Two advances in Gaussian Process-based prediction and optimization for computer experiments

David Ginsbourger ginsbourger@gmail.com
University of Neuchâtel (Institute of Mathematics & Institute of Hydrogeology)
and Ecole Nationale Supérieure des Mines de Saint-Etienne

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The approximation and optimization of costly numerical simulators often relies on a surrogate model, or *metamodel*, built on the basis of a design of experiments [6, 10]. If many kinds of approximation techniques exist [3], Gaussian Process Regression [8] (Kriging) has become very popular in computer experiments, in particular because it allows the definition of probabilistic criteria for sequential exploration [4]. For instance, Kriging-based optimization algorithms —like the *Efficient Global Optimization* algorithm (EGO [5])— take advantage of the Kriging variance in order to force exploration outside the already visited zones. After recalling some basics of Kriging and giving an illustrated introduction to the EGO algorithm, we will propose a discussion on some recent issues, respectively in Kriging model selection and in the design of probabilistic exploration criteria dedicated to parallel optimization. More precisely the two following points will be developed:

1. **Parallelizing EGO [2]:** we investigate a multipoint optimization criterion, the q-EI, aimed at choosing $q \in \mathbb{N}^*$ points at the same time. In particular, we propose different ways to parallelize EGO. Derivations are performed within the framework of Gaussian processes [8, 3]. Since directly optimizing the q-EI becomes extremely expensive as q and d (the dimension of inputs) grow, we propose two nearly optimal sequential procedures called the "Kriging Believer" and the "Constant Liar". The q-EI criterion can then be used to select between candidate designs. Finally, the efficiency of our approach is illustrated through classical optimization test problems.

2. **Taking physical symmetries into account within Kriging [1]:** Learning a deterministic function using a gaussian process relies on the selection of a covariance kernel. When some prior information is available concerning symmetries of the function to be approximated, it is clearly unreasonable not to use it in the choice of the kernel. We propose a characterization of the kernels which associated processes have their paths invariant under the action of a finite group of transformations [7].

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