PhD thesis offer

Title : Spectral methods and non-stationary kernels in computer experiments

Domain : Applied mathematics

PhD advisors:

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PhD starts: october 2012
Location: Ecole Nationale Supérieure des Mines de Saint-Etienne, Institut Camille Jordan
Salary: ~ 1600 euros/month (net)

Scientific context

Computer experiments aim at studying costly industrial computer codes such as car crash-test simulators, neutronic softwares, numerical flow simulations for aircraft design, etc. (see [Fang, Li, Sudjianto 2006], or [Santner, Williams, Notz, 2003]). For many real world problems, input space exploration, sensitivity analysis or optimization are impossible since they require too much time. An engineering method, known as surrogate modeling or response surface modeling, is then used to approximate the numerical model while being computationally cheaper to evaluate. At this point, positive definite kernels play a central role as in (general) functional approximation methods ranging from regularization techniques within the theory of RKHS (Reproducing Kernel Hilbert Spaces) to Gaussian Process Regression or Kriging. Recently, has been raised the interest of unusual spectral methods. In [Picheny, 2009], followed by [Le Gratiet et al., 2012], a close connection has been made between the design of experiments under a constant budget assumption and the spectral representation of Hilbert-Schmidt operators. In addition, promising results have been obtained with non-stationary kernels which allow taking into account some problem specificities such as symmetric response surfaces ([Ginsbourger, 2012]). In the same way, a theoretical Kriging formula for kernel-based interpolation has been given through the spectral decomposition of a Hilbert-Schmidt operator and a probability measure on the set of known function values ([Gauthier, 2012]).

Objectives

The objectives of this PhD are to extend the methodologies of response surfaces using spectral methods and non-stationary kernels. More precisely, two directions are going to

be explored:

- The spectral representation of Hilbert-Schmidt operators will be used to i) find optimal designs suited for kriging metamodeling, ii) build Gaussian process models in high dimensions
- The analysis of non-stationary kernels will be performed, allowing to add application-related knowledge to the kernel (symmetry, Dirichlet condition, …), and hence address a wider range of applications

References

- Fang, K.-T., Li R., and Sudjianto A. (2006), *Design and Modeling for Computer Experiments*, Chapman & Hall.
- Gauthier B. (2011), *Spectral Approach for kernel-base interpolation and conditional positivity*, PhD thesis, Ecole Nationale Supérieure des Mines de Saint-Etienne.
- Gauthier B., Bay X. (2012), *Spectral Approach for Kernel-based Interpolation*, The Annales de la Faculté des Sciences de Toulouse (in revision).
- Ginsbourger, D., Bay X., Roustant O., Carraro L. (2012), *Argumentwise invariant kernels for the approximation of invariant functions*, to appear in The Annales de la Faculté des Sciences de Toulouse.
- Le Gratiet, J. Garnier (2012), "Regularity dependence of the rate of convergence of the BLUP in a noisy kriging framework", Journées Mascot Num 2012, Poster, http://www.gdr-mascotnum.fr/mascot12.html
- Picheny V. (2009), *Propagation d'incertitudes dans les grands codes de calcul modélisés par surfaces de réponses*, Thèse de doctorat en co-tutelle avec l'université de Floride.
- Santner, T., Williams B., and Notz W. (2003), *The Design and Analysis of Computer Experiments*, Springer-Verlag.

Expected results

Methodological improvements in the design and modeling of computer experiments.

Candidate profile

Pure or Applied mathematics : statistics (regression, …), probability (Banach-valued random functions), functional analysis (Banach spaces theory), spectral theory of operators (Hilbert-Schmidt theory, Fourier analysis, …), complex analysis (Hardy spaces)

Programming skills (R).

Interest for computer experiments and their academic or industrial applications.