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UQ methods in DAKOTA employed by NuGET team to achieve critical QMU milestone

Uncertainty quantification (UQ) algorithms are a critical capability to perform the Quantification of Margins and Uncertainty (QMU). The UQ needs of our users, coupled with the high cost of computational simulations, have led researchers in 1411 to develop more robust and efficient UQ algorithms, delivered in the DAKOTA framework.

Second-order probability (nested sampling methods) is a differentiating capability in DAKOTA. Second-order probability allows one to propagate both aleatory (inherent variation) and epistemic (lack of knowledge) uncertainty. A common situation is where some uncertain inputs can be characterized by probability distributions, but other uncertain inputs can only be characterized with intervals (e.g., any value between an upper and lower bound is possible). In this case, the analysis is done with a nested sampling approach, where the outer loop sampling is over the epistemic variables and the inner loop sampling is over the aleatory variables. The results of second-order probability are a family or ensemble of cumulative distribution functions (CDFs), see Figure 1. Each CDF represents an inner loop sample conditioned on a possible value of the epistemic variables. The bounds on the entire family at a particular response threshold represent the epistemic uncertainty in where the true CDF value may fall. Second-order probability is being used in many Advance Simulation and Computing (ASC) milestones, for example, to assess epistemic ranges on margins at particular threshold levels.

The UQ algorithms in DAKOTA have played a crucial role in assessing uncertainties in stockpile materials, components, systems, and environments, and their effect on weapon performance, safety, and reliability. The Neutron Gamma Energy Transport (NuGET) team employed second-order probability methods for the ASC Level II Milestone titled "NuGET QMU Methodology." The goal of this milestone was to assess the influence of both aleatory and epistemic uncertainties in hostile and fratricide scenario predictions. The second-order probability method played an important role in downselecting experiments and demonstrating compliance with Stockpile-to-Target Sequence (STS) requirements. The ensembles of CDFs enabled the calculation of interval bounds on margins and failure probabilities, and demonstrated how this methodology can identify components that might have possible problems or need additional analysis to reduce epistemic uncertainty.

To help educate users about the UQ methods in DAKOTA, classes on DAKOTA 4.1 were held at SNL/NM and SNL/CA in April, training 35 users. Additional classes are planned to meet the demands of a growing user base.

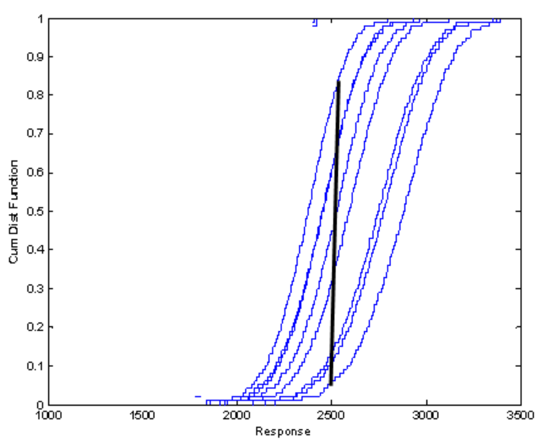

Figure 1: Ensemble of CDFs generated by second-order probability. The epistemic bounds on the probability that the response is less than 2500 are [0.04, 0.8]

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