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

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To cite this version:

Julien Bect, Nicolas Bousquet, Bertrand Iooss, Shijie Liu, Alice Mabille, et al.. Uncertainty quantification and reduction for the monotonicity properties of expensive-to-evaluate computer models. Uncertainty in Computer Models 2014 Conference, Jul 2014, Sheffield, United Kingdom. hal-01103724

HAL Id: hal-01103724
https://centralesupelec.hal.science/hal-01103724
Submitted on 16 Jan 2015

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Abstract. We consider the problem of estimating monotonicity properties of a scalar-valued numerical model—e.g., a finite element model combined with some post-processing. Several quantitative monotonicity indicators are introduced. Since the evaluation of the numerical model is usually time-consuming, these indicators have to be estimated with a small budget of evaluations.

We adopt a Bayesian approach, where the numerical model itself is modeled as a Gaussian process. We estimate the monotonicity indicators, and quantify the uncertainty surrounding them, through conditional simulations of the Gaussian process partial derivatives. The approach is illustrated with a numerical model of a passive component in a power plant.

Future work will leverage this framework together with the Stepwise Uncertainty Reduction principle to create an auxiliary discrete variable: monotonicity properties using a limited number of evaluations (runs of the code).

Partial monotonicity properties

We assume that

\[ x \in \mathbb{X} \subset \mathbb{R}^d, \]

\[ f(x) \in \mathbb{R} \text{ (scalar output),} \]

\[ f \text{ is expensive to evaluate.} \]

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

\[ \forall i < j \in I, \quad \prod_{k=i}^{j-1} [a_k, b_k], \quad x^j \rightarrow f(x) \text{ is increasing}, \]

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

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

Quantitative monotonicity indicators

Several quantities of interest (nonlinear functionals of \( f \)):

- *extrema* of the partial derivatives

\[ M_j^\ell(f) = \max_{x \in \mathbb{X}} \frac{\partial f}{\partial x^j}(x), \quad \text{and} \quad M_j^\ell(f) = \max_{x \in \mathbb{X}} \frac{\partial f}{\partial x^j}(x), \]

- “positivity rate” of the partial derivatives

\[ \alpha_j(f) = \mu \{ f_j(x) \geq 0 \}, \quad \text{where} \quad \mu \text{ is a given probability measure on } \mathbb{X}. \]

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:

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

\[ h_1, \ldots, h_d \text{ known functions, which admit first-order partial derivatives (typically, polynomial functions)} \]

\[ k_0 \text{ a stationary covariance function (for simplicity).} \]

Theorem (see, e.g., Stein, 1999). Let \( h_0(x) = h_0(x, x + h) \). The random process \( f \) is mean-square differentiable if, and only if, \( k_0 \) is twice differentiable at \( h = 0 \).

Theorem (Schauer, 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:

\[ \tilde{f}(x, j) = \left\{ \begin{array}{ll} f(x) & \text{if } j = 0, \\
\partial f/\partial x^j & \text{if } j > 0. \end{array} \right. \]

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

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 \( x_1, \ldots, x_m, m = 200 \)

- Simulation scheme

\[ R = 100 \text{ iid draws of the spatial MC \( R \)-sample,} \]

\[ S = 500 \text{ iid conditional simulations on each of them,} \]

\[ RS = 50,000 \text{ (dependent) conditional samplepaths.} \]

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 \( \alpha_j, M_j^\ell, \) or the set \( \Gamma_j \) itself!

References


