Uncertainty quantification and reduction for the monotonicity properties of expensive-to-evaluate computer models

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Understanding the structure of numerical models
Consider a (deterministic) numerical model:

\[ f(x) \]

with the following assumptions:
- \( x \in \mathbb{R}^d \)
- \( f(x) \in \mathbb{R} \) (scalar output).
- \( f \) is expensive to evaluate.

Partial monotonicity properties
We assume that:
- \( X \) is a hyper-rectangle: \( X = \prod_{j=1}^{d} [a_j, b_j] \).
- \( f \) admits (at least first-order) partial derivatives, but \( \nabla f \) is not available.

Definition (increasing case). \( f \) is said to be increasing with respect to its \( j \)th variable if:

\[ \forall x^{(j)} \in \prod_{j \neq i} [a_i, b_i], \quad x^{(i)} \mapsto f(x) \text{ is increasing}. \]

Proposition. \( f \) is increasing with respect to its \( j \)th variable if, and only if,

\[ \frac{\partial f}{\partial x^j}(x) \geq 0 \quad \forall x \in X. \]

Quantitative monotonicity indicators
Several quantities of interest (nonlinear functionals of \( f \)):

- “positivity rate” of the partial derivatives

\[ \alpha_j(f) = \mu(F_j(f)), \quad \text{where } F_j(f) = \left\{ \frac{\partial f}{\partial x^j} \geq 0 \right\}, \]

where \( \mu \) is a given probability measure on \( X \).

Proposed (Bayesian) approach:
- Endow \( f \) with a Gaussian Process prior,
- Estimate the monotonicity indicators, and quantify the uncertainty surrounding them, using conditional simulations of the partial derivatives.

Prediction and simulation of derivatives: cokriging
Consider a classical GP model:

\[ f(\beta, \theta) \sim \mathcal{GP} \left( \sum_{j=1}^{d} \beta_j h_j(\cdot), k_0(\cdot, \cdot) \right) \]

- \( h_1, \ldots, h_d \) known functions, which admit first-order partial derivatives (typically, polynomial functions)
- \( k_0 \) a stationary covariance function (for simplicity).

Theorem (see, e.g., Stein, 1999). Let \( k_0(\cdot) = k_0(x, x + h) \). The random process \( f \) is mean-square differentiable if, and only if, \( k_0 \) is twice differentiable at \( h = 0 \).

Theorem (Scheuerer, 2010). The random process \( f \) is mean-square differentiable if, and only if, the partial derivatives exist almost surely in Sobolev’s weak sense.

Useful fact. Cokriging is just a special case of kriging with an auxiliary discrete variable:

\[ \mathcal{F}(x, j) = \begin{cases} f(x) & \text{if } j = 0, \\ \frac{\partial f}{\partial x^j}(x) & \text{if } j > 0. \end{cases} \]

No need to replace your favorite kriging software (if it is flexible enough . . .)

Cokriging example: prediction and 95%-CI
The true function \( f \) (black line) is observed at six locations (red vertical dotted lines).

The kriging prediction (red line) and CI (black dashed lines) are performed using a zero-mean GP model, with a Matérn 5/2 covariance function.

Cokriging example: conditional simulations
Some setup as above. Observe that the samplepaths of \( f \) are rougher than those of \( \mathcal{F} \).

\( f \) has a Matérn 5/2 covariance function, while \( \mathcal{F} \) has a covariance function with the same regularity as a Matérn 3/2 covariance function.

Industrial test case (\( d = 7 \))
The methodology has been applied to an industrial test case proposed by EDF R&D
- Goal: assess the performance of a passive component in a power plant
- Thermomechanical numerical code, \( d = 7 \) quantitative input factors.

Implementation ⇒ discretizations
- Intractable posterior distributions for the quantitative monotonicity indicators: we rely on conditional simulations,
- Approximate computation of the indicators themselves using a Monte Carlo sample \( x_1, \ldots, x_m = 200 \)
- Simulation scheme
  - \( R = 100 \) iid draws of the spatial MC
  - \( S = 500 \) iid conditional simulations on each of them,
  - \( RS = 50000 \) (dependent) conditional samplepaths.

Future work
Work is in progress on
- Advanced simulation techniques for excursion sets (see Ginsbourger et al., 2014, for a preview): will replace the crude MC-based technique used here,
- Stepwise uncertainty reduction (using ideas from Bect et al., 2012): will be used to enrich a given initial design to learn more precisely the value of the indicators \( \alpha_j, M_j^* \) and \( M_j^* \) or, at the least, \( \Gamma_j \) itself !

References