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Maximin Design on Non-Hypercube Domain and Kernel Interpolation

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Abstract

In computer experiment framework, the choice in a design of experiments is an important concern. When there is no information about the black box function to be approximated, an exploratory design is usually taken. Two well-known exploratory criteria are minimax and maximin. In a hypercube the standard strategy consists of taking a maximin design within a class of Latin hypercube designs. However, in a non hypercubic context, it does not make sense to use the Latin hypercube sampling.
A theoretical justification to maximin and minimax criteria with regard to the kernel interpolation is first provided. Then, a simulated annealing algorithm is proposed in order to find a maximin design in any bounded connected Domain.

Keywords : maximin, minimax designs; Kernel Interpolation; Kriging; Computer experiments; simulated annealing.

1. Main text

In order to approximate an expensive black-box function, on a set $D \subset \mathbb{R}^d$, from a limited number of evaluations $\{f x_1, \dots, f x_N\}$ where $X=\{x_1 \dots x_N\}$ is a design of numerical experiments, a kernel interpolation is used. The kernel interpolant provides the same approximation than the Kriging predictor. However, the framework of kernel interpolation (see Schaback, 2007), allows to ensure a pointwise convergence under a condition on the dispersion of the points of the design X.

Let K be a positive definite kernel. $S_X^K f$ denotes the kernel interpolant of the function f on the set of points X. Thanks to works from R. Shaback and H. Wendland (Schaback, 1995 and Wendland, 2005), it is proved that for a large class of kernels defined by radial basis functions,

$$\sup_{x\in D} | f x - S_X^K f x | \leq \| f \|_K \, G_K h_X \tag{1}$$

where $\| f \|_K$ is the norm of f in the functional space associated to K, G_K is an increasing function which tends to 0 when h tends to 0 and

$$h_X = sup_{y\in D} min_{j\in\{1,\dots,N\}} \| y - x_j \|^2 \tag{2}$$

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A minimax design is defined as the design that minimizes h_X. Hence, using this kind of design with kernel interpolation guarantees the convergence of the approximation on the set D. Nevertheless, it is unfortunately too expensive to compute this criterion when the dimension is larger than 3. Thus, it is too costly to try to obtain a minimax design. It is then shown that a maximin design ensures also the convergence and that a maximin design is tractable. A design is said to be maximin if it maximizes

$$\delta_X = min_{\{i,j\in\{1,\dots,N\}\}} \parallel x_i - x_j \parallel \quad (3)$$

and the number of pairs of points which realize this distance is minimal. The convergence is ensured since $\delta_X \geq h_X$.

In the case where D is a hypercubic domain, Morris and Mitchell (1995) proposed an algorithm, based on simulated annealing, whose the goal is to reach a maximin design within a class of Latin hypercube designs. Latin hypercube sampling guarantees good projection properties on any axis and maximin designs guarantee that the point are well spread in the domain.

If D is not hypercubic but only enclosed in a hypercubic set, projection properties are not sensible. Only exploratory properties are to be focused on, that is why we propose an algorithm to achieve a maximin design in this kind of domain. This algorithm is also based on simulated annealing. The main difference between the algorithm of Morris and Mitchell and our algorithm is that their algorithm seeks a Design in a finite space of states (the Latin hypercube Designs with N points) while our algorithm has D^N as space of states. Our algorithm has a proposal distribution which is adapted to the objective function i.e. to maximize $X \to \delta_X$.

The simulated annealing aims at finding a global extremum of a function by using a Markovian kernel which is the composition of an exploratory kernel and an acceptance kernel depending on a temperature which decreases during the iterations. It is based on a Metropolis Hasting-algorithm. At a fixed temperature, the Markov chain tends to a stationary distribution which is the Gibbs measure. As the temperature decreases, the Gibbs measure concentrates on the global extremum of the function (Bartoli and Del Moral, 2001). Hence, the simulated annealing algorithm provides a Markov chain which tends to concentrate on a global extremum of the function to be optimized with a high probability. The convergence in probability of our algorithm is proved and its efficiency is tested on several examples.

2. References

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