M2 internship with possibilty of a PhD thesis
(in partnership with Transvalor)

Bayesian optimization for computer simulations and inverse problems

Nov. 2021

Keywords—Applied math.; optimization; Bayesian methods; design of numerical experiments; machine learning; non-parametric statistics; uncertainty quantification.

Context

Computer simulations are used to predict physical phenomena, or to maximize the performance of systems, to make them safer and more environmentally friendly... However, the simulation of a large system generally requires significant computing resources, and despite availability of high performance computers, the high computation times require to conduct numerical simulations sparingly and efficiently.

Gaussian process modeling [6] is a supervised learning method that can be used for predicting the results of numerical simulations at low cost, and thus enables the selection of simulations that maximize a given utility function. The principle consists in seeing a numerical simulator as a function and choosing a prior distribution for this function, expressed as a Gaussian random process. By computing posterior distributions, one can predict the result of a future numerical simulation, or estimate quantities of interest such as a probability of exceeding a threshold, or a maximum.

This approach, which is Bayesian in nature [1], is commonly used to optimize functions that are expensive to evaluate. This type of optimization method is known as *Bayesian optimization* (see for example, [2, 3, 5, 9]).

Objectives

In this internship, we shall start with a very simple problem: to predict the response of a numerical simulator modeling the physical properties of a material; this prediction is made on the basis of training data obtained from numerical simulations.

The next objective is to identify the values of the inputs of the numerical simulator that yield given outputs. This inverse problem will be formulated as an optimization problem, where Bayesian optimization techniques will be used.

From a more theoretical point of view, many results about Gaussian process come from the theory of reproducing kernel Hilbert spaces [4, 7, 8]. Here, we will be interested in the study of the convergence rates of the approximations obtained as a function of the dimension of the parameter space.

Practical information

This internship can lead to a PhD recruitment on the use of Bayesian approaches for computer experiments, optimization and inverse problems (study from both a theoretical and applied point of view, using Gaussian processes or Bayesian neural networks).

Throughout the project, regular updates will be made with Transvalor, a world leader in the simulation of material forming processes, providing funding for this internship. Transvalor is a French company, founded in 1984, whose headquarters are located in Sophia Antipolis, France.

- Duration: 5 to 6 months internship
- Place: L2S, CentraleSupelec, Paris-Saclay University, France
- Supervisors: Frédéric Magoules (Professor at MICS) and Emmanuel Vazquez (Professor at L2S)
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References

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