VALIDATION OF COMPUTER MODELS

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Abstract

We deal with validation of costly computer models $y = y_{t^*}(x)$ seen as deterministic black box models depending on both a control variable x and an unknown constant parameter t^*. The validation activities refer to the study of the predictive capability of the numerical model y with a special attention on how to take in account all sources of uncertainty. We illustrate well-known issues on toy examples, then we focus on two industrial cases motivating our study.

1. Description of a physical system with a computer model

- **A physical system** $r_\theta : x \in \mathbb{R}^n \to \mathbb{R}$ with $\theta \in \mathbb{R}^m$:
  - x is a controllable variable,
  - θ is the physical parameter,
  - physical experiments $d_z = \{z_i = r_\theta(x_i) + \epsilon_i\}_i$,
  - ϵ_i is an error term.
- **A computer model** $y_t : x \in \mathbb{R}^n \to \mathbb{R}$ with $t \in T \subset \mathbb{R}^d$; $d \leqslant m$:
  - t is a parameter of y,
  - computer experiments $d_y = \{y_{t_j}(x_i)\}_{i,j}$.
- **The true value** t^*:
  - $P : \mathbb{R}^m \to T$ the projection operator on T,
  - $t^* := P(\theta)$,
  - $y_{t^*}(x)$ is the best representation for $r_\theta(x)$.
- **Links between** y_{t^*} **and** r_θ :
  - i. y is perfect and $t^* = \theta (m = d) \implies r_\theta(x) = y_{t^*}(x)$,
  - ii. an error (bias) e exists : $t^* = \theta(m = d)$ and $r_\theta(x) = y_\theta(x) + e(x)$,
  - iii. θ is not perfectly identified by y : $t^* \neq \theta$ $(d < m)$ and $r_\theta(x) = y_{t^*}(x) + e(x)$.

2. Calibration and Validation

Calibration (or Inverse problem) It consists in estimating t^* from output data $d = (d_y, d_z)$:
- known $e(x)$ form : regression models,
- unknown $e(x)$ form : Kennedy and O'Hagan (KOH) framework [4].

Validation A framework providing predictions for r_θ in a new configuration x^*:
- the model is calibrated : cokriging emulation [3],
- the model is not calibrated : Bayarri framework [1] (similar to KOH work).

Quantities of interest:
- the *a posteriori* distribution $[t^*|d]$,
- $r_\theta(x^*)$ predictions.

Limitations:
- limited number of data d_z,
- d_y are costly.

Statistical tools Kriging emulation [5] and Bayesian inference [2].

3. Limitations of joint calibration/validation: a toy example

We apply KOH framework on a toy example.

Model and data:
- $r_{\theta=-9}(x) = 10x^2 - 9x + 3$ for $x \in [0, 1]$,
- $y_t(x) = 10x^2 + tx$ for $x \in [0, 1]$, $t \in [-20, 20]$,
- $\text{card}(d_y) = 150$ and $\text{card}(d_z) = 10$.

***A priori* hypothesis**:
- $[t^*] \sim \mathcal{N}(0, 100)$,
- kriging model on both $y_t(x)$ and $e(x)$,
- a polynomial of degree 2 for $y_t(x)$ mean.

Case 1 : Added *a priori* hypothesis : A polynomial of degree 2 for $e(x)$ mean

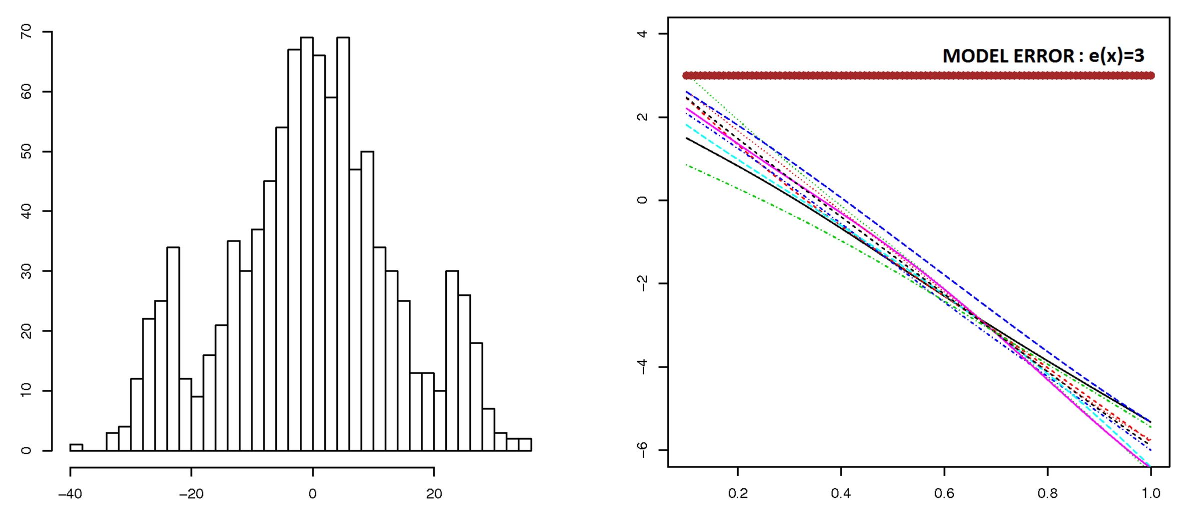

Figure 1: *On the left side : the a posteriori distribution* $[t^*|d]$. *On the right side: posterior sample of* $\hat{e}_{\hat{t}^*}(x)$ *paths (with* $\hat{t}^* = \mathbb{E}[t^*|d]$*).*

Case 2 : Added *a priori* hypothesis : A constant $e(x)$ mean

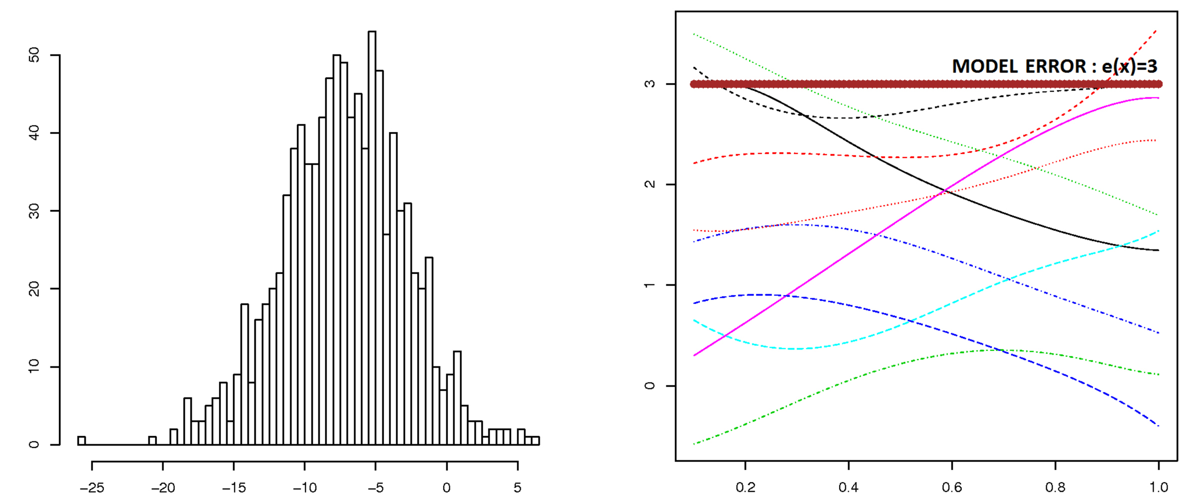

Figure 2: *On the left side : the a posteriori distribution* $[t^*|d]$. *On the right side: posterior sample of* $\hat{e}_{\hat{t}^*}(x)$ *paths (with* $\hat{t}^* = \mathbb{E}[t^*|d]$*).*

Conclusions The *posterior* distribution of both $[t^*|d]$ and $[e(x)|d]$ strongly depend on the *prior*, due to non-identifiability. Joint calibration and validation of a computer model is an ill-posed problem. In practice, each task must be performed separately.

4. Thermal performance of buildings

The case deals with the electric consumption $r_\theta(x)$ of a building. A constant temperature is held inside an experimental cell (see figure 3).

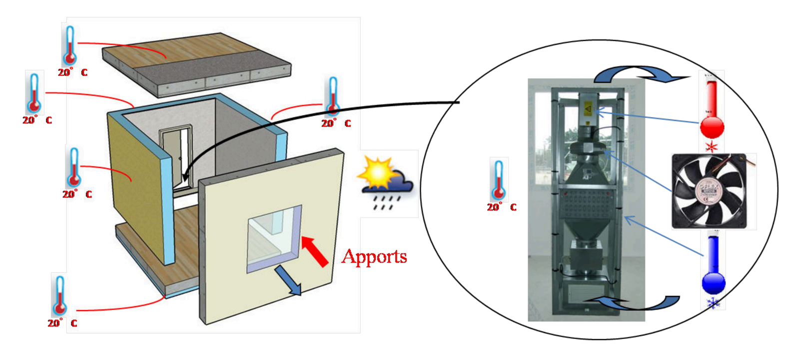

Figure 3: *Experimental cells measuring how well a building is insulated from the external weather conditions*

Material and data:
- an experimental cell,
  $\implies$ measures z_i
- a numerical sofware Dymola,
  $\implies$ computer experiments $y_{t_j}(x_i)$

Aims:
- explain both x and t,
- calibrate y,
- predict $r_\theta(x^*)$.

5. A 2D fluids mechanics case

This example deals with tuning parameters Ψ : indeed, the implemented solution $\hat{y}_{t^*,\Psi}(x)$ is often a discrete approximation of the unknwon analytic solution $y_{t^*}(x)$. Here, the model output is the fluid velocity in any point P inside the cavity (see figure 4).

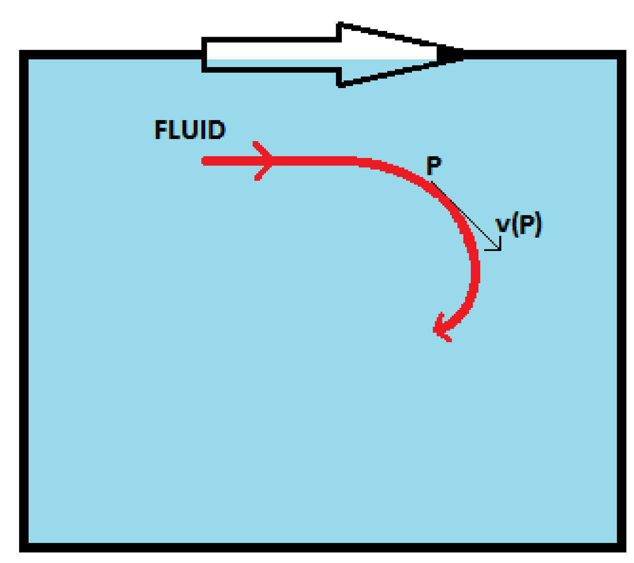

Figure 4: *The case deals with water laminar flow through a square cavity in* $2D$ *with the upper wall is moving forward.*

Hypothesis:
- x includes the cavity length and initial fluid velocity,
- $t^* = \theta$ (including mass density, viscosity, Reynolds number) is supposed exactly known (no uncertainty),
- $e(x) = 0 \implies y_{t^*}(x) = r_\theta(x)$,
- $\{\Psi\}$ is a discrete set.

Aim: estimate the best value Ψ^* in a sense to define.

Idea: a metric between r_θ and $\hat{y}_{t^*,\Psi}$,

$$\Psi^* = \underset{\Psi}{\text{argmin}} \, \|r_\theta(x) - \hat{y}_{t^*,\Psi}(x)\|.$$

Main issue: huge number of possible configurations Ψ, making exhaustive exploration impossible.

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