Calibration of computer models with Bayesian global optimization
Project for MSc Scientific Computing and Data Analysis (G5K609)

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Description

Computer experiments often use computer models (simulators) to simulate the behavior of a complex real system under consideration. Simulators often include additional calibration parameters that regulate their behavior. It is important to find optimal values for these parameters, as well as to quantify their uncertainty through probabilities, in order to improve the predictive ability of the simulator, or in order to better understand a physical phenomenon associated with a specific parametrization. Such computer models are expensive to run several times, and hence traditional optimisation algorithms cannot be applied. Here, by expensive, we mean in time, money, etc...

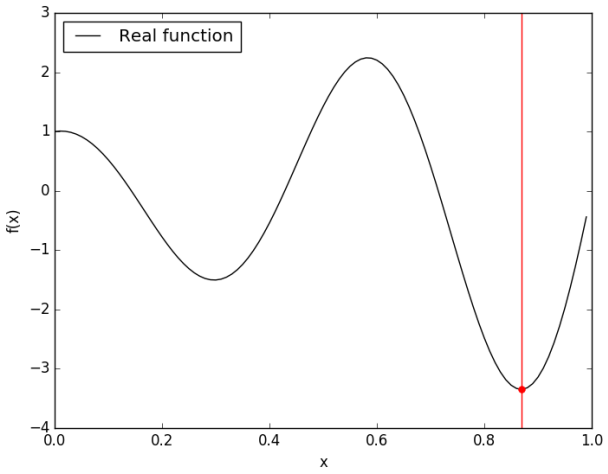
Bayesian global optimization (BGO) aims at optimizing objective functions which are extremely expensive to be directly evaluated many times, and whose analytic expression and derivatives may not be available. Hence, BGO is an important tool for the calibration and analysis of real world applications in engineering, biology, etc....

- Consider a function $f(x) = \exp(1.4x)\cos(3.5\pi x)$ with minimum $f_{\min} \approx -3.3470$ at location $x_{\min} \approx 0.8686$.

  on the right $\longrightarrow$

- Pretend, we do not know the equation of $f(\cdot)$.
- Assume that we wish itsto find its minimum and minimum location by BGO.
- To see the BGO in action, discovering the global minimum and recovering the real function, click [HERE].

  Red dots: the samples; Blue lines: the recovered function and error bounds; red line: the acquisition function.



Anticipated Outcomes:

Students who will work on this project are expected to be able to:

- work in the Bayesian statistics framework
- explain, design, and apply Gaussian Process emulators
- calibrate expensive computer models against data-sets
- implement Python and use modules such as pyMC, GPy

References

- Brochu, E., Cora, V. M., & De Freitas, N. (2010). A tutorial on Bayesian optimization of expensive cost functions, with application to active user modeling and hierarchical reinforcement learning. arXiv preprint arXiv:1012.2599. [LINK]
- Snoek, J., Larochelle, H., & Adams, R. P. (2012). Practical Bayesian optimization of machine learning algorithms. In Advances in neural information processing systems (pp. 2951-2959) [LINK]
- Mockus, J. (1975). On Bayesian methods for seeking the extremum. In Optimization Techniques IFIP Technical Conference (pp. 400-404). Springer Berlin Heidelberg. [LINK]