# Notes on Bayesian Optimization for Multi-Objective Optimization

compiled by D. Gueorguiev 12/25/23

## Overview of Bayesian Optimization in Single- and Multi- Objective Optimization Problems

Mathematical Formulation:

We are considering the problem of finding a global maximizer (or minimizer) of an unknown objective function :

(1)

where is some design space of interest; In global optimization, is often a compact subset of but the Bayesian optimization framework can be applied to diverse search spaces which involve categorical or conditional inputs or even combinatorial search spaces with multiple categorical inputs.

Furthermore, we will assume that the unknown aka *blackbox* function has no simple closed form, but it can be evaluated at any arbitrary query point in the domain . This evaluation produces noise-corrupted (stochastic) outputs such that . In other words, we can only observe the function through unbiased noisy point-wise observations .

We notice that in order to solve (1) we need to know something about .

Although, this is the minimum requirement for Bayesian optimization, when gradients are available, they can be incorporated in the algorithm as well. If we apply the Bayes theorem for the two random quantities and we can write:

(2)

Notice that the factor is subsumed in the right-hand side of (2).

Out prior belief about how likely various functions are, and our collection of observations of the function, which give us insight into the specific we are dealing with. We can use the accumulating knowledge about to find the that solves out problem. More realistically, we can use the knowledge to help us approximately solve our problem , or perhaps just get ourselves headed in the right direction.

The Optimization methods that take this probabilistic approach are known as “Bayesian optimization” methods. These methods are unique in that they retain all accumulated data about the function and use all of it to determine where to search next.

### A bit of Background on classical Optimization

As we mentioned earlier, the original problem posed with (1) is too broad for our purposes. We will restrict ourselves to and . We will suppose that is compact, and that is Lipschitz-continuous i.e. , for some constant . This is sufficient to guarantee that a solution exists, i.e. .

# Bibliography

Bobak Shahriari, e. a. (2016). *Taking the Human Out of the Loop: A Review of Bayesian Optimization.* Retrieved from www.cs.ox.ac.uk: https://github.com/dimitarpg13/optimization\_classification\_regression/blob/main/literature/articles/multi-objective\_Bayseian\_optimization/Taking\_the\_Human\_Out\_of\_the\_Loop-A\_Review\_of\_Bayesian\_Optimization\_Shahriari\_UBC\_2016.pdf

Lizotte, D. J. (2008, Sep 1). *Practical Bayesian Optimization .* Retrieved from https://www.csd.uwo.ca/~dlizotte/publications: https://github.com/dimitarpg13/optimization\_classification\_regression/blob/main/literature/articles/multi-objective\_Bayseian\_optimization/PracticalBayesianOptimization\_lizotte\_phd\_thesis\_2008.pdf

Majid Abdolshah, e. a. (2019, Dec 8). *Multi-objective Bayesian optimisation with preferences over objectives.* Retrieved from https://proceedings.neurips.cc/: https://github.com/dimitarpg13/optimization\_classification\_regression/blob/main/literature/articles/multi-objective\_Bayseian\_optimization/NeurIPS-2019-multi-objective-bayesian-optimisation-with-preferences-over-objectives-Paper.pdf

Shinya Suzuki, S. T. (2020, July 13). *Multi-objective Bayesian Optimization using Pareto-frontier Entropy.* Retrieved from https://proceedings.mlr.press/: https://github.com/dimitarpg13/optimization\_classification\_regression/blob/main/literature/articles/multi-objective\_Bayseian\_optimization/Multi-objective\_Bayesian\_Optimization\_using\_Pareto-frontier\_Entropy\_Suzuki\_ICML\_2020.pdf

Takashi Wada, H. H. (2019, May 7). *Bayesian Optimization for Multi-objective Optimization and Multi-point Search.* Retrieved from arxiv.org: https://github.com/dimitarpg13/optimization\_classification\_regression/blob/main/literature/articles/multi-objective\_Bayseian\_optimization/Bayesian\_Optimization\_for\_Multi-objective\_Optimization\_and\_Multi-point\_Search\_Wada\_KobeSteel\_2019.pdf