Gaussian processes for computer experiments with monotonicity information

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Abstract:

Recently, statistical researchers have shown increased interest in Gaussian process modeling with monotonicity constraints (see [2], [4] and [5]). In computer experiments, the true function (scalar output) may be known to be monotone with respect to some or all input variables. We propose a new methodology based on the Bayesian Gaussian process metamodeling to sample from posterior distribution including monotonicity information in the monovariate case.
Let $y = f(x)$ be a monotonic increasing function where the input x is assumed to be scalar and in the domain $[0, 1]$. We consider a set of computer experiments $\{(x_i, y_i) \mid i = 1, \cdots, n\}$ of size n and assume that

$$y_i = f(x_i),\ 1 \leq i \leq n. \tag{1}$$

Also suppose that $\mathcal{M}$ is the space of increasing functions and $(Y_x)_{x\in[0,1]}$ is a zero-mean Gaussian process (GP) with kernel $k(x, x')$ given by a priori knowledge about the relationship between the input x and the output y. The following experimental results (see figures below) are obtained with the classical Gaussian kernel.
We are interested in the simulation of the conditional (or posterior) distribution of the GP Y given data and monotonicity information

$$\begin{array}{l} Y_{x_i} = y_i,\ 1 \leq i \leq n, \\ Y \in \mathcal{M}. \end{array} \tag{2}$$

The important step is to approximate the GP by a finite-dimensional GP Y^N

$$Y_x^N = \sum_{j=1}^{N} \xi_j \phi_j(x), \tag{3}$$

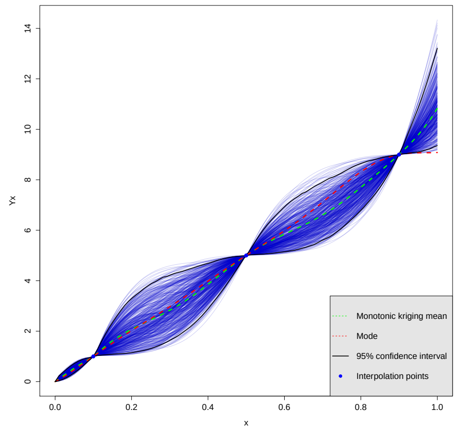
in which $\xi = \begin{pmatrix} \xi_1 \\ \vdots \\ \xi_N \end{pmatrix}$ is a zero-mean Gaussian random vector with covariance matrix Γ_N.

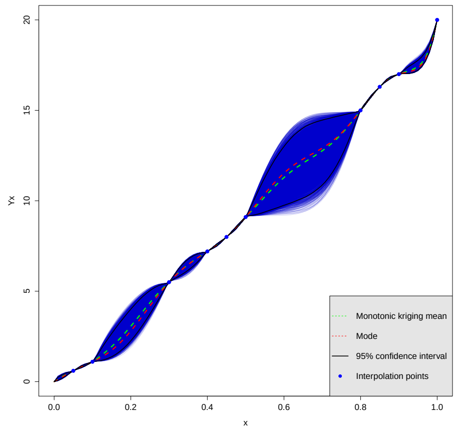
Such a decomposition can be seen as a Karhunen-Loève approximation of the process Y where the deterministic basis functions ϕ_j $(1 \leq j \leq N)$ are chosen in the space $\mathcal{M}$ of increasing functions and where random coefficients ξ_j partially reflect the randomness of the Gaussian process Y.
Due to the special choice of the basis functions ϕ_j, the crucial property here is that Y^N should be a monotonic increasing function **if and only if** the N coefficients ξ_j are all nonnegative. Now, we are

mainly interested in the new formulation of the problem : simulate the conditional distribution of the random Gaussian vector ξ given

$$\begin{array}{ll} \sum_{j=1}^{N} \xi_j \phi_j(x_i) = y_i,\ 1 \leq i \leq n & \text{(n interpolation linear equations)} \\ \xi_j \geq 0,\ 1 \leq j \leq N & \text{(N inequality conditions)} \end{array} \quad (4)$$

The advantage of such a methodology is that any posterior sample of the vector ξ leads to a monotone interpolating function. By a Monte Carlo technique, the conditional mean value of the function could be computed and be thought as the conditional monotone kriging mean. The conditional monotone kriging variance and confidence bounds can be calculated as well.





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