Introduction to Bayesian Optimization

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Contents

1 Introduction

Bayesian optimization refers to an optimization approach that uses Bayesian inference to guide the optimizer to make "better" decisions based on *uncertainty*. In addition, this approach provides a framework that enables us to strategically tackle the uncertainty inherent in all optimization decisions. One particularly attractive property of this framework is its *unparalleled* sample efficiency, a property we will discuss more in-depth later.

In these notes, the goal is to introduce Bayesian optimization from a high-level perspective and introduce the components involved in the "Bayesian optimization workflow". Additional notes discussing the components and related topics in detail are available in the `bayesian-optimization` repository and are linked below. We will begin with the motivation behind Bayesian optimization, primarily focusing on the theoretical motivation and examples of real-world Bayesian optimization applications.

1.1 Additional Notes

The links below lead to other notes in the `bayesian-optimization` repo, discussing the components in and topics related to Bayesian optimization.

- **Bayesian Decision Theory**
- **Gaussian Processes**
- **Covariance Functions and Kernels**
- **Model Evaluation and Selection**
- **Utility Functions**
- **Acquisition Functions**
- **Computing Acquisition Functions**
- **GP Regression**
- **GP Classification**

2 Motivation

2.1 Theoretical Motivation

First, we consider the theoretical motivation for the Bayesian optimization approach. Typically, the theoretical motivation steps from the form or type of *objective* (the "function" we are aiming to optimize). Note that the list below is by no means exhaustive; there exists additional theoretical motivation but these are seemingly the most common, particularly with regard to the form and characteristics of the objective.

- **Black-box objective functions** are functions that we can only interact with via its inputs and outputs meaning classical, analytical methods do not work. However, we can usually use Bayesian optimization to approximate such an objective and manage the inherent uncertainty.
- **Expensive-to-evaluate objective functions** are functions that require significant computation effort to obtain their output. However, just as with black-box objectives, we can use Bayesian optimization to approximate and model these efficiently.
- More generally, this approach is very useful when the objectives lack analytical evaluation (or, if analytical evaluation is expensive).
- In some spaces such as the discrete or combinatorial ones, the objective may not have efficient gradients (if they exist). Thus, classical gradient-based optimization methods are incompatible.

2.2 Applications

The application potential of Bayesian optimization can be seen across several critical domains, especially those attempting to accelerate the identification of solutions to real-world scientific and engineering problems. Some of these applications include:

- Drug discovery
- Molecule/protein discovery
- Materials design
- AutoML (i.e., hyperparameter tuning)
- Engineering decisions
- Many more...

The diagrams in the next few sections are there to illustrate how the Bayesian optimization approach is used in real-world applications. There will also be commentary explaining why the approach is so useful in these applications. Just as with the list above, this is not (in any way) an exhaustive review of applications. Rather, the point of these sections is to showcase the real-world motivation for this optimization approach.

Application: Drug Discovery

Figure 1 below shows an example of a chemical process optimization problem, common in drug discovery. In the left half of the figure, four common (classical) approaches are shown but these approaches are expensive. Alternatively, the Bayesian optimization approach is shown in the right half. That approach uses data from previous experiments to locate points that may optimize the unknown objective, while strategically handling uncertainty in the model. The located points will usually be used to plan future experiments as they represent samples of *high utility* (i.e., the point should be useful in optimizing the reaction parameter).

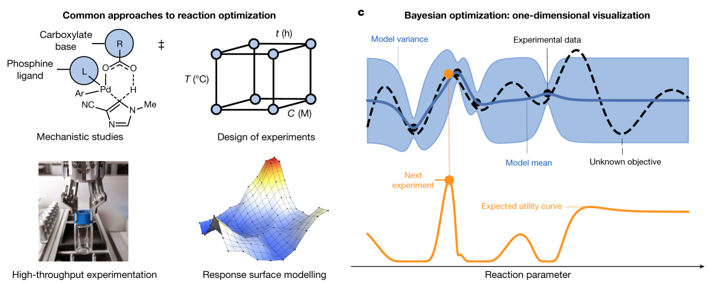


Figure 1: From *Bayesian optimization as a tool for chemical synthesis* by Shields et al. (2021)

Application: Molecule/Protein Discovery

In the field of molecule and protein design, there are similar considerations to the ones in the previous application: experiments are costly. Figure 2 shows the integration of the Bayesian optimization approach with experimentation. In most environments, scientists synthesize and test several different formulations to obtain a dataset. This dataset is used to help model the underlying objective and can be used to suggest new, promising formulations. Then, as shown in the figure, the new formulations are synthesized, tested, and added to the dataset so as to inform the model and optimizer of formulations to suggest next.

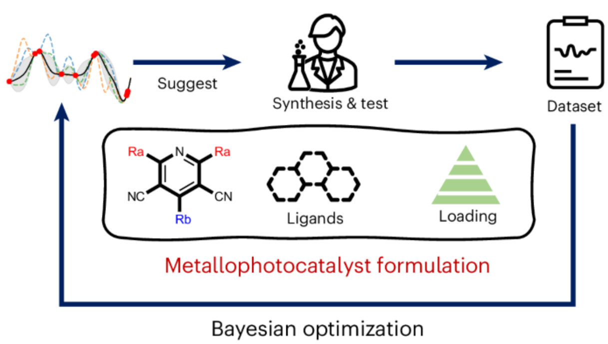


Figure 2: From *Sequential closed-loop Bayesian optimization as a guide for organic molecular metallophotocatalyst formulation discovery* by Li et al. (2024)

Application: Materials Discovery

Figure 3 is similar to the one for molecule/protein discovery but now it is showcasing some additional details specific to materials design and discovery. Again, the initial dataset is used to model the underlying objective and inform design exploration, with results from design exploration being used to augment the dataset. Additionally, in this particular example, the researchers also use the experiments to assist in calibrating a simulation of designs, another application of Bayesian optimization.

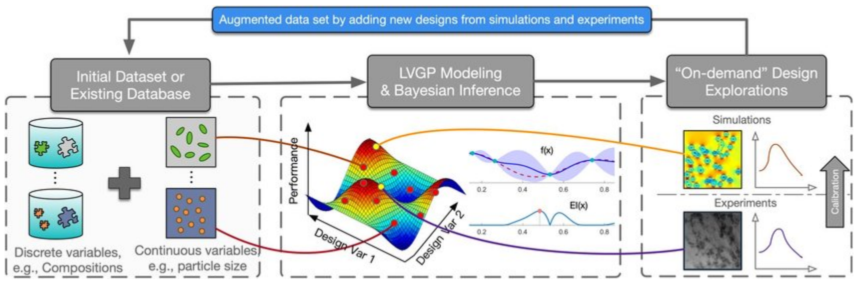


Figure 3: From *Bayesian optimization for Materials Design with Mixed Quantitative and Qualitative Variables* by Zhang et al. (2020)

Application: AutoML

Figure 4 shows a workflow to tune neural network hyperparameters using Bayesian optimization, specifically using a Gaussian process as a surrogate model. AutoML is the process of automating the machine learning workflow and typically includes tuning models' hyperparameters. We can use Bayesian optimization to perform this tuning in a more efficient manner by identifying the next set of promising hyperparameters based on the current model and its uncertainty.

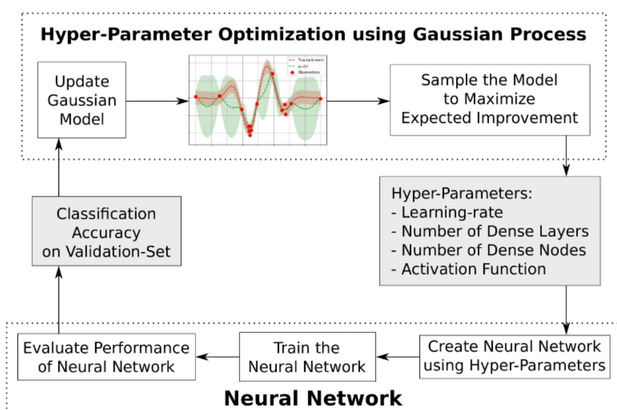


Figure 4: From *Achieve Bayesian optimization for tuning hyperparameters* by Edward Ortiz on *Medium* (2020)

Application: Engineering Decisions

Figure 5 shows how Bayesian optimization can be used to calibrate a particle accelerator in a similar manner to the previous applications. The "operator" inputs the target beam parameters while a camera inputs the observed beam parameters. Then, Bayesian optimization determines the changes (i.e., the next set of beam parameters) to ideally improve the calibration of the particle accelerator.

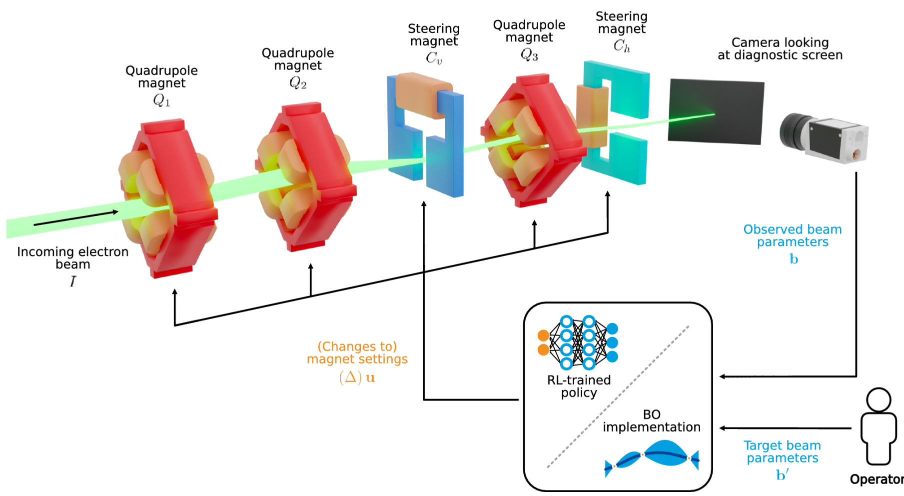


Figure 5: From *Reinforcement learning-trained optimizers and Bayesian optimization for online particle accelerator tuning* by Kaiser et al. (2024)

3 Optimization Foundations

Optimization is a process and field of study that aims to efficiently locate the optimal objective value and/or its location from the search domain and its corresponding objective values. In this section, we will introduce the foundations of optimization to understand the ideas that Bayesian optimization builds on. For a more thorough review of optimization, see Nocedal and Wright's *Numerical Optimization* book (in the Springer Series in Operations Research).

3.1 Formalization of Optimization

Let's first formalize a typical optimization problem. This formulation is a simple and flexible one for global optimization and is not inherently Bayesian. Additionally, it is also formulating a *continuous* optimization problem but there exists other "types" of optimization other than just continuous.

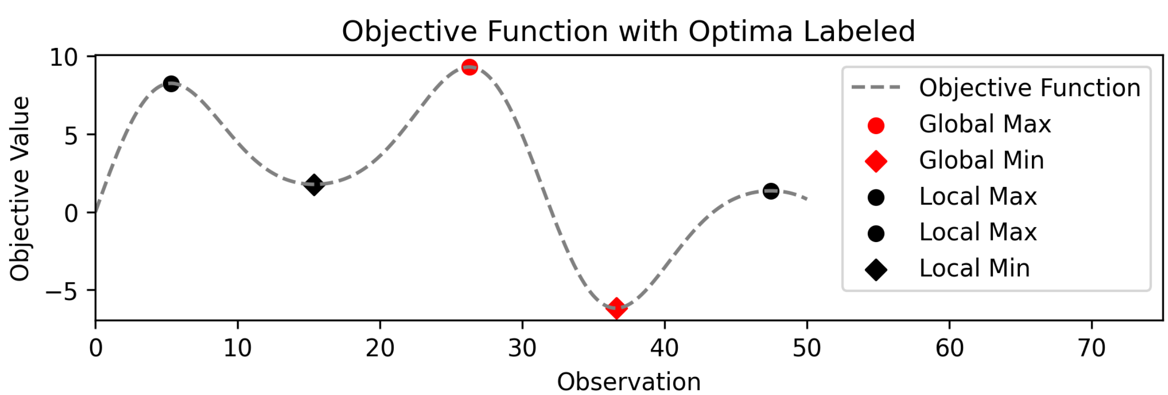
$$x^* \in \arg\max_{x \in \mathcal{X}} f(x) \qquad\qquad f^* = \max_{x \in \mathcal{X}} f(x) = f(x^*)$$

where $f : \mathcal{X} \to \mathbb{R}$ is a real-valued *objective function* on some domain $\mathcal{X}$, x^* is the point that obtains the global maximum value f^*. Note that the max versus min is arbitrary and depends on the specific problem.

Black-box optimization arises from the fact that we do not need to have an explicit objective function f but rather only some information about the objective at identified points.

The plot below shows an objective function with its *optima* labeled. **Optima** are the points that either maximize or minimize (optimize) the objective function. The objective function plotted below is given by

$$f(x) = 10\sin(0.2x)\cos(0.1x) + \sin(0.5x) + 0.05x$$

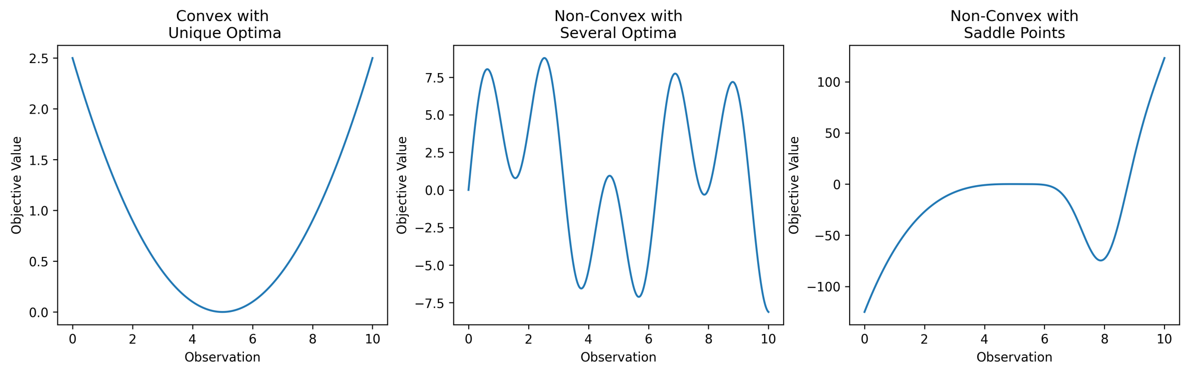


In the plot on the previous page, the optima were found by obtaining the values of the objective at every point in the *domain*. However, in optimization, we typically want to avoid such computations due to its expensiveness and rather use methods to find the optima in a more efficient manner. Furthermore, in the event we are dealing with *black-box optimization*, recall that we don't necessarily have an explicit objective but rather inputs and their corresponding outputs. That means that evaluating the objective function at each point in the domain is not only inefficient but effectively impossible.

3.2 Objective Functions

The **objective function** is the function that we want to optimize. For some problems, there is a mathematical model that can be developed to describe the objective. However, in many real-world applications, there is no analytical or mathematical model to describe the objective (one of the motivations for Bayesian optimization).

Some objective functions are convex with only a single, unique global minimum or maximum. Other functions are non-convex and might have several local optima or a flat region with many saddle points. The plot below shows these three general types of objectives.



While the plots showing non-convex objective functions pose difficulty to efficiently optimize such functions, there are other characteristics (listed below) of objective functions common in Bayesian optimization that also lead to issues.

- The objective is considered to be a *black-box* function meaning we can only interact with the objective via its inputs and outputs.
- The objective's returned value is *corrupted* by some sort of noise and does not represent the exact true objective value at that location.
- The objective has a *high cost* of evaluation and requires a sample efficient method to avoid expensive probing.
- There *do not exist gradients* (if we did, efficient gradient-based methods could be employed to locate and evaluate optima).

3.3 Observation Models

Observation models are similar to the idea of surrogate models used in the Bayesian optimization workflow but there are some key differences. The observation model is used to describe how the true objective is *observed*, usually accounting for some form of (additive) noise. On the other hand, the surrogate model is a probabilistic model (i.e., Gaussian process) used to approximate the unknown objective function.

Specifically, the **observation model** is an approach to formalize the relationship between the true objective function, the actual observation, and the noise. This is rather important since the model used to relate the true objective and actual observations must account for uncertainty due to noise. Mathematically, this is the probability distribution of y given the sample location x and true objective function f:

$$p(y|f, x)$$

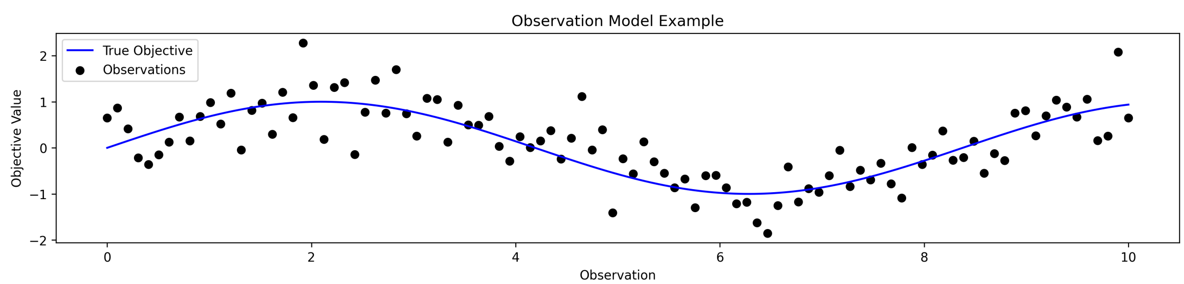
To account for uncertainty, we assume that the observations are *stochastically* dependent on the objective. Mathematically, we assume an additive noise term ε:

$$y = f(x) + \varepsilon$$

Let $\varepsilon \sim \mathcal{N}(0, \sigma^2)$. Then, the model becomes:

$$p(y|x, f, \sigma) = \mathcal{N}(y; f, \sigma^2)$$

Thus, the observation y at sample location x is treated as a *random variable* which follows a Gaussian, or normal, distribution with mean f and variance σ^2. This leads to the distribution of y being centered around the true objective value at sample location x, $f(x)$.



In the plot above, the true objective is shown in addition to 100 observations that have an additive term of random (Gaussian, or normal) noise. The observation model will need to take this into account since noise, often called *uncertainty* in Bayesian optimization, is inherent in real-world problems. It can come from measurement errors, environmental factors, or simply the randomness in the system being optimized.

3.4 Optimization Policies

In simple terms, the optimization policy handles the repeated interactions between the "inner-workings" of the policy and the environment, with the environment typically being *noise-corrupted* (hence the need for an observation model).

More definitively, a **policy** is a mapping function that takes in a new input observation plus any existing observations and uses a *principled* sampling approach to output the next observation location. It will also decide if it should perform another iteration (select a new observation) or terminate the optimization process (see *Termination Policies* below).

For most applications, we want the policy to ideally be learning and improving such that it will guide the search toward the global optimum more effectively. Furthermore, the iterative policy improvement should lead to a good policy that retains the (typically limited) sampling budget for more promising candidate points. A policy that does not consider observed data are known as a *non-adaptive* policy and is not ideal for costly observations.

Note that in some literature, there is little distinction between the optimization policy and the termination policy (discussed next). To be clear, the termination policy is one of the several components that make up the optimization policy. This lack of distinction is not unreasonable but rather something to be aware of when reviewing the vast literature on optimization.

3.5 Termination Policies

A **termination policy** is the final decision in the optimization loop. The policy decides whether to terminate immediately or continue with another observation (continue to optimize the objective). Such policies can be *deterministic* or *stochastic*.

- A **deterministic termination policy** is one that will stop the optimization process after reaching a goal or exhausting a pre-defined search budget.
- A **stochastic termination policy** is one that will depend on the observed data and some level of randomness or probability.

Note that this piece of the optimization process can be handled by an external agent or be dynamic (i.e., a deterministic or stochastic termination policy). For the purposes of this notebook, we will not focus on specific termination policies here. This is primarily due to the fact that the termination policy depends heavily on the approach or method and the problem/application.

3.6 Diagram of the Optimization Process

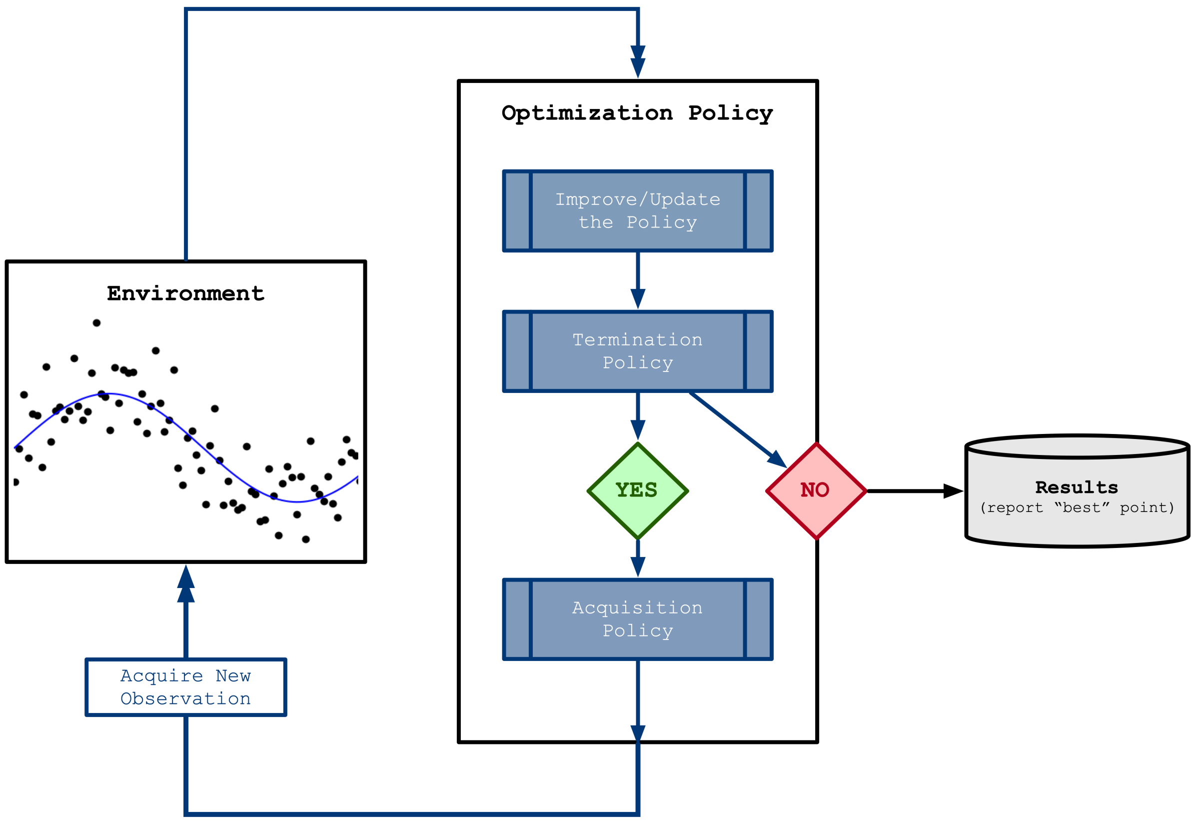


Figure 6: General Optimization Process Diagram

4 Bayesian Foundations

Before we venture into the world of Bayesian optimization, we must first review some foundations of Bayesian statistics. For a more comprehensive examination of Bayesian statistics, the reader is referred to *Mathematical Statistics and Data Analysis* by John A. Rice or *Bayesian Optimization* by Roman Garnett (which provides an optimization-focused review).

4.1 Bayesian Statistics

Bayesian statistics provide us with a systematic and quantitative approach to reason about uncertainty using probabilities. Thus, in *Bayesian* optimization, we use *Bayesian* statistics to reason about uncertainty in the observation (or surrogate) model.

One of the central concepts in Bayesian statistics is **Bayesian inference**. Bayesian inference uses Bayes' theorem to reason about how the prior distribution $p(\theta)$, the likelihood $p(\text{data}|\theta)$, and the posterior distribution $p(\theta|\text{data})$ interact with each other. Note that θ represents the parameter of interest.

Recall **Bayes' theorem**:

$$p(\theta|\text{data}) = \frac{p(\text{data}|\theta)p(\theta)}{p(\text{data})}$$

Let's take a step back and break this down. First, Bayesian inference is a framework that allows us to infer uncertain features of a system of interest from observations using the laws of probability. Thus, within this framework, all unknown quantities are denoted by *random variables*. This is convenient as we can express our beliefs using probability distributions reflecting plausible values.

The **prior distribution**, $p(\theta)$, represents our beliefs before we observe any data. For instance, if we believe that the data is normally distributed then we would likely define the prior distribution to be the Gaussian normal distribution with mean μ and standard deviation σ.

Then, we can refine our initial beliefs once we have observed some data using the **likelihood function**, $p(\text{data}|\theta)$. The likelihood function, or likelihood, provides the distribution of observed values (y) given the location (x), and values of interest (θ).

Finally, using the observed value y, we can derive the **posterior distribution**, $p(\theta|\text{data})$, using Bayes' theorem (defined above) where $\text{data} = (x, y)$. This so-called posterior distribution acts as a "compromise" between our initial beliefs from the prior and our observations from the likelihood. It is at the heart of Bayesian optimization and is used to update the surrogate model as we acquire additional observations.

4.2 Bayesian Inference of the Objective Function

The primary use of Bayesian inference in Bayesian optimization is to reason about the uncertainty in the objective function. Specifically, the probabilistic belief we use over the objective function is called a *stochastic process*. A **stochastic process** is a probability distribution over an infinite collection of random variables, for example, the objective function value at each point in the domain.

We will use a **prior process**, $p(f)$, to express our assumptions (beliefs) that we may have about the objective function. Then, we can define a stochastic process using the distribution of the function values $\boldsymbol{\phi}$ given a finite set of points $\boldsymbol{x}$:

$$p(\boldsymbol{\phi}|\boldsymbol{x})$$

The "gold standard" stochastic process used in Bayesian optimization is the **Gaussian process** due to its expressivity and flexibility, in addition to the fact that many of these finite-dimensional distributions are multivariate Gaussian (or approximately so).

Let's now return to discussing how Bayesian inference is applied over the objective. Suppose we make a set of observations at locations $\boldsymbol{x}$ with corresponding values $\boldsymbol{y}$. Let $\mathcal{D} = (\boldsymbol{x}, \boldsymbol{y})$ be the dataset of aggregated observations. Bayesian inference will account for these observations via the formation of the **posterior process**, akin to the posterior predictive distribution:

$$p(f|\mathcal{D}) = \int p(f|\boldsymbol{x}, \boldsymbol{\phi}) p(\boldsymbol{\phi}|\mathcal{D}) \, \mathrm{d}\boldsymbol{\phi}$$

5 The Bayesian Approach

The "Bayesian approach", particularly in the context of optimization, refers to a philosophical approach that uses Bayesian inference to reason about uncertainty. Specifically, the Bayesian approach enables us to tackle the inherent uncertainty in optimization decisions which is crucial since our decisions will determine our success. This is accomplished through a systematic reliance on probability laws and Bayesian inference during optimization.

Recall that the objective function is viewed as a random variable that will be informed by our prior expectations and posterior observations. The Bayesian approach will play an active role in the optimization process to guide the optimization policy by evaluating the merit of a candidate observation. This results in **uncertainty-aware optimization policies**.

5.1 Uncertainty-Aware Optimization Policies

The optimization policy determines the decisions made during the optimization process. To reasonably handle the uncertainty of the objective function, the policy should use the available data to determine the successive observation locations optimally. There is only one requirement from ourselves: we need to establish our preferences for what data or what "kind" of data we want to acquire. Then, we design the policy to maximize such preferences.

Clearly, this will require some sort of framework to make decisions in this way, especially in the face of uncertainty. A natural choice is **Bayesian decision theory** which will be discussed in more detail in another set of notes (see the *Additional Notes* section).

As we continue to explore Bayesian optimization and uncertainty-aware policies, a common theme will begin to emerge: all Bayesian optimization policies handle the uncertainty in the objective function in a uniform manner, a property that is defined implicitly within an optimal *acquisition function*.

6 Bayesian Optimization Workflow

The Bayesian optimization workflow consists of two main *primitives*: the surrogate model and the acquisition function. In this section, we will briefly discuss these two primitives to understand how they fit into this workflow. Note that these topics will be discussed in-depth in other notes (see the *Additional Notes* section).

6.1 Surrogate Models

Surrogate models are the models we use in Bayesian optimization to express our beliefs and knowledge about the objective function. While in certain literature the term *observation model* is used interchangeably with *surrogate model*, they are distinguishable. For instance, if we have a mathematical formulation of the objective then we refer to the model that relates the observations and the objective as an *observation model*. However, if we do not know the underlying structure of the objective then we refer to the model as a *surrogate model* since it acts as a surrogate and "takes the place" of the objective function. The surrogate model is used within the posterior process to quantify the probabilities of observations in conjunction with utility functions. Therefore, it is a powerful tool when we are reasoning about both the uncertainty and utility of candidate observations.

As mentioned before, we use a *stochastic process* to characterize the objective function and the gold standard in Bayesian optimization is the *Gaussian process*. In fact, one of the most common choices for surrogate models is the Gaussian process due to its flexibility, expressivity, and sufficient uncertainty quantification properties. We will discuss Gaussian processes in greater detail in other notes (see *Additional Notes* section).

6.2 Acquisition Functions

Acquisition functions assign a score to candidate observations where the score represents an observation's potential benefit during optimization. Ideally, acquisition functions are cheap to evaluate and address the *exploitation-exploration tradeoff*. In the context of optimization, *exploitation* refers to sampling where the objective value is expected to be large whereas *exploration* refers to sampling where we are more uncertain about the objective value. Another useful property of an acquisition function is it vanishes at pre-existing observations as there is no sense in sampling twice.

There are two main types of acquisition functions: myopic and look-ahead. Myopic acquisition functions consider only the immediate utility while look-ahead acquisition functions consider longer-term utility. This will be discussed further in the notes covering Bayesian decision theory. Regardless of the type, the optimization policy should be designed to maximize the acquisition function such that the candidate observation with the most potential benefit is selected.

7 References

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

[2] Peng Liu. 2023. *Bayesian optimization : Theory and practice using python.* Apress, New York, NY.

[3] Carl Edward Rasmussen and Christopher K. I Williams. 2019. *Gaussian processes for machine learning.* The MIT Press.