Calibration of computer models

Introduction

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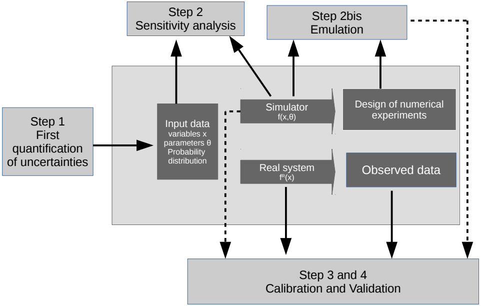
Uncertainty Quantification / Model Uncertainty



In this course, we will focus on calibration and validation.

Calibration of a computer code

Computer experiments:

Computer model (simulator) $(\mathbf{x}, \boldsymbol{\theta}) \mapsto f(\mathbf{x}, \boldsymbol{\theta}) \in \mathbb{R}^s$ where

- **physical parameters**: $\mathbf{x} \in \mathbb{X} \subset \mathbb{R}^p$ observable and often controllable inputs
- **simulator parameters**: $\boldsymbol{\theta} \in \Theta \subset \mathbb{R}^d$ non-observable parameters, required to run the simulator.

  2 types:
  - "calibration parameters": physical meaning but unknown, necessary to make the code mimic the reality,
  - "tuning parameters": no physical interpretation.

Goal:
Calibrate the code: finding "best" or "true" $\boldsymbol{\theta}$ from real observations / field data (provided by physical experiments):

$$\mathbf{y}^e = \{y_1^e = \zeta(\mathbf{x}_1^e) + \epsilon_1, \ldots, y_n^e = \zeta(\mathbf{x}_{n_e}^e) + \epsilon_{n_e}\},$$

where ζ is the real physical phenomenon.

Validation

- Validation (rather than verification) is considered,
- Does the computer simulator correspond to field data?

$$\exists \boldsymbol{\theta}^*?, \ \text{s.t.}, \ \forall \mathbf{x}, \quad f(\mathbf{x}, \boldsymbol{\theta}^*) \approx y(\mathbf{x})$$

- This question is related with intended use of the simulator: range of $\mathbf{x}$, required precision...
- Biased computer model, no setting of calibrated parameters leads to outputs close to field data
  $\Rightarrow$ discrepancy.
- Do we want to validate the computer model itself or the computer model with the bias / discrepancy correction?

Framework

KOH framework chosen for this course:
[Kennedy and O'Hagan, 2001, Higdon et al., 2004, Bayarri et al., 2007] and many papers after.

History Matching not consider but may be relevant depending on the objective
[Craig et al., 1997, Vernon et al., 2010, Boukouvalas et al., 2014, Andrianakis et al., 2017]

Deterministic or stochastic simulator

In most contributions, f is considered to be deterministic.

But some recent work considered f as stochastic [Baker et al., 2022]:

- f uses stochastic approximations (MC,...) but the modeled phenomenon is deterministic ζ...
- f models a stochastic phenomenon $\zeta(\cdot)$ is stochastic.

Notations

- $\zeta(\mathbf{x})$ real physical or biological phenomenon,
- $f(\mathbf{x}, \boldsymbol{\theta})$ numerical code/model with $\mathbf{x}$ observable or controllable input variable, $\boldsymbol{\theta}$ model parameter (no counterpart in the real phenomenon),
- DoNE: Design of Numerical Experiments: $D^c = \{(\mathbf{x}_1, \boldsymbol{\theta}_1), \dots, (\mathbf{x}_N, \boldsymbol{\theta}_N)\}$ with corresponding evaluations of the computer model (time-consuming):

$$\mathbf{y}^c = f(D^c) = \{f(\mathbf{x}_1, \boldsymbol{\theta}_1), \dots, f(\mathbf{x}_N, \boldsymbol{\theta}_N)\},$$

- DoFE: Design of Field Experiments: $D^e = \{\mathbf{x}_1^e, \dots, \mathbf{x}_{n_e}^e\}$ with corresponding noisy observation of ζ:

$$\mathbf{y}^e = \{y_1 = \zeta(\mathbf{x}_1^e) + \epsilon_1, \dots, y_n = \zeta(\mathbf{x}_{n_e}^e) + \epsilon_{n_e}\}.$$

Outline

1. Calibration KOH and extensions
2. Sequential design of experiments
3. Focus on the discrepancy function and validation
4. Extensions to calibration of stochastic simulator

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