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3.8 Proposed Approach to Uncertainty Quantification and Sensitivity Analysis in the next PA

Recommendation #62, 93, 153, 154, 155, 156

Performance Assessment Error Analysis and Resource Management

Scope Abstract: This memorandum builds upon Section 3.8 of SRNL (2016) and Flach (2017) by defining key error analysis, uncertainty quantification, and sensitivity analysis concepts and terms, in preparation for the next E-Area Performance Assessment (WSRC 2008) revision.

Results / Conclusions: This memorandum 1) reviews how mean squared error between a model prediction and reality can be separated into systemic bias / epistemic uncertainty and stochastic uncertainty / aleatory uncertainty components, 2) reviews how stochastic uncertainty can be approximately decomposed into contributions from each input parameter, 3) defines two sensitivity analysis concepts, 4) distinguishes between error analysis and stochastic uncertainty analysis, and 5) discusses efficient use of resources based on sensitivity analysis.

Discussion

Model error (composed of bias and uncertainty)

For a given physical model, let the true input values be denoted by x_j, the true output value by y, and the true relationship (function) between x_j and y by

$$y = f(x_1, x_2, \cdots) = f(x_j) \tag{1}$$

Similarly, let the estimates of these entities be denoted by a circumflex accent:

$$\hat{y} = \hat{f}(\hat{x}_j) \tag{2}$$

Modeling error is

$$e = \hat{y} - y \tag{3}$$

The expected (average, mean) value of the squared error is

$$\begin{aligned} E[(\hat{y} - y)^2] &= E\left[\{(\hat{y} - E[\hat{y}]) - (y - E[\hat{y}])\}^2\right] \\ &= E[(\hat{y} - E[\hat{y}])^2] - E[2(\hat{y} - E[\hat{y}])(y - E[\hat{y}])] + E[(y - E[\hat{y}])^2] \\ &= E[(\hat{y} - E[\hat{y}])^2] - 0 + (y - E[\hat{y}])^2 \\ &= (y - E[\hat{y}])^2 + E[(\hat{y} - E[\hat{y}])^2] \end{aligned} \tag{4}$$

(https://en.wikipedia.org/wiki/Mean_squared_error) where $E[\cdot]$ denotes the mathematical expected value operator. The expected value of a random variable X is defined by

$$E[X] = \begin{cases} \sum_x x f(x) & \text{if } X \text{ is discrete} \\ \int_{-\infty}^{+\infty} x f(x) dx & \text{if } X \text{ is continuous} \end{cases} \tag{5}$$

where $f(x)$ is the distribution of X. The first term of the mean squared error is the squared difference between the true output value and the expected (or average) estimated output value, and a measure of model bias, β^2:

$$\beta^2 \equiv (y - E[\hat{y}])^2 \tag{6}$$

The second term is recognized as the definition of variance of the estimated output value, $\sigma_{\hat{y}}^2$:

$$\sigma_{\hat{y}}^2 \equiv E[(\hat{y} - E[\hat{y}])^2] = E[\hat{y}^2] - E[\hat{y}]^2 \tag{7}$$

If the expected squared error is abbreviated as

$$e_{\hat{y}}^2 \equiv E[(\hat{y} - y)^2] \tag{8}$$

Equation (4) becomes

$$e_{\hat{y}}^2 = \beta^2 + \sigma_{\hat{y}}^2 \tag{9}$$

That is, the average squared error is the sum of model *systemic bias* (due to limited data and knowledge) and *stochastic uncertainty* (due to the probabilistic variability) components. *Epistemic uncertainty* and *aleatory uncertainty* are alternative terms, respectively.

<u>Model variance</u>

Model output uncertainty σ_y^2 can be decomposed into contributions associated with each parameter by approximating Equation (2) with the first two terms of a Taylor series about the expected (average) values of input parameters

$$\hat{y} \cong \hat{f}\left(E[\hat{x}_j]\right) + \frac{\partial \hat{f}}{\partial \hat{x}_j}\left(\hat{x}_j - E[\hat{x}_j]\right) \tag{10}$$

Summation over the index j is implied in this expression. Equation (9) is exact for linear functions of the model input parameters. Using this linear approximation (in general), the expected value of the model input becomes

$$E(\hat{y}) = \hat{f}\left(E[\hat{x}_j]\right) + \frac{\partial \hat{f}}{\partial \hat{x}_j} \cdot 0 = \hat{f}\left(E[\hat{x}_j]\right) \tag{11}$$

Returning to Equation (6) and using Equations (9) and (10) yields:

$$\begin{aligned} \sigma_{\hat{y}}^2 &= E[(\hat{y} - E[\hat{y}])^2] \\ &\cong E\left[\left(\frac{\partial \hat{f}}{\partial \hat{x}_j}\right)^2 \left(\hat{x}_j - E[\hat{x}_j]\right)^2\right] \\ &= \left(\frac{\partial \hat{f}}{\partial \hat{x}_j}\right)^2 E\left[\left(\hat{x}_j - E[\hat{x}_j]\right)^2\right] \\ &= \left(\frac{\partial \hat{f}}{\partial \hat{x}_j}\right)^2 \sigma_{\hat{x}_j}^2 \end{aligned} \tag{12}$$

or in explicit form

$$\sigma_{\hat{y}}^2 \cong \left(\frac{\partial \hat{f}}{\partial \hat{x}_1}\right)^2 \sigma_{\hat{x}_1}^2 + \left(\frac{\partial \hat{f}}{\partial \hat{x}_2}\right)^2 \sigma_{\hat{x}_2}^2 + \cdots \tag{13}$$

That is, the model output uncertainty (expressed as a variance) is approximately (exact for linear systems) the sum of contributions from each input parameter, with each contribution being the square of the gradient times the variance of the input parameter. Equation (12) can be abbreviated as

$$\sigma_{\hat{y}}^2 \equiv \sigma_{\hat{y}1}^2 + \sigma_{\hat{y}2}^2 + \cdots \tag{14}$$

and Equation (8) becomes (approximately)

$$e_{\hat{y}}^2 \cong \beta^2 + \sigma_{\hat{y}1}^2 + \sigma_{\hat{y}2}^2 + \cdots \tag{15}$$

Sensitivity analysis (SA)

Equation (12) can be used to rank input parameters according to the sensitivity of the model output to its inputs, an exercise termed *sensitivity analysis* (Saltelli 2002). One approach is to rank parameters in the order $k, \ell, \cdots$ according to the criterion

$$\left(\frac{\partial \hat{f}}{\partial \hat{x}_k}\right)^2 > \left(\frac{\partial \hat{f}}{\partial \hat{x}_\ell}\right)^2 > \cdots \tag{16}$$

Note that criterion (15) does not consider input parameter uncertainty. A second, and generally preferred, method is to rank inputs according the criterion

$$\left(\frac{\partial \hat{f}}{\partial \hat{x}_k}\right)^2 \sigma_{\hat{x}_k}^2 > \left(\frac{\partial \hat{f}}{\partial \hat{x}_\ell}\right)^2 \sigma_{\hat{x}_\ell}^2 > \cdots \tag{17}$$

which can be written more compactly using Equation (13) as

$$\sigma_{\hat{y}k}^2 > \sigma_{\hat{y}\ell}^2 > \cdots \tag{18}$$

Uncertainty quantification (UQ)

The systemic difference between physical reality and average model prediction, or model bias, is generally unknowable, but can potentially be estimated. As examples, an abstracted model might be compared to a higher-fidelity model that is believed to be relatively unbiased, model validation data might indicate the level of model basis, or expert elicitation might be used. Considering the challenges of estimating bias, quantitative error analysis is often limited to (stochastic) *uncertainty quantification* (UQ). UQ may use linear approximations (Equation (12)) or other techniques (e.g. Monte Carlo) to quantify uncertainty.

Management of model biases and uncertainties

Equation (14) can be rewritten as

$$e_{\hat{y}}^2 \cong \sigma_{\hat{y}}^2 \left(\frac{\beta^2}{\sigma_{\hat{y}}^2} + \frac{\sigma_{\hat{y}k}^2}{\sigma_{\hat{y}}^2} + \frac{\sigma_{\hat{y}\ell}^2}{\sigma_{\hat{y}}^2} + \cdots + \frac{\sigma_{\hat{y}m}^2}{\sigma_{\hat{y}}^2} + \cdots \right) \tag{19}$$

where the uncertainty contributions are ordered according to Criterion (17). Input parameters associated with the term $\sigma_{\hat{y}m}^2/\sigma_{\hat{y}}^2$ and beyond might be neglected in UQ and SA, if uncertainty contributions are rapidly descending and

$$\frac{\sigma_{\hat{y}m}^2}{\sigma_{\hat{y}}^2} < \varepsilon \cdot max\left(\frac{\beta^2}{\sigma_{\hat{y}}^2}, 1\right) \tag{20}$$

where ε is some selected cutoff value. If uncertainty contributions decline more gradually, then

$$\frac{\sigma_{\hat{y}m}^2}{\sigma_{\hat{y}}^2} + \cdots < \varepsilon \cdot max\left(\frac{\beta^2}{\sigma_{\hat{y}}^2}, 1\right) \tag{21}$$

may be more appropriate. As noted above, the bias term may be poorly known.

The concepts embodied in Equations (19) and (20) provide a rationale for managing model biases and uncertainties by focusing resources (funding, schedule, effort) only on those input parameters that contribute significantly to squared error $e_{\hat{y}}^2$.

Summary of key concepts

- Model error is the concern, not just stochastic uncertainty.
- Squared model error is composed of deterministic bias (epistemic uncertainty) and stochastic uncertainty (aleatory uncertainty).
- Output variance can be decomposed (at least approximately) into contributions associated with each random input parameter.
- Sensitivity analysis takes two main forms: gradient-only versus gradient times variance.
- Analysts need to be clear about which form is being used.
- The “gradient times variance” form is generally preferred.
- Quantitative error analysis is typically restricted to defining the stochastic component, even though error contains a deterministic bias too.

- Resources should be focused on those attributes of the overall PA analysis that contribute most significantly to error.

- Model bias can be large compared to stochastic uncertainty.

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