Optimization Under Uncertainties for Multi-Fidelity Black-Box Simulators

G. Pierron[†,1,2], M. R. El Amri[✠,2], C. Helbert[§,1], G. Perrin[§,3], D. Sinoquet[✠,2]

[†] PhD student (presenting author). [§] PhD supervisor. [✠] PhD advisor.

PhD expected duration: Oct. 2025 – Sep. 2028

[1] Institut Camille Jordan, Centrale Lyon
{celine.helbert, guillaume.pierron}@ec-lyon.fr

[2] IFP Énergies Nouvelles
{mohamed-reda.el-amri, guillaume.pierron, delphine.sinoquet}@ifpen.fr

[3] Université Gustave Eiffel
guillaume.perrin@univ-eiffel.fr

Abstract

We consider a complex physical system $\mathcal{S}$, depending on a controllable parameter $\mathbf{x} \in \mathcal{D}_X \subset \mathbb{R}^{d_X}$ and on an uncontrollable parameter $\mathbf{u} \in \mathcal{D}_U \subset \mathbb{R}^{d_U}$. We consider that $\mathbf{u}$ is an output of a random variable $\mathbf{U}$, defined on a universe $(\Omega, \mathcal{A}, \mathbb{P})$ and with support equal to D_U.

We want to optimize the system $\mathcal{S}$, by tuning the parameter $\mathbf{x}$. More precisely, we consider a feature $F^{(\infty)}(\mathbf{x}, \mathbf{u})$ of our system, and we aim to solve the optimization problem (1).

$$\arg\min_{\mathbf{x} \in \mathcal{D}_{\mathbf{X}}} \mathbb{E}\left[F^{(\infty)}(\mathbf{x}, \mathbf{U})\right] \tag{1}$$

For a given $(\mathbf{x}, \mathbf{U})$, we cannot directly compute $F^{(\infty)}(\mathbf{x}, \mathbf{U})$ as long as it depends on the system $\mathcal{S}$, whose physical equations are too complex to solve in closed form. Thus we must approximate our function of interest $F^{(\infty)}$ through a set of computer codes $\left(F^{(1)}, \cdots, F^{(L)}\right)$, so that, for $\ell \in \{1, \cdots, L\}$, the code $F^{(\ell)}$ simulates $F^{(\infty)}$ with the fidelity level ℓ, with the associated computational cost w_ℓ. We assume that $w_1 < \cdots < w_L$ (the lower the fidelity, the cheaper the simulator evaluation).

The practical optimization problem that we will try to solve is the following (2).

$$\arg\min_{\mathbf{x} \in \mathcal{D}_{\mathbf{X}}} \mathbb{E}\left[F^{(L)}(\mathbf{x}, \mathbf{U})\right] \tag{2}$$

An existing algorithm to address such a problem is a combination of two intricated loops :

- an outer optimization loop, which relies on the Efficient Global Optimization (EGO, developed in [2]) with objective function $f^{(L)} = \mathbb{E}\left[F^{(L)}(\cdot, \mathbf{U})\right]$, using a metamodel that can integrate uncertainties on each new observation (as we never can compute the exact value of the desired expectation).
- an inner estimation loop, which aims to estimate $f^{(L)}(\mathbf{x})$ for a new point $\mathbf{x}$, reducing the uncertainty of the estimation by evaluating many times the (costly) simulator $F^{(L)}$.

This methodology is very costly. The goal of this thesis is to learn how to use the low-fidelity codes, in order to have a better control on the uncertainties with the same computational expense for each iteration and to have better optimization results with the same total cost.

Several strategies could allow us to make use of these lower-fidelity simulators.
One possible way could be the modelization of all the fidelity levels, taking into account the difference of costs, in a mutli-fidelity metamodel (similar to that introduced in the PhD thesis of Loic Le Gratiet [3]) on which it could be possible to build specific acquisition functions.

Another approach keeps stucking to the only modelization of $F^{(L)}$, but uses the low-fidelity codes as control variates [1]. The first part of my PhD work is to explore this approach. An existing elegant method, named Multi-Fidelity Monte-Carlo (MFMC), and developed in [4], allows to minimize the variance of the estimator of our objective function, with a fixed cost budget, by tuning a control-variate coefficent and an allocation of the budget to the different fidelity levels. We want to plug this method in our Bayesian optimization loop.

This existing method assumes that we already know at least some coefficients of the covariance matrix of the random vector $\left(F^{(\ell)}(\mathbf{x}, \mathbf{U})\right)$ for any design point $\mathbf{x}$. We will try to move beyond this strong hypothesis, and we aim to see if it is still possible to obtain better optimization results than with the simple Monte-Carlo method on the high-fidelity simulator.

Short biography (PhD student)

My background is a master's degree on statistics and probability. My PhD thesis is partly funded by the CIROQUO consortium, which is a partnership between researchers and industrial companies to address issues raised by the high costs of data in optimization and uncertainty quantification. I am an employee of IFP Énergies Nouvelles for 3 years, and I am also enrolled as a PhD student in Centrale Lyon.

References

[1] Zdravko Botev and Ad Ridder. Variance Reduction. In *Wiley StatsRef: Statistics Reference Online*, pages 1–6. John Wiley & Sons, Ltd, Chichester, England, UK, November 2017.

[2] Donald R. Jones, Matthias Schonlau, and William J. Welch. Efficient Global Optimization of Expensive Black-Box Functions. *J. Global Optim.*, 13(4):455–492, December 1998.

[3] Loic Le Gratiet. *Multi-fidelity Gaussian process regression for computer experiments.* PhD thesis, Université Paris-Diderot - Paris VII, Paris, France, October 2013.

[4] B. Peherstorfer, K. Willcox, and M. Gunzburger. Optimal Model Management for Multifidelity Monte Carlo Estimation. *SIAM J. Sci. Comput.*, 2016.