Acquisition Functions

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Contents

1 Introduction **2**

2 Decision-Theoretic Acquisition Functions **3**

2.1 Expected Improvement (EI) 3

2.2 Probability of Improvement (PI) 3

2.3 Knowledge Gradient (KG) 3

2.4 Mutual Information (MI) and Entropy Search (ES) 3

3 Related Topics from Optimization **4**

3.1 Multi-Armed Bandits 4

3.2 Statistical Upper Bound (UCB) 4

3.3 Thompson Sampling 4

4 Constructing Acquisition Functions **5**

5 References **6**

1 Introduction

At the core of optimization is the **acquisition function** (also referred to as the **policy**) that decides where to observe next based on the available data. Since we are focusing on Bayesian optimization, we will consider acquisition functions that refer to our probabilistic beliefs about the objective function when making decisions likely to result in favorable outcomes. In previous notes, we examined utility functions which are used to assist the acquisition function evaluate candidate observations based on their potential to aid the optimization process. In these notes, we will discuss acquisition functions with a particular focus on the acquisition functions frequently used in Bayesian optimization and the common themes in their design.

In Bayesian optimization, there are two main approaches used in acquisition function design: decision-theoretic and multi-armed bandit-inspired. The **decision-theoretic** approach uses Bayesian decision theory and is the most prevalent approach in Bayesian optimization, see the *Bayesian Decision Theory* notes for background. Recall that Bayesian decision theory provides us with a framework to derive the (exact) optimal policy, although typically these are intractable and have little practical value. However, there are approximations to the optimal policy that are both tractable and practical and we will use those ideas to design acquisition functions that are also both tractable and practical.

Alternatively, we can apply algorithms for **multi-armed bandits** to the optimization setting. A multi-armed bandit is a finite-dimensional model of sequential optimization with noisy observations. In particular, we have an "agent" faced with a finite set of "arms" representing potential actions and corresponding stochastic rewards from unknown distributions for each arm. The agent must select a sequence of arms from the set with the sequence yielding the cumulative reward. Thus, we aim to design a policy that sequentially selects arms in a manner that maximizes the expected cumulative reward. We will extend this to model optimization such that algorithms with strong performance guarantees for multi-armed bandits can inspire high-performing acquisition functions for Bayesian optimization.

2 Decision-Theoretic Acquisition Functions

2.1 Expected Improvement (EI)

2.2 Probability of Improvement (PI)

2.3 Knowledge Gradient (KG)

2.4 Mutual Information (MI) and Entropy Search (ES)

3 Related Topics from Optimization

3.1 Multi-Armed Bandits

3.2 Statistical Upper Bound (UCB)

3.3 Thompson Sampling

4 Constructing Acquisition Functions

5 References

[1] Roman Garnett. 2023. *Bayesian optimization.* Cambridge University Press, Cambridge, United Kingdom ;