Bayesian Mixture of Gaussian Processes in Computer Experiments

Ofir Harari, David M. Steinberg

September 4, 2011

Consider a model of the form

$$Y(x) = \mu + Z(x) \ ,$$

where

$$Z(x) = pZ_1(x) + (1-p)Z_2(x) \ , \ \ 0 \leq p \leq 1$$

is a mixture of two independent stationary Gaussian processes, having the same marginal variance σ^2. Such a model could be appropriate when there is some uncertainty regarding the family of correlations to be used, or more importantly: we believe the underlying function follows a global trend - characterized by a small correlation parameter θ_1 - as well as many fine details, expressed by using a secondary process with a large correlation parameter θ_2.

By assigning a prior, $(p, \theta_1, \theta_2) \sim \pi(p, \theta_1, \theta_2)$, we may use MCMC methods to draw samples from the posterior distribution $\pi\left(p, \theta_1, \theta_2 \middle| \mathbf{y}\right)$ and consequently, for a new site x_0, draw a sample from the posterior predictive distribution $\pi\left(y(x_0) \middle| \mathbf{y}\right)$. This provides us with an estimate of $\widehat{y}(x_0) = \mathbb{E}\left[y(x_0) \middle| \mathbf{y}\right]$ as well as Bayesian credible intervals based on the empirical quantiles.

So far simulations have been performed for several univariate and bivariate functions, and the results seem promising, especially for functions of higher curvature.

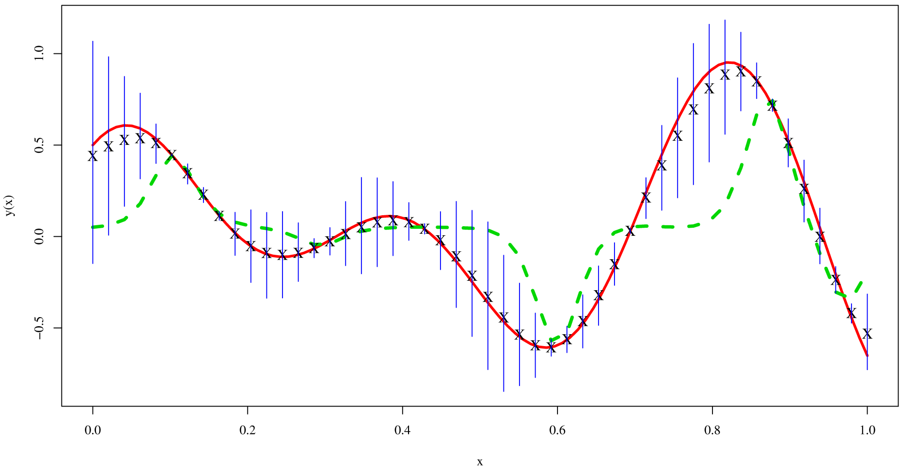


Figure 1: Mixed Gaussian process model predictions (marked by '**x**') and 95% credible intervals (vertical lines) vs. ordinary Kriging (dashed line) for $y(x) = \dfrac{\sin 10x + \cos 15x}{2}$. The solid line is the true function.

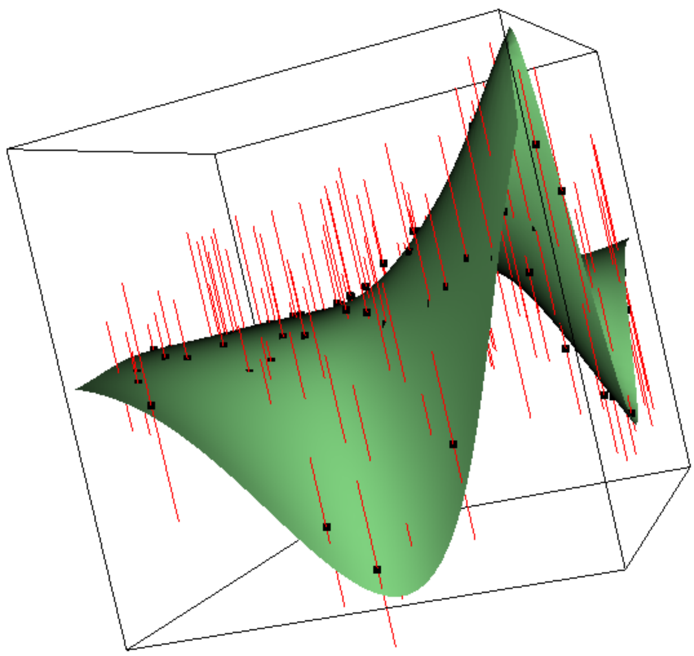


Figure 2: Mixed GP model predictions and credible intervals for
$f(x,y) = \left[\left(x-\frac{1}{5}\right)^2 - \left(y-\frac{7}{10}\right)^2\right] \cos\left((10x-5)\,y\right) \exp\left\{-5\left[\left(x-\frac{4}{5}\right)^2 + \left(y-\frac{1}{10}\right)^2\right]\right\}$

1. Calibration parameters are unknown model parameters in deterministic computer simulator that are fixed in analogous physical experiment.
2. Calibration parameters are well-defined if deterministic simulator can match mean physical response.
3. Calibration is process of using computer simulator and physical experiment data to:
    - make inference about unknown calibration parameters in (2)
    - in any case, provide (bias-corrected) estimates of mean physical response and quantify uncertainty in these estimates.

Our Goals:

- Case 1 - Computer simulator matches mean physical response

  Identify physical experiment designs that yield small bias and mean square prediction errors (MSPEs) for calibration parameters.

- Case 2 - No choice of calibration parameters allows computer simulator to match mean physical response

  Identify physical experiment designs that yield small bias and MSPEs for predictions of mean physical response.

Optimal design for models of computer experiments

Andrey Pepelyshev

Consider the linear regression model

$$y_j = y_j(t_j) = \theta_1 f_1(t_j) + \ldots + \theta_m f_m(t_j) + \varepsilon_j$$

where $t_j \in [-T, T]$, $j = 1, \ldots, N$ and $\mathbf{E}\varepsilon_j \varepsilon_i = K(t_j, t_i)$.
Let an optimal design minimize $\mathrm{Var}(\hat{\theta}_{\mathrm{OLS}})$.

- Necessary optimality conditions are derived
- Optimality of the uniform and arcsine designs is established for some models

Models when the arcsine design is optimal

Consider the polynomial regression model with

$$f(x) = (1, x, x^2, \ldots, x^{m-1})^T,$$

$x \in [-1, 1]$, and the covariance function is

$$K(u, v) = \gamma - \beta \ln(u - v)^2$$

with $\gamma \geq 0$, $\beta > 0$.

Then the design with the arcsine density satisfies the necessary conditions for universal optimality.

Models when the uniform design is optimal

From the Merser theorem we have

$$K(u,v) = \sum_{j=1}^{\infty} \lambda_j \, \varphi_j(u) \, \varphi_j(v).$$

Consider the regression model with

$$f(x) = (\varphi_{i_1}(x), \dots, \varphi_{i_m}(x))^T,$$

$i_j \neq i_l$, and the covariance kernel $K(x,u)$.

Then the design with uniform density satisfies the necessary conditions for universal optimality.

OpenTURNS, an Open Source Uncertainty Engineering Software

Poster session

Anne-Laure Popelin

Accelerating Industrial Productivity
via Deterministic Computer Experiments
and Stochastic Simulation Experiments.

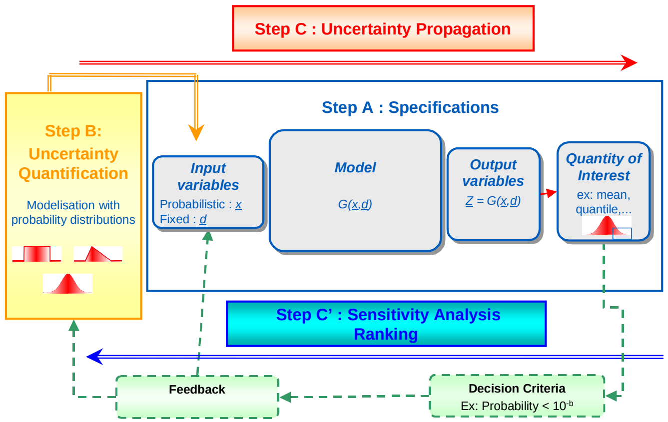
Cambridge, Sept. 2011

CHANGER L'ÉNERGIE ENSEMBLE

Open TURNS – The software implementation of the uncertainty methodology

- Partnership EDF R&D – EADS IW – Phimeca since 2005

- TURNS : Treatments of Uncertainties, Risk'n Statistics
- Open : Open source : LGPL (code), FDL (doc.)
  - Environment : Linux, Windows
  - Languages : C++ (libraries), Python (command scripts)
  - IHM "Eficas"
- Included in the Debian distribution
- Modular structure



- Diffusion:
  - Complete documentation
  - Website: http://www.openturns.org/
  - Training and annual users day

Open TURNS

Main features in OpenTURNS

- Use of non-intrusive techniques → generic

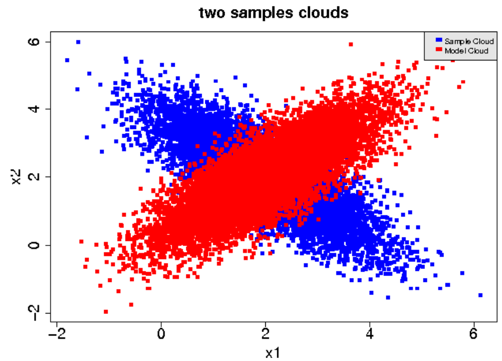
- Wrapping of external codes, considered as mathematical functions in OpenTurns

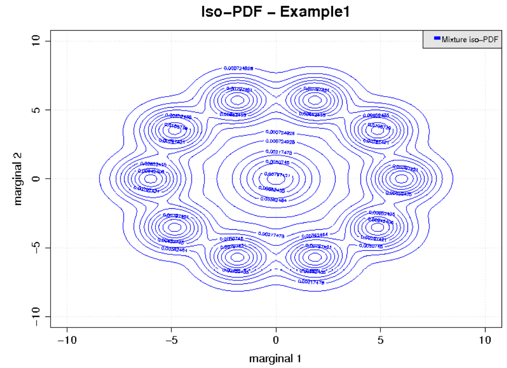
- <u>Step B: modeling uncertainty of inputs</u>
  - With data: parametric & non-parametric stats
  - Dependence: definition by marginals + copula

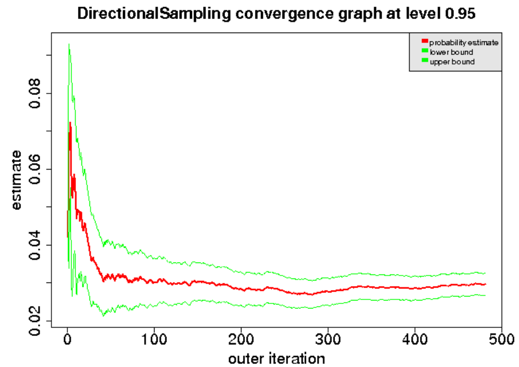
- <u>Step C: Uncertainty propagation</u>
  - Standard and advanced Monte Carlo techniques (Importance sampling, directional sampling …)
  - FORM-SORM method

- <u>Metamodels</u>: Polynomials, polynomial chaos expansion

- <u>Step C': Sensitivity analysis</u> - Linear & rank regression, Sobol, polynomial chaos, reliability importance factors







FAST and RBD revisited

J.-Y. Tissot C. Prieur

University of Grenoble – INRIA

DAE Workshop – September 5th-9th, 2011 – Cambridge, UK

FIELD: global sensitivity analysis

TOOLS: functional analysis of variance, harmonic analysis

METHODS OF INTEREST (FAST and RBD): estimating partial variances of a multivariate continuous function/model.

1. Why are (some) people interested in FAST and RBD?

   (+) efficiency (accurate estimates, low computational cost)

   but

   (−) no strong theoretical basis (unusual designs of experiments)

2. Our work aims to:
   - provide a new introduction to these methods using classical designs (based on cyclic groups and orthogonal arrays)
   - derive theoretical results on the estimation error
   - propose some directions for future research (improvements and generalizations)