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An Introduction to Bayesian Optimization

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In this talk, we delve into the foundational principles of Bayesian optimization, a method particularly well-suited for optimizing deterministic or stochastic functions, whether scalar or vectorial, especially when the evaluation of the function is computationally expensive and no gradient information is available.

Bayesian optimization is particularly relevant in the domains of Design and Analysis of Computer Experiments (DACE) and Uncertainty Quantification (UQ). In these areas, it is typically applied to minimize costs or maximize performance through complex computer simulations, including those utilizing Partial Differential Equations and finite element methods. Additionally, Bayesian optimization has become increasingly popular in Machine Learning and Artificial Intelligence for optimizing parameters in learning procedures, highlighting its versatility and effectiveness across a range of fields.

At the core of Bayesian optimization is the practice of modeling the target function using the Gaussian process framework. This modeling approach enables the construction of a sampling criterion, also known as an acquisition function. We will examine various classic sampling criteria, including the widely-used Expected Improvement (EI) criterion, and discuss the concept of Stepwise Uncertainty Reduction (SUR). Our discussion will focus on how Bayesian optimization effectively manages the balance between exploration and exploitation.

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