

PhD Offer

Metamodeling and robust optimization – application to ideotype design under climatic uncertainty

General information

- Period : October 2016 – October 2019
- Location: MIA-T, INRA (Toulouse)
- Advisors: Victor Picheny and Robert Faivre (INRA Toulouse) and Aurélien Garivier (IMT, Université Paul Sabatier, Toulouse)
- Contacts : victor.picheny@toulouse.inra.fr, robert.faivre@toulouse.inra.fr, aurelien.garivier@math.univ-toulouse.fr
- Funding : of the order of 24K€ / year gross salary

Applicant Profile

Candidates should have completed a Master in applied mathematics, statistics, machine learning, or engineering with a mathematical background. The applicant should demonstrate both theoretical and computational skills. Implementations in R are expected.

Key-words

Surrogate model – Gaussian process- Bayesian optimization – EGO – computer experiments – noise

Context and motivation

Using complex numerical models for prediction, risk assessment or design has become an essential tool in numerous fields, including engineering, economy or in natural sciences. Often times, the modeled systems depend on uncertain environments that greatly influence the quantities of interest : typically in agronomy, an annual yield or environmental impact depend on the climatic conditions at hand [1]. It is then necessary to design methods that account for uncertain environments, in particular by integrating risk-aversion concepts.

This PhD focuses on metamodel-based optimization (also referred to as Bayesian optimization), and in particular on Gaussian process regression, which efficiency has been empirically demonstrated numerous times over the last 15 years [2]. The research domain is hence multi-disciplinary, at the intersection between applied mathematics, statistics and *machine learning*.

PhD objectives

Metamodel-based optimization under uncertainty has retained a growing attention over the past few years, following the emergence of complex simulators that depend on stochastic processes. However, if several solutions have been proposed when average performances are optimized [3], solutions are scarce as soon as risk-aversion strategies are sought.

The objective of this PhD is first to propose new metamodeling approaches allowing to consider either several risk levels at once, or the entire distribution of the quantity of interest. Among possible starting points, the student may focus on vectorial prediction for several risk indices (*co-kriging*, [4]), or functional predictors [5]. Secondly, sampling strategies based on these metamodels may be developed to achieve optimization. Those approaches could either be heuristic (in the spirit of [2,3]) or based on recent convergence results [6,7].

The approaches developed may be validated on an agronomical problem : the ideotype design of sunflower crops, based on the SUNFLO model [8].

References

- [1] Debaeke P. et Quilot-Turion B. (eds) (2014). Conception d'idéotypes de plantes pour une agriculture durable. Collection École-chercheurs INRA, FormaSciences, FPN, INRA-CIRAD (ISBN 2-7380-1347-3), 254p.
- [2] Jones, D. R. (2001). A taxonomy of global optimization methods based on response surfaces. *Journal of global optimization* 21, 345–383
- [3] Picheny, V., Wagner, T., Ginsbourger, D., (2013). A benchmark of kriging-based infill criteria for noisy optimization. *Structural and Multidisciplinary Optimization*, 48(3), 607-626
- [4] Rougier, J., (2008). Efficient emulators for multivariate deterministic functions. *Journal of Computational and Graphical Statistics*, 17(4), 827-843
- [5] Plumlee, Matthew, and Rui Tuo. "Building accurate emulators for stochastic simulations via quantile Kriging." *Technometrics* 56.4 (2014): 466-473.
- [6] Srinivas N., Krause A., Kakade S. and Seeger M. (2012), Information-Theoretic Regret Bounds for Gaussian Process Optimization in the Bandit Setting, *IEEE Transactions on Information Theory*, 58(5),3250-3265
- [7] Bubeck S., Munos R., Stoltz G., Szepesvari C. (2011), X-armed bandits, *Journal of Machine Learning Research*, 12, 1655-1695
- [8] Casadebaig P., Guilioni L., Lecoœur J., Christophe A , Champolivier L., Debaeke P., (2010). SUNFLO, a model to simulate genotype-specific performance of sunflower crop in contrasting environments. *Agricultural Forest Meteorology*, 151(2), 163-178