Utility Functions

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1 Introduction

In the Bayesian decision theory notes, one of the mechanisms crucial to making optimal decisions was the **utility function**. The utility function evaluates the quality of the dataset returned by the optimization process based on the preferences we express via the utility function itself. Given a model of the objective, the utility function allows us to derive the optimal policy very simply: maximize the expected utility of each observation and consequently maximize the expected utility of the returned dataset. Therefore, we can identify very clearly what is required of us: define a model that is consistent with our beliefs about the objective and define a utility function that expresses our preferences across outcomes.

However, while we can clearly identify *what* we need to do, the *how* we do it is not exactly trivial. For instance, as Garnett points out, our beliefs and preferences are innately internalized which makes it difficult to break them down into mathematical expressions. Luckily, there are avenues we can take to mathematically express our beliefs and preferences using surrogate models (i.e., Gaussian processes) and utility functions (i.e., expected improvement), respectively. In these notes, we focus on how to define utility functions that are consistent with our preferences, including a review of utility functions frequently used in Bayesian optimization. Many of these utility functions' underlying motivation often contribute to novel approaches. Finally, we follow Garnett's position when delving into utility functions: while Gaussian processes are common in Bayesian optimization, we will not assume that the surrogate model is a Gaussian process.

2 Expected Utility of the Final Recommendation

Simply put, the purpose of optimization is to search the space of candidates for the best candidate that we implicitly decide to use, often in another routine. Recall the applications provided in the *Introduction to Bayesian Optimization* notes: when applying (Bayesian) optimization for AutoML purposes, we are searching the space of candidate *hyperparameters* that will be used to train a neural network—in hopes that when the network is re-evaluated its performance (i.e., classification accuracy) improves. However, as we have seen, the best candidate is typically found closer to the termination of the optimization process meaning that for the most part, the dataset that we acquire during optimization is only used to guide us towards the best candidate.

Clearly, the selection of the "best candidate" can be regarded as another **decision**. Thus, if the goal of optimization is to guide us to the optimal final decision then the optimization policy should be designed to maximize the expected utility of the final decision. In this section, we will focus on (1) defining the "final recommendation" as a decision, (2) selecting an action space to move across, and (3) selecting a utility function to use when evaluating candidate observations.

2.1 Defining the Final Recommendation Decision

We stated previously that the best candidate is typically viewed as the "final" recommendation for another system and can thus be regarded as a decision. Here, we will define the final recommendation decision in a mathematical manner such that it becomes evident how the utility function aids this decision. Note that in some literature, the terms *final recommendation* and *terminal recommendation* are used interchangeably.

First, suppose that our optimization process returned an arbitrary dataset $\mathcal{D} = (\mathbf{x}, \mathbf{y})$. Then, suppose that we aim to use this returned dataset to recommend a candidate $x \in \mathcal{X}$ that will be used in another, external routine. In this external routine, the performance is quantified by the underlying objective function value denoted $\phi = f(x)$. Once again, this recommendation is regarded as a **decision under uncertainty** about the objective value that is informed by the posterior predictive distribution denoted by $p(\phi|x, \mathcal{D})$.

Recall that in order to completely define the decision problem, we must identify the action space $\mathcal{A} \subset \mathcal{X}$ for our recommendation and identify a utility function $v(\phi)$ to evaluate a recommendation post-hoc based on the objective value ϕ. Once these are defined, a **rational** recommendation should maximize the expected utility:

$$x \in \underset{x' \in \mathcal{A}}{\arg\max}\, \mathbb{E}\left[v(\phi')|x', \mathcal{D}\right]$$

Notice that the recommendation's expected utility above is only dependent on the returned dataset from the optimization process. This property brings about a natural utility that we can use in optimization. The **natural utility** function computes the expected quality of an optimal final recommendation given the returned dataset $\mathcal{D}$:

$$u(\mathcal{D}) = \max_{x' \in \mathcal{A}} \mathbb{E}\left[v(\phi')|x', \mathcal{D}\right]$$

Furthermore, the recommendation's expected utility will also not depend on the optimal recommendation itself (i.e, x') since we are selecting the maximal expected objective function value. Thus, since we are computing the expectation of the objective function value given the candidate and returned dataset, the expected utility will not depend on the optimal recommendation's objective value either.

Referencing the depiction of the sequential decision tree in Figure 5.4, Garnett notes that the utility function will effectively "collapse" the expected utility of a final decision into a utility of the returned dataset. This means that we are able to select the action space and utility function for the final recommendation based purely on the problem at hand. We will consider Garnett's advice for these selections next.

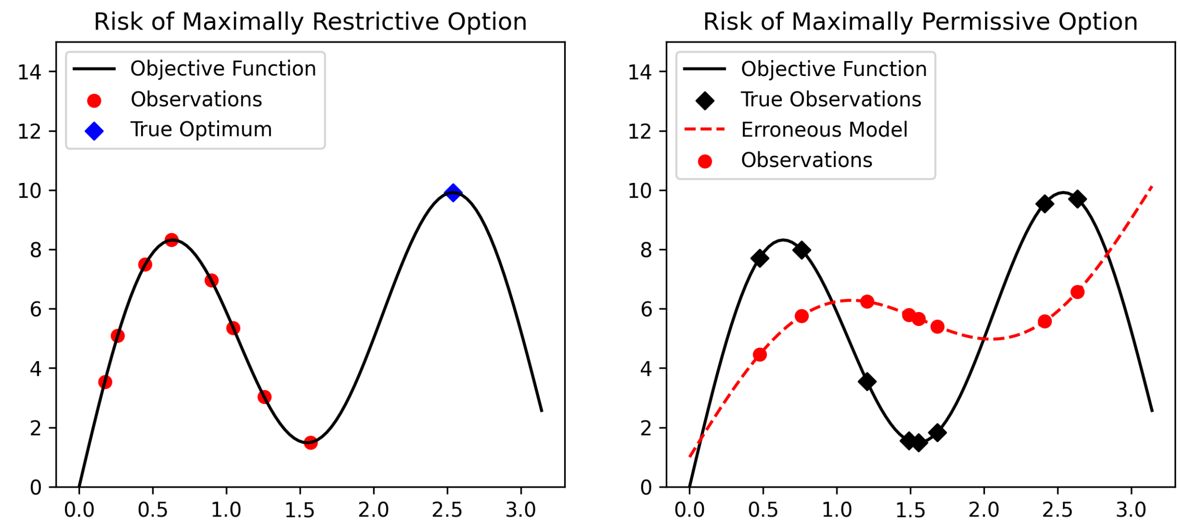
2.2 Selecting an Action Space

We need to select an action space for our recommendation, denoted by $\mathcal{A} \subset \mathcal{X}$. Let's take a look at two extreme options with one being maximally restrictive and the other being maximally permissive.

- The **maximally restrictive** option restricts our recommendation choices to only the points visited during optimization, $\mathbf{x}$. Although this option will ensure that we have at least some knowledge of the objective function at our recommended point, it does not allow for any exploration. In other words, we may not have visited the best point so it will not be contained in $\mathbf{x}$ and we are therefore unable to recommend it.
- The **maximally permissive** option defines the action space to be the entire domain $\mathcal{X}$. However, opting to have the entire domain be our action space will require us to have faith in the objective function model's belief, particularly when recommending an unvisited point. In other words, while it gives us more freedom to explore, it also means we have to be careful about where our model has higher uncertainty.

The plots on the following page provide examples of these two extreme options. On the left, the plot shows an example of the maximally restrictive option that only allows visited points to be recommended. Clearly, our observations denoted by the red markers do not include the true optimum denoted by the blue marker.

On the other hand, the plot to the right shows an example of the maximally permissive option that denotes the entire domain to be the action space. As shown by the dashed red line, our model is very erroneous and does not capture the underlying objective. In particular, we could end up recommending points that have the highest model value but not the highest objective model. While these examples themselves are extreme and a bit exaggerated, they represent the risks present if we use either extreme to select an action space.



While these are the extreme options that one could take to select an action space, there have been some more reasonable suggestions in the literature. One reasonable suggest is shown in Osborne et al. and is essentially a compromise between the two extremes. Specifically, the final recommendation choice is restricted to points where the objective value is known within some acceptable tolerance. Osborne et al. defined a parametric and data-dependent action space (with form given below) to achieve this compromise.

$$\mathcal{A}(\varepsilon; \mathcal{D}) = \{x | \text{std}\left[\phi | x, \mathcal{D}\right] \leq \varepsilon\}$$

In the expression above, ε denotes a threshold for the highest amount of acceptable uncertainty in the objective function value. This approach should, for the most part, avoid issues of recommending points at locations where the objective function is not sufficiently known while allowing for some exploration beyond the points visited during optimization.

2.3 Selecting a Utility Function

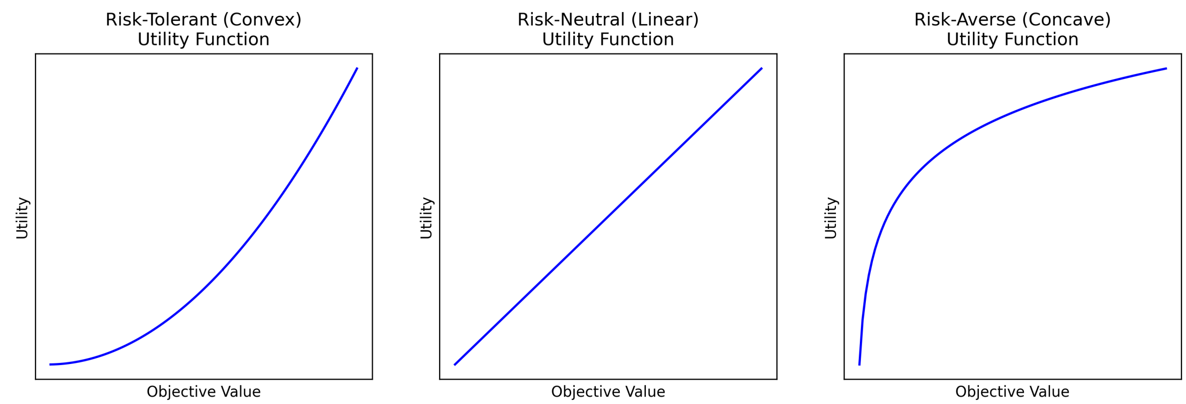
In addition to selecting an action space for our recommendation, we also need to select a utility function $v(\phi)$ that will evaluate a recommendation x after we observe its corresponding objective function value ϕ. For our purposes, we have been focusing on maximization so the utility function should be **monotonically increasing** in ϕ. This means that as the objective value ϕ increases, its utility $v(\phi)$ should also increase.

- Remember that if the decision problem calls for it, it is fairly trivial to change the focus and setup from maximization to minimization, and vice versa.

While we know that the utility function should always be increasing in ϕ, there is still the question of what shape the function ought to assume. The answer to this question will depend on our **risk tolerance**. Risk tolerance refers to the tradeoff between potentially obtaining a higher expected value but with greater uncertainty thereby imposing some risk in our recommendation. Alternatively, we could have a lower expected value with lower uncertainty making it a safer recommendation.

- A **risk-tolerant** (convex) utility function will allow for more risk to potentially attain greater reward (i.e., higher expected value but higher uncertainty).
- A **risk-neutral** (linear) utility function is indifferent between points with equal expected value without regard to their uncertainty.
- A **risk-averse** (concave) utility function will avoid risk and err towards lower risk even if it means a lower reward (i.e., lower uncertainty but lower expected value).

The plots below illustrate the shape the utility function would take based on the risk tolerance.



The most simple and commonly used utility function in Bayesian optimization is a risk-neutral, linear utility function:

$$v(\phi) = \phi$$

When the utility function is linear, the expected utility from recommending x is simply the posterior mean of ϕ:

$$\mathbb{E}\left[v(\phi)|x, \mathcal{D}\right] = \mu_{\mathcal{D}}(x)$$

Recall that the risk-neutral, linear utility function does not consider the uncertainty in the objective function when making a decision. While this type of utility is simple and therefore computationally convenient, it may not truly be consistent with our preferences.

In addition to expressing our risk preferences, we can reason about them using the **certainty equivalent**. The certainty equivalent is an objective value that corresponds to a (hypothetically) risk-free alternative recommendation to which our preferences would be indifferent. For instance, suppose that we have a risky potential recommendation x where we do not know its true corresponding value of the objective function. Then, the certainty equivalent for x is an objective function value ϕ' such that

$$v(\phi') = \mathbb{E}\left[v(\phi)|x, \mathcal{D}\right]$$

When using a risk-neutral utility, the certainty equivalent of some point x is its expected value: $\phi' = \mu_{\mathcal{D}}(x)$. Therefore, we would only abandon one recommendation in favor of another if the if the latter had a higher expected value without considering risk. Alternatively, we may want to express our risk-aware preferences using **nonlinear** utility functions.

3 A Note on Nonlinear Utility Functions

As mentioned in the previous section, we may wish (or even truly need) to express our risk-aware preferences using nonlinear utility functions. To illustrate this, let's consider a scenario where our preferences lean more towards risk aversion. With these preferences, we may accept a recommendation point with a lower expected value if it also results in less risk. From our previous discussion on the shape of utility functions based on risk tolerance, we should express these preferences using a concave utility function. Garnett uses Jensen's inequality as an example of a utility function expressing risk averse preferences:

$$v(\phi') = \mathbb{E}\left[v(\phi)|x, \mathcal{D}\right] \leq v\left(\mathbb{E}\left[\phi|x, \mathcal{D}\right]\right) = v(\mu_{\mathcal{D}}(x))$$

With this utility function, the certainty equivalent of a risky recommendation will be less than its expected value. On the other hand, we could express risk-seeking preferences using a convex utility function. In such a case, the certainty equivalent of a risky recommendation will be greater than its expected value. Then, our preferences will implicitly push toward gambling. For obvious reasons, literature on economic and decision theory have proposed several risk-averse utility functions although these (and risk-seeking utility functions) are not typically used in Bayesian optimization. Note that these types of utilities can be useful in certain settings, especially where risk neutrality is questionable.

Before continuing, let's review a natural approach to quantify the risk associated with a recommendation of an uncertain value ϕ. To do this, we simply use its standard deviation:

$$\sigma = \mathrm{std}\left[\phi|x, \mathcal{D}\right]$$

Then, we can establish our preferences for potential recommendations using a weighted combination of a point's expected reward and its risk:

$$\mu_{\mathcal{D}}(x) + \beta\sigma = \mu + \beta\sigma$$

where β represents a tunable risk-tolerance parameter with $\beta < 0$ penalizing risk (inducing risk-averse behavior), $\beta > 0$ rewarding risk (inducing risk-seeking behavior), and $\beta = 0$ inducing risk neutrality. This framework serves as the base for two common utility functions in Bayesian optimization: *simple reward* and *global reward*. We will discuss these next.

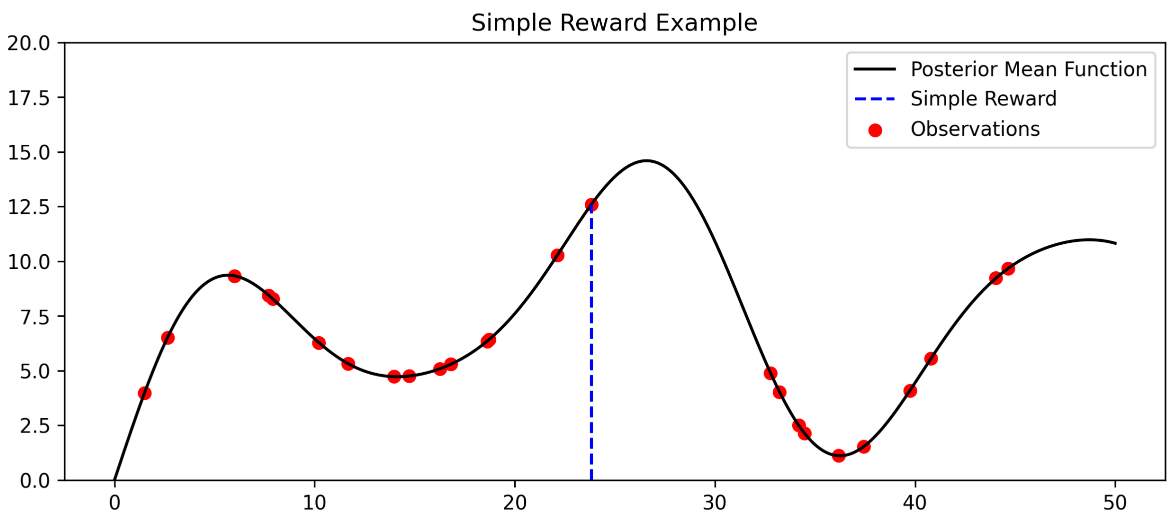
4 Common Utility Functions

In this section, we review utility functions common in Bayesian optimization literature and practice. This is by no means an exhaustive review of each and every utility function out there but rather an exposition of the utility functions frequently used in Bayesian optimization.

4.1 Simple Reward

The **simple reward** is named as such since it assumes that we are risk-neutral and thus limit the action space to only points visited during optimization. Suppose an optimization process returned dataset $\mathcal{D}(\mathbf{x}, \mathbf{y})$ to guide the final recommendation made using the risk-neutral utility function $v(\phi) = \phi$. Then, the expected utility of the optimal recommendation is:

$$u(\mathcal{D}) = \max \mu_{\mathcal{D}}(\mathbf{x})$$



There is one technical caveat that Garnett points out: if the returned dataset is empty, then the maximum degenerates and results in $u(\emptyset) = -\infty$. Furthermore, in the special case where we have exact observations (i.e., $\mathbf{y} = f(\mathbf{x}) = \boldsymbol{\phi}$), the simple reward will reduce to the maximal objective value observed during optimization:

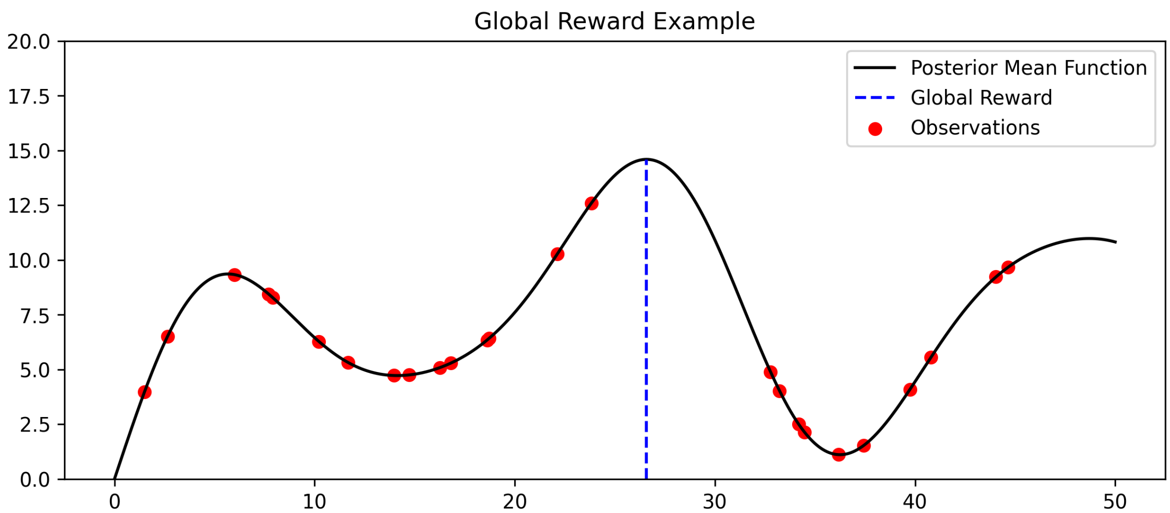
$$u(\mathcal{D}) = \max \boldsymbol{\phi}$$

4.2 Global Reward

The **global reward** is similar to the simple reward in that it assumes we are risk-neutral but now we allow the action space to be the entire domain $\mathcal{X}$. Then, the expected utility of the optimal recommendation is the global maximum of the posterior mean:

$$u(\mathcal{D}) = \max_{x \in \mathcal{X}} \mu_{\mathcal{D}}(x)$$

Recall that when the action space is expanded to include the entire domain, we inherently include points that were unseen about during the optimization process. Therefore, these "unseen" points are points where we are more uncertain about the objective value and can lead to a different and potentially more risky recommendation.



In the plot above, both the posterior mean function and observations denoted by the solid black line and red markers, respectively, are the same from the previous plot for the simple reward. However, with the global reward, we expand the action space to include the entire domain so the global reward is simply the globally maximal posterior mean value denoted by the vertical dashed blue line.

4.3 A Tempting, Nonsensical Alternative to Simple Reward

Before we discuss other commonly used utility functions, let's review the tempting, but not exactly rational alternative to the simple reward that Garnett mentions. We are referring to an alternative utility function that is deceptively similar to the simple reward: the maximum noisy observed value in the dataset:

$$u(\mathcal{D}) = \max \mathbf{y}$$

Notice that if we specify the maximum **noisy** observed value in the dataset. This is because we assume that there is some sort of noise which leads to uncertainty in the objective function. If we are in the special case of dealing with exact observations then this utility function will reduce to the simple reward defined previously. However, when dealing with inexact or noisy observations (much more common), this utility is absurd.

Garnett notes that the absurdity of the utility function is increased when the observed noisy maximum value is more reflective of noise than actual optimization progress. To that end, if the **signal-to-noise ratio** is relatively high (i.e., the noise is not extreme) then this utility function can be used as an approximation to the simple reward. See Figure 6.2 in Garnett's text for an extreme but helpfully illustrative example.

4.4 Cumulative Reward

The **cumulative reward** differs from both the simple and global rewards in that it accounts for the objective value of every point in the dataset. Specifically, it rewards the acquisition of observations with high average objective values. Furthermore, in comparison to the simple and global rewards which operate under the notion that the goal is to find the best point from the search space, the cumulative reward is useful when the objective values of all observations in the dataset are important. This is common in applications where our optimization routine may be responsible for controlling a critical, external system.

Given a returned dataset $\mathcal{D} = (\mathbf{x}, \mathbf{y})$, the cumulative reward is given by the sum of the observed objective values $\mathbf{y}$:

$$u(\mathcal{D}) = \sum_i y_i$$

With regard to the practical usage of the cumulative reward, Garnett points out one notable use case: **active search**. Active search is a model for scientific discovery where we select points for evaluation in a successive manner with the goal of identifying as many points as possible in a rare, valuable class denoted $\mathcal{V} \subset \mathcal{X}$. To accomplish this, when we make an observation at location $x \in \mathcal{X}$, it will yield a binary observation representing whether or not the observation is in the desired class (i.e., $y = [x \in \mathcal{V}]$).

4.5 Information Gain

The premise behind **information gain** is that we can evaluate the quality or utility of a dataset based on the quantitative amount of information it provides about a random variable of interest. In that respect, we will prefer datasets that contain more knowledge about the random variable of interest. This type of approach is referred to as *information-theoretic* and originates from the domain of *information theory*. Furthermore, it serves as an alternative approach to the simple, global, and cumulative rewards that evaluate datasets based on the objective values they contain.

Let ω be a random variable of interest we want to learn more about as we observe data during optimization. As noted by Garnett, the choice of ω is open-ended and depends on the application. However, there do exist some natural choices for ω such as the location of the global optimum x^* and the maximum objective value f^*. Below, we will review how to quantify the information about ω contained in a dataset $\mathcal{D}$ using Garnett's notation.

To begin, we will quantify our initial uncertainty about ω using the differential **entropy** of its prior distribution $p(\omega)$:

$$H\left[\omega\right] = -\int p(\omega) \log p(\omega) \, \mathrm{d}\omega$$

From this, the **information gain** provided by a dataset $\mathcal{D}$ is given by the different in entropy between the prior and posterior distribution:

$$u(\mathcal{D}) = H\left[\omega\right] - H\left[\omega|\mathcal{D}\right]$$

where $H\left[\omega|\mathcal{D}\right]$ is the differential entropy of the posterior.

Be aware that Garnett's notation is not standard and there is one particular caveat with such notation. The notation for the conditional entropy of ω given $\mathcal{D}$ is exactly the same as the notation we use here for the differential entropy of the posterior: $H\left[\omega|\mathcal{D}\right]$. However, for our purposes, this is perfectly fine. Furthermore, as Garnett notes, if necessary we will denote the conditional entropy with an explicit expectation: $\mathbb{E}\left[H\left[\omega|\mathcal{D}\right]|\mathbf{x}\right]$.

Furthermore, there is also an alternative definition of information gain used in literature that could be a point of confusion. The alternative definition of information gain is the **Kullback-Leibler (KL) divergence** between the posterior and prior distributions:

$$u(\mathcal{D}) = D_{\mathrm{KL}}\left[p(\omega|\mathcal{D})||p(\omega)\right] = \int p(\omega|\mathcal{D}) \log \frac{p(\omega|\mathcal{D})}{p(\omega)} \, \mathrm{d}\omega$$

The expressions from the previous page enable us to quantify the amount of information a dataset contains based on how our prior belief in ω changes after it is collected. In addition, the Kullback-Leibler divergence definition for information gain has some convenient properties compared to the definition before it: the KL divergence definition is **invariant** to reparameterization of ω and is always nonnegative. These properties are useful in cases when unexpected observations are collected and could cause the other definition to become negative (and therefore unintuitive).

Luckily for us, the connection between these two definitions for information gain are surprisingly strong, especially for sequential decision making. Specifically, the expectation with respect to observations are equal which means that when we maximize the expected utility using either definition, it will lead to the same decisions.

4.6 Comparison of Utility Functions

Having reviewed several utility functions that quantitatively evaluate a returned dataset from an optimization process, we can begin to examine the subtle differences between their respective approaches. Since the simple reward is the most common utility function in Bayesian optimization, we will compare it to the other utility functions we presented earlier. Its popularity comes from its frequent use in conjunction with the prevalent **expected improvement (EI)** acquisition function. One key distinction between it and the others is that its approach considers only the local properties of the objective function posterior distribution to evaluate the data. This local approach is both rational and convenient computationally since it only considers the points visited during optimization.

Alternatively, the global reward utility function uses the global properties of the objective function. This stems from the decision to denote the entire domain as the action space meaning that the utility function will consider the entire posterior mean. Furthermore, it also means that this type of utility function has the option to recommend a point that was unobserved during optimization. In an entire different direction from the objective value-based approaches, information gain uses information theory to evaluate a dataset based on the change in knowledge it provides. This kind of approach considers the posterior entropy of the variable of interest and thus relies on the global properties of the objective function.

Finally, since some utility functions consider the local properties and others consider the global properties, there can be disagreement between the simple reward and other utility functions. Garnett provides some examples of datasets that have a good global outcome but poor local outcome, and vice versa. It is recommended to page through the last few pages of Chapter 6 to read about these examples and connect these concepts to their visual counterparts.

5 Relationship Between the Model of the Objective Function and Utility Function

After surveying the utility functions frequently used in Bayesian optimization, one hopefully recognizes the relationship between the model of the objective function and utility function: most of the utility functions are dependent on the underlying model of the objective function. In this section, we will formalize this idea.

Consider the first two utility functions (the simple and global rewards). Both are defined using the posterior mean function $\mu_{\mathcal{D}}$. On the other hand, information gain relies on the posterior belief about the location and value of the optimum $p(x^*, f^*|\mathcal{D})$. Recognize that the posterior mean and the posterior beliefs are byproducts of the posterior distribution of the objective function (the model of the objective function).

However, this is not always ideal and there are approaches that mitigate the dependence of the utility function on the model of the objective function. One approach is a computational mitigation strategy using **model averaging**. Recall that model averaging is a process where we marginalize the model with respect to the model posterior. Another approach is to define model-agnostic utility functions that are based on the data alone (i.e., no relation to a model) but this is fairly limited under the assumption that the utility should be sensible.

- One example of the latter approach is the cumulative reward since it is only defined based on the observed values $\mathbf{y}$.
- Another example of the latter approach is the maximum function value utility but as noted previously, that utility's rationale diminishes if observation values are noisy.

Alternatives defined in the same manner as the examples above often have similar difficulties: noise will bias many natural measures such as the order statistics (i.e., minimum, maximum, etc.) of the observations. In particular, while for additive noise with zero mean, we would expect that the noise would not impact the cumulative reward at all it would still affect the aforementioned order statistics.

6 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.