6.6.36) of the TSURFER code documentation [7].

is the posterior covariance matrix of generalized data, $\mathbf{z}$, and $\mathbf{\Lambda}$ and $\tilde{\mathcal{S}}$ are given by Eqs. (13) and (5), respectively. Inserting the expression for $\mathbf{\Lambda}$ from Eq. (13) into Eq. (17) yields the posterior generalized covariance matrix stated in Eq. (6). The expression for posterior expectation values of generalized data, $\langle\mathbf{z}\rangle'$, taken from [1] is

$$\langle\mathbf{z}\rangle' = \langle\mathbf{z}\rangle + \tilde{\mathbf{C}}_{\mathbf{zz}}\tilde{\mathcal{S}}\tilde{\mathbf{C}}_{\mathbf{dd}}^{-1}(\langle\tilde{\mathbf{d}}\rangle' - \langle\tilde{\mathbf{d}}\rangle), \tag{18}$$

where angular brackets explicitly denote expectation values. Eq. (7) is obtained by replacing $\langle\tilde{\mathbf{z}}\rangle', \langle\tilde{\mathbf{z}}\rangle, \langle\tilde{\mathbf{d}}\rangle', \langle\tilde{\mathbf{d}}\rangle$ in Eq. (18) by $\tilde{\mathbf{z}}', \tilde{\mathbf{z}}, \tilde{\mathbf{d}}', \tilde{\mathbf{d}}$, respectively.

The conventional GLLS solution is recovered for $\langle\tilde{\mathbf{d}}\rangle' = \mathbf{0}$ and $\tilde{\mathbf{C}}_{\mathbf{d}'\mathbf{d}'} = \mathbf{0}$, for which $\lambda = \mathbf{0}$ and $\mathbf{\Lambda} \to \mathbf{0}$, that is, the likelihood function in Eq. (9) becomes $\delta_{\text{Dirac}}(\mathbf{k}(\alpha) - \mathbf{m})$. Data $\mathbf{m}$ could then be marginalized by integrating them out of the posterior PDF to yield a posterior PDF of model parameters, $\boldsymbol{\alpha}$, alone:

$$\begin{aligned} p'\Big(\alpha|\langle\tilde{\mathbf{d}}\rangle' = \mathbf{0}, \tilde{\mathbf{C}}_{\mathbf{d}'\mathbf{d}'} = \mathbf{0}, \langle\mathbf{z}\rangle, \tilde{\mathbf{C}}_{\mathbf{zz}}\Big) \\ \propto p((\mathbf{z}|_{\mathbf{m}=\mathbf{k}(\alpha)})|\langle\mathbf{z}\rangle, \tilde{\mathbf{C}}_{\mathbf{zz}}) \\ \propto e^{-\frac{1}{2}\chi^2(\alpha)} \end{aligned} \tag{19}$$

where

$$\chi^2(\boldsymbol{\alpha}) = (\mathbf{z}|_{\mathbf{m}=\mathbf{k}(\alpha)} - \langle\mathbf{z}\rangle)^\intercal \tilde{\mathbf{C}}_{\mathbf{zz}}^{-1}(\mathbf{z}|_{\mathbf{m}=\mathbf{k}(\alpha)} - \langle\mathbf{z}\rangle) \tag{20}$$

is a conventional cost function, and

$$\mathbf{z}|_{\mathbf{m}=\mathbf{k}(\alpha)} \equiv \begin{pmatrix} \boldsymbol{\alpha} \\ \mathbf{k}(\boldsymbol{\alpha}) \end{pmatrix}. \tag{21}$$

Finally, the form of the cost function minimized by the TSURFER formalism, and the solution thereof, is recovered for $\tilde{\mathbf{C}}_{\mathbf{m}\alpha} = \mathbf{0}$ in Eq. (4).

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