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INNOVATION CHALLENGE

The NASA Langley UQ Challenge on Optimization under Uncertainty

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This paper presents an Uncertainty Quantification (UQ) challenge problem focusing on key aspects of model calibration, uncertainty reduction, and reliability-based design subject to aleatory and epistemic uncertainty.

I. Introduction

NASA missions often involve the development of new vehicles and systems that must be designed to operate in harsh domains with a wide array of operating conditions. These missions involve high-consequence and safety-critical systems for which quantitative data is either very sparse or prohibitively expensive to collect. Limited heritage data may exist, but is also usually sparse and may not be directly applicable to the system of interest, making uncertainty quantification extremely challenging. NASA modeling and simulation standards require estimates of uncertainty and descriptions of any processes used to obtain these estimates. The NASA Langley Research Center has developed a UQ challenge problem in an effort to focus a community of researchers towards common goals. The challenge features key issues in UQ using a discipline-independent framework. While the formulation is indeed discipline-independent, the underlying application is consistent with the complexities found in realistic systems.

II. Uncertainty Classification

This challenge problem adopts the generally accepted classification of uncertainty referred to as aleatory and epistemic [1, 2, 3]. *Aleatory* uncertainty (also called irreducible uncertainty, or stochastic uncertainty) is uncertainty due to inherent variation or randomness. An aleatory variable is often modeled by a probability distribution. In contrast, *epistemic* uncertainty arises due to a lack of knowledge. Epistemic uncertainty is not an inherent property of the system, but instead it represents the state of knowledge of the analyst on the value of a parameter. In the context of this challenge, an epistemic variable can take any fixed value within a bounded set. According to its physical origin, the value of a parameter can be either fixed (e.g., the mass of a specific element produced by a manufacturing process) or varying (e.g., the mass of any element that can be produced by a manufacturing process). The physical origin of a parameter as well as the knowledge we have about it must be used to create an Uncertainty Model (UM) for it. Intervals, fuzzy sets, random variables, probability boxes [4], etc., are different classes of uncertainty models. Because most models, especially those characterizing uncertainty, are imperfect; the possibility of improving them always exists. A reduction of the uncertainty in an epistemic variable e is attained by reducing the size of the set where the true value of such a variable is expected to be. This reduction can be attained by performing additional experiments or doing better computational simulations. Conversely, an irreducible model remains fixed throughout the UQ process.

III. Framework

A computational model of a physical system will be used to evaluate and improve its reliability. Denote by $\delta \in \mathbb{R}^{n_\delta}$ a parameter of the model whose value is uncertain, and by $\theta \in \mathbb{R}^{n_\theta}$ a design variable to be prescribed. The parameter δ is comprised of elements of a and e, where $a \in \mathbb{R}^{n_a}$ and $e \in \mathbb{R}^{n_e}$ are aleatory an epistemic variables respectively. The UM for a will be denoted as $a \sim f_a(a)$, where $f_a(a)$ is a joint density supported in the set A. In contrast, the UM for e will be denoted as $e \sim E$, where E is a hyper-rectangular set. Hence, the UM of δ is fully prescribed by the pair $\langle f_a(a), E \rangle$. In this challenge the functional form of $f_a(a)$ and the geometry of E are to be chosen by the respondents.

The system of interest is modeled as a set of interconnected subsystems. However, the uncertain parameter δ is concentrated onto a single subsystem. This subsystem is modeled by the function $y(a, e, t)$, where $y : \mathbb{R}^{n_a} \times \mathbb{R}^{n_e} \times [0, T] \rightarrow \mathbb{R}$ and t is time. The integrated system is modeled by $z\,(a, e, \theta, t)$, where $z : \mathbb{R}^{n_a} \times \mathbb{R}^{n_e} \times \mathbb{R}^{n_\theta} \times [0, T] \rightarrow \mathbb{R}^2$. Hence, the output of the subsystem is a function of time, whereas the output of the integrated system are two functions of time. Each of these functions will be given as a discrete time history, e.g., $y(t) = [y(0), \ldots, y(T)]$.

The goal of the designer is to find a design point θ that yields a fast-decaying response $z_1(t)$ while keeping $z_2(t)$ below a given threshold. These design objectives will be cast as a set of reliability requirements. These requirements are fully prescribed by the performance functions $g(a, e, \theta)$, where $g : \mathbb{R}^{n_a} \times \mathbb{R}^{n_e} \rightarrow \mathbb{R}^{n_g}$. The system will be regarded as requirement compliant when $g(a, e, \theta) < 0$. For fixed values of θ and e, the set of a points where $g < 0$ is called the *safe domain*, whereas its complement set is the *failure domain*. In this application the requirements define competing design objectives: design points that contract the failure domain corresponding to one requirement might also expand the failure domain corresponding to another. When e and θ are fixed, and $a \sim f_a(a)$, the probability of failure can be readily estimated. When $e \sim E$, θ is fixed, and $a \sim f_a(a)$ the probability of failure varies in a range.

An overview of the key goals of this challenge is as follows:

- Create an UM of δ according to observations of the subsystem.
- Choose a limited number of epistemic variables to refine.
- Perform a reliability analysis of a given design point.
- Seek a design point θ with improved reliability.
- Improve the UM of δ and θ according to observations of the integrated system.

- Improve θ by accepting a small risk.

IV. Problem Statement

The NASA UQ challenge is divided into the six subproblems described below. The numerical setup is $n_a = 5$, $n_e = 4$, $n_\theta = 9$, $n_g = 3$, $T = 5$, $B = [0,2]^{n_a}$, $E_0 = [0,2]^{n_e}$, $n_1 = 100$, $n_2 = 100$ and $\hat{r} = 0.05$. Requirement $g_1 < 0$ is needed for the system to be stable, requirement $g_2 < 0$ with

$$g_2 = \max_{t \in [T/2, T]} |z_1(a, e, \theta, t)| - 0.02, \tag{1}$$

for the settling time of the new response to be sufficiently fast, and requirement $g_3 < 0$ with

$$g_3 = \max_{t \in [0, T]} |z_2(a, e, \theta, t)| - 4, \tag{2}$$

for the energy consumption to be acceptable. The dataset, the baseline design, the computational models, and means to evaluate g can be downloaded from the website provided below.

A. Model Calibration & Uncertainty Quantification of a Subsystem

Here we seek the characterization of the parameters of the subsystem according to a limited number of observations of the physical system.

A.1) Given the data sequence $D_1 = \{y^{(i)}(t)\}$ for $i = 1, \ldots n_1$, create an UM for δ such that $a \sim f_a(a)$ for $a \in A \subseteq B$, and $e \sim E \subseteq E_0$.

A.2) Explain the rationale that led you to chose a particular distribution class for a. Why is that distribution better than any other? Evaluate the degree of dependency among the parameters of the identified $f_a(a)$. Explain the rationale that led you to chose the geometry of E. Evaluate the extent by which the identified UM underfits/overfits the data. How does the value of n_1 impact your answers?

B. Uncertainty Reduction

B.1) Rank the epistemic parameters according to their ability to improve the predictive ability of the computational model of the subsystem.

B.2) Chose $k \leq 4$ epistemic variables for refinement[a]. Ask the NASA hosts for a refined UM of them. Denote the reduced epistemic space E_1.

B.3) Update the UM of δ and the parameter ranking such that $e \sim E \subseteq E_1$.

C. Reliability Analysis of Baseline Design

Here we evaluate the reliability of a given design point θ_{baseline} for the current UM.

[a]Another opportunity for refinement will be available in Subproblem E. The total number of refinements a group can request shall not exceed 4. The same epistemic parameter can be refined multiple times.

C.1) Evaluate the range of the failure probability for each individual requirement,

$$R_i(\theta) = \left[\min_{e\in E} \mathbb{P}[g_i(a,e,\theta) \geq 0],\ \max_{e\in E} \mathbb{P}[g_i(a,e,\theta) \geq 0]\right], \tag{3}$$

for $i = 1, \ldots n_g$, where $\mathbb{P}[\cdot]$ is the probability operator.

C.2) Evaluate the range of the failure probability for all requirements,

$$R(\theta) = \left[\min_{e\in E} \mathbb{P}\left[g(a,e,\theta) \geq 0\right],\ \max_{e\in E} \mathbb{P}\left[g(a,e,\theta) \geq 0\right]\right]. \tag{4}$$

C.3) Rank the epistemic uncertainties according to the contraction of $R(\theta)$ that might result from their reduction.

C.4) Identify representative realizations of $\delta \in A \times E$ having a comparatively large likelihood near the failure domain. Use these points to characterize qualitatively different transitions to failure. Show the corresponding time responses of the integrated system.

C.5) Evaluate the severity of each individual requirement violation, as measured by

$$s_i(\theta) = \max_{e\in E} \left\{\mathbb{E}[\ g_i(a,e,\theta) \mid g_i(a,e,\theta) \geq 0\ ]\, \mathbb{P}[g_i(a,e,\theta) \geq 0]\right\}, \tag{5}$$

where $i = 1, \ldots n_g$ and $\mathbb{E}[\cdot|\cdot]$ is the conditional expectation.

D. Reliability-Based Design

Here we seek to improve the reliability of the system by identifying a new design point.

D.1) Find a reliability-optimal design point θ_{new}.

D.2) Perform the analysis of θ_{new} described in Subproblem C for the current UM.

E. Model Update and Design Tuning

Here we seek to improve the UM and the design by using observations of the physical, integrated system corresponding to θ_{new}.

E.1) Provide θ_{new} to the NASA hosts, who will give you the corresponding data sequence $D_2 = \{z^{(i)}(t)\}$ for $i = 1, \ldots n_2$.

E.2) Use this sequence to update the UM and tune your design.

E.3) Chose $4 - k$ epistemic variables for refinement. Ask the hosts for their refined UMs. Denote the reduced epistemic space E_2.

E.4) Update the UM of δ and further improve the design such that $e \sim E \subseteq E_2$. Denote the resulting design point θ_{final}.

E.5) Perform the analysis of θ_{final} described in Subproblem C for the current UM.

E.6) Compare θ_{baseline}, θ_{new} and θ_{final} using the figures of merit in (3), (4) and (5).

F. Risk-Based Design (Optional)

Here we seek a design point that only accounts for $(100 - r)\%$ of the volume of E, where $r \in [0, 100)$ is called risk.

F.1) Propose a metric to quantify the gain, ℓ, resulting from taking the risk $r = \hat{r}$.

F.2) Find a design point that maximizes $\ell(\hat{r})$ and denote it as $\theta_{\hat{r}\%\text{risk}}$. Explain the process by which the portion of E being ignored was chosen.

F.3) Compare $\theta_{\hat{r}\%\text{risk}}$ and θ_{final} using the figures of merit above. Is it worth taking this risk?

F.4) Evaluate $\ell(r)$ for a few values in $r \in [0, 20]$ to determine an optimal risk value (if any).

V. Conference Paper

Responses to the challenge will be part of a dedicated session of the ESREL 2020 conference (*https://www.esrel2020-psam15.org/*) to be held in Venice, Italy, from June 21st to June 26, 2020. Each participating group must first register via *http://uqtools.larc.nasa.gov/nasa-uq-challenge-problem-2020/*. In the process, the work email addresses of *all* coauthors must be provided. All interactions with the NASA hosts must be made by the corresponding author of the paper using this website. For the sake of a fairness, we request each team to work independently from the other teams. Therefore, **no exchanges of information between teams is allowed**. Furthermore, co-authors of registered groups can not be part of any other future group.

Extended abstracts **not exceeding 8 pages** must be submitted by January 15, 2020 according to the guidelines given in *https://www.esrel2020-psam15.org/authors.html*. Abstracts will be evaluated based on their technical merit, adherence to the challenge's goals, and clarity. Notifications of acceptance will be given by the end of January. Please use the notation introduced herein, justify the approaches chosen, and comment on those that did not work. We request you not to specify the refined UMs nor your design points in the article. However, please send us your final UM, θ_{final} and $\theta_{5\%\text{risk}}$ by the final paper's deadline. The authors of high-quality papers will be invited to contribute to a special journal edition, in which a full disclosure of results is expected.

VI. Software

The computational models of the subsystem and of the integrated system as well as the data will be given as MATLAB® files. These files, namely `yfun.m` (the subsystem), `zfun.m` (the integrated system), `gfun.m` (the performance functions), `baseline-design.mat` (the baseline design) and `D1.mat` (n observations of the response of the subsystem), can be downloaded from the website above. The use of the functions, which require the Control Systems Toolbox to run, is exemplified in `test.m`.

References

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