# **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 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 , a corresponding calculated value of , and their evaluation uncertainty , which is the sum of two uncertainty sources, i.e., the Monte-Carlo uncertainty and benchmark uncertainty in Figure 1. Let the bias[[1]](#footnote-2) be given as . Thus, each experiment defines its own PDF of expected deviations between measured and predicted values, defined as a normal distribution with the mean value , denoted as the experimental bias, and uncertainty is given by the standard deviation , which leads to the parametric bias, written as:

|  |  |  |
| --- | --- | --- |
|  |  | (10) |

where

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

|  |  |  |
| --- | --- | --- |
|  |  | (11) |

And the pooled variance , that employs the concept of inverse-variance weighting, is defined as the sum of the weighted bias variance which explains the spread of experimental biases, and the arithmetic average of the evaluation variances such as

|  |  |  |
| --- | --- | --- |
|  |  | (12) |

where

|  |  |  |
| --- | --- | --- |
|  |  | (13) |
|  |  | (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:

|  |  |  |
| --- | --- | --- |
|  | for the parametric method | (15) |

|  |  |  |
| --- | --- | --- |
|  | for the non-parametric method | (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 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 for each experiment for its weight estimation. The first step is to calculate the required weight by the selected function that is:

|  |  |  |
| --- | --- | --- |
|  |  | (17) |

where and are heuristic constants that are set to be 25 and 100 for this analysis, respectively, and is the maximum value of the selected benchmark experiments. The sum of individual weight factors should be the same as the required weight calculated in Eq. (17), such as:

|  |  |  |
| --- | --- | --- |
|  |  | (18) |

and the individual weight factors also satisfy the following linear relation with an appropriately selected acceptance , , such that

|  |  |  |
| --- | --- | --- |
|  |  | (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 is set to be zero to maximize the required weight , if Eq. (18) does not meet.

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

|  |  |  |
| --- | --- | --- |
|  |  | (20) |
|  |  | (21) |

Eq. (20) and (21) imply that the samples are taken in proportion and the samples corresponding the other proportion 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 samples for the selected experiments can be presented in a matrix form such that:

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

|  |  |  |
| --- | --- | --- |
|  |  | (22) |

An analytical form of the maximum values 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 is the product of the individual experimental CDFs

and the corresponding PDF is

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.

A graph of a normal distribution

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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 and , 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

where is an aggregated form of the sensitivity profiles of the selected experiments and the application introduced in Section 2.2, i.e., whose last row vector is the sensitivity profile for the application, and 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 , which can also be represented by with degree of freedom, such as

|  |  |  |
| --- | --- | --- |
|  |  | (23) |

where is a prior calculated *keff* vector, is an adjusted, i.e., posterior, *keff* vector, and is a measurement *keff* vector.

The minimizer of this objective function above may be given by

|  |  |  |
| --- | --- | --- |
|  |  | (24) |

where , and is the discrepancy vector, .

The posterior covariance matrix for the *keff* is given by

|  |  |  |
| --- | --- | --- |
|  |  | (25) |

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

A diagram of a triangle

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**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 in that the square sum of the uncertainty reduction ratio and 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.

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. [↑](#footnote-ref-2)