ST 441: Probability, Computing and Simulation, Fall 2020

Exploratory Bayesian Optimization

Project Proposal

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I. Research Objectives

The purpose of this project is to gain a deeper understanding of Bayesian Optimization and its practical application in data analysis and simulation. Bayesian Optimization is an increasingly popular topic in the field of Machine Learning. It allows us to find an optimal hyperparameter configuration for a particular machine learning algorithm without too much human intervention. Bayesian Optimization has several advantages compared to other optimization algorithm. The first advantage of Bayesian Optimization is that it does not require hand-tuning or expert knowledge, which makes it easily scalable for larger, more complicated analysis. The second advantage of Bayesian Optimization is when evaluations of the fitness function are expensive to perform. If the fitness function f is cheap to evaluate we could sample at many points e.g. via grid search, random search or numeric gradient estimation. However, if function evaluation is expensive e.g. tuning hyperparameters of a deep neural network, probe drilling for oil at given geographic coordinates or evaluating the effectiveness of a drug candidate taken from a chemical search space then it is important to minimize the number of samples drawn from the black box function f.

II. Outline of Approach

Here are the steps that I'm going to approach this project:

1) **Gaussian Process:** First, I'm going to do a research about Gaussian Processes and find an implementation of the algorithm.
2) **Bayesian Optimization**: Next, I'm going to get a better understanding of the relationship between Gaussian Process and Bayesian Optimization and implement it as well.
3) **Dummy function:** After that, I'm going to test my implementation of Bayesian Optimization on a dummy fitness function f, to check if it's working correctly.
4) **Practical Application:** Finally, I'm going to apply my implemented Bayesian Optimization on a real world problem.

REFERENCES

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[3] Donald R. JonesMatthias SchonlauWilliam J. Welch, “Efficient Global Optimization of Expensive Black-Box Functions.“

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