Appendix

Brief descriptions are offered to provide the fundamentals of two standard methods, i.e., the parametric and nonparametric, and two S/U-based advanced methods, i.e., Whisper and GLLSM.

Parametric and nonparametric methods

If either the calculated or the collected responses have a shape of Gaussian PDF, the first considerable consolidation method is the parametric/non-parametric methods. Consider conducting N experiments, each with a different gradient vector, and assume the application gradient is not included in the analysis. Each experiment records a measured value of m_i, a corresponding calculated value of k_i, and their evaluation uncertainty σ_{e_i}, which is the sum of two uncertainty sources, i.e., the Monte-Carlo uncertainty and benchmark uncertainty in Figure 1. Let the bias[1] be given as $\beta_i = k_i - m_i$. Thus, each experiment defines its own PDF of expected deviations between measured and predicted values, defined as a normal distribution with the mean value β_i, denoted as the experimental bias, and uncertainty is given by the standard deviation σ_{e_i}, which leads to the parametric bias, written as:

$$\beta_p = \bar{k} - \bar{m} \tag{10}$$

where

$$\bar{k} = \sum_{i=1}^{N} \left(\frac{k_i}{\sigma_{e_i}^2} \right) / \sum_{i=1}^{N} \left(\frac{1}{\sigma_{e_i}^2} \right)$$

$$\bar{m} = \sum_{i=1}^{N} \left(\frac{m_i}{\sigma_{e_i}^2} \right) / \sum_{i=1}^{N} \left(\frac{1}{\sigma_{e_i}^2} \right)$$

while the non-parametric approach takes the minimum experimental bias, i.e., the worst case, as the application bias β_{np} such as:

$$\beta_{np} = \min\{k_i - m_i\} \tag{11}$$

And the pooled variance σ_p^2, that employs the concept of inverse-variance weighting, is defined as the sum of the weighted bias variance s^2 which explains the spread of experimental biases, and the arithmetic average of the evaluation variances $\bar{\sigma}^2$ such as

$$\sigma_p^2 = s^2 + \bar{\sigma}^2 \tag{12}$$

where

$$s^2 = \frac{N}{N-1} \sum_{i=1}^{N} \left(\frac{\beta_i - \beta_p}{\sigma_{e_i}} \right)^2 / \sum_{i=1}^{N} \left(\frac{1}{\sigma_{e_i}^2} \right) \tag{1}$$

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[1] In some renditions, the bias is standardized by the measured or calculated value; this subtlety however is discarded here as it does not add much value to the discussion.

$$\bar{\sigma}^2 = N\left(\sum_{i=1}^{N}\left(\frac{1}{\sigma_{\bar{e}_i}^2}\right)\right)^{-1} \tag{14}$$

Therefore, the pooled variance can be interpreted as the combined effect of two statistical properties, one is the inverse-variance weighted mean, i.e., the weighted average, and the other is the variance of the means, i.e., the weighted spread of the experimental biases. Finally, the posterior application distributions for the parametric and non-parametric methods can be statistically written as:

$$\mathcal{N}\left(k_{app} - \beta_p, \sigma_p\right) \text{ for the parametric method} \tag{15}$$

$$\mathcal{N}\left(k_{app} - \beta_{np}, \sigma_p\right) \text{ for the non-parametric method} \tag{16}$$

Whisper

Los Alamos National Laboratory researchers have developed the Whisper method. It is claimed to have the following two main characteristics: a) it employs the EV theorem to determine the posterior application distribution; and b) it employs similarity c_k leveraged by a heuristic formula for weighting to reduce the number of samples generated from low-relevance experiments in an attempt to reduce their impact.

Whisper requires to pre-calculate similarity values $c_{k,i}$ for each experiment for its weight estimation. The first step is to calculate the required weight by the selected function that is:

$$w_{req} = w_{min} + w_{penalty}\left(1 - c_{k,max}\right) \tag{17}$$

where w_{min} and $w_{penalty}$ are heuristic constants that are set to be 25 and 100 for this analysis, respectively, and $c_{k,max}$ is the maximum c_k value of the selected benchmark experiments. The sum of individual weight factors w_i should be the same as the required weight w_{req} calculated in Eq. (17), such as:

$$w_{req} = \sum_i w_i \tag{18}$$

and the individual weight factors also satisfy the following linear relation with an appropriately selected acceptance c_k, $c_{k,acc}$, such that

$$w_i = \max\left\{0, \frac{c_{k,i} - c_{k,acc}}{c_{k,max} - c_{k,acc}}\right\} \tag{19}$$

In case of that, the number of similar benchmarks in the selected set is too few so that the criterion (18) cannot be met, Whisper offers an additional interpolation recipe. To focus on the net effect of its weighting scheme, this interpolation technique is not applied, instead acceptance c_k is set to be zero to maximize the required weight w_{req}, if Eq. (18) does not meet.

Next, generate K samples from each experimental bias PDF with a mean of the bias β_i and the standard deviation of the evaluation uncertainty σ_{e_i} given weight w_i. The PDF and CDF that the samples are to be drawn from can be written analytically such as:

$$f_i(x) = \begin{cases} 1 - w_i & , \quad x = -\infty \\ \dfrac{w_i}{\sqrt{2\pi\sigma_{e_i}^2}} e^{-\frac{1}{2}\left(\frac{x+\beta_i}{\sigma_{e_i}}\right)^2} & , \quad \text{otherwise} \end{cases} \tag{20}$$

$$F_i(x) = (1 - w_i) + \frac{w_i}{2}\left[1 + \text{erf}\left(\frac{x + \beta_i}{\sqrt{2\sigma_{e_i}^2}}\right)\right] \tag{21}$$

Eq. (20) and (21) imply that the samples are taken in proportion w_i and the samples corresponding the other proportion $1 - w_i$ are set to be negative infinity. For example, with unit weight, i.e., a perfect relevant experiment, all samples are generated from the original bias PDF. Conversely, a zero value of the weight, i.e., an irrelevant experiment, implies that all samples are negative infinity, hence allowing the analyst to remove the impact of that irrelevant experiment on the Whisper validation analysis. An example of the K samples for the N selected experiments can be presented in a matrix form such that:

$$X = \begin{bmatrix} X_1^{(1)} & X_1^{(2)} & \cdots & X_1^{(K)} \\ X_2^{(1)} & X_2^{(2)} & \cdots & X_2^{(K)} \\ \vdots & \vdots & \ddots & \vdots \\ X_N^{(1)} & X_N^{(2)} & \cdots & X_N^{(K)} \end{bmatrix}$$

Once the samples have been generated according to their weights, Whisper takes the maximum values of each column of X matrix.

$$Y = \left[\max\left\{X_1^{(1)}, \dots, X_N^{(1)}\right\} \quad \max\left\{X_1^{(2)}, \dots, X_N^{(2)}\right\} \quad \cdots \quad \max\left\{X_1^{(K)}, \dots, X_N^{(K)}\right\}\right] \tag{22}$$

An analytical form of the maximum values Y in (22) is unknown, however, it can be approximated by the histogram with enough samples, roughly more than 10,000 samples are recommended.

If the experimental PDF/CDF are all the same and the weights are unity, the EV CDF $F(x)$ is the product of the individual experimental CDFs $F_i(x)$

$$F(x) = \prod_{i=1}^{N} F_i(x)$$

and the corresponding PDF is

$$f(x) = F(x) \sum_{i=1}^{N} \frac{f_i(x)}{F_i(x)}$$

As a result of this process, the mass of the EV PDF is towards the right, when a larger number of experiments are involved as shown in Figure 14.

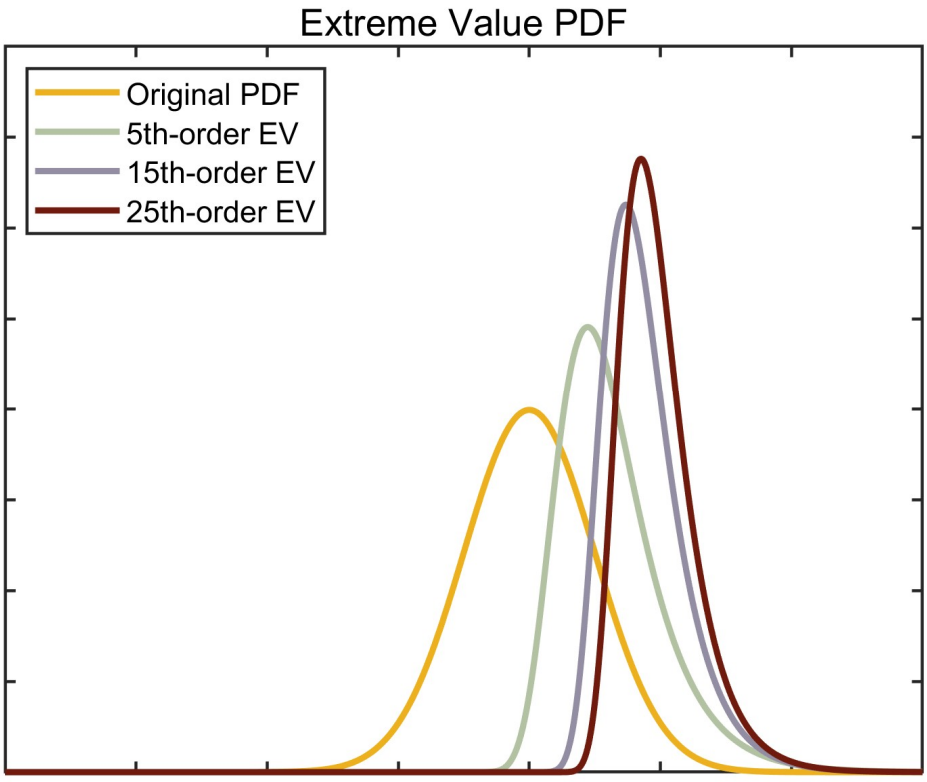

Figure 14. Change in maximum value PDF with an increasing number of experiments

The Whisper weighting scheme introduced through (17) to (19) constraints a maximum threshold on the weights to ensure that the EV PDF does not toward the right indefinitely with an increasing number of experiments.

Standard GLLSM

The standard GLLSM differs from the other three methods, as it quantifies the uncertainty in the calculated responses of each experiment and provides a mathematically justifiable uncertainty reduction procedure. It allows the analyst to take credit for the uncertainty reduction by solving a mathematical minimization problem to find optimal adjustments for the cross-sections and to present the results as a conditional probability based on the Bayesian Theorem.

Let the covariance matrix for the calculated and measured responses be $\mathbf{C_k}$ and $\mathbf{C_m}$, respectively. If adjoint capabilities are available, i.e., sensitivity profiles are applicable, the covariance matrix for the calculated responses can be obtained by the so-called sandwich rule such as

$$\mathbf{C_k} = \mathbf{S}\mathbf{C_\alpha}\mathbf{S^T}$$

where $\mathbf{S}$ is an aggregated form of the sensitivity profiles of the selected experiments and the application introduced in Section 2.2, i.e., $\mathbf{S} = [s_1 \quad s_2 \quad \cdots \quad s_{N+1}]^T \in \mathbb{R}^{(N+1)\times n}$ whose last row vector is the sensitivity profile for the application, and $\mathbf{C_\alpha} \in \mathbb{R}^{n\times n}$ is nuclear data prior covariance.

If adjoint capabilities are not readily available, the analyst may consult with a non-intrusive approach to estimate the covariance matrix for calculated responses [29].

GLLSM solves a minimization problem in which the objective function subject to the constraint $k'(\alpha') = m'$, which can also be represented by χ^2 with N degree of freedom, such as

$$\chi_N^2(\alpha') = [k' - k]^T \mathbf{C_k^{-1}} [k' - k] + [m' - m]^T \mathbf{C_m^{-1}} [m' - m] \tag{23}$$

where k is a prior calculated k_{eff} vector, k' is an adjusted, i.e., posterior, k_{eff} vector, and m is a measurement k_{eff} vector.

The minimizer of this objective function above may be given by

$$\Delta k = -\mathbf{C_k}(\mathbf{C_k} + \mathbf{C_m})^{-1} d \tag{24}$$

where $\Delta k = k' - k$, and d is the discrepancy vector, $d = k - m$.

The posterior covariance matrix for the k_{eff} is given by

$$\mathbf{C_{k'}} = \mathbf{C_k} - \mathbf{C_k}(\mathbf{C_k} + \mathbf{C_m})^{-1} \mathbf{C_k} \tag{25}$$

The diagonal elements of this matrix represent the adjusted uncertainty in k_{eff}. The application bias and the posterior uncertainty can be found as the last element of Eq. (24) and (25), respectively.

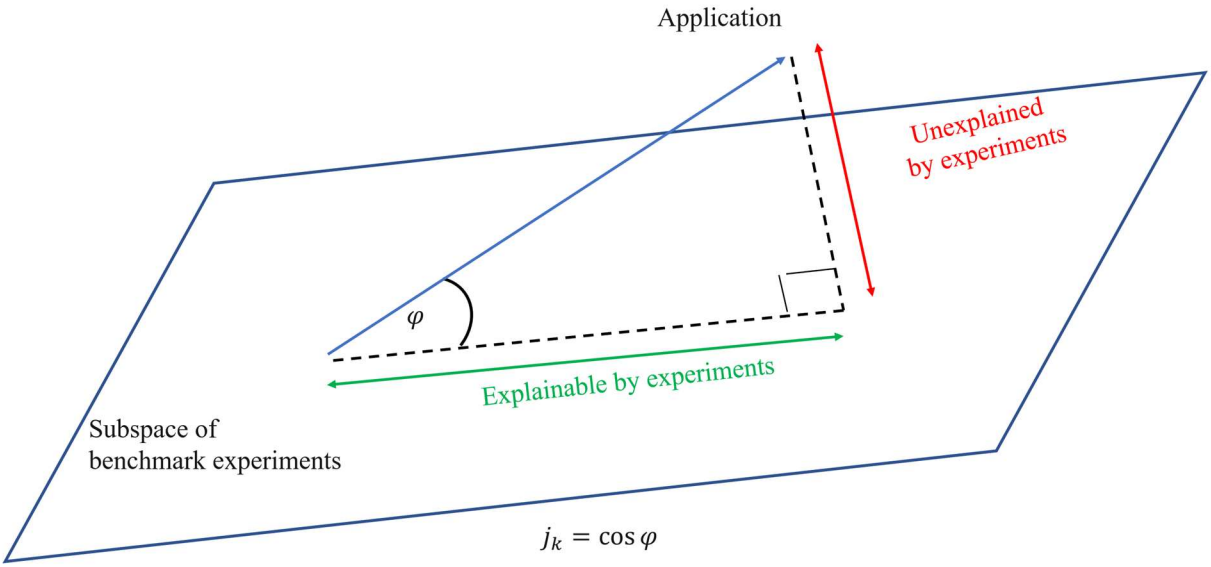

Figure 15. Graphical interpretation of GLLSM procedure

As earlier presented in Section 2.3, the uncertainty reduction of the GLLSM process is related to the relevance index j_k in that the square sum of the uncertainty reduction ratio and j_k value is always unity. The GLLSM procedure that maps biases from experimental to application conditions can be graphically interpreted by distinguishing the application conditions in terms of the explainable and unexplainable parts by the selected experiments as shown in Figure 15.

j_k relevance index

Although it is well summarized in already published papers, this section briefly outlines a more efficient method for calculating c_k similarity and j_k relevance. It should be noted that in the referenced papers, c_k refers to similarity, while relevance is denoted as the j_k index.

For the calculation of the c_k indices, all coefficients can be computed at once from the calculated response covariance matrix $\mathbf{C_k}$, which includes both experiments and applications. Initially, sensitivity profiles of experiments and applications $\mathbf{S}$, along with the covariance matrix of nuclear data $\mathbf{C_\alpha}$, are collected. Subsequently, the calculated response covariance matrix for experiments and applications can be computed using the sandwich equation such as:

$$\mathbf{C_k} = \mathbf{S}\mathbf{C_\alpha}\mathbf{S^T}$$

where $\mathbf{S}$ is an aggregated form of the sensitivity profiles of the selected experiments and the application.

Consider our $\mathbf{C_k}$ is a form of:

$$\mathbf{C_k} = \begin{bmatrix} \sigma_{c_1}^2 & \rho_{c_{1,2}}\sigma_{c_1}\sigma_{c_2} & \cdots & \rho_{c_{1,m}}\sigma_{c_1}\sigma_{c_m} & \rho_{c_{1,app}}\sigma_{c_1}\sigma_{c_{app}} \\ \rho_{c_{1,2}}\sigma_{c_1}\sigma_{c_2} & \sigma_{c_2}^2 & \cdots & \rho_{c_{2,m}}\sigma_{c_2}\sigma_{c_m} & \rho_{c_{2,app}}\sigma_{c_2}\sigma_{c_{app}} \\ \vdots & \vdots & \ddots & \vdots & \vdots \\ \rho_{c_{1,m}}\sigma_{c_1}\sigma_{c_m} & \rho_{c_{2,m}}\sigma_{c_2}\sigma_{c_m} & \cdots & \sigma_{c_m}^2 & \rho_{c_{m,app}}\sigma_{c_m}\sigma_{c_{app}} \\ \rho_{c_{1,app}}\sigma_{c_1}\sigma_{c_{app}} & \rho_{c_{2,app}}\sigma_{c_2}\sigma_{c_{app}} & \cdots & \rho_{c_{m,app}}\sigma_{c_m}\sigma_{c_{ap}} & \sigma_{c_{app}}^2 \end{bmatrix}$$

Take its diagonal elements and square-root of it:

$$\mathbf{\Sigma_c} = \mathrm{diag}([\sigma_{c_1} \quad \sigma_{c_2} \quad \cdots \quad \sigma_{c_m} \quad \sigma_{c_{app}}])$$

Finally, the normalized calculated response covariance matrix becomes:

$$\mathbf{R_c} = \mathbf{\Sigma_c^{-1}}\mathbf{C_k}\mathbf{\Sigma_c^{-1}} = \begin{bmatrix} 1 & \rho_{c_{1,2}} & \cdots & \rho_{c_{1,m}} & \rho_{c_{1,app}} \\ \rho_{c_{1,2}} & 1 & \cdots & \rho_{c_{2,m}} & \rho_{c_{2,app}} \\ \vdots & \vdots & \ddots & \vdots & \vdots \\ \rho_{c_{1,m}} & \rho_{c_{2,m}} & \cdots & 1 & \rho_{c_{m,app}} \\ \rho_{c_{1,app}} & \rho_{c_{2,app}} & \cdots & \rho_{c_{m,app}} & 1 \end{bmatrix}$$

The last column of the last row of $\mathbf{R_c}$, except for the last element, is the collection of the experiments' c_k values, i.e., $[\rho_{c_{1,app}} \quad \rho_{c_{2,app}} \quad \cdots \quad \rho_{c_{m,app}}]$. According to the conventional experiment selection method, one may sort experiments based on these calculated c_k values.

On the other hand, to calculate the j_k relevance index, in addition to the calculated response covariance matrix, a measured response covariance matrix, denoted by $\mathbf{C_m} \in \mathbb{R}^{(m+1)\times(m+1)}$, needs to be prepared. Note that measured responses are usually considered independent of each other, so a measured response covariance matrix often appears as a diagonal matrix. Also, there is no measurement available for the application, the elements of its last column and row are all zero.

$$\mathbf{C_m} = \begin{bmatrix} \sigma_{e_1}^2 & 0 & \cdots & 0 & 0 \\ 0 & \sigma_{e_2}^2 & \cdots & 0 & 0 \\ \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & \cdots & \sigma_{e_m}^2 & 0 \\ 0 & 0 & \cdots & 0 & 0 \end{bmatrix}$$

where $\sigma_{e_i}^2$ is the variance of the *i*-th measured response. Since the application does not have measurement information, the last element is set to be zero.

The prior bias is derived from the difference between calculated responses and measured responses. Therefore, according to the error propagation, the prior bias or discrepancy covariance matrix can be obtained as the sum of these two matrices, such that:

$$\mathbf{C_d} = \mathbf{C_k} + \mathbf{C_m} = \begin{bmatrix} \sigma_{c_1}^2 + \sigma_{e_1}^2 & \rho_{c_{1,2}}\sigma_{c_1}\sigma_{c_2} & \cdots & \rho_{c_{1,m}}\sigma_{c_1}\sigma_{c_m} & \rho_{c_{1,app}}\sigma_{c_1}\sigma_{c_{app}} \\ \rho_{c_{1,2}}\sigma_{c_1}\sigma_{c_2} & \sigma_{c_2}^2 + \sigma_{e_2}^2 & \cdots & \rho_{c_{2,m}}\sigma_{c_2}\sigma_{c_m} & \rho_{c_{2,app}}\sigma_{c_2}\sigma_{c_{app}} \\ \vdots & \vdots & \ddots & \vdots & \vdots \\ \rho_{c_{1,m}}\sigma_{c_1}\sigma_{c_m} & \rho_{c_{2,m}}\sigma_{c_2}\sigma_{c_m} & \cdots & \sigma_{c_m}^2 + \sigma_{e_m}^2 & \rho_{c_{m,app}}\sigma_{c_m}\sigma_{c_{app}} \\ \rho_{c_{1,app}}\sigma_{c_1}\sigma_{c_{app}} & \rho_{c_{2,app}}\sigma_{c_2}\sigma_{c_{app}} & \cdots & \rho_{c_{m,app}}\sigma_{c_m}\sigma_{c_{app}} & \sigma_{c_{app}}^2 + \sigma_{e_{app}}^2 \end{bmatrix}$$

Then, take its diagonal elements and square-root of them:

$$\mathbf{\Sigma_d} = \mathrm{diag}\left(\left[\sqrt{\sigma_{c_1}^2 + \sigma_{e_1}^2} \quad \sqrt{\sigma_{c_2}^2 + \sigma_{e_2}^2} \quad \cdots \quad \sqrt{\sigma_{c_m}^2 + \sigma_{e_m}^2} \quad \sqrt{\sigma_{c_{app}}^2 + \sigma_{e_{app}}^2}\right]\right)$$

By analogy, normalize the discrepancy covariance matrix by the square-rooted matrix $\mathbf{\Sigma_d}$:

$$\mathbf{R_d} = \mathbf{\Sigma_d^{-1} C_d \Sigma_d^{-1}} = \begin{bmatrix} 1 & \rho_{d_{1,2}} & \cdots & \rho_{d_{1,m}} & \rho_{d_{1,app}} \\ \rho_{d_{1,2}} & 1 & \cdots & \rho_{d_{2,m}} & \rho_{d_{2,app}} \\ \vdots & \vdots & \ddots & \vdots & \vdots \\ \rho_{d_{1,m}} & \rho_{d_{2,m}} & \cdots & 1 & \rho_{d_{m,app}} \\ \rho_{d_{1,app}} & \rho_{d_{2,app}} & \cdots & \rho_{d_{m,app}} & 1 \end{bmatrix}$$

where

$$\rho_{d_{i,j}} = \frac{\rho_{c_{i,j}}\sigma_{c_i}\sigma_{c_j}}{\sqrt{\sigma_{c_i}^2 + \sigma_{e_i}^2}\sqrt{\sigma_{c_j}^2 + \sigma_{e_j}^2}}$$

Now, $\mathbf{R_d}$ may be subgrouped, as follows:

$$\mathbf{R_d} = \begin{bmatrix} \mathbf{R_x} & \mathbf{R_w} \\ \mathbf{R_w^T} & 1 \end{bmatrix}$$

where $\mathbf{R_w} \in \mathbb{R}^m$ is the last column of $\mathbf{R_d}$ except for the last element, and $\mathbf{R_x} \in \mathbb{R}^{m \times m}$ is the remaining square matrix. Finally, the j_k relevance is calculated as a matrix-vector product, such as:

$$j_k = \sqrt{\mathbf{R_w R_x^{-1} R_w}}$$