Non-stationary Gaussian process modelling and sequential design of experiments for exploration of high variation regions

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Abstract:

Gaussian Process (GP) models are commonly used for predicting response surfaces of expensive computer experiments $f : D \in \mathbb{R}^d \to \mathbb{R}$. The model is obtained by conditioning the prior distribution of a GP on a set of evaluations. Appropriate prior covariances allow to incorporate certain types of information in the model [5]. Besides, GP models are very useful in sequential design of experiments, notably using variance-based criteria for choosing the next evaluations. Standard settings, i.e. with a stationary GP model and a variance based criterion, do not account for heterogeneous variations of the response across the input space. In this work, we focus on approximating functions with heterogeneous variations, a situation encountered in many cases, for instance in mechanical test cases addressed by IRSN in nuclear safety contexts, where responses can behave very differently depending on regions of the input space. We develop methods that involve kernel as well as criterion aspects.

Our first contribution is the development of a new family of non-stationary covariance functions for GP modelling in cases where the function's behaviour varies along unknown preferential axes. The structure of the covariance is based on a warping T of the input space (non-linear map method [6], [1]): $c(\boldsymbol{x}, \boldsymbol{x}') = k_\beta(T(\boldsymbol{x}), T(\boldsymbol{x}'))$, with k_β a covariance function on $\mathbb{R}^p \times \mathbb{R}^p$, usually stationary, and T a function from D to $\mathbb{R}^p$. Without restrictions on T, model estimation becomes a numerical burden as d increases. Our model generalises two existing ones, axial warping [8] and Multiple Index Model (MIM) [7]. We investigate mathematical properties of the kernel and propose a heuristic for building the model in a high dimension case. Results show that the model is able to capture orientation and size of regions with high variations.

We also propose criteria functions based on the distribution of the gradient of the GP model. These new criteria, named GNV and IGNV for (Integrated) Gradient Norm Variance, allow a trade-off between focusing in high variation zones and making a global exploration. Analytical calculations are performed and complemented by efficient approximations where necessary, in order to mitigate the computational burden of criteria maximization.

Finally we apply all combinations of the considered criteria and models on a test case from a simulator of fracture dynamics [4] (see the figure). Two associations take out in terms of prediction quality: our new model with classical variance-based criteria (MSE and IMSE) and a stationary model with the proposed gradient-based criteria. Our model was compared with the efficient method of Bayesian Treed Gaussian Process model (TGP [2]). In this case, validation procedures show that our model is the most reliable. But in a fluid dynamics application of higher dimension

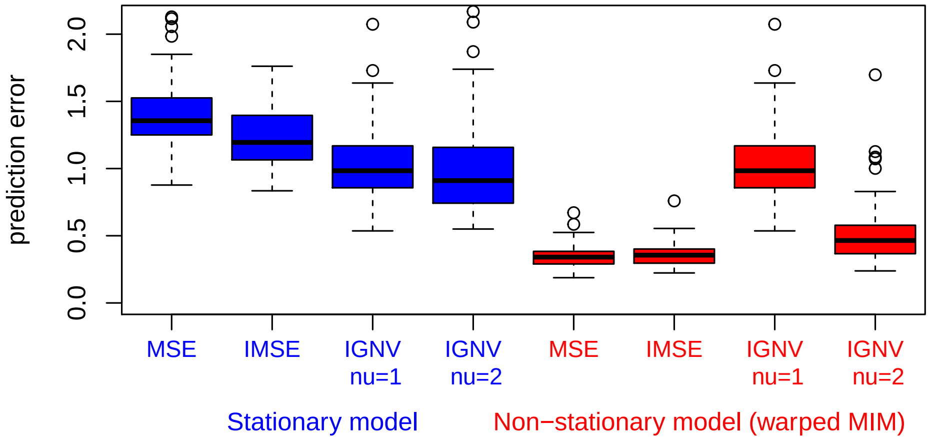

Figure: Prediction error (IRSN test case), after sequential designs of experiments. Results vary according to the model (stationary or the proposed non-stationary model), and to the criterion. Ten points are added to initial space-filling designs of size 20. The quantiles correspond to the random drawing of 100 initial designs.

from NASA [3], TGP remains the best competitor in most configurations, which suggests directions of improvement for our proposed model, some of which being currently investigated.

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Short biography – I have studied engineering and applied mathematics at École des Mines de Saint-Étienne. I am doing a joint Ph.D. between University of Bern and École Centrale Marseille, funded by the IRSN. After a year at the Institute of Mathematical Statistics and Actuarial Science in Bern (IMSV), I am now continuing my research activities in a laboratory of the IRSN (LIMAR, Cadarache, France).