SAND2014-2200P

Optimal Selection of Calibration and Validation Test Samples under Uncertainty

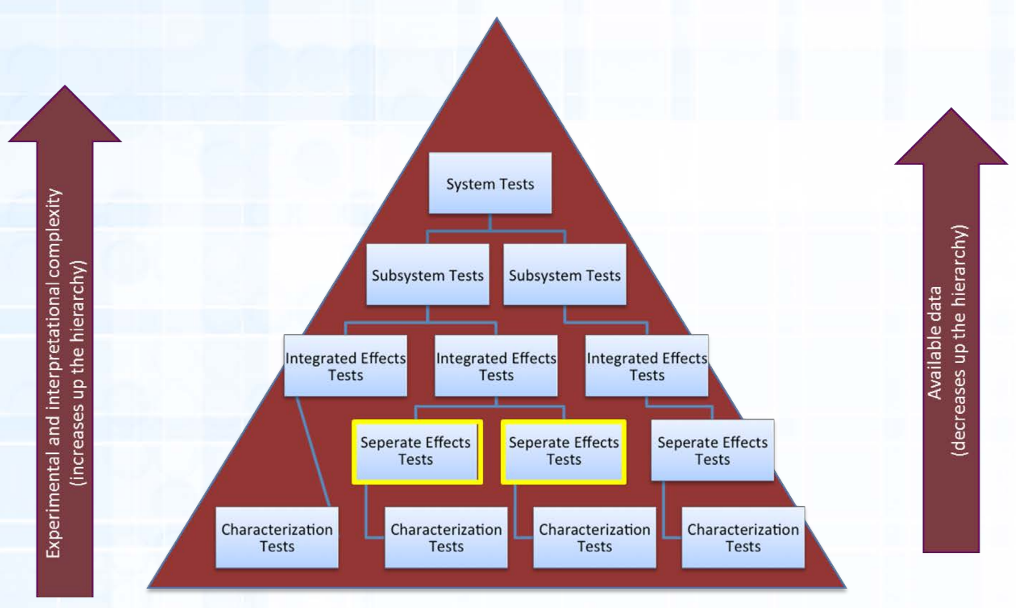
Angel Urbina • Sandia National Laboratories

Joshua Mullins, Chenzhao Li & Sankaran Mahadevan • Vanderbilt University

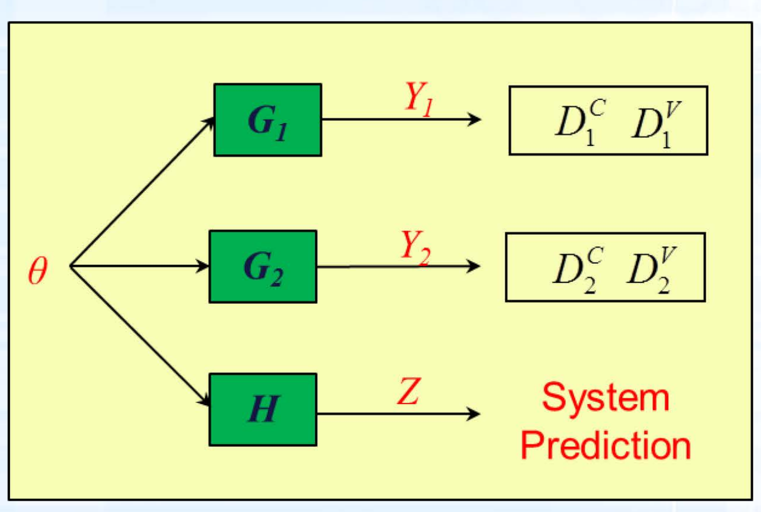
Validation Hierarchy or Pyramid

Problem Description (within the context of a validation hierarchy):

- Determine where and how much data to collect in each of the boxes (or nodes) in the hierarchy to characterize the uncertainty in the parameters needed for system-level prediction
- No experimental data available at the system level



Problem Statement



- D_1^C, D_1^V and $Y_1 = 10X + 2X^2 + 0.5X^3$
- D_2^C, D_2^V and $Y_2 = 10X + 2X^2 + X^3$
- $Z = 10X + 2X^2 + 2X^3$

- Given two "nodes" in the validation hierarchy and a system level model,
- Predict the optimal number of calibration and validation experiments that will simultaneously:
  - Minimize prediction uncertainty by parameter uncertainty reduction (calibration) and
  - allowing conservatism for epistemic uncertainties from models and data (validation)

Optimal Test Selection Framework

Discrete optimization

(simulated annealing)

- Select an initial iterate for the decision variables and take random walks
- Accept all new iterates with smaller objective function values and accept larger objective function values with probability according to

$$P = exp(-\frac{\Delta f}{T})$$

- Reduce temperature (T) at each iteration such that the probability of accepting worse iterates decreases

$$T = T_0\left(1 - \frac{k}{K}\right)^{\alpha}$$

Δf: Change in obj. function
T_0: Initial temperature
k: Current iteration no.
K: Total no. of iterations
α: Rate of temp. decrease

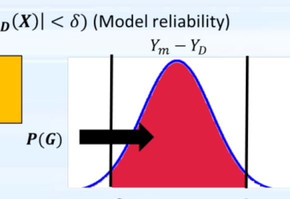
Probabilistic validation

(model reliability metric for sparse data)

- Calibrated models may be overconfident
- Perform validation to assess model performance outside domain
- Use probabilistic validation to incorporate the result into predictions

$P(G) = P(|Y_m(X,\theta) - Y_D(X)| < \delta)$ (Model reliability)

$P(G)$: Model reliability
δ: Chosen tolerance



Bayesian calibration

(parameter uncertainty including data uncertainty)

- Difference between prediction and observation described by measurement error (may also include model discrepancy)

$$Y_D(X) = Y_m(X,\theta) + \varepsilon_m$$

- Update distribution of θ with data

$$\pi(\theta|Y_D) = \frac{\Pr(Y_D|\theta)\pi(\theta)}{\int \Pr(Y_D|\theta)\pi(\theta)d\theta}$$

- Additional observations tend to reduce parameter uncertainty

$X \rightarrow$ model inputs
$\theta \rightarrow$ model parameters
$Y_m \rightarrow$ model output
$\varepsilon_m \rightarrow$ measurement noise
$Y_D \rightarrow$ measurement data

Objective Function Formulation

Calibration

$$\min_{n_1,n_2,n_3,n_4} E(E[Var(Z)])$$

Validation

$$\min_{n_1,n_2,n_3,n_4} E(Var[E(Z)])$$

$$s.t. \sum_{i=1}^{4} c_i n_i \leq budget$$

- Motivation
  - **Calibration**: minimize expected prediction uncertainty
  - **Validation**: minimize uncertainty in the model reliability computation
  - Calibration decreases prediction uncertainty while validation may expand it within this integration framework

Framework Implementation

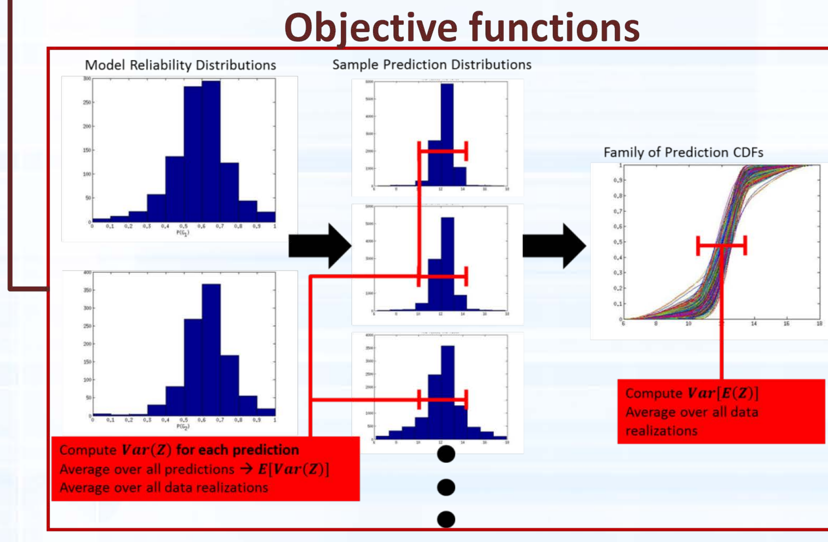
Simulated Annealing
Design variables:
$n_{c1}, n_{c2}, n_{v1}, n_{v2}$

Bayesian calibration

1) Sample vectors $D_1^{C^i}, D_1^{V^i}, D_2^{C^i}, D_2^{V^i}$ of lengths $n_{c1}, n_{v1}, n_{c2}, n_{v2}$ respectively
2) Perform three calibrations

$$\pi(\theta|Y_D) = \frac{\Pr(Y_D|\theta)\,\pi(\theta)}{\int \Pr(Y_D|\theta)\,\pi(\theta)d\theta}$$

Objective functions



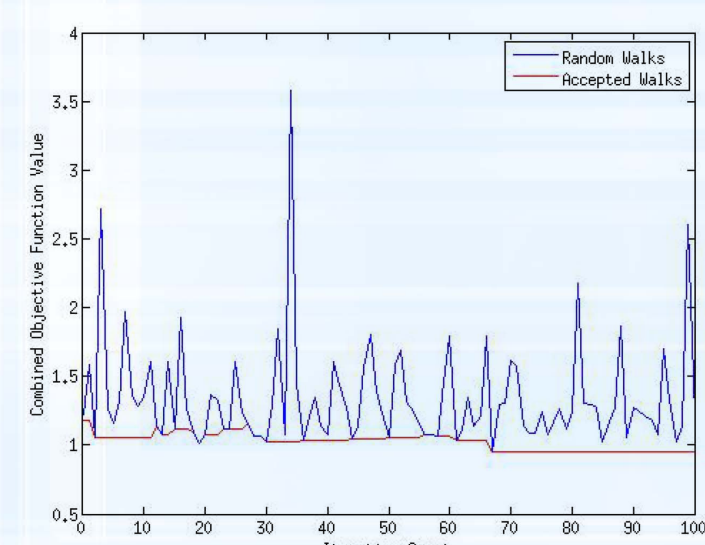
Incorporate validation

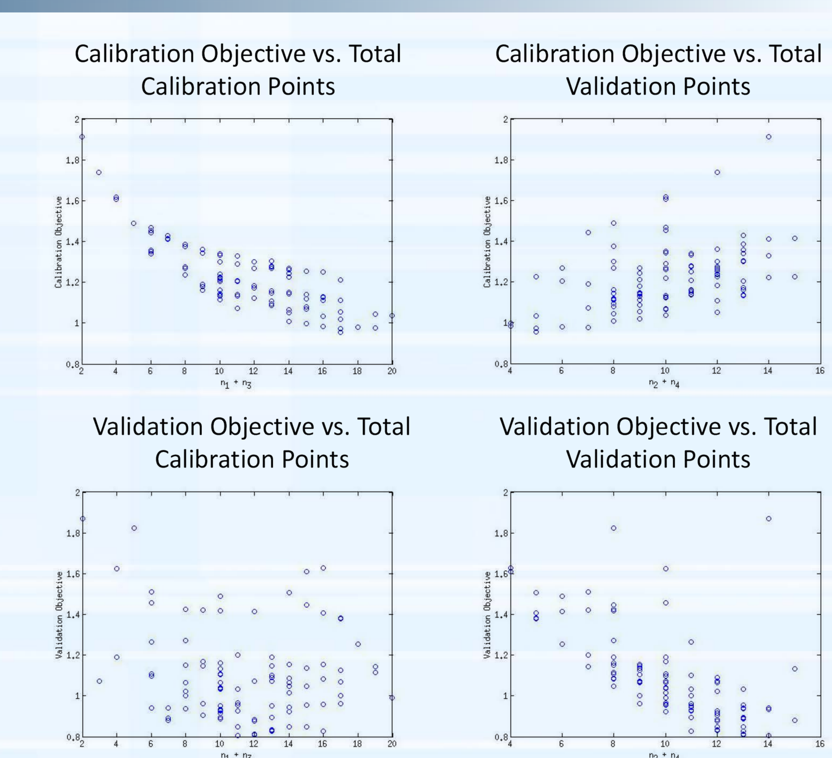
- After calibration, perform validation
- Calculate $P(G_1)$ and $P(G_2)$
- Modify PDF of θ
- Propagate through H

Predictive Parameter PDF

$$\begin{aligned} f(\theta \mid D_1^C, D_2^C, D_1^V, D_2^V) &= P(G_1)P(G_2)f(\theta \mid D_1^C, D_2^C) \\ &+ P(G_1')P(G_2)f(\theta \mid D_2^C) \\ &+ P(G_1)P(G_2')f(\theta \mid D_1^C) \\ &+ P(G_1')P(G_2')f(\theta) \end{aligned}$$

Optimization Results





The formulation drives the optimization to [10, 9, 2, 4]

- 10 calibration at level 1
- 9 validation at level 1
- 2 calibration at level 2
- 4 validation at level 2

The goals of calibration and validation are balanced

Conclusions and Path Forward

- This framework enables a decision maker to:
  - understand the trade-offs between the number of experiments at different levels of a hierarchy and
  - the effect on uncertainty in the predictions space
- High level observations are made relative to this example:
  - Additional calibration data points reduce uncertainty in the prediction by reducing parameter uncertainty
  - Additional validation points reduce the epistemic uncertainty about the prediction arising from inability to assess the model with sparse data
- Path forward:
  - Connect experimental decision making with model improvement decisions
  - Connect framework to system-level risk decision making
    - How much UQ is enough (budget selection)?
    - What is the appropriate validation tolerance?

Publications

- J. Mullins, C. Li, S. Mahadevan, and A. Urbina, Test Selection for Prediction Uncertainty Quantification and Reduction, manuscript in preparation
- Mullins, J., Chenzhao, L., Mahadevan, S., and Urbina, A., "Optimal Selection of Calibration and Validation Test Samples under Uncertainty", 2014 International Modal Analysis Conference, Orlando, Florida.
- Mullins, J., Li., C., Sankararaman, S., Mahadevan, S., and Urbina, A., "Uncertainty Quantification Using Multi-Level Calibration and Validation Data," *Proceedings of the 54th AIAA/ASME/ASCE/AHS/ASC Structures, Structural Dynamics and Materials Conference*, Boston, MA, 2013.
- Urbina, A. Mahadevan, S. and Paez, T.L., "Resource Allocation using Quantification of Margins and Uncertainty", 51th AIAA/ ASME/ASCE/AHS/ASC Structures, Structural Dynamics, and Materials Conference, Orlando, Florida, April 2010.
- Urbina, Angel, "Uncertainty Quantification and Decision Making in Hierarchical Development of Computational Models." Ph.D. Dissertation, Vanderbilt University, 2009 .

This work is supported by the Division of Chemical Sciences, Geosciences, and Biosciences, the Office of Basic Energy Sciences, the U. S. Department of Energy.

Sandia National Laboratories is a multi-program laboratory managed and operated by Sandia Corporation, a wholly owned subsidiary of Lockheed Martin Corporation, for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-AC04-94AL85000.

SAND2013-XXXXX Sandia Creative Group 284-2905 LW-04-13

U.S. DEPARTMENT OF ENERGY

National Nuclear Security Administration

Sandia National Laboratories