Bayesian Optimization with Expensive Integrands

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Abstract

We propose a Bayesian optimization algorithm for objective functions that are sums or integrals of expensive-to-evaluate functions, allowing noisy evaluations. These objective functions arise in multi-task Bayesian optimization for tuning machine learning hyperparameters, optimization via simulation, and sequential design of experiments with random environmental conditions. Our method is average-case optimal by construction when a single evaluation of the integrand remains within our evaluation budget. Achieving this one-step optimality requires solving a challenging value of information optimization problem, for which we provide a novel efficient discretization-free computational method. We also provide consistency proofs for our method in both continuum and discrete finite domains for objective functions that are sums. In numerical experiments comparing against previous state-of-the-art methods, including those that also leverage sum or integral structure, our method performs as well or better across a wide range of problems and offers significant improvements when evaluations are noisy or the integrand varies smoothly in the integrated variables.

1 Introduction

We consider two closely-related derivative-free black-box global optimization problems with expensive-to-evaluate objective functions,

$$\max_{x \in A \subset \mathbb{R}^d} G(x) := \max_{x \in A \subset \mathbb{R}^d} \sum_{w=1}^{n} F(x, w) p(w)$$

(1)

and

$$\max_{x \in A \subset \mathbb{R}^d} G(x) := \max_{x \in A \subset \mathbb{R}^d} \int F(x, w) p(w) dw,$$

(2)

where $A$ is a simple compact set (e.g., a hyperrectangle, simplex, or finite collection of points); $w$ is a vector belonging to a set $W$; $p$ is finite and inexpensive to evaluate with a known analytic form; and $F$ is expensive to evaluate, does not provide derivatives with its evaluations, and may be observable either directly or with independent normally distributed noise. We also assume in (2) that $F(x, \cdot)p(\cdot)$ is integrable for each $x$. Here, “expensive-to-evaluate” functions are ones that consume a great deal of time per evaluation, e.g., minutes or hours each, or whose number is otherwise severely restricted (see, e.g., Sacks et al. [1989], Booker et al. [1998]).

We treat $F$ as a black box and assume that it is continuous in $x$ and also in $w$ in problem (2) and well-represented by a Gaussian process prior (Rasmussen and Williams [2006]) as described below, but make no other assumptions on its structure.

This pair of closely related problems arises in three settings:

1. First, both (1) and (2) arise when optimizing average-case performance of an engineering system or business process across environmental conditions, where $F(x, w)$ is the performance of system design $x$
under environmental condition \( w \), and \( p(w) \) represents the fraction of time that condition \( w \) occurs. This arises, for example, when choosing the shape of an aircraft’s wing \cite{Liem et al. 2014}, the configuration of a cardiovascular bypass graft \cite{Sankaran and Marsden 2010}, or the parameters of an algorithm that dispatches cars in a ride-sharing service.

2. Second, both (1) and (2) arise when we wish to optimize the expected value of a system modeled by a discrete-event simulation \( f(x, \omega) \), where \( \omega \) is random. In this setting, we may choose a random variable \( w \) whose distribution \( p(w) \) we know, and for which we can simulate \( \omega \) given \( w \). We may then define \( F(x, w) = E[f(x, \omega)|w] \). Our objective \( E[f(x, \omega)] \) becomes either \( \sum_{w=1}^{n} F(x, w)p(w) \) if \( w \) is discrete or \( \int F(x, w)p(w)dw \) if \( w \) is continuous, and we can obtain noisy observations of \( F(x, w) \) by simulating \( f(x, \omega) \) with \( \omega \) drawn from its conditional distribution given \( w \). This arises, for example, when building a transportation system to maximize expected service quality subject to stochastic patterns of arrivals through the day \( \omega \), which we can simulate given the total number of arrivals in a day \( w \). When used for variance reduction in simulation rather than optimization, this technique is known as stratification \cite{Glasserman 2003}.

3. Third, (1) arises when tuning a machine learning algorithm’s hyperparameters by using k-fold cross-validation. In this application, \( F(x, w) \) is the error on fold \( w \) using hyperparameters \( x \) and our goal is to minimize \( \sum_{w} F(x, w) \). This problem arises more generally when optimizing average performance across multiple prediction tasks \cite{Bardenet et al. 2013, Hutter et al. 2011, Swersky et al. 2013} and is called multi-task Bayesian optimization \cite{Swersky et al. 2013}. Although (1) and (2) can be considered jointly as maximization of an objective \( \int F(x, w)d\mu(w) \) where \( \mu \) is a measure, and our theoretical analysis will at times take this view, (1) and (2) have very different properties computationally and have been considered separately in the literature so we refer to them separately here.

Potential Solution Approaches: Problems (1) and (2) may be solved by optimizing \( G(x) \) directly with a method designed for derivative-free black box global optimization of expensive and possibly noisy functions. These methods include Bayesian optimization methods \cite{Jones et al. 1998, Forrester et al. 2008, Brochu et al. 2010} and other surrogate-based optimization methods \cite{Barthelemy and Haftka 1993, Dennis and Torczon 1997, Mueller and Shoemaker 2014}. Indeed, \( G(x) \) can be evaluated using multiple evaluations of \( F(x, w) \) by summing in (1) or with numerical quadrature in (2). However, the expense of evaluating \( G(x) \) is many times larger than for \( F(x, w) \), especially if \( n \) in (1) is large or numerical quadrature in (2) is performed accurately. This approach is inefficient because it is unable to adjust the computational effort spent on evaluating \( G(x) \): it either evaluates it fully or not at all. This inefficiency is most apparent when the first evaluations of \( F(x, w) \) at \( x \) indicate \( G(x) \) is substantially sub-optimal: the extra expense of fully evaluating \( G(x) \) is wasted.

These problems may also be solved by applying a black box global optimization method to noisy observations of \( G(x) \) obtained via Monte Carlo sampling. One may sample \( w_1, \ldots, w_m \) from \( p \) and use \( \frac{1}{m} \sum_{i=1}^{m} F(x, w_i) \) as a noisy estimate of \( G(x) \). This approach is inefficient because it ignores information about \( w \) when building its surrogate for \( G \). This inefficiency is most apparent when the first two evaluations of \( F(x, w) \) are at the same or very similar \( w \). If \( F \) is free from noise and varies slowly with \( w \), the second such evaluation provides little information beyond the first. This inefficiency could perhaps be mitigated by using Quasi Monte Carlo (QMC; see, e.g., \cite{Glasserman 2003} together with an optimization method (ideally a multifidelity one, e.g., \cite{Forrester et al. 2007}) that is tolerant to bias in its noisy observations, but even this would become inefficient when most of \( G(x) \)’s variability is driven by values of \( w \) not sampled until later in the QMC sequence.

These inefficiencies in optimization based on surrogate models of \( G \) suggest one may create a more efficient method through surrogate models of \( F \), coupled with intelligent selection of points \( x \) and \( w \) at which to evaluate \( F \). \cite{Williams et al. 2000} and \cite{Swersky et al. 2013} developed methods of this type for solving (1), and \cite{Groot et al. 2010, Xie et al. 2012} for solving (2). While these approaches can improve performance over modeling \( G \) alone, we show in this article that they leave substantial room for improvement. Indeed, all of these previous
approaches except [Xie et al. (2012)] use heuristic two-step rules that choose \( x \) first without considering \( w \), and then choose \( w \) with \( x \) fixed. As we show below, not considering \( x \) and \( w \) together causes these methods to perform poorly in certain settings, even sometimes failing to be asymptotically consistent. Moreover, these previous methods are insufficiently general: [Xie et al. (2012)] requires \( p \) and the kernel of the covariance of the Gaussian process to be Gaussian, and all previous methods require evaluations of \( F \) to be free from noise, significantly restricting their applicability.

**Contributions:** In this paper, we significantly generalize and improve over this previous work by developing a novel method, Bayesian Quadrature Optimization (BQO), that uses a one-step value of information analysis to select the pair of points \( x, w \) at which to evaluate \( F \). This method is general and supports solving either (1) or (2) with noisy or noise-free evaluations of \( F \), and this support for noisy observations significantly expands the applicability of our approach within optimization via simulation. This algorithm is Bayes-optimal by construction when only a single evaluation of \( F \) may be made. We also prove that it provides a consistent estimator of the global optimum of \( G \) as the number of samples allowed extends to infinity in both the finite and continuum domain settings for the finite sum problem (1). Performing the one-step value of information analysis at the heart of BQO requires solving a challenging optimization problem, and we present novel computational methods that solve this problem efficiently, including a novel discretization-free method for estimating the gradient of the value of information, a new convergence analysis of a different and less efficient discretized scheme more closely related to past work, and a novel transformation that provides a more computationally convenient form of \( F \). We demonstrate that our algorithm substantially outperforms state-of-the-art Bayesian optimization methods when observations are noisy or the integrand varies smoothly in the integrated variables, and performs as well as state-of-the-art methods in the remaining settings. Our demonstrations use a variety of problems from optimization via simulation and hyperparameter tuning in machine learning. We also provide a robust implementation of our method at https://github.com/toscanosaul/bayesian_quadrature_optimization.

Our method improves over the previous literature in three ways: First, it is more general, as it is the first to allow noise in the evaluation of \( F \), the first to simultaneously support solving both (1) and (2), and allows general \( p \) in contrast with [Groot et al. (2010)] and [Xie et al. (2012)]’s requirement that \( p \) be a normal density. Second, it is more well-supported theoretically, as its one-step optimality justification contrasts with the heuristic justification offered in [Williams et al. (2000)], [Groot et al. (2010)] and [Swersky et al. (2013)]. (Xie et al. (2012) is one-step Bayes-optimal for the special case of (2) that it considers.) Also none of these previous methods come with a proof of consistency, and Williams et al. (2000) may fail to be consistent if a poor tie-breaking rule is chosen as we note below. Third, it provides better empirical performance in problems with noisy evaluations or when the integrand varies smoothly in the integrated variables, and performs comparably in other problems. We discuss this previous literature in more detail below.

This paper significantly extends the conference paper [Toscano-Palmerin and Frazier (2016)], where an early version of the BQO method was referred to as Stratified Bayesian Optimization (SBO). We have re-named our method to reflect its more general ability to solve problems beyond the second use-case based on stratification described at the start of this section. Beyond that conference paper, the current paper includes proofs of consistency for both finite and continuum domains for the finite sum problem (1), a proof of convergence of the discretized computational method used in that paper, a new discretization-free computational method that is substantially more efficient in higher dimensions, and additional numerical experiments on new problems with new benchmark algorithms.

**Detailed Discussion of Related Work:** [Williams et al. (2000)] considers the problem (1) when \( F \) is noiseless, and uses a small modification of the well-known expected improvement acquisition function [Mockus 1989, Jones et al. 1998]. Their acquisition function is a two step procedure which first uses expected improvement to choose \( x \in A \) by maximizing the conditional expectation of \( \max \{ 0, G(x) - \max_{1 \leq i \leq n} G(x_i) \} \) given the past \( n \) observations, and then chooses \( w \in W \) by minimizing the posterior mean squared prediction error. This
algorithm is not consistent for finite \( A \) for the following reason: After \( F(x,w) \) has been evaluated for all \( x \in A \), (but not necessarily all \( w \in W \)), \( G(x) - \max_{x \in A} G(x) \leq 0 \) almost surely. This implies that the conditional expectation of \( \max \{ 0, G(x) - \max_{x \in A} G(x) \} \) is 0 for all \( x \). If the tie-breaking rule used chooses the same \( x \) on each iteration, then this method will fail to evaluate each \( x \) infinitely often. \cite{lehman} considers minor modifications of the previous algorithm, and their M-robust algorithm can also fail to be consistent with a poor tie-breaking rule.

\cite{groot} considers problem (2) when \( F \) is noiseless, \( p(w) \) is Gaussian, and the kernel of the Gaussian process on \( F \) is the squared exponential kernel. Its acquisition function is a minor modification of the active learning method ALC (\cite{cohn}). Numerical experiments in that paper do not demonstrate an improvement over evaluating \( G \) directly. While the method proposed for choosing \( x, w \) is motivated by minimizing the expected variance of the objective \( G \) after one evaluation, it does not do so optimally. Instead, like \cite{williams}, it chooses \( x \) ignoring what \( w \) will be chosen, and then chooses \( w \) with \( x \) fixed. This is in contrast with our approach, which chooses \( x \) and \( w \) jointly in a one-step optimal way.

\cite{swersky} considers problem (1) when \( F \) is noiseless, and uses a small modification of the expected improvement acquisition function (\cite{jones}). Like \cite{williams} and \cite{groot}, and in contrast with our joint optimization approach, it first chooses \( x \) ignoring \( w \), and then in a second step it chooses \( w \) with \( x \) fixed. Although one should typically choose \( w \) to reduce uncertainty about \( G(x) \), \cite{swersky} instead chooses \( w \) using an expected improvement criterion over \( F(x,w) \) even though we are not maximizing over \( w \). This can select points whose posterior mean of \( F(x,w) \) is high but posterior variance is extremely low, essentially wasting a measurement. This leads in turn to examples where the policy repeatedly samples the same \( x \) and under-explores, as we discuss in the appendix (\S D). Our numerical experiments show this method can perform well in problems with a small number of homogeneous tasks, but tends to underperform significantly as the number of tasks increase.

\cite{xie} considers problem (2) when \( F \) is noiseless, \( p \) is Gaussian and independent, and the Gaussian process on \( F \) has a squared exponential kernel. BQO generalizes the method in that paper to the significantly more applicable setting where \( F \) can be noisy (required for application to optimization via simulation), with any \( p \) (required for applications to cross-validation in machine learning) and any kernel (required for good performance on a wider variety of problems). These generalizations significantly increase the difficulty of the problem, because they preclude closed-form expressions used in \cite{xie}. We also provide significantly improved computational methods: the discretized method used in \cite{xie} to optimize the acquisition function requires computation that scales exponentially in the dimension, preventing its use for more than 3 dimensions, while our discretization-free method has sub-exponential scaling and numerical experiments demonstrate excellent performance on problems in up to 7 dimensions. Although \cite{xie} does not provide theoretical analysis, one can see our convergence proof for the discretized method as addressing theoretical questions left unanswered by that previous work. We also go beyond \cite{xie} in extending our methodology to be fully Bayesian by sampling Gaussian process hyperparameters from their posterior distribution using slice sampling.

Other related work includes \cite{marzat}, which considers a related but different formulation of (1) based on maximizing worst-case performance over a discrete set of environmental conditions. \cite{lam} considers a modification of \cite{williams} where the criterion used is for response surface model fit instead of global optimization.

Our consistency proof for the finite sum problem (1) is the first for any algorithm that evaluates \( F \) instead of \( G \). Consistency of some Bayesian optimization algorithms that evaluate \( G \) have, however, been shown in the literature. \cite{frazier} proved consistency of the knowledge gradient algorithm for any Gaussian process for finite domains. Later \cite{bull} proved consistency of expected improvement for functions that belong to the reproducing kernel Hilbert space (RKHS) of the covariance function. The recent working paper \cite{bect} also contains consistency results for knowledge gradient and expected improvement over any Gaussian process with continuous paths.

Our BQO algorithm can be considered to be within the class of knowledge gradient policies (\cite{powell} and...
Our BQO algorithm relies on a Gaussian process (GP) model of the underlying function $F$, which then implies a Gaussian process model over $G$. Before presenting BQO in §3, we present this statistical model to provide notation used through the rest of the paper. The first part of our development is standard in Bayesian optimization (Jones et al. 1998) and Bayesian quadrature (O’Hagan 1991), while the second part, in which a Gaussian process on the function’s integral or sum is obtained, is only standard in Bayesian quadrature.

We suppose that observing $F$ at $x, w$ provides an observation $y(x, w)$ equal to $F(x, w)$ optionally perturbed by additive independent normally distributed noise with mean 0 and variance $\lambda_{(x,w)}$. To permit estimation, we require one of two additional assumptions on this noise: either that $\lambda_{(x,w)}$ is constant across the domain; or that observing at $x,w$ also provides an observation of $\lambda_{(x,w)}$. The first assumption has been shown to be effective in a wide range of applications in the Bayesian optimization literature (Snoek et al. 2012). The second is reasonable in discrete-event simulation applications in which $y(x, w)$ is the average of a large batch of independent replications. In such applications, the difference between $y(x, w)$ and its mean $F(x, w)$ converges to a normal distribution by the central limit theorem as the batch size grows large, and $\lambda_{(x,w)}$ can be estimated by dividing the sample variance of these samples by their number (Kim and Nelson 2007).

We assume that the function $F$ follows a Gaussian process prior distribution:

$$ F (\cdot, \cdot) \mid \theta \sim GP (\mu_0 (\cdot, \cdot; \theta), \Sigma_0 (\cdot, \cdot; \cdot; \theta)),$$

where $\mu_0$ is a real-valued function taking arguments $x, w$ (the mean function), $\Sigma_0$ is a positive semi-definite function taking arguments $x, w, x’, w’$ (the kernel), and $\theta$ are the hyperparameters of the mean function and kernel. $\theta$ contains $\lambda_{(x,w)}$ when the variance of the observational noise is assumed to be unknown and constant. Common choices for $\mu_0$ and $\Sigma_0$ from the Gaussian process regression literature (Rasmussen and Williams 2006, Murphy 2012, Goovaerts 1997, Seeger et al. 2005, Bonilla et al. 2007) include setting $\mu_0$ to a constant and letting $\Sigma_0$ be the squared exponential or Matérn 5/2 kernel. In the case of the finite sum (1), kernels from the intrinsic model of coregionalization are appropriate (Seeger et al. 2005, Goovaerts 1997, Bonilla et al. 2007) and will be discussed in §6.

Following work on fully Bayesian inference in GP regression (Neal 1997), we additionally place a Bayesian prior distribution $\pi$ on $\theta$. This prior can regularize values of $\theta$ used in inference, pushing them toward regions of the space of hyperparameters believed to best correspond to the data. The prior can also be set constant if there is enough data to obviate such regularization.

We now discuss inference supposing that we have $n$ points in the historical data $H_n := (y_1, \ldots, y_{1,n})$, where $y_i = y(x_i, w_i)$ is a (possibly noisy) observation of $F(x_i, w_i)$ with the conditional distribution given $x_i, w_i$ described above. Within our inference procedure we sample $\theta$ from its posterior distribution given $H_n$ via slice sampling (Neal 2003). One may also replace this sampling-based fully Bayesian treatment of $\theta$ by using the maximum a posteriori estimate (MAP), which sets $\theta$ to its posterior mode (Murphy 2012). This is less
computationally intensive, but tends to be less accurate. The maximum likelihood estimate (MLE) of $\theta$ is a particular case of the MAP when the prior distribution on $\theta$ is flat.

Using this procedure to sample $\theta$, we now describe computation of the posterior distribution on both $F$ and $G$ given $\theta$. The posterior distribution on $F$ given $\theta$ at time $n$ is

$$F(\cdot, \cdot; \theta) | H_n, \theta \sim GP(\mu_n(\cdot, \cdot; \theta), \Sigma_n(\cdot, \cdot, \cdot; \theta)),$$

where the parameters $\mu_n$, $\Sigma_n$ can be computed using standard results from Gaussian process regression (Rasmussen and Williams 2006). To support later analysis, we provide these expressions here, suppressing dependence on $\theta$ in our notation:

$$\mu_n(x, w) = \mu_0(x, w) + \left[ \Sigma_0(x, w, x_1, w_1) \cdots \Sigma_0(x, w, x_n, w_n) \right] A_n^{-1} \begin{pmatrix} y_1 - \mu_0(x_1, w_1) \\ \vdots \\ y_n - \mu_0(x_n, w_n) \end{pmatrix}$$

(3)

$$\Sigma_n(x, w, x', w') = \Sigma_0(x, w, x', w') - \left[ \Sigma_0(x, w, x_1, w_1) \cdots \Sigma_0(x, w, x_n, w_n) \right] A_n^{-1} \begin{pmatrix} \Sigma_0(x', w', x_1, w_1) \\ \vdots \\ \Sigma_0(x', w', x_n, w_n) \end{pmatrix}$$

(4)

where

$$A_n = \begin{bmatrix} \Sigma_0(x_1, w_1, x_1, w_1) & \cdots & \Sigma_0(x_1, w_1, x_n, w_n) \\ \vdots & \ddots & \vdots \\ \Sigma_0(x_n, w_n, x_1, w_1) & \cdots & \Sigma_0(x_n, w_n, x_n, w_n) \end{bmatrix} + \text{diag}(\lambda(x_1, w_1), \ldots, \lambda(x_n, w_n)).$$

We now describe the posterior distribution on the objective function $G$ given $\theta$. We assume that $G$ is written in its integral form $\int F(x, w)p(w)dw$. Results for $H_n$ are similar, where the resulting expressions are obtained by replacing integration over $w$ by a sum over $w$ (or equivalently Lebesgue integration with respect to a counting measure). We denote by $E_n$, Cov$_n$, and Var$_n$ the conditional expectation, conditional covariance, and conditional variance with respect to the Gaussian process posterior given $H_n$ and $\theta$. By results from Bayesian quadrature (O’Hagan 1991), for $G(x) := \int F(x, w)p(w)dw$, we have that

$$E_n[G(x)] = \int \mu_n(x, w)p(w)dw := a_n(x; \theta),$$

(5)

$$\text{Cov}_n(G(x), G(x')) = \int \int \Sigma_n(x, w, x', w')p(w)p(w')dwdw'.$$

(6)

Ignoring some technical details, the first line is derived using interchange of integral and expectation, as in $E_n[G(x)] = E_n[\int F(x, w)p(w)dw] = \int E_n[F(x, w)p(w)]dw = \int \mu_n(x, w)p(w)dw$. The second line is derived similarly, though with more effort, by writing the covariance in terms of the expectation and interchanging expectation and integration.

The posterior distributions of $F$ and $G$ given $H_n$ and marginalizing over $\theta$ are infinite mixtures of Gaussian processes. Means of these posterior distributions can be obtained by averaging (3) or (5) with respect to the posterior on $\theta$.

### 3 Conceptual Description of the BQO Algorithm

Our BQO algorithm uses the statistical model described in §2 and samples $F$ sequentially. It chooses where to sample $F$ using a value of information analysis (Howard 1966). This analysis measures the expected quality of the best solution we can provide to (1) or (2) after $n$ samples, and how this quality improves with an additional
sample of \(F(x, w)\). In this section we describe this value of information analysis from a conceptual perspective in preparation for describing in §4 the novel computational methodology we create to make its implementation possible. This conceptual value of information analysis echoes the use of value of information in Bayesian optimization in works on knowledge-gradient methods (Frazier et al. 2009) and in problem (2) by Xie et al. (2012). The value of information analysis we describe here generalizes Xie et al. (2012) to support noisy observations, integrals with dependent normally distributed densities, non-normally distributed densities, and sums, and general kernels. While the generalization of the conceptual form of the value of information analysis from Xie et al. (2012) to handle this richer class of problems is straightforward, it presents a host of new computational challenges that requires new methodology, as fully described in §4.

We conduct our value of information analysis assuming the hyperparameters \(\theta\) are given, as is common practice in Bayesian optimization (Swersky et al. 2013, Shahriari et al. 2016). Then, in the implementation of the BQO algorithm, because \(\theta\) is unknown, we average this \(\theta\)-dependent value of information over the posterior on \(\theta\). While in principle one could instead conduct the full value of information analysis acknowledging that \(\theta\) is unknown, proceeding as we do provides substantial computational benefits.

To conduct this analysis, we first study the expected quality of the best solution we can provide. Given \(n\) samples, \(\theta\), and a risk-neutral utility function, we would choose as our solution to (1) or (2),

\[
x_{n, \theta}^* \in \arg\max_{x \in A} E_n[G(x) \mid \theta] = \arg\max_{x \in A} a_n(x; \theta),
\]

where \(a_n(x; \theta) := E_n[G(x) \mid \theta]\). This solution has expected value (again, with respect to the posterior after \(n\) samples given \(\theta)\),

\[
a_{n, \theta}^* := E_n[G(x_{n, \theta}^*) \mid \theta] = \max_x E_n[G(x) \mid \theta] = \max_x a_n(x; \theta).
\]

Consequently, the improvement in expected solution quality resulting from a sample at \((x, w)\) at time \(n\) is

\[
V_n(x, w; \theta) = E_n[a_{n+1, \theta}^* - a_{n, \theta}^* \mid x_{n+1} = x, w_{n+1} = w],
\]

and we refer to this quantity as the value of information. Our Bayesian Quadrature Optimization (BQO) algorithm then is defined as the algorithm that samples where this value of information (marginalized over \(\theta\)) is maximized,

\[
(x_{n+1}, w_{n+1}) \in \arg\max_{x, w} E[V_n(x, w; \theta) \mid H_n].
\]

Here, the expectation is over the posterior on \(\theta\), as indicated by the subscript.

This policy is one-step Bayes optimal in the known-hyperparameter case (i.e., the prior on \(\theta\) is concentrated on a single value), in the sense that if we can take one more sample before reporting a final solution then its sampling decision maximizes the expected value of \(G\) at this reported final solution. It is not necessarily Bayes-optimal if we can take more than one sample, but we argue that it remains a reasonable heuristic, and our numerical experiments in §6 support this. It is also Bayes-optimal for the problem (1) in the known-hyperparameter case when the number of iterations converge to infinity, as we show in §5.

Figure 1 illustrates BQO, showing one step in the algorithm applied to a simple analytic test problem

\[
\max_{x \in [-\frac{1}{2}, \frac{1}{2}]} E[zx^2 + w],
\]

where \(w \sim N(0, 1)\), \(z \sim N(-1, 1)\), and \(F(x, w) = E[zx^2 + w \mid w] = -x^2 + w\). Direct computation shows \(G(x) = -x^2\). In the figure, we fix \(\theta\) to a maximum likelihood estimate obtained using 15 training points.

The figure’s first row shows the contours of \(F(x, w)\) (left panel) and BQO’s estimate (right panel) after evaluating \(F\) at points chosen uniformly at random in an initial training phase, and at an additional \(n = 9\) points chosen by BQO. The second row’s left panel shows the value of information \(V_n(x, w; \theta)\). The value of information is small near where BQO has already sampled, because it has less uncertainty about \(F(x, w)\) in this region. BQO’s value of information is also small for extreme values of \(x\), because its posterior on \(G\)
(a) The contours of $F(x,w)$. $G$ is determined from $F$ by $G(x) = \int F(x,w)p(w)dw$.

(b) The contours of BQO’s estimate $\mu_n(x,w;\theta)$ of $F(x,w)$ after $n = 9$ evaluations of $F$ by BQO.

(c) The contours of BQO’s value of information $V_n(x,w;\theta)$ versus $x$ and $w$. $F$ was evaluated previously at the red points, chosen according to a random uniform design in an initial phase of training, and at $n = 9$ black points, chosen by BQO.

(d) The objective $G(x)$, BQO’s estimate $a_n(x;\theta)$ of $G(x)$, and BQO’s 95% credible interval for $G(x)$ after $n = 9$ evaluations of $F$ by BQO. The estimate of $G$ is extremely close to its true value, especially near its maximum.

Figure 1: Illustration of the BQO algorithm on an analytic test problem after evaluating $F$ at points chosen uniformly at random in an initial phase of training and $n = 9$ points chosen by BQO.
suggests that these \( x \) are far from its maximum, and small for extreme values of \( w \) because \( p(x,w) \) is small there. BQO’s value of information is thus largest for points that are far from previous samples, relatively close to the maximizer of \( G \)’s posterior mean, and have moderate values of \( w \). BQO samples next at the point with the largest value of information, near \( x = -0.2 \) and \( w = 1.8 \). The second row’s right panel shows the posterior on \( G \). This posterior is accurate and almost perfectly estimates \( G \)’s maximizer.

Figure 2 shows equivalent quantities for the knowledge-gradient (KG) method (Frazier et al. 2009), after noisy evaluations of \( G \) at points chosen uniformly at random in an initial training phase, and at an additional \( n = 9 \) points chosen by KG. Like other traditional Bayesian optimization methods, KG models \( G(x) \) directly, ignoring valuable information from \( w \), and computes a value of information as a function of \( x \) only while leaving the choice of \( w \) to chance. As a consequence, KG’s estimates of \( G \) and its maximizer have significantly more error than BQO’s estimates.

Figure 2: Illustration of a traditional Bayesian optimization algorithm in the same problem setting as Figure 1. The algorithm pictured is the knowledge gradient (KG) method (Frazier et al. 2009). This algorithm evaluates \( G \), unlike BQO’s evaluations of \( F \). As a consequence, it tends to provide lower-quality estimates of \( G \) within a given sampling budget.

4 Computation of the BQO Algorithm

In this section we develop methods to compute the value of information (7) and its gradient, to support implementation of the BQO algorithm. We introduce a new and powerful method in §4.2 for computing unbiased stochastic estimators of the gradient of the value of information, which we refer to more briefly as stochastic gradients. These stochastic gradients are used within a stochastic gradient ascent method to optimize the value of information.

We also show in §4.4 how a deterministic discretized method for approximating the value of information and its gradient, first developed in Xie et al. (2012) for the setting without noise and independent Gaussian \( p(w) \) and kernel, can be extended to our more general setting. When it was first proposed in Xie et al. (2012) it lacked a theoretical analysis of its discretization error. To address this shortcoming, we demonstrate that this discretization error vanishes asymptotically when the discretizations are sufficiently well-designed. We refer to this method as the “discretized method,” and refer to the first method (which does not rely on discretization) as the “discretization-free method.”
We provide an analysis of the computational complexity of each method, showing that the time and space complexity of the discretization-free method scale better in the dimension of $x$. In concert with this theoretical observation, empirical observations show that the discretized method is fastest when $x$ has one or two dimensions but is too slow to be practical in higher dimensions. In contrast, our numerical experiments (§6) show that our novel discretization-free method is practical in dimensions as large as 7.

To simplify proofs, we assume that $G$ has the integral form defined in (2). As we mentioned in §2, results for (1) are similar, where the resulting expressions are obtained by replacing integration over $w$ by a sum. We also assume in our computation of the value of information that $\theta$ is given, as discussed in §3, and drop the dependence on $\theta$ from our notation (except in §4.3 where we write it explicitly to support a high-level summary of the BQO algorithm). Table 1 summarizes notation used in this section, including both notation introduced in previous sections and new notation defined later in this section.

Table 1: Table of Notation.

| Symbol | Definition |
|--------|------------|
| $G(x)$ | $\sum_{w=1}^{m} F(x, w) p(w)$ or $\int F(x, w) p(w)dw$ |
| $V_n(x)$ | Value of information at time $n$ |
| $a_n(x)$ | Kernel of the Gaussian process prior distribution over the function $F$ |
| $H_n$ | History observed by time $n$ |
| $\Sigma_0$ | Variance of the noise in evaluations of $F(x, w)$ |
| $\Sigma_i(x, i)$ | $\sum \Sigma_0(x, w, x_i, w_i) p(w)dw$ if $G(x) = \int F(x, w) p(w)dw$, or $\sum_{w=1}^{m} \Sigma_0(x, w, x_i, w_i) p(w)$ if $G(x) = \sum_{w=1}^{m} F(x, w) p(w)$ for $i = 1, \ldots, n + 1$ |
| $\gamma$ | $\Sigma_0(x_{n+1}, w_{n+1}, x_1, w_1), \ldots, \Sigma_0(x_{n+1}, w_{n+1}, x_n, w_n))^T$ |
| $\lambda_{(x, w)}$ | Value of information at time $n$ |
| $A_n$ | $\Sigma_0(x_i, w_i, x_j, w_j)_{i, j=1}^{n} + \text{diag} \left( \left( \lambda_{(x, w)} \right)_{i=1}^{n} \right)$ |
| $\delta_n^2(x, x_{n+1}, w_{n+1})$ | $\text{Var}_n[G(x)] - \text{Var}_{n+1}[G(x)|x_{n+1}, w_{n+1}]$ |
| $\text{Var}_n$ | Conditional variance given $H_n$ |

4.1 Preliminary Representation of the Value of Information

In this section, we find a useful representation of the value of information (7) that will allow us to develop the discretization-free (§4.2) and discretized (§4.4) methods to approximate it and its gradient. We first observe that we can rewrite the value of information (7) as

$$V_n(x_{n+1}, w_{n+1}) = \text{max}_{x' \in A} a_{n+1}(x') | x_{n+1}, w_{n+1} | - \text{max}_{x' \in A} a_{n}(x').$$

(10)

This expression is not directly useful from a computational perspective, so we take one step further and find the joint distribution of $a_{n+1}(x)$ across all $x$ conditioned on $x_{n+1}, w_{n+1}$ and $H_n$ for any $x$. This is provided by the following lemma. The lemma is a generalization of Section 2.1 in Frazier et al. (2009), and we include the proof in the appendix (§A).

**Lemma 1.** There exists a random variable $Z_{n+1}$, whose conditional distribution given $H_n$ is standard normal, such that $a_{n+1}(x) = a_n(x) + \delta_n(x, x_{n+1}, w_{n+1}) Z_{n+1}$ for all $x$, with

$$\delta_n^2(x, x_{n+1}, w_{n+1}) := \text{Var}_n[G(x)] - \text{Var}_{n+1}[G(x)|x_{n+1}, w_{n+1}].$$

The posterior mean $a_n(x)$ of $G(x)$ can be represented by

$$a_n(x) = \int \mu_0(x, w) p(w)dw + [B(x, 1) \cdots B(x, n)] A_{n+1}^{-1} \begin{pmatrix} y_1 - \mu_0(x_1, w_1) \\ \vdots \\ y_n - \mu_0(x_n, w_n) \end{pmatrix},$$

(11)
where $B(x, i) := \int \Sigma_0 (x, w, x_i, w_i) p(w) \, dw$ for $1 \leq i \leq n$. We also have that

$$
\tilde{\sigma}_n (x, x_{n+1}, w_{n+1}) = \frac{B(x, n+1) - [B(x, 1) \cdots B(x, n)] A_n^{-1} \gamma}{\sqrt{\Sigma_0 (x_{n+1}, w_{n+1}, x_{n+1}, w_{n+1})}} \times 1\{ \lambda(x_{n+1}, w_{n+1}) > 0 \text{ or } (x_{n+1}, w_{n+1}) \notin \{(x_i, w_i) : i \leq n\} \},
$$

where $\gamma^T := (\Sigma_0(x_{n+1}, w_{n+1}, x_1, w_1), \ldots, \Sigma_0(x_{n+1}, w_{n+1}, x_n, w_n))$.

The expressions in this lemma require that $\lambda(x_{n+1}, w_{n+1})$ be known to compute the value of information. This is seldom true in practice, but this quantity can be estimated and the estimate used in its place. If the noise is homogeneous then it can be estimated by including it as a hyperparameter in our Gaussian-process-based inference. If each observation is an average of many i.i.d. replications, allowing the variance of the noise in each observation to be estimated with high accuracy, and we believe that the noise does not change abruptly in the domain, then we can use the mean of the variance estimates from previous observations as our estimator of $\lambda(x_{n+1}, w_{n+1})$. Finally, if we are in neither of these situations, then we can use the approach developed in Kersting et al. (2007) in which a Gaussian process is used to estimate the variance of heteroscedastic noise across the domain.

We now use Lemma 1 to estimate the value of information and its gradient in the next subsection.

### 4.2 Discretization-Free Computation of the Value of Information and its Gradient

In this subsection, we provide unbiased and strongly consistent Monte Carlo estimators of the value of information and its gradient. Our techniques use the envelope theorem (Milgrom and Segal 2002) and were inspired by Wu et al. (2017), which uses this theorem to build an unbiased estimator of the gradient of the knowledge-gradient in a different setting.

First, Lemma 1, equation (10), and the strong law of large numbers show that if $\{Z_i\}_{i=1}^{\infty}$ are independent standard normal random variables, then

$$
\hat{V}_{n,m}(x, w) := \frac{1}{m} \sum_{i=1}^{m} \left[ \max_{x' \in A} \left( a_n(x') + \tilde{\sigma}_n(x', x, w) Z_i \right) - \max_{x' \in A} a_n(x') \right]
$$

is an unbiased and strongly consistent estimator of the value of information $V_n(x, w)$. The inner optimization problems $\max_{x' \in A} \left( a_n(x') + \tilde{\sigma}_n(x', x, w) Z_i \right)$ can be solved using standard optimization methods such as LBFGS (Zhu et al. 1997) or Newton methods (if the Hessian of the kernel exists). Gradients of the inner optimization problem’s objective can be computed using (15).

We now build an unbiased and strongly consistent estimator of $\frac{\partial}{\partial w} V_n(x, w)$ where $x = (x_1, \ldots, x_d), w = (w_1, \ldots, w_p)$, $r \in \{x_i : 1 \leq i \leq d\} \cup \{w_i : 1 \leq i \leq p\}$, and give sufficient conditions for existence of $\frac{\partial}{\partial r} V_n(x, w)$. We use the envelope theorem (Milgrom and Segal 2002), along with the following lemma, which shows some smoothness properties of $a_n$ and $\tilde{\sigma}_n$. The proof of this lemma may be found in Appendix A.

**Lemma 2.** We assume $\mu_0$ is constant, and the kernel $\Sigma_0$ of the prior distribution on $F$ is continuously differentiable and bounded. We also suppose there is a non-negative function $h$ such that $\int h(x, w', x') p(w') \, dw'$ is finite for all $x, x' \in A$, and $\left| \frac{\partial \Sigma_0(x, w, x', w')}{\partial w} \right| < h(x, w', x')$ for all $x, x' \in A$ and $w, w' \in W$. Then:

1. $a_n$ and $\tilde{\sigma}_n(\cdot, x, w)$ are both continuously differentiable for any $x, w$ if $\Sigma_n(x, w, x, w) > 0$.

2. For any $x'$, $\tilde{\sigma}_n(x', x, w)$ is continuously differentiable with respect to $x, w$ if $\Sigma_n(x, w, x, w) > 0$ and $\lambda_{(x, w)}$ is continuously differentiable.
The condition $\Sigma_n(x, w, x, w) > 0$ in the previous lemma is always true in the noisy case, as shown by (4). In the noiseless case, $\Sigma_n(x, w, x, w)$ can be zero only if $x, w$ is a previously measured point.

The following lemma shows how to compute stochastic gradients of $V_n(x, w)$ and allows us to optimize $V_n$ with a stochastic gradient ascent method.

**Lemma 3.** Suppose that the hypotheses of Lemma 2 on $\Sigma_0$ and $p$ are satisfied. Also assume that for a given $(x_{n+1}, w_{n+1})$, $\arg\max_{x' \in A} (a_n(x') + \sigma_n(x', x_{n+1}, w_{n+1}) Z)$ is almost surely a singleton, where $Z$ is a standard normal random variable. Also assume $\Sigma_n(x_{n+1}, w_{n+1}, x_{n+1}, w_{n+1}) > 0$ and $\lambda_{(x, w)}$ is continuously differentiable at $x = x_{n+1}$ and $w = w_{n+1}$. Let \( \{Z_i\}_{i=1}^{\infty} \) be independent standard normal random variables. Then

$$\nabla V_n(x_{n+1}, w_{n+1}) = \frac{1}{m} \sum_{i=1}^{m} \nabla (x_{n+1}, w_{n+1}) \sigma_n(y_i, x_{n+1}, w_{n+1}) Z_i \quad \text{a.s.,}$$

where $y_i = \arg\max_{x' \in A} (a_n(x') + \sigma_n(x', x_{n+1}, w_{n+1}) Z)$. Furthermore, $E \left[ \nabla (x_{n+1}, w_{n+1}) \sigma_n(y_i, x_{n+1}, w_{n+1}) Z_i \right] = V_n(x_{n+1}, w_{n+1})$ for all $i$.

**Proof.** Let $Z$ be a standard normal random variable, and $f(x', (x, w)) := a_n(x') + \sigma_n(x', x, w) Z$ where $x', x \in A$ and $w \in W$. By Lemma 2, $f$ is continuously differentiable, and so by the envelope theorem (Milgrom and Segal 2002 Corollary 4),

$$\nabla (x_{n+1}, w_{n+1}) f(y, (x_{n+1}, w_{n+1})) = \nabla (x_{n+1}, w_{n+1}) (a_n(y) + \sigma_n(y, x_{n+1}, w_{n+1}) Z) = \nabla (x_{n+1}, w_{n+1}) \sigma_n(y, x_{n+1}, w_{n+1}) Z \quad \text{a.s.,}$$

where $y = \arg\max_{x' \in A} (a_n(x') + \sigma_n(x', x_{n+1}, w_{n+1}) Z)$ and the dependence of $y$ on $x_{n+1}, w_{n+1}$ is ignored when taking the gradient.

We now show that $\nabla V_n(x_{n+1}, w_{n+1}) = E_n \left[ \nabla (x_{n+1}, w_{n+1}) \max_{x' \in A} (a_n(x') + \sigma_n(x', x_{n+1}, w_{n+1}) Z) \right]$. First observe that if $z$ is a real number such that $\arg\max_{x' \in A} (a_n(x') + \sigma_n(x', x_{n+1}, w_{n+1}) z) = \{y_z\}$, by the envelope theorem, we then have that

$$\nabla (x_{n+1}, w_{n+1}) \max_{x' \in A} (a_n(x') + \sigma_n(x', x_{n+1}, w_{n+1}) z) = \nabla (x_{n+1}, w_{n+1}) (a_n(y_z) + \sigma_n(y_z, x_{n+1}, w_{n+1}) z).$$

Furthermore, we have that

$$\left| \nabla (x_{n+1}, w_{n+1}) (a_n(y_z) + \sigma_n(y_z, x_{n+1}, w_{n+1}) z) \right| = \left| \nabla (x_{n+1}, w_{n+1}) (\sigma_n(y_z, x_{n+1}, w_{n+1}) z) \right| \leq L_{(x_{n+1}, w_{n+1})} |z|$$

where $L_{(x_{n+1}, w_{n+1})} = \sup_{x' \in A} \left| \nabla (x_{n+1}, w_{n+1}) \sigma_n(x', x_{n+1}, w_{n+1}) \right|$, which is finite because $\sigma_n(\cdot, x_{n+1}, w_{n+1})$ is continuously differentiable and $A$ is a compact set. Consequently, $E_n \left[ L_{(x_{n+1}, w_{n+1})} Z \right] < \infty$.

By Corollary 5.9 of Bartle (1966), $\nabla V_n(x, w) = E_n \left[ \nabla (x_{n+1}, w_{n+1}) \max_{x' \in A} (a_n(x') + \sigma_n(x', x_{n+1}, w_{n+1}) Z) \right]$.

Finally, the first claim of the lemma follows from the strong law of large numbers. \qed

As a reminder, we assumed that the objective function $G$ has the integrated form at the beginning of the section. In the case of the finite sum (1), the assumptions we have made in Lemma 3 and Lemma 2 may no longer hold. In particular, $\frac{\partial}{\partial w_j} \Sigma_0(x, w, x', w)$ will typically not exist for $1 \leq j \leq p$ where $w = (w_1, \ldots, w_p)$, and so $\frac{\partial}{\partial w_j} V_n(x, w)$ may not exist either (see Lemma 1). However, our approach remains applicable in this setting: we use $\nabla V_n(x, w)$ to maximize $V_{n, x}(x, w)$ for each $w \in W$, and then easily solve $\max_{w \in W} V_n^x(w) = \max_{w \in W} \left[ \max_{x \in A} V_n(x, w) \right]$ observing that $W$ is a finite set. Using $\nabla V_n(x, w)$ in this way requires showing similar results to the ones presented in this section to compute stochastic gradients of $V_n(x, w)$ with respect to $x$ for any fixed $w$, under the assumption that $\Sigma_0(\cdot, w, \cdot, w')$ and $\lambda_{(x, w)}$ are sufficiently smooth for any $w, w' \in W$. We do not include these results here, because their proofs follow the same ideas already presented.
4.3 Computation and Complexity of the BQO Algorithm

In this section, we summarize computation of the BQO algorithm, which combines the tools developed in previous sections, and discuss its complexity. First, recall we previously described methods for obtaining unbiased samples of $V_n$ and $\nabla V_n$ using a fixed value of $\theta$. Because $\theta$ was fixed, we suppressed it in our notation, but here we indicate it explicitly, writing these values as $V_n(\theta)$ and $\nabla V_n(\theta)$ and their estimators as $\hat{V}_n(\theta)$ and $\hat{\nabla V}_n(\theta)$ respectively. We will use these within a stochastic gradient algorithm, ADAM (Kingma and Ba 2014), for solving problem (8), i.e., for maximizing $E[V_n(\theta) \mid H_n]$. Within this stochastic gradient algorithm, each stochastic gradient is obtained by first taking $J$ independent samples $\hat{\theta}_j : j = 1, \ldots, J$ from the posterior distribution on $\theta$ given $H_n$ using slice sampling, and then computing $\frac{1}{J} \sum_{j=1}^{J} \hat{\nabla} V_n(\hat{\theta}_j)$, where each $\hat{\nabla} V_n(\theta)$ uses a single independent standard normal random variable (so $m = 1$ as defined Lemma 3). We use a similar approach in the final step of our algorithm to select a point with maximal posterior mean $E[a_N(x; \theta) \mid H_N]$, except that the only source of randomness in our stochastic gradient estimator is $\theta$.

The BQO algorithm using this approach is summarized in Algorithm 1.

Algorithm 1 BQO Algorithm

1: Evaluate $F$ at $n_0$ points, chosen uniformly at random from $A \times W$.
2: for $n = 0$ to $N-1$ do
3: Use the multi-start ADAM algorithm to maximize $E[V_n(\theta) \mid H_n]$, using the stochastic gradient estimator $\frac{1}{n_0 + n} \sum_{j=1}^{J} \hat{\nabla} V_n(\hat{\theta}_j)$ on each iteration using independent samples $\hat{\theta}_j$ from the posterior on $\theta$. Include all $n_0 + n$ samples of $F$ when computing the posterior. Let $(x_{n+1}, w_{n+1})$ be the resulting maximizer.
4: Sample $F(x_{n+1}, w_{n+1})$ to obtain $y_{n+1}$.
5: end for
6: Use the multi-start ADAM algorithm to maximize $E[a_N(x; \theta) \mid H_N]$ using the stochastic gradient estimator $\frac{1}{J} \sum_{j=1}^{J} \nabla a_N(x; \hat{\theta}_j)$, using independent samples $\hat{\theta}_j$ from the posterior on $\theta$. Return $x^* \in \text{argmax}_{x \in A} E[a_N(x; \theta) \mid H_N]$.

Observe that in the noise-free case, $V_n(x, w)$ is not differentiable at any previously evaluated point $x, w$, as shown by the last equation of Lemma 1. The set of previously evaluated points, however, is finite and so we can still use ADAM by perturbing the algorithm’s current iterate whenever it resides at a non-differentiable point. A similar idea can be found in Jin et al. 2017. Finally we discuss BQO’s time and space complexity, assuming we use it to select $N$ points $(x, w)$ to sample. To select each point $(x, w)$ to sample, we use Algorithm 1 which runs the ADAM algorithm for $T$ iterations. Each iteration requires a stochastic gradient computed using $J$ independent standard Gaussian random variables, $J$ independent samples $\hat{\theta}_j$ from the posterior on $\theta$ (let $Q$ be the number of iterations of slice sampling used for each), and $J$ runs of LBFGS to maximize $(a_n(x') + \hat{\sigma}_n(x', x_{n+1}, w_{n+1}) Z_i)$. Let $K$ be the number of steps in a single run of LBFGS, where each step requires an evaluation of $a_n$, $\hat{\sigma}_n$, and their gradients. Let $O(L)$ be the complexity of computing the kernel and its gradient, and let $O(S)$ be the complexity of computing $(\nabla V_n + I) B(x, n+1)$, and $B(x, i)$ for all $i \leq n$.

With this notation, we show in the appendix (§B) that the BQO algorithm has time complexity $O(JQN^3 + JQLN^3 + JT(\text{SN}^2 + \text{N}^3) + JTLN^2)$ and space complexity $O(N^2)$.

The integrals in (15), $\nabla V_n + I) B(x, n+1)$, and $B(x, i)$ do not necessarily have closed-form expressions. While we might estimate them via Monte Carlo or numerical integration, this can be inconvenient and increase computational cost. Consequently it may be better to first perform a change of variables from $w$ to another $w'$ for which integrals may be evaluated in closed form. One such transformation, to the Gaussian distribution, is discussed in the appendix §C. In addition, a change of variables from $w$ to $w'$ induces a change from $F(x, w)$ to some other $F'(x, w')$, which might change more slowly with $w'$ (requiring fewer samples to model it) or be better modeled by a Gaussian process. We illustrate this change of variable technique in our numerical experiments, in the inventory (§6.6) and Citi Bike (§6.3) problems.
4.4 Discretized Computation of the Value of Information and its Gradient

In this section we describe an alternate approach to that in §4.2 for estimating the value of information and its gradient. It uses a discretization of $A$. Although this approach was already considered in [Xie et al., 2012], which presents a particular case of our method for the integral objective (2) in the noise-free setting with an independent Gaussian $p$ and Gaussian kernel, we extend this analysis by generalizing it to our setting and showing that a sequence of increasingly fine discretizations produces a sequence of estimators whose estimates converge to the value of information. Thus, these estimators, while biased, are strongly consistent. In practice, computational intractability limits this approach when $A$ has more than 3 dimensions. This lack of scalability is also demonstrated by a complexity analysis we present at the end of this subsection.

**Lemma 4.** We assume that $\Sigma_0(\cdot, w,w',x',w')$ is continuous for all $w,w' \in W$, $x' \in A$, $\Sigma_0$ is bounded, and $\mu_0$ is a constant. Suppose that we have an increasing sequence of finite discretizations $\{A_L^\ell\}_{L=1}^\infty$ of $A$, such that $\bigcup_{L=1}^\infty A_L^\ell$ is dense in $A$. Then

$$V_n(x_{n+1},w_{n+1}) = \lim_{L \to \infty} \left( E_n \left[ \max_{x \in A_L^\ell} \left( a_n(x) + \hat{\sigma}(x,x_{n+1},w_{n+1})Z_{n+1} \right) \right] - \max_{x \in A_L^\ell} a_n(x) \right).$$

The proof of this lemma may be found in §A. A sequence of discretizations that satisfy the properties of the lemma can be built by considering the rationals, as we do in the proof of Theorem 5.

Using the previous lemma, we have that $V_n(x_{n+1},w_{n+1}) = \lim_{L \to \infty} h(a_n(A_L^\ell), \hat{\sigma}_n(A_L^\ell,x_{n+1},w_{n+1}))$, where $a_n(A_L^\ell) = (a_n(x_i))_{i=1}^L$, $\hat{\sigma}_n(A_L^\ell,x) = (\hat{\sigma}_n(x_i,x,w))_{i=1}^L$, and $h : \mathbb{R}^L \times \mathbb{R}^L \to \mathbb{R}$ is defined by

$$h(a,b) = E \left[ \max_i a_i + b_i | Z \right] - \max_i a_i,$$

where $a$ and $b$ are any deterministic vectors, and $Z$ is a one-dimensional standard normal random variable. We can then approximate the value of information by $h(a_n(A_L^\ell), \hat{\sigma}_n(A_L^\ell,x_{n+1},w_{n+1}))$ for some $L$. By convenience, we denote $a_n(x_i)$ by $q_i$ and $\hat{\sigma}_n(x_i,x,w)$ by $r_i$ for each $i$ in $\{1,\ldots,L\}$. If $A = A_L^\ell$, which is possible if $A$ is a finite set, then the approximation is exact.

Algorithm 1 of [Frazier et al., 2009] applied to $h$, gives a subset of indexes $\{j_1,\ldots,j_\ell\}$ from $\{1,\ldots,L\}$, such that $V_n(x_{n+1},w_{n+1}) = h(a_n(A_L^\ell), \hat{\sigma}_n(A_L^\ell,x_{n+1},w_{n+1})) = \sum_{i=1}^{\ell-1} (r_{j_{i+1}} - r_{j_i}) f(-|c_i|)$, where $f(z) := \varphi(z) + z\Phi(z)$, $c_i := \frac{q_{i+1} - q_i}{r_{j_{i+1}} - r_{j_i}}$ for $1 \leq i \leq \ell - 1$, and $\varphi, \Phi$ are the standard normal cdf and pdf, respectively. This shows how to approximate the value of information $V_n$ using the discretization $A_L^\ell$ of $A$.

We now show how to approximate the gradient of the value of information $V_n$ using the discretization $A_L^\ell$ of $A$. Observe that if $\ell = 1$, $V_n(x,w) = 0$ and so $\nabla V_n(x,w) = 0$. On the other hand, if $\ell > 1$, one can show via direct computation that $\nabla V_n(x,w) = \sum_{i=1}^{\ell-1} (-\nabla r_{j_i} + \nabla r_{j_{i+1}}) \varphi(|c_i|)$. Consequently, we only need to compute $\nabla r_{j_i}$ for each $i$ in $\{1,\ldots,\ell\}$. Another direct computation shows that $\nabla (x_{n+1},w_{n+1}) \hat{\sigma}_n(x,x_{n+1},w_{n+1}) = \beta_1 \beta_3 - \frac{1}{2} \beta_1^2 \beta_2 [\beta_5 - \beta_4]$, where

$$\beta_1 = \left[ \Sigma_0(x_{n+1},w_{n+1},x_{n+1},w_{n+1}) - \gamma^T A_n^{-1} \gamma \right]^{-1/2},$$
$$\beta_2 = B(x,n+1) - [B(x,1) \cdots B(x,n)] A_n^{-1} \gamma,$$
$$\beta_3 = \left( \nabla B(x,n+1) - \nabla (\gamma^T) A_n^{-1} [B(x,1),\cdots,B(x,n)]^T \right),$$
$$\beta_4 = 2 \nabla (\gamma^T) A_n^{-1} \gamma,$$
$$\beta_5 = \nabla \Sigma_0(x_{n+1},w_{n+1},x_{n+1},w_{n+1}).$$
Complexity of the Discretized Version of the BQO Algorithm. Here we discuss the time and space complexity of a version of BQO based on discretized computation of the value of information and its gradient. We use the same notation and a similar analysis to that in the previous section. As a reminder, $O(L)$ is the complexity of the computation of the kernel and its gradient, and $O(S)$ is the complexity of computing $\nabla_{n+1} B(x, n+1)$, and $B(x, i)$ for all $i \leq n$. We sample $J$ parameters $(\tilde{\theta}_1, \cdots, \tilde{\theta}_J)$ from the posterior on $\theta$, running slice sampling for at most $Q$ iterations for each, and we optimize the value of information with the ADAM algorithm for at most $T$ iterations. If we use a uniform discretization of size $E^d$ where $d$ is the dimension of $A$, the time complexity of the BQO algorithm run for $N$ iterations is $O(E^d TJ(SN^2 + N^3) + JTLN^2 + JQLN^3 + JQN^d)$, and the space complexity is $O(N^2 + E^d)$. Thus if $E$ increases, the time complexity and space complexity increase exponentially. This makes this method impractical when $d > 3$.

5 Asymptotic Analysis for BQO

In this section, we show consistency of BQO. We show that if $p$ and $W$ are finite, $A$ is finite or a closed box in $\mathbb{R}^d$, the integrand function $F$ follows a Gaussian process prior with continuous paths for a fixed $w$, and the prior on the hyperparameters of the kernel is concentrated on a single value, then as the number of iterations of the algorithm tends to infinity, the optimal solution given by the BQO algorithm converges in expectation to an optimal solution $\arg\max_{x \in A} G(x)$. We omit the explicit dependence of the expressions on $\theta$ since the prior on $\theta$ is assumed concentrated on a single value.

We state two consistency results, one for continuum $A$ (Theorem 1) and the other for finite $A$ (Theorem 2). The proofs for both results may be found in the appendix. The proof for finite $A$ has a similar structure to the proof of consistency for the knowledge-gradient method for finite domains in problems without integrated objectives from Frazier et al. (2009). We present a proof for the finite case partly because finite $A$ arises in practice, and partly because it is substantially simpler than the continuum case and provides a starting point for understanding the continuum proof. Our proof for the continuum goes substantially beyond the techniques required for the finite case, and develops techniques that may also be useful for proving consistency of other Bayesian optimization methods in continuum settings. Consistency of Bayesian optimization in continuum settings has been largely unexplored, with the authors being aware of only two other papers on this topic: The working paper Bect et al. (2016) contains consistency results for Bayesian optimization algorithms over Gaussian processes with continuous paths in the continuum setting; and Bull (2011) proved consistency of expected improvement for functions that belong to the reproducing kernel Hilbert space (RKHS) of the covariance function in the continuum setting, though Driscoll’s Theorem (Lukić and Beder 2001) shows that, under some regularity conditions, sample paths of the Gaussian process almost surely do not belong to the RKHS.

We first introduce notation needed for the theorems. Define $A' = A \times W$. Define the set $\mathcal{H} := D(A') \times D_{\text{kernel}}(A' \times A')$, where $D(A')$ is the set of functions defined on $A'$, and $D_{\text{kernel}}(A' \times A')$ is the set of positive semidefinite functions defined on $A' \times A'$. We define the set $\mathcal{H}_i \subset \mathcal{H}$ as

$$\{ (\mu, \Sigma) : \mu \equiv 0, \Sigma_{w,w'}(x,y) := \Sigma(x,w,y,w') \text{ is in } C^1(\mathbb{R}^d \times \mathbb{R}^d) \text{ and is isotropic for all } w, w' \in W \}.$$ 

We first state our result for continuum $A$ and prove it in the appendix §E.2.

**Theorem 1.** Suppose that $A = [a_1, b_1] \times \cdots \times [a_d, b_d] \subset \mathbb{R}^d$, $a_i < b_i$ for all $i$, $W$ is a finite set, and the probability space is complete. Assume $(\mu_0, \Sigma_0) \in \mathcal{H}_i$. We assume that the function $g_w(x) := \lambda(x,w)$ is continuous in $A$ for all $w \in W$, and there exists $k_{\lambda}, K_{\lambda} > 0$ such that $k_{\lambda} < \lambda(x,w) < K_{\lambda}$ for all $w \in W$ and $x \in A$. Then

$$\lim_{N} E_{BQO}^{N} \left[ \max_{x \in A} a_N(x) \right] = E \left[ \max_{x \in A} G(x) \right],$$

where $E_{BQO}^{N}$ indicates expectation with respect to the distribution over sampling decisions induced by BQO.
We also state our result for finite $A$ and prove it in the appendix §E.1.

**Theorem 2.** Suppose that $A$ and $W$ are finite. Assume $(\mu_0, \Sigma_0) \in \mathcal{H}$. We have that

\[
\lim_N E^{BQO}[\max_{x \in A} a_N(x)] = E[\max_{x \in A} G(x)].
\]

### 6 Numerical Experiments

In this section we present numerical experiments motivated by applications in operations research and machine learning. We compare the BQO algorithm against baseline Bayesian optimization algorithms and algorithms from the literature designed for the specific problems considered. These experiments illustrate how the BQO algorithm can be applied in practice, and demonstrate it performs at least as well as these benchmarks on all problems considered, and often much better.

We compare on seven test problems: a test problem with a simple analytic form (§6.1); a composition of Branin functions (§6.2) used in Williams et al. (2000); a realistic problem arising in the design of the New York City’s Citi Bike system (§6.3); cross-validation of convolutional neural networks (§6.5) and recommendation engines (§6.4); an inventory problem with substitution (§6.6); and a collection of problems simulated from Gaussian process priors (§6.7) that provide insight into how the benefit provided by BQO is determined by problem characteristics, and that identify problems where BQO is most helpful.

As benchmark algorithms we consider the multi-task algorithm in Section 3.2 of Swersky et al. (2013) and the algorithm of Williams et al. (2000), which both place a Gaussian process prior on $F(x, w)$, as BQO does. In addition, we consider two baseline Bayesian optimization algorithms: the knowledge-gradient (KG) policy of Frazier et al. (2009) and the Expected Improvement criterion of Jones et al. (1998), which both place the Gaussian process prior directly on $G(x)$. The KG policy is equivalent to BQO in problems where all components of $w$ are moved into $x$. We also solved the problems from §6.1 and §6.3 with Probability of Improvement (PI) (Brochu et al. 2010), but do not include these results because both KG and EI significantly outperform PI.

We now discuss the kernels used in these experiments. When implementing BQO and the benchmark algorithms in the Branin (§6.2) and inventory (§6.6) problems, we use the 5/2-Matérn kernel $\Sigma_0(x, w, x', w') = \sigma^2 \left(1 + \sqrt{5}r + \frac{\sqrt{5}}{3}r^2\right) \exp\left(-\sqrt{5}r\right)$, where $r = \sqrt{\sum_{k=1}^n \alpha_k^2 \left|x_k - x'_k\right|^2}$, $n$ is the number of tasks, and $\{\sigma_{t, t'}\}_{t, t' \in \{1, \ldots, n\}}$ are real numbers, such that $\sigma_{t, t'} = \sigma_{t', t}$ whenever $t_1 \neq t_2'$ and $t_2 \neq t'$, and the matrix $(\sigma_{t, t'} : t, t' \in \{1, \ldots, n\})$ is symmetric and positive definite.

In the cross-validation problems (§6.4, §6.5), we use the expected improvement algorithm with the 5/2-Matérn kernel and the BQO algorithm (Algorithm 1 in §3) and multi-task Bayesian algorithm with the task kernel (Swersky et al. 2013), which is the Kronecker product of a 5/2-Matérn kernel and a kernel defined only over the finite set $W$. Specifically this kernel is defined by $\Sigma_0(x, t, x', t') = \sigma_{t, t'} \left(1 + \sqrt{5}r + \frac{\sqrt{5}}{3}r^2\right) \exp\left(-\sqrt{5r}\right)$, where $r = \sqrt{\sum_{k=1}^n \alpha_k^2 \left|x_k - x'_k\right|^2}$, $n$ is the number of tasks, and $\{\sigma_{t, t'}\}_{t, t' \in \{1, \ldots, n\}}$ are real numbers, such that $\sigma_{t, t'} = \sigma_{t', t}$ whenever $t_1 \neq t_2'$ and $t_2 \neq t'$, and the matrix $(\sigma_{t, t'} : t, t' \in \{1, \ldots, n\})$ is symmetric and positive definite.

In the analytic test problem (§6.1), Citi Bike problem (§6.3), and the problems simulated from Gaussian process priors (§6.7), we implemented BGO and the benchmark algorithms with the squared exponential kernel $\Sigma_0(x, w, x', w') = \sigma_0^2 \exp\left(-\sum_{k=1}^n \alpha_k^{(1)} \left|x_k - x'_k\right|^2 - \sum_{k=1}^d \alpha_k^{(d)} \left[w_k - w'_k\right]^2\right)$, where $\alpha_0^2$ is the common prior variance and $\alpha_1^{(1)}, \ldots, \alpha_n^{(n)}, \alpha_2^{(1)}, \ldots, \alpha_2^{(d)} \in \mathbb{R}_+$ are the length scales parameters.

In the majority of our experiments (§6.2 and §6.4, §6.6) we implement BGQO using the discretization-free approach with fully Bayesian inference over hyperparameters (Algorithm 1 in §3). In the analytic test problem (§6.1), the Citi Bike problem (§6.3), and the problems simulated from Gaussian process priors (§6.7), we use the discretized version (4.4) of the BQO algorithm. In these problems we also calculate the hyperparameters of the kernels, $\sigma^2$ and $\mu_0$, using maximum likelihood estimation following the first stage of samples. We do not
use the discretization-free version of BQO in these problems because they were performed as part of an initial conference paper version of this work (Toscano-Palmerin and Frazier 2016), and only the discretized version of BQO existed at that time. Benchmark algorithms in each problem were implemented using the same approach to hyperparameter estimation as used by BQO.

6.1 An Analytic Test Problem

In our first example, we consider the problem (9) stated in §3. BQO is well-suited to this problem because evaluations of $F(x, w)$ have much lower noise than those of $G(x)$. We do not compare against the multi-task algorithm (Swersky et al. 2013) and SDE algorithm (Williams et al. 2000) because they can only be applied when the objective function is a finite sum. We do not compare against Xie et al. (2012) because this problem has noisy evaluations. Figure 3 compares the performance of BQO, KG and EI on this problem, plotting the number of samples beyond the first stage on the $x$ axis, and the average true quality of the solutions provided, $G(\arg\max_x E_n[G(x)])$, averaging over 3000 independent runs of the three algorithms. We see that BQO substantially outperforms both benchmark methods. This is because BQO reduces the noise in its observations by conditioning on $w$, allowing it to more swiftly localize the objective’s maximum.

Figure 3: Performance comparison between BQO and two Bayesian optimization benchmark, the KG and EI methods, on the analytic test problem (9) from §3, as described in §6.1.

6.2 Branin Function

In this example problem we compare BQO against the SDE (Williams et al. 2000) and multi-task (Swersky et al. 2013, Section 3.2) algorithms. We consider the Branin problem proposed in Williams et al. (2000) where

$$F(x_1, x_2, x_3, x_4) = y_b(15x_1 - 5, 15x_2)y_b(15x_3 - 5, 15x_4),$$

is the Branin function and $x_1, x_2, x_3, x_4 \in [0, 1]$. We define $x := (x_1, x_4)$ and $w := (x_2, x_3)$. The joint distribution $p$ of $w$ is defined in Table 2. We maximize the function $G(x_1, x_4) := \sum_{(x_2, x_3) \in \{0.25, 0.5, 0.75\} \times \{0.2, 0.4, 0.6, 0.8\}} p(x_2, x_3) F(x_1, x_2, x_3, x_4)$.

Figure 4 compares the performance of BQO, SDE and the multi-task algorithm on this problem, plotting the number of samples beyond the first stage on the $x$ axis, and the average true quality of the solutions provided, $G(\arg\max_x E_n[G(x)])$. We average over 100 independent runs of the BQO algorithm, 126 independent runs of
| $x_2/x_3$ | 0.2 | 0.4 | 0.6 | 0.8 |
|-----------|-----|-----|-----|-----|
| 0.25      | 0.0375 | 0.0875 | 0.0875 | 0.0375 |
| 0.5       | 0.0750 | 0.1750 | 0.1750 | 0.0750 |
| 0.75      | 0.0375 | 0.0875 | 0.0875 | 0.0375 |

Table 2: Probability distribution of $w = (x_2, x_3)$ for the Branin problem from §6.2.

the multi-task algorithm, and 230 independent runs of the SDE algorithm. We see that BQO substantially outperforms both the SDE and multi-task optimization benchmarks, despite the fact that these competing methods also model $F$. We believe this is because SDE and the multi-task optimization algorithm both choose points using a heuristic rule that performs poorly in certain settings, as explained in the introduction, rather than using a one-step optimality analysis like BQO.

Figure 4: Performance comparison between BQO, the SDE algorithm (Williams et al. 2000), and the multi-task algorithm (Swersky et al. 2013) on the Branin problem from §6.2.

6.3 New York City’s Citi Bike System

We now consider a queuing simulation based on New York City’s Citi Bike system in which system users may remove an available bike from a station at one location within the city and ride it to a station with an available dock in some other location. The optimization problem that we consider is the allocation of a constrained number of bikes (6000) to available docks within the city at the start of rush hour, so as to minimize, in simulation, the expected number of potential trips in which the rider could not find an available bike at their preferred origination station, or could not find an available dock at their preferred destination station. We call such trips “negatively affected trips.”

We simulate the demand for bike trips on days from January 1st to December 31st between 7:00am and 11:00am. We use 329 actual bike stations, locations, and numbers of docks from the Citi Bike system. In our simulator, we choose a day at random from the 365 days of the year and then simulate the demand for trips between each pair of bike stations on that day using an independent Poisson process whose rate is given by historical data from that day in 2014 available from Citi Bike’s website (Motivate International 2015). Travel times between pairs of stations are modeled using an exponential distribution with parameters estimated from this same dataset. If a potential trip’s origination station has no available bikes, then that trip does not occur, and we increment our count of negatively affected trips. If a trip does occur, and its preferred destination station
does not have an available dock, then we also increment our count of negatively affected trips, and the bike is returned to the closest bike station with available docks.

We divide the bike stations into 4 groups using k-nearest neighbors, and let \( x \) be the number of bikes in each group at 7:00 AM. We suppose that bikes are allocated uniformly among stations within a single group. The random variable \( w \) is the total demand for bike trips during the period of our simulation, summed over all pairs of bike stations. The distribution of \( w \) is a mixture of Poisson distributions. Evaluations of \( F(x; w) \) for \( w \) fixed are noisy due to additional sources of randomness beyond \( w \) within our simulation.

We solve this problem with BQO, KG, EI and the multi-task algorithm. The multi-task algorithm cannot solve problems where the objective function is an infinite sum, as it is in this problem, so we modify the objective function it uses to a truncated expectation over finitely many values of \( w \). Because implementing the multi-task algorithm become computationally intractable when there are thousands of tasks, we restrict this truncated expectation to 181 values of \( w \).

Figure 5a compares the performance of BQO, KG, EI and the multi-task algorithm, plotting the number of samples beyond the first stage on the \( x \) axis, and the average true quality of the solutions provided, \( G(\text{argmax}_{x} E_{w}[G(x)]) \), averaging over 300 independent runs of BQO, EI and KG, and 100 independent runs of the multi-task algorithm. We see that BQO quickly finds an allocation of bikes to groups that attains a small expected number of negatively affected trips. We believe that multi-task does poorly because of the large number of tasks, and its inability to leverage information across related tasks.

![Figure 5a](image1.png)

(a) Performance comparison between BQO and two Bayesian optimization benchmark, the KG and EI methods, on the Citi Bike Problem from §6.3

Figure 5: Performance results for the Citi Bike problem (plot a), and a screenshot from our simulation of the Citi Bike problem (plot b), as described in §6.3

6.4 Hyperparameter Tuning in Recommender Systems

In this subsection and the following we consider optimization of a machine learning model’s hyperparameters where error is evaluated using cross-validation. Cross-validation is a method for estimating a machine learning model’s error. In more detail, \( n \)-fold cross-validation randomly splits the training data into \( n \) datasets of roughly equal size. Then, for each dataset (or “fold”), it trains the machine learning model holding out that data, and evaluates the error of the resulting estimates on the held out data. The average of these errors is called the cross-validation error, and is used as an objective in optimization of a machine learning model’s hyperparameters. In this approach, we minimize \( \frac{1}{n} \sum_{i=1}^{n} L(x; D_i) \) over \( x \), where \( L(x; D_i) \) is the error of the model with hyperparameters \( x \) evaluated on the \( i \)-th dataset \( D_i \).
In this subsection we consider the problem of optimizing hyperparameters for probabilistic matrix factorization (PMF) models used in recommender systems (Mnih and Salakhutdinov 2008). We apply this PMF model to a dataset from arxiv.org (Cornell University Library 2017), with information about downloads from 2752 users on 2018 papers. We treat a user as providing a positive binary rating for a paper if that user downloaded the paper, which creates 263,238 positive binary ratings.

We use 5-fold cross-validation to provide an estimate of the test error as a function of four PMF model hyperparameters: the learning rate, the $\ell_2$ regularizer, the number of epochs, and the matrix rank. We then use EI, BQO and the multi-task algorithm to choose these hyperparameters to minimize this cross-validation error. EI simply selects a set of hyperparameters $x$ at each step and evaluates all 5 folds, while BQO and the multi-task algorithm select an $x$ and a fold $w$.

Figure 6a compares the cross-validation error of these algorithms, plotting the number of folds queried beyond the first stage on the $x$ axis, and the best error obtained, averaging over 35 independent runs of BQO and multi-task, and 65 of EI. We see that BQO and multi-task perform similarly, and both outperform EI. We conjecture that multi-task’s competitive performance in this problem is due to the small number of tasks and the homogeneity of the folds.

![Figure 6a](image)

(a) Performance comparison between BQO and two Bayesian optimization benchmark, the multi-task and EI methods, on the recommender system problem §6.4

![Figure 6b](image)

(b) Performance comparison between BQO and two Bayesian optimization benchmark, the multi-task and EI methods, on the convolutional neural network problem §6.5

Figure 6: Performance results for the recommender system (plot a) and convolutional neural network (plot b) problems.

6.5 Hyperparameter Tuning in Convolutional Neural Networks

We consider the problem of training convolutional neural networks (CNNs) to classify images (Krizhevsky et al. 2012). We use 5-fold cross validation on the CIFAR10 dataset (Krizhevsky et al. 2018), which consists of 10 classes and 50,000 training images. We choose the network architecture described in the pytorch tutorial (PyTorch core team 2018), which consists of two convolutional layers, two fully connected layers, and on top of them a softmax layer for final classification. We tune the following hyperparameters: the number of epochs, the batch size, the learning rate, the number of channels in the first convolutional layer, the size of the kernel in the convolutional layers, and the number of hidden units in the first fully connected layer. The number of channels in the second convolutional layer is the number of channels in the first convolutional layer plus 10, and the number of hidden units in the second fully connected layer is 84.

Figure 6b compares the performance of EI, BQO and the multi-task algorithm, plotting the number of folds queried beyond the first stage on the $x$ axis, and the best error obtained, averaging over 90 independent runs of...
BQO and the multi-task algorithm, and 75 of EI. We see that BQO and multi-task perform similarly, but better than EI. As in the recommender system problem, we conjecture that multi-task is competitive because of the small number of tasks and their homogeneity.

6.6 Newsvendor Problem under Dynamic Consumer Substitution

The newsvendor problem under dynamic consumer substitution is adapted from [Mahajan and van Ryzin 2001], and was considered in [Henderson and Pasupathy 2018]. In this problem, we choose the initial inventory levels of the products sold, each with given cost $c_j$ and price $p_j$. Our goal is to optimize profit.

A sequence of $T$ customers indexed by $t$ arrive in order and either buy an in-stock product, or decide to not buy anything. Here, $T$ is known. Customer $t$ assigns a utility $U^j_t$ to each product $j$, and to the no-purchase option (indexed by $j = 0$). Customer $t$ decides which product to buy, if any, by choosing the $j$ with the largest $U^j_t$ among the in-stock $j$ and the no-purchase option. Utilities for products ($j > 0$) are modeled with the multinomial logit model, where $U^j_t = u^j + \xi^j_t$, $u^j$ is constant, and $\{\xi^j_t\}$ are mutually independent Gumbel random variables with distribution function $P(\xi^j_{st} \leq z) = \exp\left(-e^{-(z/\mu + \gamma)}\right) =: \Psi^j_t(z)$ where $\gamma$ is Euler’s constant. The utility for the no-purchase option is $U^0_t = 0$. In this problem, the objective function $G(x)$ is defined as the expected overall profit considering the $T$ customers starting from a vector $x$ of initial inventory positions for each product. This profit is computed as sum of the prices of the products sold minus the cost of the initial inventory.

We consider the setting where there are 1000 customers and 2 products whose costs are 5 and 10 dollars respectively and prices are 8 and 18 dollars respectively. We assume that $u_i$ is equal to 1 for all $j > 0$.

We now describe how we use BQO in this problem. Fix a product $j$. Observe that since $\xi^j_t$ for $j > 0$ follows a Gumbel distribution with cdf $\Psi^j_t$, then $\Psi^j_t(Z)$ is uniformly distributed on $[0,1]$. Consequently, $\gamma^{-1}\left(\Psi^j_t\left(\xi^j_{st}\right)\right)$ follows a gamma distribution where $\gamma$ is the gamma cumulative distribution function. Now define the vector $W := (W_1, W_2)$ where $W_j = \sum_{t=1}^{T} \gamma^{-1}\left(\Psi^j_t\left(\xi^j_{st}\right)\right)$. It is straightforward to simulate $\xi = (\xi^j : t, j)$ given $W$, for example by noting that the distribution of $(\gamma^{-1}(\Psi^j_t(\xi^j_{st}))/W_j : t \geq 1)$ is Dirichlet and independent of $W_j$ (see Theorem 2.1 of Section 2.1.2 of Ng et al. 2011). Thus, simulating from this Dirichlet and multiplying by the given value of $W_j$ provides a sample of $\xi^j$ given $W_j$. Alternatively, we can use a simple modification of Example 10e in Section 10.2 of Ross (2012). We can also simulate $\xi^j$ given that $W^j$ resides in an interval by acceptance-rejection sampling, or by simulating $W^j$ from a truncated gamma distribution, and then simulating $\xi^j$ conditioned on $W^j$.

We then apply BQO with $F(x,w)$ equal to the conditional expectation of the profit given $W = w$ and the initial inventory levels $x$ for each product. To observe this conditional expectation we average results from 25 independent simulations, where the collection of values for $\xi^j$ are simulated conditioned on $W$.

We similarly apply the multi-task algorithm with $F(x,i)$ equal to the conditional expectation of the profit given the initial inventory level $x$ and that $W \in R_i$. Here, each $R_i$ is a rectangular region of values for $W_j$ given by $R_1 = [0,q_{1/2}]^2$, $R_2 = (q_{1/2},\infty)^2$, $R_3 = [0,q_{1/2}] \times (q_{1/2},\infty)$, and $R_4 = (q_{1/2},\infty) \times [0,q_{1/2}]$, where $q_{1/2}$ is the median of $W_j$ (this is the same for $j = 1$ and $j = 2$). For each observation of this conditional expectation we average 25 independent simulations. The EI algorithm observes the profit without conditioning, averaging 25 independent simulations.

In Figure 7[we compare the performance of EI, BQO and the multi-task algorithm, plotting the number of samples beyond the first stage on the $x$ axis, and the best profit obtained, averaging over 100 independent runs of BQO, 80 of multi-task, and 230 of EI. We see that BQO outperforms the benchmark algorithms, and the multi-task algorithm underperforms the other algorithms considered.
6.7 Problems Simulated from Gaussian Process Priors

We now compare the performance of BQO against a benchmark Bayesian optimization algorithm on synthetic problems drawn at random from Gaussian process priors. By varying the parameters of the Gaussian process prior, we study how BQO’s performance relative to a benchmark (the KG algorithm) varies with problem characteristics, offering insight into the types of real-world problems on which BQO is likely to provide the most substantial benefit in comparison with using a traditional Bayesian optimization method.

These experiments show that the most important factor influencing BQO’s relative performance is the speed with which $F(x, w)$ varies with $w$. BQO provides the most value when this variation is large enough to influence performance, and small enough to allow $F(x, w)$ to be modeled with a Gaussian process. Thus, users of BQO should choose a $w$ that plays a big role in overall performance, and whose influence on performance is smooth enough to support predictive modeling. These experiments also show that when settings are favorable, BQO provides substantial benefit, in some cases offering an improvement of almost 1000%. On those few problems in which BQO underperforms the benchmark, it underperforms by a much smaller margin of less than 50%.

We now construct these problems in detail. Let $f(x, w, z) = h(x, w) + r(z)$ on $[0, 1]^2 \times \mathbb{R}$, where: $r(z)$ is drawn, for each $z$ in a fine discretization of $[0, 1]$, independently from a normal distribution with mean 0 and variance $\alpha_d$ (we could have set $r$ to be an Ornstein-Uhlenbeck process with large volatility, and obtained an essentially identical result); and $h$ is drawn from a Gaussian Process with mean 0 and Gaussian covariance function $\Sigma((x, w), (x', w')) = \alpha_h \exp \left(-\beta \| (x, w) - (x', w') \|^2_2 \right)$. We then define $F$ by $F(x, w) = E[f(x, W, Z) | W = w]$ where the expectation is over $Z$, and $G$ by $G(x) = E[f(x, W, Z)]$. We then define $F$ by $F(x, w) = E[f(x, W, Z) | W = w]$ where the expectation is over $Z$, and $G$ by $G(x) = E[f(x, W, Z)]$, where the expectation is over both $W$ and $Z$, $W$ is drawn uniformly from $\{0, 1/49, 2/49, \ldots, 1\}$ and $Z$ is drawn uniformly from the discretization of $[0, 1]$. To observed $F$, we draw 1 sample of $W$ and $Z$ and average $f(x, W, Z)$. (We also performed experiments, not shown here, that observed $F$ by averaging multiple samples, and found the same qualitative behavior.)

We thus have a class of problems parametrized by $\alpha_h$, $\alpha_d$, $\beta$, and an outcome measure determined by the overall number of samples. Before displaying results, we reparametrize the dependence on $\alpha_h$ and $\alpha_d$ in what will be a more interpretable way. We first set $\text{Var}[f(x, W, Z) | W, Z] = \alpha_h + \alpha_d$ to 1, as multiplying both $\alpha_h$ and $\alpha_d$ by a scalar simply scales the problem. Then, the variance reduction ratio $\frac{\text{Var}[f(x, W, Z) | W]}{\text{Var}[f(x, W, Z)]}$ achieved by BQO in conditioning on $W$ is approximately $\alpha_h / (\alpha_d + \alpha_h)$, with this estimate becoming exact as $\beta$ grows large and the values of $h(x, w)$ become uncorrelated across $w$. We define $A = \alpha_h / (\alpha_d + \alpha_h)$ equal to this approximate variance reduction ratio. Thus, our problems are parametrized by the approximate variance reduction ratio $A$, the overall number of samples, and by $\beta$, which measures the speed with which $F(x, w)$
varies with $w$.

Given this parametrization, we sampled problems from Gaussian process priors using all combinations of $A \in \{\frac{1}{2}, \frac{1}{4}, \frac{1}{8}, \frac{1}{16}\}$ and $\beta \in \{2^{-4}, 2^{-3}, \ldots, 2^9, 2^{10}\}$. We also performed additional simulations at $A = \frac{1}{2}$ for $\beta \in \{2^{11}, \ldots, 2^{15}\}$. Figure 8 shows Monte Carlo estimates of the normalized performance difference between BQO and KG for these problems, as a function of $\log(\beta)$ (log is the natural logarithm), $A$, and the number of samples taken overall. The normalized performance difference is estimated for each set of problem parameters by taking a randomly sampled problem generated using those problem parameters, discretizing the domain into 2500 points, running each algorithm independently 500 times on that problem, and averaging $(G(x^*_\text{BQO}) - G(x^*_\text{KG})) / |G(x^*_\text{KG})|$ across these 500 samples, where $x^*_\text{BQO}$ is the final solution calculated by BQO, and similarly for $x^*_\text{KG}$.

Figure 8: Normalized performance difference between BQO and KG in problems simulated from a Gaussian process, as a function of $\beta$, which measures how quickly $F(x, w)$ varies with $w$, the approximate variance reduction ratio $A$, and the overall number of samples. BQO outperforms KG over most of the parameter space, and is approximately 10 times better when $\beta$ is near $\exp(4)$.

The normalized performance difference is robust to $A$ and the overall number of samples, but is strongly influenced by $\beta$. BQO is always better than KG whenever $\beta \geq 1$. Moreover, it is substantially better than KG when $\log(\beta) \in (3, 5)$, with BQO outperforming KG by as much as a factor of 10. For larger $\beta$, BQO remains better than KG, but by a smaller margin. This unimodal dependence of the normalized performance difference on $\beta$ can be understood as follows: BQO provides value by modeling the dependence of $F(x, w)$ on $w$. Modeling this dependence is most useful when $\beta$ takes moderate values because it is here where observations of $F(x, w)$ at one value of $w$ are most useful in predicting the value of $F(x, w)$ at other values of $w$. When $F$ varies very quickly with $w$ (large $\beta$), it is more difficult to generalize, and when $F$ varies very slowly with $w$ ($\beta$ close to 0), then modeling dependence on $w$ is comparable with modeling $F$ as constant.

7 Conclusions

We have presented a new Bayesian optimization algorithm, Bayesian Quadrature Optimization, designed for objectives that are sums or integrals of expensive-to-evaluate integrands. This method is derived from a conceptual one-step optimality analysis for which we provide novel computational techniques that support efficient implementation. We demonstrated that this method is consistent when the objective is a finite sum, and showed
via extensive numerical experiments that it performs as well or better than the state of the art, providing substantial value when evaluations are noisy or the integrand varies smoothly in the integrated variables.

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### Appendix

#### A Proofs of Results in Section 4

**Proof of Lemma 1.**

**Proof.** Recall that we assume throughout §4 that \( G \) has the integrated form (2). Results for (1) are similar with the resulting expressions obtained by replacing integration over \( w \) by a sum. By equation (5),

\[
a_{n+1}(x) = \int \mu_{n+1}(x, w) p(w) dw \\
= \int \mu_0(x, w)p(w) dw + \left[ B(x, 1) \cdots B(x, n+1) \right] A_{n+1}^{-1} \begin{pmatrix}
y_1 - \mu_0(x_1, w_1) \\
\vdots \\
y_{n+1} - \mu_0(x_{n+1}, w_{n+1})
\end{pmatrix},
\]

(13)

where \( B(x, i) := \int \Sigma_0(x, w, x_i, w_i) p(w) dw \) for \( 1 \leq i \leq n+1 \).

Since \( y_{n+1} \) conditioned on \( H_n, x_{n+1}, w_{n+1} \) is normally distributed, then \( a_{n+1}(x) \mid H_n, x_{n+1}, w_{n+1} \) is also normally distributed. By the tower property,

\[
E_n \left[ a_{n+1}(x) \mid x_{n+1}, w_{n+1} \right] = E_n \left[ E_{n+1} \left[ G(x) \right] \mid x_{n+1}, w_{n+1} \right] = E_n \left[ G(x) \right] = a_n(x),
\]

and by the law of total variance,

\[
\sigma_n^2(x, x_{n+1}, w_{n+1}) := \text{Var}_n \left[ a_{n+1}(x) \mid x_{n+1}, w_{n+1} \right] \\
= \text{Var}_n \left[ E_{n+1} \left[ G(x) \right] \mid x_{n+1}, w_{n+1} \right] = \text{Var}_n \left[ G(x) \right] - E_n \left[ \text{Var}_{n+1} \left[ G(x) \right] \mid x_{n+1}, w_{n+1} \right].
\]
Using the equation (13) and the previous expressions, we get the following formula for $a_{n+1}$

$$a_{n+1}(x) = a_n(x) + \tilde{\sigma}_n(x, x_{n+1}, w_{n+1})Z$$

(14)

where $Z \sim N(0,1)$ conditioning on $H_n$, and $\tilde{\sigma}_n(x, x_{n+1}, w_{n+1}) = \pm \sqrt{\text{Var}_n[a_{n+1}(x) \mid x_{n+1}, w_{n+1}]}$, which ends the proof of the first part of the lemma.

Finally, we only need to show the last claim of the lemma. We have that if $\lambda_{(x_{n+1}, w_{n+1})} > 0$, or $(x_{n+1}, w_{n+1})$ is not in $H_n$, then $\Sigma_{n+1}(x_{n+1}, w_{n+1}, x_{n+1}, w_{n+1}) > 0$, and then

$$\tilde{\sigma}_n^2(x, x_{n+1}, w_{n+1}) = \text{Var}_n[G(x)] - E_n[\text{Var}_{n+1}[G(x) \mid x_{n+1}, w_{n+1}]]$$

$$= \int \int \Sigma_n(x, w, x', w') p(w) p(w') dw dw' - \int \int \Sigma_{n+1}(x, w, x', w') p(w) p(w') dw dw'$$

$$= \int \int \Sigma_n(x, w, x_{n+1}, w_{n+1}) \Sigma_n(x_{n+1}, w_{n+1}, x_{n+1}, w_{n+1}) + \lambda_{(x_{n+1}, w_{n+1})}$$

$$= \left[ \frac{\int \Sigma_n(x, w, x_{n+1}, w_{n+1}) p(w) dw}{\sqrt{\Sigma_n(x_{n+1}, w_{n+1}, x_{n+1}, w_{n+1}) + \lambda_{(x_{n+1}, w_{n+1})}}} \right]^2$$

$$= \left[ \frac{B(x, n+1) - [B(x, 1) \ldots B(x, n)] A_n^{-1} \gamma}{\sqrt{\Sigma_0(x_{n+1}, w_{n+1}, x_{n+1}, w_{n+1}) + \gamma^T A_n^{-1} \gamma + \lambda_{(x_{n+1}, w_{n+1})}}} \right]^2,$$

where $\gamma^T := (\Sigma_0(x_{n+1}, w_{n+1}, x_{n+1}, w_{n+1}), \ldots, \Sigma_0(x_{n+1}, w_{n+1}, x_{n+1}, w_{n+1}))$. Observe that in (14) the distribution of the left-hand side does not depend on the sign of $\tilde{\sigma}_n$. Thus, without loss of generality, we define $\tilde{\sigma}_n(x, x_{n+1}, w_{n+1})$ equal to $\frac{B(x, n+1) - [B(x, 1) \ldots B(x, n)] A_n^{-1} \gamma}{\sqrt{\Sigma_0(x_{n+1}, w_{n+1}, x_{n+1}, w_{n+1}) + \gamma^T A_n^{-1} \gamma + \lambda_{(x_{n+1}, w_{n+1})}}}$. If $\lambda_{(x_{n+1}, w_{n+1})} = 0$ and $(x_{n+1}, w_{n+1})$ is in $H_n$, then it is easy to see that $\tilde{\sigma}_n^2(x, x_{n+1}, w_{n+1}) = 0$ because $\Sigma_n = \Sigma_{n+1}$.

\end{proof}

\begin{proof}
We first show that $a_n(\cdot)$ and $\tilde{\sigma}_n(\cdot, x_{n+1}, w_{n+1})$ are continuously differentiable for each $(x_{n+1}, w_{n+1})$. In Lemma 1, we show that

$$a_n(x) = \int \mu_0(x, w) p(w) dw - [B(x, 1), \ldots, B(x, n)] A_n^{-1} \begin{bmatrix} y_1 - \mu_0(x_1, w_1) \\ \vdots \\ y_n - \mu_0(x_n, w_n) \end{bmatrix}$$

and

$$\tilde{\sigma}_n(x, x_{n+1}, w_{n+1}) = \frac{B(x, n+1) - [B(x, 1) \ldots B(x, n)] A_n^{-1} \gamma}{\sqrt{\Sigma_0(x_{n+1}, w_{n+1}, x_{n+1}, w_{n+1}) + \gamma^T A_n^{-1} \gamma + \lambda_{(x_{n+1}, w_{n+1})}}}.$$ 

Thus we only need to show that $B(x, i)$ for all $1 \leq i \leq n$ and $\int \mu_0(x, w) p(w) dw$ are continuously differentiable on $x$. $\int \mu_0(x, w) p(w) dw$ is continuously differentiable because $\mu_0$ is constant.

We now show that $B(x, i)$ is continuously differentiable for any $1 \leq i \leq n$. $\Sigma_0$ is bounded, and so for $x \mapsto \Sigma_0(x, w', y, w) p(w')$ is integrable with respect to $w'$ for any $(y, w)$ because $p$ is integrable with respect to $w'$.
Moreover, $\Sigma_0(x, w', y, w)$ is differentiable with respect to $x$, and $\frac{\partial \Sigma_0(x, w', y, w)}{\partial x}$ is continuous on $x$, and so it is bounded for any $y, w, w'$ fixed because $A$ is compact. Consequently, 
\begin{equation}
\frac{\partial B(x, i)}{\partial x} = \int \frac{\partial \Sigma(x, w', x_i, w_i)}{\partial x} p(w') \, dw'
\end{equation}
for all $i$ by Corollary 5.9 of Barle (1966). Moreover, by Corollary 5.8 of Barle (1966), $\frac{\partial B(x, i)}{\partial x}$ is continuous on $x$. This proves the first part of the lemma.

We now prove the second part of the lemma. Using a similar argument with the hypothesis that $|\frac{\partial \Sigma_0(x, w', x', w)}{\partial w}| < h(x, w', x')$, and Corollaries 5.8 and 5.9 of Barle (1966), we can show that $(y, w) \mapsto \int \Sigma_0(x, w', y, w) p(w') \, dw'$ is continuously differentiable for any $x$. Thus, using that $\lambda_{(x, w)}$ is continuously differentiable, we can conclude that $\tilde{\sigma}_n(x', x, w)$ is continuously differentiable with respect to $(x, w)$.

Proof of Lemma 4

Proof. First, we show $a_n(x)$ and $\tilde{\sigma}_n(\cdot, x_{n+1}, w_{n+1})$ are both uniformly continuous in $A$. By Lemma 1

\[ a_n(x) = \int \mu_0(x, w) p(w) \, dw - \left[ B(x, 1), \ldots, B(x, n) \right] A_n^{-1} \begin{bmatrix} y_1 - \mu_0(x_1, w_1) \\ \vdots \\ y_n - \mu_0(x_n, w_n) \end{bmatrix} \]

and

\[ \tilde{\sigma}_n(x, x_{n+1}, w_{n+1}) = \frac{B(x, n+1) - \left[ B(x, 1), \ldots, B(x, n) \right] A_n^{-1} \gamma}{\sqrt{\Sigma_0(x_{n+1}, w_{n+1}, x_{n+1}, w_{n+1}) - \gamma^T A_n^{-1} \gamma + \lambda_{(x_{n+1}, w_{n+1})}}} \]

Thus we only need to show that $B(x, i)$ is continuous for all $1 \leq i \leq n$ because $A$ is compact. The continuity follows from the Corollary 5.7 of Barle (1966).

$a_n(x)$ and $\tilde{\sigma}_n(x, x_{n+1}, w_{n+1})$ are both bounded on $x$ because they are both continuous on a compact set, and so $E_n[\sup_{x\in A} a_{n+1}(x)] < \infty$. Consequently by the monotone convergence theorem,

\[ \lim_{L \to \infty} E_n \left[ \max_{x \in A_L} \left( a_n(x) + \tilde{\sigma}(x, x_{n+1}, w_{n+1}) Z_{n+1} \right) \right] = E_n \left[ \lim_{L \to \infty} \max_{x \in A_L} \left( a_n(x) + \tilde{\sigma}(x, x_{n+1}, w_{n+1}) Z_{n+1} \right) \right]. \quad (16) \]

Furthermore, by a trivial modification to our Lemma 10 using the uniform continuity of $a_n(x)$ and $\tilde{\sigma}_n(\cdot, x_{n+1}, w_{n+1})$, we can see that $\lim_{L \to \infty} \max_{x \in A_L} a_n(x) = \max_{x \in A} a_n(x)$, and

\[ \lim_{L \to \infty} \max_{x \in A_L} \left( a_n(x) + \tilde{\sigma}(x, x_{n+1}, w_{n+1}) Z_{n+1} \right) = \max_{x \in A} \left( a_n(x) + \tilde{\sigma}(x, x_{n+1}, w_{n+1}) Z_{n+1} \right) \text{a.s.} \quad (17) \]

Thus, using the two previous equations and (16), we conclude the proof of the lemma.\[ \square \]

B BQO’s Time and Space Complexity

In this section, we discuss BQO’s time and space complexity, assuming we use it to select $N$ points $(x, w)$ to sample. To select each point $(x, w)$ to sample, we use Algorithm 1, which runs the ADAM algorithm for $T$ iterations. Each iteration requires a stochastic gradient computed using $J$ independent standard Gaussian random variables, $J$ independent samples from the posterior on $\theta$, and $J$ runs of LBFGS to maximize
where we use the squared exponential kernel \( \Sigma((x, z), (y, w)) = \sigma_0^2 \exp\left(-\sum_{k=1}^n \alpha_1^{(k)} [x_k - y_k]^2 - \sum_{k=1}^d \alpha_2^{(k)} [w_k - z_k]^2\right) \), and

\[
p(w) = \Pi_{i=1}^n \phi_t(w_i)
\]

(18)

where \( w = (w_1, \ldots, w_n) \), and \( \phi_t \) is the density of a normal random variable with mean \( \mu_t \) and variance \( \sigma_t^2 \).

C Closed-Form Expressions for the Gaussian and Squared Exponential Kernel Case

In this section we give closed-form expressions for \( B \) and its gradient to compute BQO and its gradient when we use the squared exponential kernel \( \Sigma((x, z), (y, w)) = \sigma_0^2 \exp\left(-\sum_{k=1}^n \alpha_1^{(k)} [x_k - y_k]^2 - \sum_{k=1}^d \alpha_2^{(k)} [w_k - z_k]^2\right) \), and
The previous assumptions are quite common, for example they are assumed in Xie et al. (2012). Moreover, we can always transform a problem of the form \( \int F(x,w)dp(w)dw \) to a new problem of the form \( \int F'(x,w)p'(w)dw \) where \( p' \) is of the form given in [18] under suitable conditions. The procedure and necessary conditions are:

- Denote the continuous density of \( W \) by \( p \), where \( W \) is a random vector such that \( P[W = w] = p(w) \).
- Assume that we can compute or estimate the marginals of the random vector \( W \): \( F_i(w_i) := P(W_i \leq w_i) \) for all \( i \).
- Denote the inverse of the distribution function of a standard Gaussian random variable by \( h \). We have that \( h(F(W)) \sim N(0,1) \) for all \( i \). Thus,

\[
h(F(W)) = (h(F_1(W_1)), \ldots, h(F_n(W_n))) \sim N(0,\Sigma).
\]

- We assume that \( \Sigma \) is positive definite, and can be computationally estimated.
- We have that \( \Sigma^{-1/2}h(F(W)) \sim N(0,I) \).
- Define \( Y = \Sigma^{-1/2}h(F(W)) = (h_1(W), \ldots, h_n(W)) \), where \( h_i(w) = \left[ \Sigma^{-1/2}h(F(W)) \right]_i \) is the \( i \)th component of the vector \( \Sigma^{-1/2}h(F(W)) \) for all \( i \). Let \( J_i \) denote the Jacobian computed from \( h_i \). Assume that \( J_i \) does not vanish identically. By the change of variables theorem, we have that

\[
\int F(x,w)p(w)dw = \int F'(x,y)p'(y)dy
\]

where \( F'(x,y) = F(x,F_1^{-1}(h_1^{-1}\left[ \Sigma^{1/2} \right]_1), \ldots, F_n^{-1}h_1^{-1}\left[ \Sigma^{1/2}y \right]_n))|J_i| \) and \( \left[ \Sigma^{1/2}y \right]_i \) is the \( i \)th entry of \( \Sigma^{1/2}y \).

This shows how to transform a general problem to a problem with density given by (18), and the conditions under which this is possible. However, we do not always want to use this transformation because the correlation between \( F'(x,w) \) and \( F'(x',w') \) can be too small, which may not be optimal for BQO as we discuss in §6.7.

We now compute the closed-form expressions of \( B \) and its gradient. We have that

\[
B(x,i) = \int \Sigma_0 (x,w,x_i,w_i)p(w)dw = \sigma_0^2 \exp \left( -\sum_{k=1}^n \alpha_1^{(k)}[x_k-x_{ik}]^2 \right) \prod_{k=1}^d \int \exp \left( -\alpha_2^{(k)}[w_k-w_{ik}]^2 \right) \varphi_k(w_k)dw_k
\]

for \( i = 1, \ldots, n \). Thus, we only need to compute \( \int \exp \left( -\alpha_2^{(k)}[w_k-w_{ik}]^2 \right) \varphi_k(w_k)dw_k \) for any \( k \) and \( i \), which is given by the following equations,
\[ \int \exp \left( -\alpha_2^{(k)} [w_k - w_{ik}]^2 \right) \phi_k (w_k) d (w_k) = \frac{1}{\sqrt{2\pi} \sigma_k} \int \exp \left( -\alpha_2^{(k)} [z - w_{ik}]^2 - \frac{[z - \mu_k]^2}{2\sigma_k^2} \right) dz \]

\[ = \frac{1}{\sqrt{2\pi} \exp \left( -\alpha_2^{(k)} (w_{ik})^2 - \frac{\mu_k^2}{2\sigma_k^2} - \frac{2\alpha_2^{(k)} w_{ik}}{4(\alpha_2^{(k)} - \frac{1}{2\sigma_k^2})} \right) \times \int \exp \left( -\left( \alpha_2^{(k)} + \frac{1}{2\sigma_k^2} \right) [z - \frac{\mu_k}{2(\alpha_2^{(k)} - \frac{1}{2\sigma_k^2})}]^2 \right) dz \]

\[ = \frac{1}{\sqrt{2\sigma_k} \sqrt{\alpha_2^{(k)} + \frac{1}{2\sigma_k^2}}} \times \exp \left( -\frac{\mu_k^2}{2\sigma_k^2} - \alpha_2^{(k)} (w_{ik})^2 - \frac{\mu_k^2 + 2\alpha_2^{(k)} w_{ik}}{4\left(\alpha_2^{(k)} - \frac{1}{2\sigma_k^2}\right)} \right). \]

This shows how to compute \( B \). We now compute the gradient of \( B \). Observe that

\[ \nabla_{x_{n+1},j} \Sigma_0 (x_{n+1}, w_{n+1}, x_i, w_i) = \begin{cases} 0, & i = n + 1 \\ -2\alpha_1^{(j)} [x_{n+1, j} - x_{i, j}] \Sigma_0 (x_{n+1}, w_{n+1}, x_i, w_i), & i < n + 1 \end{cases} \]

\[ \nabla_{w_{n+1},j} \Sigma_0 (x_{n+1}, w_{n+1}, x_i, w_i) = \begin{cases} 0, & i = n + 1 \\ -2\alpha_2^{(j)} [w_{n+1, j} - w_{i, j}] \Sigma_0 (x_{n+1}, w_{n+1}, x_i, w_i), & i < n + 1 \end{cases} \]

where \( \nabla_{x_{n+1},j} \) is the derivative respect to the \( j \)th entry of \( x_{n+1} \). Consequently,

\[ \nabla_{x_{n+1},j} B (x, n + 1) = -2\alpha_1^{(j)} (x_j - x_{n+1, j}) B (x, n + 1) \]

\[ \nabla_{w_{n+1},k} B (x, n + 1) = \sigma_0^2 \exp \left( -\sum_{i=1}^{n} \alpha_1^{(i)} [x_i - x_{n+1, i}]^2 \right) \prod_{j \neq k} \exp \left( -\alpha_2^{(j)} [w_j - w_{n+1, j}]^2 \right) \phi_j (w_j) d (w_j) \]

\[ \times \int \left( -2\alpha_2^{(k)} (w_k - w_{n+1, k}) \right) \exp \left( -\alpha_2^{(k)} [w_k - w_{n+1, k}]^2 \right) \phi_k (w_k) d (w_k), \]
\[
\int w_k \exp \left( -\alpha_2^{(k)} [w_k - w_{n+1,k}]^2 \right) \varphi_k (w_k) d (w_k) = \frac{1}{\sqrt{2\pi}\sigma_k} \int \exp \left( -\alpha_2^{(k)} [z - w_{ik}]^2 - \frac{[z - \mu_k]^2}{2\sigma_k^2} \right) dz \\
= \frac{1}{\sqrt{2\pi}\sigma_k} \exp \left( -\frac{\mu_k^2}{2\sigma_k^2} - \alpha_2^{(k)} (w_{ik})^2 - \frac{\left( \frac{\mu_k}{\sigma_k} + 2\alpha_2^{(k)} w_{ik} \right)^2}{4 \left( -\alpha_2^{(k)} - \frac{1}{2\sigma_k^2} \right)} \right) \\
\times \int \exp \left( -\left( \alpha_2^{(k)} + \frac{1}{2\sigma_k^2} \right) \left[ z - \frac{\mu_k}{\sigma_k} + 2\alpha_2^{(k)} w_{ik} \right] \right)^2 dz \\
= \frac{1}{\sqrt{2\sigma_k}} \exp \left( -\frac{\mu_k^2}{2\sigma_k^2} - \alpha_2^{(k)} (w_{ik})^2 - \frac{\left( \frac{\mu_k}{\sigma_k} + 2\alpha_2^{(k)} w_{ik} \right)^2}{4 \left( -\alpha_2^{(k)} - \frac{1}{2\sigma_k^2} \right)} \right) \\
\times \left( \frac{\mu_k}{\sigma_k} + 2\alpha_2^{(k)} w_{ik} \right) \left( \frac{2}{1 + \frac{1}{2\sigma_k^2}} \right),
\]

which shows how to compute the gradient of \( B \).

## D Illustration of Poor Performance of the Multi-Task Algorithm

In this section we give an example where the average multi-task algorithm presented in Section 3.2 of [Swersky et al. (2013)] is inefficient, and we show that the BQO algorithm does not have that problem.

Let \( A = \{1, 2\}, W = \{1, \ldots, M\} \), and \( w_1 = 0.5, w_i = \frac{0.5}{M-1} \) if \( i > 1 \). We want to maximize

\[
G (x) = \sum_{i=1}^{M} w_i F (x, i).
\]

We assume that \( F (1, 1) = \cdots = F (1, M) = L > 0 \), and \( F (1, 1) = L > 0 \) has been evaluated. In addition, we suppose that \( F (x, i) \sim N (0, M-1) \) for \( i > 1 \), \( F (2, 1) \sim N (0, \nu^2) \) for some \( \nu^2 > 1 \), and their correlation is equal to zero. By equation 15 in [Jones et al. (1998)] we have that

\[
EI_n (x) = (a_n (x) - \max_{i\leq n} a_n (x_i)) \Phi (z_n) + \sqrt{\Sigma_n (x,x)} \phi (z_n)
\]

if \( \Sigma_n (x,x) > 0 \), where \( z_n = (a_n (x) - \max_{i\leq n} a_n (x_i)) / \sqrt{\Sigma_n (x,x)} \), and \( \Sigma_n (x,x) \) is the posterior variance of \( G (x) \). Consequently,

\[
EI_1 (1) = \frac{1}{\sqrt{2\pi}} \sqrt{\frac{1}{4 (M-1)^2}} M-1 = \frac{1}{\sqrt{2\pi}} \sqrt{\frac{1}{4 (M-1)}}
\]

and

\[
EI_1 (2) = \phi (z_{1,2}) \sqrt{\frac{1}{4 (M-1) + \frac{\nu^2}{4}}} + \Phi (z_{1,2}) \left( -\frac{L}{2} \right)
\]

where \( z_{1,2} = \frac{\sqrt{\frac{1}{4 (M-1) + \frac{\nu^2}{4}}}}{\sqrt{\pi \nu^2}} \).
Suppose that in the next iteration we choose again a point of the form \((1, i)\), and \(F(1, i) = L_i\), thus we have that

\[
EI_2(1) = \frac{1}{\sqrt{2\pi}} \sqrt{\left(\frac{1}{4(M-1)^2}\right)(M-2)}
\]

and

\[
EI_2(2) = \phi(z_{2,2}) \sqrt{\left(\frac{1}{4(M-1)} + \frac{v^2}{4}\right) + \Phi(z_{2,2})\left(-\frac{L}{2} - \frac{1}{2(M-1)L}\right)}
\]

where \(z_{2,2} = \frac{-L - \frac{1}{2(M-1)}}{\sqrt{\frac{1}{4(M-1)} + \frac{v^2}{4}}}\). Similarly, we can see that if we keep choosing points of the form \((1, i)\), we are going to have that

\[
EI_n(1) = \frac{1}{\sqrt{2\pi}} \sqrt{\left(\frac{1}{4(M-1)^2}\right)(M-n)}
\]

and

\[
EI_n(2) = \phi(z_{n,2}) \sqrt{\left(\frac{1}{4(M-1)} + \frac{v^2}{4}\right) + \Phi(z_{n,2})\left(-\frac{L}{2} - \frac{n-1}{2(M-1)L}\right)}
\]

where \(z_{n,2} = \frac{-L - \frac{n-1}{2(M-1)}}{\sqrt{\frac{1}{4(M-1)} + \frac{v^2}{4}}}\) if \(n \leq M\).

Observe that

\[
\phi\left(\frac{-L - \frac{n-1}{2(M-1)}}{\sqrt{\frac{1}{4(M-1)} + \frac{v^2}{4}}}\right) \rightarrow 0
\]

uniformly on \(n < M\) if \(L \rightarrow \infty\). Consequently, for \(L\) large, we have that

\[
EI_n(2) < EI_n(1)
\]

if \(n < M\), and so we can only choose a point of the form \((2, j)\) until we have evaluated all the \(M\) different points of the form \((1, i)\), which is clearly inefficient when \(M\) is large.

We now show that the BQO algorithm does not have that problem. Observe that if \(i > 1\),

\[
\left(\frac{\sum_j w_j \Sigma(1, i, 1, j) - \sum_j w_j \Sigma(1, i, 2, j)}{\Sigma(1, i, 1, i)}\right)^2 = \left(\frac{1}{M-1}\right)^2 < \left(\frac{\frac{v^2}{2}}{M-1}\right)^2 = \left(\frac{\sum_j w_j \Sigma(2, 1, 1, j) - \sum_j w_j \Sigma(2, 1, 2, j)}{\Sigma(2, 1, 2, 1)}\right)^2
\]

and by Theorem\(\ref{theo:3}\) we have that \(BQO((1, i)) < BQO((2, 1))\) for all \(i\), and thus the BQO algorithm chooses to evaluate \((2, 1)\).
Theorem 3. We have that

\[ BQO_n(t,s) \geq BQO_n(z,w') \]

if for all \( x, y \)

\[
\left( \frac{\int \Sigma_n(x,w,z,w') dp(w) - \int \Sigma_n(y,w,z,w') dp(w)}{\sqrt{\Sigma_n(z,w',z,w')}} \right)^2 \leq \left( \frac{\int \Sigma_n(x,w,t,s) dp(w) - \int \Sigma_n(y,w,t,s) dp(w)}{\sqrt{\Sigma_n(t,s,t,s)}} \right)^2
\]

Proof. The proof is a direct consequence of Lemma 1 and the Vitale’s extension of the Sudakov-Fernique inequality (Vitale 2000).

\[ \square \]

E Consistency of BQO

In this section, we prove the two consistency results: Theorem 1 and Theorem 2 of §5. To support the proofs of our theorems, we embed BQO within a controlled Markov process framework. We denote the probability space by \((\Omega, \mathcal{F}, P)\), and assume it is complete. The action space is the domain of \(F\), which is \(A \times W\), where \(W\) is a subset of \(\mathbb{R}^\ell\). The state space is the set of possible parameters of the Gaussian process on \(F\). More formally, if we denote \(A \times W\) by \(A'\), the state space is defined by \(\mathcal{H} := D(A') \times D_{\text{kernel}}(A' \times A')\), where \(D(A')\) is the set of functions defined on \(A'\), and \(D_{\text{kernel}}(A' \times A')\) is the set of positive semidefinite functions defined on \(A' \times A'\).

The discrete-time dynamic system, which shows how the posterior parameters change when a new observation is obtained, is given by

\[
S_{n+1} := (\mu_{n+1}, \Sigma_{n+1}) = f_n((\mu_n, \Sigma_n), u_n, Z_n)
\]

where \(u_n\) is the chosen point to measure at stage \(n\), \(Z_n \sim N(0,1)\), and \(f_n\) is defined by

\[
\mu_{n+1}(x',w') = \mu_n(x',w') + \frac{\Sigma_n((x',w'), u_n)}{\sqrt{\Sigma_n(u_n,u_n) + \lambda_{u_n}}} Z_n
\]

and

\[
\Sigma_{n+1}((y,r),(z,s)) = \Sigma_n((y,r),(z,s)) + \frac{\Sigma_n((y,r),u_n) \Sigma_n((z,s),u_n)}{\Sigma_n(u_n,u_n) + \lambda_{u_n}}
\]

where \(\lambda_{u_n}\) is the variance of the sample \(y_{u_n}\) of \(F(u_n)\), e.g. \(y_{u_n} = F(u_n) + \varepsilon_n\) where \(\varepsilon_n \sim N(0,\lambda_{u_n})\).

We now define a sequence of value functions \(V^n : \mathcal{H} \rightarrow \mathbb{R}\) by

\[
V^n(s) := \sup_{\pi \in \Pi} E^\pi [\max_{x \in A} a_N(x) \mid S^n = s]
\]

where \(N\) is the number of times that we can evaluate \(F\), \(\Pi\) is the class of admissible policies (a policy is a sequence of maps \(\pi = (\pi_1, \ldots, \pi_N)\), where each \(\pi_i\) maps parameters of the Gaussian process into the domain of \(F\), and conditioning on \(S^n = s\) means that \(F \sim GP(s)\) where \(s = (\mu, \Sigma)\).

Similarly, we define the value of a policy \(\pi \in \Pi\) as

\[
V^{\pi,n}(s) := E^\pi [V^n(S^n) \mid S^n = s] = E^\pi [\max_{x \in A} a_N(x) \mid S^n = s].
\]

An optimal policy given \(s\) optimizes \(V^{\pi,0}(s)\).

We denote the weighted sum of a function over \(W\) by its Lebesgue integral respect to \(p\). Given \(s\), we denote the parameters of the induced GP on \(G\) by \(T(s)\), where the mean is \(a(x) = \int_w \mu(x,w) dp(w)\) and the covariance is \(\alpha(x,y) = \int_w \int_w \Sigma((x,w),(y,w')) dp(w) dp(w')\). Observe that the integrals are sums because \(W\) is finite.
We define the set \( \mathcal{H} \subset \mathcal{H} \) as
\[
\{ (\mu, \Sigma) : \mu \equiv 0, \Sigma, w' (x,y) := \Sigma (x,w,y,w') \text{ is in } C^1 (\mathbb{R}^n \times \mathbb{R}^n) \text{ for all } w, w' \in W, \text{ and } \Sigma \text{ is isotropic} \}.
\]
We summarize the notation that is used in this section:

\[
\begin{aligned}
V^n (s) &= \sup_{\pi \in \Pi} E^\pi [\max_{x \in A} a_N (x) \mid S^n = s] =: V^n (s; N)
U (s) &= E [\max_{x \in A} G (x) \mid S^0 = s]
V^{\pi,n} (s; N) &= E^\pi [\max_{x \in A} a_N (x) \mid S^n = s] := V^{\pi,n} (s)
R^n (s; (x, w)) &= E [V^{n+1} (S^{n+1}) \mid S^n = s, (x_{n+1}, w_{n+1}) = (x, w)]
\mathcal{F}^n &= \text{ the smallest sigma-algebra generated by the observations obtained by time } n
\mathcal{F}^\infty &= \text{ the smallest sigma-algebra generated by } \{ \mathcal{F}^n \}_n
\mu_n (x, w) &= E [F (x, w) \mid \mathcal{F}^n] \text{ for } 0 \leq n \leq \infty
\Sigma_n (x, w, x', w') &= \text{ Cov} [F (x, w), F (x', w') \mid \mathcal{F}^n] \text{ for } 0 \leq n \leq \infty.
\end{aligned}
\]
Observe that
\[
\begin{aligned}
V^N (s) &= \max_{x \in A} a_N (x) = \max_{x \in A} \int_w \mu_N (x, w) \, dp (w),
R^{N-1} (s; (x, w)) &= E [V^N (S^N)] \mid S^{N-1} = s, (x_N, w_N) = (x, w).
\end{aligned}
\]
We do not write the specific dependence on a policy \( \pi \) when there is no confusion.

### E.1 Consistency of BQO for Finite Domains

In this subsection, we prove a slightly stronger result (Theorem 4) whose proof implies Theorem 2. All the results of this subsection assume that both \( A \) and \( W \) are finite.

**Theorem 4.** Suppose that \( A \) and \( W \) are finite. For each \( s \in \mathcal{H} \), we have that
\[
\lim_{N \to \infty} V^0 (s; N) = \lim_{N \to \infty} V^{BQO,0} (s; N).
\]

**Proof.** We first note that the limit of \( S^n \) exists by Lemma 5. Denote it by \( S^\infty \). Furthermore, \( V^{BQO,0} (s; N) \) is non-decreasing in \( N \) and bounded above by Lemma 7 and so by Fatou’s lemma we have that \( \lim_{N \to \infty} V^{BQO,0} (s; N) = V^{BQO,0} (s; \infty) \). By Lemma 6 under the BQO policy \( V^N (S^\infty) = U (S^\infty) \) a.s. for all \( N \). Thus,
\[
\begin{aligned}
V^{BQO,0} (s; \infty) &= E^{BQO} [V^N (S^\infty) \mid S^0 = s] \\
&= E^{BQO} [U (S^\infty) \mid S^0 = s] \\
&= E^{BQO} [E [\max_{x \in A} G (x) \mid S^0 = S^\infty] \mid S^0 = s] \\
&= E [\max_{x \in A} G (x) \mid S^0 = s] \\
&= U (s)
\end{aligned}
\]
and \( U (s) \geq V^0 (s; \infty) \) by Lemma 7. This ends the proof because \( V^0 (s; \infty) \geq V^{BQO,0} (s; \infty) \).

**Lemma 5.** For any \( s = (\mu, \Sigma) \in \mathcal{H} \), and policy \( \pi \), we have that \( (S^n) \) converges almost surely pointwise to \( S^\infty = (\mu_\infty, \Sigma_\infty) \in \mathcal{H} \), where \( \mu_\infty (x, w) = \lim_n \mu_n (x, w) \) and \( \Sigma_\infty ((x, w), (x', w')) = \lim_n \Sigma_n ((x, w), (x', w')) \).
Proof. This is proof is strongly based on [Frazier et al. (2009)]. We first show that the limit exists for any pair of points \((x, w), (x', w')\). Let \(M^n = (\mu^n, \Sigma^n + \mu^n(\mu^n'))\) where \(\mu^n = (\mu_n(x, w), \mu_n(x', w'))\), and

\[
\Sigma^n := \left( \begin{array}{cc} \Sigma_n((x, w), (x, w)) & \Sigma_n((x, w), (x', w')) \\ \Sigma_n((x', w), (x, w)) & \Sigma_n((x', w), (x', w')) \end{array} \right).
\]

We only need to show that \(M^n\) converges a.s. since \((\mu^n, \Sigma^n)\) is a linear transformation of \(M^n\). We may write the components of \(M^n\) as the conditional expectation of an integrable random variable with respect to \(F^n\) (the smallest \(\sigma\)-algebra generated by the information at time \(n\)) by \(\mu^n = E_n[(F(x, w), F(x', w'))]\) and \(\Sigma^n + \mu^n(\mu^n') = E_n[(F(x, w), F(x', w'), (F(x, w), F(x', w'))]\). Thus \(M^n\) is a uniformly integrable martingale and hence converges a.s. (see Kallenberg [1997]). Thus the limit exists a.s. because the domain of \(F\) is finite. Furthermore, since the limit of kernels is a kernel, we must have that \(\Sigma\) is semi-positive definite.

Lemma 6. Under the BQO policy, if \(s = (\mu_0, \Sigma_0) \in \mathcal{H}_1\) and \(A\) is finite, then \(V^N(S^\infty) = U(S^\infty)\) a.s. where \(S^\infty\) is the limit of \((S^n)\), and

\[
V^n(s) = \sup_{\pi \in \Pi} E^{\pi} \left[ \max_{x \in A} a_N(x) \mid S^n = s \right]
\]

\[
U(s) = E \left[ \max_{x \in A} G(x) \mid S^0 = s \right].
\]

Proof. Define the events \(H(x,w) := \{R^{N-1}(S^\infty; (x, w)) > V^N(S^\infty)\}\) for any \(x \in A, w \in W\), where \(S^\infty\) is the limit of the parameters of the GP model, and define the Q-factors

\[
R^{N-1}(s; (x, w)) := E \left[ V^N(S^N) \mid S^{N-1} = s, (x_N, w_N) = (x, w) \right].
\]

For any \(B \subset A \times W\), we define the events:

\[
H_B := \left[ \bigcap_{(x, w) \in B} H(x,w) \right] \bigcap \left[ \bigcap_{(x, w) \notin B} H(x,w) \right].
\]

By Proposition 2, \(R^{N-1}(s; (x, w)) \geq V^N(s)\), and so \(H_B\) is the event that \(R^{N-1}(S^\infty; (x, w)) > V^N(S^\infty)\) for \((x, w) \in B\), and \(R^{N-1}(S^\infty; (x, w)) = V^N(S^\infty)\) for \((x, w) \notin B\). We will show that \(P[H_B] = 0\) if \(B \neq \emptyset\), and so we will have that \(P[H_0] = 1\).

Let \(B \neq \emptyset\). Assume that \(P[H_0 \cap \{S^n \rightarrow S^\infty\}] > 0\). By contraposition of Lemma 8, there exists a measurable set \(\mathcal{L}\) such that \(P[\mathcal{L}] > 0\), and for each \(\omega \in \mathcal{L} \cap \{S^n \rightarrow S^\infty\}\), we have that there exists \(K_{(x,w)}(\omega) \in \mathbb{N}\) for each \((x, w) \in B\) such that the BQO policy does not sample \((x, w)\) for \(n > K_{(x,w)}(\omega)\).

Fix \(\omega \in \mathcal{L} \cap \{S^n \rightarrow S^\infty\}\), and define \(K(\omega) := \max_{(x,y) \in B} K_{(x,w)}(\omega)\). Given that \(S^n \rightarrow S^\infty\) and \(R^{N-1}(S^\infty; (x, w)) > V^N(S^\infty) = R^{N-1}(S^\infty; (y, r))\) for \((x, w) \in B\) and \((y, r) \notin B\), there exists \(n > K(\omega)\), such that

\[
\min_{(x, w) \in B} R^{N-1}(S^n(\omega); (x, w)) > \max_{(x, w) \notin B} R^{N-1}(S^n(\omega); (x, w)).
\]

Thus the BQO policy must sample from \((x, w) \in B\) at time \(n\), which contradicts that the BQO policy never samples from \((x, w) \in B\) at time \(n\). Consequently, \(P[H_0] = 1\), and so \(R^{N-1}(S^\infty; (x, w)) = V^N(S^\infty)\) for all \((x, w)\) almost surely. By Lemma 9, we conclude that \(V^N(S^\infty) = U(S^\infty)\) almost surely, as we wanted to prove.

Lemma 7. \(\sup_{\pi} E^{\pi} \left[ \max_{x \in A} a_N(x) \mid S^0 = s \right]\) is non-decreasing in \(N\) and is bounded above. For any policy \(\pi\), \(E^{\pi} \left[ \max_{x \in A} a_N(x) \mid S^0 = s \right]\) is non-decreasing in \(N\) and is bounded above. Furthermore, \(V^0(s; N) \leq U(s)\).
Proof. First, we prove that \( V^0(s;N) = \sup_{\pi} E^\pi \left[ \max_{x \in A} a_N(x) \mid S^0 = s \right] \) is non-decreasing in \( N \) and bounded above. Observe that \( V^0(s;N-1) = \sup_{\pi} E^\pi \left[ \max_{x \in A} a_{N-1}(x) \mid S^0 = s \right] = V^1(s;N) \), then

\[
V^0(s;N) - V^0(s;N-1) = V^0(s;N) - V^1(s;N),
\]

and this difference is not negative by Proposition 1. This shows that \( V^0 \) is non-decreasing.

Now, we show that \( V^0(s;N) \leq U(s) \). We have that for any policy \( \pi \),

\[
E^\pi \left[ \max_{x \in A} a_N(x) \mid S^0 = s \right] = E^\pi \left[ \max_{x \in A} E_N^\pi G(x) \mid S^0 = s \right] \leq E^\pi \left[ E_N^\pi \left[ \max_{x \in A} G(x) \mid S^0 = s \right] \right] = E^\pi \left[ \max_{x \in A} G(x) \mid S^0 = s \right] = E \left[ \max_{x \in A} G(x) \mid S^0 = s \right] = U(s),
\]

and then \( V^0(s;N) \leq U(s) \).

We now show that \( V^\pi,0(s;N) = E^\pi \left[ \max_{x \in A} a_N(x) \mid S^0 = s \right] \) is non-decreasing in \( N \) for any stationary policy. We have that \( V^\pi,0(s;N-1) = E^\pi \left[ \max_{x \in A} a_{N-1}(x) \mid S^0 = s \right] = V^\pi,1(s;N) \), and then

\[
V^\pi,0(s;N) - V^\pi,0(s;N-1) = V^\pi,0(s;N) - V^\pi,1(s;N),
\]

and this difference is not negative by Proposition 2.

\( \square \)

**Proposition 1.** For \( s = (\mu, \Sigma) \in \mathcal{H} \) and \( x \in A, w \in W \), we have that \( R^{n-1}(s; (x, w)) \geq V^n(s) \) for all \( 0 \leq n < N \). Furthermore, \( V^{n+1}(s;N) \leq V^n(s;N) \) for all states \( s \).

**Proof.** This proof is based on a similar proposition in Frazier et al. (2009). We first show that \( R^{n-1}(s; (x, w)) \geq V^n(s) \). We proceed by induction on \( n \). For \( n = N - 1 \), we have that \( V^N(s) = \max_{x \in A} a(x) \), and by Jensen’s inequality

\[
R^{N-1}(s; (x, w)) = E \left[ V^N(S^N) \mid S^{N-1} = s, (x_N, w_N) = (x, w) \right] = E \left[ \max_{z \in A} a_N(z) \mid S^{N-1} = s, (x_N, w_N) = (x, w) \right] \geq \max_{z \in A} E \left[ a_N(z) \mid S^{N-1} = s, (x_N, w_N) = (x, w) \right] = \max_{z \in A} E \left[ \int \mu(z, r) dp(r) + \sigma(z, x, w) Z \right] = V^N(s),
\]

where the penultimate equality follows by Lemma 1.

Now, we prove the induction step. For \( 0 \leq n < N - 1 \),

\[
R^n(s; (x, w)) = E \left[ V^{n+1}(S^{n+1}) \mid S^n = s, (x_{n+1}, w_{n+1}) = (x, w) \right] = E \left[ \sup_{(x', w')} R^{n+1}(s^{n+1}; (x', w')) \mid S^n = s, (x_{n+1}, w_{n+1}) = (x, w) \right] \geq \sup_{(x', w')} E \left[ R^{n+1}(s^{n+1}; (x', w')) \mid S^n = s, (x_{n+1}, w_{n+1}) = (x, w) \right] = \sup_{(x', w')} E \left[ V^{n+2}(s^{n+2}) \mid S^n = s, (x_{n+1}, w_{n+1}) = (x, w), (x_{n+2}, w_{n+2}) = (x', w') \right]
\]

where the second equality follows from the dynamic programming principle.
In the last equation both points \((x, w)\) and \((x', w')\) are inerchangeable, in the sense that it does not matter the order in which \((x, w)\) and \((x, w)\) are chosen. Thus, we have that

\[
R^n(s; (x, w)) \geq \sup_{(x', w')} E \left[ V^{n+2}(s^{n+2}) \mid S^n = s_n, (x_{n+1}, w_{n+1}) = (x', w'), (x_{n+2}, w_{n+2}) = (x, w) \right]
\]

\[
= \sup_{(x', w')} E \left[ V^{n+2}(s^{n+2}) \mid S^n = s, (x_{n+1}, w_{n+1}) = (x', w'), (x_{n+2}, w_{n+2}) = (x, w) \mid Z_2 \right]
\]

\[
= \sup_{(x', w')} E \left[ R^{n+1}(f_n(s, (x', w'), Z_2); (x, w)) \right]
\]

where \(Z_2 \sim N \left( 0; \Sigma_n ((x', w'), (x', w')) \right) + \lambda((x', w')) \), and \(f_n(s, (x', w'), Z_2)\) are the new parameters of the posterior Gaussian process after observing \(Z_2\) and choosing \((x', w')\).

By the induction hypothesis,

\[
R^n(s; (x, w)) \geq \sup_{(x', w')} E \left[ V^{n+2}(f_n(s, (x', w'), Z_2)) \right]
\]

\[
= \sup_{(x', w')} R^{n+1}(s; (x', w'))
\]

\[
= V^{n+1}(s)
\]

as we wanted to prove.

Finally, take the extra measurement \((x, w)\) to be the measurement made by the optimal policy in state \(s\), and thus by the first part of the proposition we conclude that \(V^{n+1}(s; N) \leq V^n(s; N)\).

\[\square\]

**Proposition 2.** Let \(\pi\) be a stationary policy, and \(s = (\mu, \Sigma)\). We have that \(V^{\pi, n}(s; N) \geq V^{\pi, n+1}(s; N)\).

**Proof.** We proceed by induction on \(n\). Consider the base case, \(n = N - 1\). By Jensen’s inequality we have

\[
V^{\pi, N-1}(s; N) = E \left[ \max_{x \in A} \left( \int \mu(x, w) dp(w) + \frac{\int \Sigma((x, w), \pi(s)) dp(w)}{\Sigma(\pi(s), \pi(s)) + \lambda(\pi(s))} Z \right) \right]
\]

\[
\geq \max_{x \in A} E \left[ \left( \int \mu(x, w) dp(w) + \frac{\int \Sigma((x, w), \pi(s)) dp(w)}{\Sigma(\pi(s), \pi(s)) + \lambda(\pi(s))} Z \right) \right]
\]

\[
= \max_{x \in A} a(x)
\]

\[
= V^{\pi, N}(s; N)
\]

where \(Z \sim N \left( 0, \Sigma((\pi(s), \pi(s)) + \lambda(\pi(s))) \right)\), and \(\lambda(\pi(s))\) is the variance of the observations of \(F(\pi(s))\).

Now consider the induction step. For \(n < N - 1\), we assume that if \(n \leq m\), we have that \(V^{\pi, m}(s; N) \geq V^{\pi, m+1}(s; N)\) for all parameters \(s\). Thus,

\[
V^{\pi, n}(s; N) = E^{\pi} \left[ \max_{x \in A} a_n(x) \mid S^n = s \right]
\]

\[
= E^{\pi} \left[ E^{\pi} \left[ \max_{x \in A} a_n(x) \mid S^n = s, Z_{n+1}, (x_{n+1}, w_{n+1}) = \pi(s) \right] \right]
\]

\[
\geq E \left[ E^{\pi} \left[ \max_{x \in A} a_n(x) \mid S^{n+1} = s, Z_{n+2}, (x_{n+2}, w_{n+2}) = \pi(s) \right] \right]
\]

\[
= E^{\pi} \left[ \max_{x \in A} a_n(x) \mid S^{n+1} = s \right]
\]

\[
= V^{\pi, n+1}(s; N),
\]

as we wanted to prove.

\[\square\]

**Lemma 8.** If the policy \(\pi\) samples from \((x, w)\) infinitely often almost surely, then \(R^{N-1}(S^\infty, (x, w)) = V^N(S^\infty)\) almost surely under \(\pi\).
Proof. Note that there exists a sequence of i.i.d. normal random variables \( \{ \varepsilon_k \}_k \) with mean zero and variance \( \lambda_{(x,w)} \) such that we observe \( F(x, w) + \varepsilon_k \) the \( k \)-th time that \( F(x, w) \) is queried. By the strong law of large numbers, we have that there exists a measurable set \( \mathcal{L} \) of probability one such that \( \frac{1}{m} \sum_{k=1}^{m} \varepsilon_k \) converges to the zero random variable as \( m \) goes to infinity. By hypothesis, there exists a measurable set \( \mathcal{F} \) with probability one such that \( \pi \) samples from \( (x, w) \) infinitely often. Consequently, \( \mathcal{F} \cap \mathcal{L} \) has probability one.

Fix \( \omega \in \mathcal{F} \cap \mathcal{L} \). Consider the observations \( \{ y_{nm} \}_{m \geq 0} \) where \((x_{nm}, w_{nm}) = (x, w)\), and \( y_{nm} := F(x, w) + \varepsilon_m \). So, we have that \( y_{nm} \) converges to \( F(x, w) \), and then the posterior distribution of \( G \) given \( \mathcal{F}^\infty \) does not depend on the noisy observations of \( F(x, w) \). Consequently, we have that if \( \varepsilon \sim N(0, \lambda_{(x,w)}) \), then

\[
R^{N-1}(S^\infty; (x, w)) = E \left[ \max_x E \left[ G(x') \mid \mathcal{F}^\infty, F(x, w) + \varepsilon \right] \mid \mathcal{F}^\infty \right] = E \left[ \max_x E \left[ G(x') \mid \mathcal{F}^\infty \right] \mid \mathcal{F}^\infty \right] = \max_x E \left[ G(x') \mid \mathcal{F}^\infty \right] = V^N(S^\infty).
\]

This ends the proof. \( \square \)

Lemma 9. Let \( S = (\mu, \Sigma) \in \mathcal{H} \). If \( A \) is finite and \( R^{N-1}(S; (x, w)) = V^N(S) \) for all \((x, w)\), then \( V^N(S) = U(S) \).

Proof. Suppose that \( A = \{x_1, \ldots, x_M\} \) and \( W = \{w_1, \ldots, w_M\} \). Fix any \( x \in A \) and \( w \in W \). We will show that \( \sigma_i(\Sigma, (x, w)) = \sigma_1(\Sigma, (x, w)) \) for every \( i \), where

\[
\sigma_i(\Sigma, (x, w)) = \frac{\int \Sigma((x, r), (x, w)) dp(r)}{\sqrt{\Sigma((x, w), (x, w)) + \lambda_{(x,w)}}}.
\]

We reorder the index set \( \{1, \ldots, M\} \) such that \( a(x_1) = \max_i a(x_i) = V^N(s) \). For a standard univariate normal random variable \( Z \), we have that

\[
0 = R^{N-1}(S; (x, w)) - V^N(S) = E \left[ \max_i (a(x_i) + \sigma_i(\Sigma, (x, w))) \right] - a(x_1)
\]

\[
= E \left[ \max_i (a(x_i) + \sigma_i(\Sigma, (x, w))) \right] - a(x_1) + E \left[ \sigma_1(\Sigma, (x, w)) \right] + E \left[ \sigma_1(\Sigma, (x, w)) \right] = E \left[ \sigma_1(\Sigma, (x, w)) \right] + E \left[ \sigma_1(\Sigma, (x, w)) \right] = E \left[ \sigma_1(\Sigma, (x, w)) \right] = E \left[ \sigma_1(\Sigma, (x, w)) \right] = E \left[ \sigma_1(\Sigma, (x, w)) \right].
\]

Thus, using that \( \max_i [a(x_i) - a(x_1) + (\sigma_i(\Sigma, (x, w))) - \sigma_1(\Sigma, (x, w))] \geq 0 \), we have that

\[
\int_0^\infty P(\max_i [a(x_i) - a(x_1) + (\sigma_i(\Sigma, (x, w))) - \sigma_1(\Sigma, (x, w))] \geq u) du = 0
\]

which implies that \( P(\max_i [a(x_i) - a(x_1) + (\sigma_i(\Sigma, (x, w))) - \sigma_1(\Sigma, (x, w))] \geq u] = 0 \) for almost every \( u \) in \([0, \infty)\). Taking the limit as \( u \to 0 \), by the bounded convergence theorem, we have that

\[
0 = \lim_{u \to 0} \int_0^\infty P(\max_i [a(x_i) - a(x_1) + (\sigma_i(\Sigma, (x, w))) - \sigma_1(\Sigma, (x, w))] \geq u] du = \int_0^\infty P(\max_i [a(x_i) - a(x_1) + (\sigma_i(\Sigma, (x, w))) - \sigma_1(\Sigma, (x, w))] > 0] du = \int_0^\infty P(\max_i [a(x_i) - a(x_1) + (\sigma_i(\Sigma, (x, w))) - \sigma_1(\Sigma, (x, w))] > 0] du
\]

and so \( \max_i [a(x_i) - a(x_1) + (\sigma_i(\Sigma, (x, w))) - \sigma_1(\Sigma, (x, w))] = 0 \) a.s., which implies that \( \sigma_i(\Sigma, (x, w)) = \sigma_1(\Sigma, (x, w)) \).

For all \( y, w, x_i, x_j \), we have that

\[
\int \Sigma((y, w), (x_i, r)) dp(r) = \int \Sigma((y, w), (x_j, r)) dp(r)
\]
and so
\[
\int \Sigma_1 ((y, w), (x_i, r)) \, dp(r) = \int \Sigma((y, w), (x_i, r)) \, dp(r) - \frac{\Sigma((y, w), (x_1, w_1)) \int \Sigma((x_1, w_1), (x_i, r)) \, dp(r)}{\sqrt{\Sigma((x_1, w_1), (x_1, w_1)) + \lambda_{(x_1, w_1)}}} \\
= \int \Sigma((y, w), (x_i, r)) \, dp(r) - \frac{\Sigma((y, w), (x_1, w_1)) \int \Sigma((x_1, w_1), (x_i, r)) \, dp(r)}{\sqrt{\Sigma((x_1, w_1), (x_1, w_1)) + \lambda_{(x_1, w_1)}}} \\
= \int \Sigma_1 ((y, w), (x_i, r)) \, dp(r).
\]

By recursion, we conclude that for all \( n \leq N, y, w, x_i, x_j \), we have that
\[
\int \Sigma_n ((y, w), (x_i, r)) \, dp(r) = \int \Sigma_n ((y, w), (x_i, r)) \, dp(r).
\]

Consequently, we have that for all \( y, x_i, x_j \)
\[
\int \int \Sigma_n ((y, w), (x_i, r)) \, dp(r) \, dp(w) = \int \int \Sigma_n ((y, w), (x_i, r)) \, dp(r) \, dp(w).
\]

Denote \( (x_N, w_N) \) by \( (x, w) \), we have that for all \( x_i, x_j, x' \),
\[
\int \int \Sigma_n ((x, w), (x_i, r)) \, dp(r) \, dp(w) = \int \int \Sigma_n ((x, w), (x_i, r)) \, dp(r) \, dp(w),
\]
\[
\int \int \Sigma_n ((x', w), (x_i, r)) \, dp(r) \, dp(w) = \int \int \Sigma_n ((x, w), (x_i, r)) \, dp(r) \, dp(w)
\]
\[
= \int \int \Sigma_n ((x, w), (x, r)) \, dp(r) \, dp(w)
\]

Consequently, the vector \( (G(z) : z \in A) \) has a covariance matrix with all entries equal to
\[
\int \int \Sigma_N ((x, w), (x, r)) \, dp(r) \, dp(w).
\]

Now define a normal random vector \( W(y) = a_N(y) - a_N(x) + G(x) \). Conditioned on \( \mathcal{F}^N \), it has mean vector \( a_N \), and covariance matrix with all entries equal to \( \int \int \Sigma_N ((x, u), (x, s)) \, dp(u) \, dp(s) \). Consequently, \( W \) is equal in distribution to \( (G(y) : y \in A) \).

We then have that
\[
U(S^N) = E_N \left[ \max_{x \in A} G(x) \right] = E_N \left[ \max_{y \in A} W(y) \right] = E_N \left[ \max_{y \in A} (a_N(y) - a_N(x) + G(x)) \right]
\]
\[
= E_N \left[ \max_{y \in A} a^N(y) \right] = \max_{y \in A} a^N(y) = V^N(S^N).
\]

Then
\[
V^N(S) = R^{N-1}(S; (x, w)) = E \left[ V^N(S^N) \mid x_N = x, w_N = w, S^{N-1} = S \right]
\]
\[
= E \left[ U(S^N) \mid x_N = x, w_N = w, S^{N-1} = S \right]
\]
\[
= E \left[ E_N \left[ \max_{x \in A} G(x) \right] \mid x_N = x, w_N = w, S^{N-1} = S \right]
\]
\[
= E \left[ \max_{x \in A} G(x) \mid x_N = x, w_N = w, S^{N-1} = S \right]
\]
\[
= U(S),
\]

which ends the proof.
\[\square\]
E.2 Consistency of BQO for Continuum Domains

In this subsection, we prove a slightly stronger result (Theorem 5) whose proof implies Theorem 1.

**Theorem 5.** Suppose that $A = [a_1, b_1] \times \cdots \times [a_d, b_d] \subset \mathbb{R}^d$, $a_i < b_i$ for all $i$, and $|W| = m$. Let $s = (\mu, \Sigma) \in \mathcal{H}_r$. We assume that the function $g_w(x) := \lambda_{(w,x)}$ is continuous in $A$ for all $w \in W$, and there exist $k_\lambda, K_\lambda > 0$ such that $k_\lambda < \lambda_{(w,x)} < K_\lambda$ for all $w \in W$ and $x \in A$. We then have that

$$\lim_{N \to \infty} V^0(s;N) = \lim_{N \to \infty} V^{BQO,0}(s;N)$$

As we did in the appendix §E.1, we analyze the problem with a dynamic programming framework, and use the same notation defined there. In addition, we assume without loss of generality that $\int p(w)dw = 1$. All the results of this subsection assume that $W$ is finite.

We introduce the following notation:

- $Q$ is a finite set of $A$
- $V^n_Q(s) = \sup_{\pi \in \Pi} E_\pi \left[ \max_{x \in Q} a_N(x) \mid S^n = s \right] := V^n_Q(s;N)$
- $U_Q(s) = E \left[ \max_{x \in Q} G(x) \mid S^0 = s \right]$
- $V^{\pi,n}_Q(s;N) = E_\pi \left[ \max_{x \in Q} a_N(x) \mid S^n = s \right] := V^{\pi,n}_Q(s)$
- $R^{n}_Q(s; (x, w)) = E \left[ V^{n+1}_Q \left( S^{n+1} \right) \mid S^n = s, x_{n+1} = x, w_{n+1} = w \right]$
- $\mu_Q$ is the function $\mu$ where the first entry is restricted to $Q$
- $S_Q = (\mu_Q, \Sigma)$
- $L_n(x, y, z) = \int \Sigma_n(x, w, y, z) dp(w)$

Observe that

$$V^n_Q(s) = \max_{x \in Q} a_N(x)$$

$$V^{\pi,n}_Q(s;N) = V^{\pi,n}_Q(s_Q;N)$$

$$R^{n-1}_Q(s; (x, w)) = E \left[ V^n_Q \left( S^n \right) \mid S^{n-1} = s, x_N = x, w_N = w \right].$$

We should note that Lemma 7 proved in the appendix §E.1 under the assumption that we can only choose a finite number of alternatives, holds under the assumption that we are optimizing over a finite set and we can choose any alternative in a compact set.

**Proof of Theorem 5**

*Proof.* Assume without loss of generality that $A = [0, 1]$. Let $\{Q_m\}_{m \geq 1}$ be an increasing sequence of sets defined by

$$Q_m = \bigcup_{n \geq 1} \bigcup_{i=0}^{n} \left\{ \frac{i}{n} \right\} \subset A.$$

It is clear that $\bigcup_{m \geq 1} Q_m = \mathbb{Q} \cap [0, 1]$, and $|Q_m| < \infty$. Let $\{b(m, N, \pi)\}_{N \geq 0, m \geq 1, \pi \in \Pi}$ be a sequence of real numbers defined by

$$b(m, N, \pi) = E_\pi \left[ \max_{x \in Q_m} a_N(x) \mid S^0 = s \right].$$

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By Lemma \[10\] and the Monotone Convergence Theorem applied to \{\max_{x \in Q_m} a_N(x) - \max_{x \in Q_1} a_N(x)\} we have that (note that the expectation of \(\max_{x \in Q_m} a_N(x)\) is finite by Lemma \[11\])

\[
\lim_N \sup_{\pi} E^\pi \max_{x \in A} a_N(x) \mid S^0 = s = \lim_N \sup_{\pi} E^\pi \lim_m \max_{x \in Q_m} a_N(x) \mid S^0 = s = \lim_N \sup_{\pi} \lim_m \max_{x \in Q_m} a_N(x) \mid S^0 = s = \lim_N \sup_{\pi} \max_{x \in Q_m} a_N(x) \mid S^0 = s = \lim_N \lim_m \sup_{\pi} b(m, N, \pi)
\]

By Lemma \[7\], we have that

\[
\lim_N \lim_m \sup_{\pi} b(m, N, \pi) = \sup_N \sup_m \sup_{\pi} b(m, N, \pi)
\]

and then

\[
\lim_N \lim_m \sup_{\pi} b(m, N, \pi) = \lim_m \lim_N \sup_{\pi} b(m, N, \pi), \tag{19}
\]

thus by Theorem \[6\] and Lemma \[7\]

\[
\lim_N \sup_{\pi} E^\pi \max_{x \in A} a_N(x) \mid S^0 = s = \lim_m \lim_N \sup_{\pi} b(m, N, \pi) = \lim_m \lim_N b(m, N, BQO) = \sup_m \sup_N b(m, N, BQO) = \lim_N \lim_m b(m, N, BQO).
\]

By the Monotone Convergence Theorem applied to \{\max_{x \in Q_m} a_N(x) - \max_{x \in Q_1} a_N(x)\} and by Lemma \[10\] we have that

\[
\lim_N \sup_{\pi} E^\pi \max_{x \in A} a_N(x) \mid S^0 = s = \lim_N E^{BQO} \lim_m \max_{x \in Q_m} a_N(x) \mid S^0 = s = \lim_N E^{BQO} \max_{x \in A} a_N(x) \mid S^0 = s.
\]

\[\square\]

**Lemma 10.** Assume that \(A = [0, 1]\), and \(|W| < \infty\). \(E^\pi \left[ \lim_m \max_{x \in Q_m} a_N(x) \mid S^0 = s \right] = E^\pi \left[ \max_{x \in A} a_N(x) \mid S^0 = s \right] \) where \(\{Q_m\}_m\) are the sets defined in the proof of Theorem \[5\].

**Proof.** Let \(\omega \in \Omega\) and \(\varepsilon > 0\). There exists \(x_0 \in A\) such that

\[
\max_{x \in A} a_N(x) = a_N(x_0)
\]

because \(a_N\) is a continuous function in a compact set. Let \(\delta > 0\) such that \(|a_N(x_0) - a_N(x)| < \varepsilon\) whenever \(|x_0 - x| < \delta\). Using the completeness of the rationals, we have that there exist \(M, \{q_m\}_{m \geq 0} \subset \mathbb{Q} \cap [0, 1]\), and \(\{r_m\}_{m \geq 1} \subset \mathbb{N}\) such that \(q_m \in Q_{r_m}, r_m \leq r_{m+1}\), and if \(m \geq M\),

\[
|q_m - x_0| < \delta,
\]

and then

\[
|a_N(x_0) - a_N(q_m)| < \varepsilon,
\]

which implies that if \(m \geq r_M\),

\[
|\max_{x \in Q_m} a_N(x) - \max_{x \in A} a_N(x)| < \varepsilon,
\]

and then \(\max_{x \in Q_m} a_N(x) \rightarrow \max_{x \in A} a_N(x)\) almost surely.

\[\square\]
Lemma 11. Let $\pi$ be an admissible policy, and $s_0 \in A$. We have that, given a finite or compact set $Q$ of $A$ and $|W| < \infty$,

$$E^\pi \left[ \sup_{x \in Q} a_N(x) \right] < \infty.$$

Proof. Let $\phi_i(z_i)$ be the density of a normal random variable with mean zero and variance $\Sigma_{i-1}(x_i, w_i, x_i, w_i) + \lambda_{(x_i, w_i)}$ where $(x_i, w_i)$ is the point chosen by $\pi$ at iteration $i$, we have that

$$E^\pi \left[ \sup_{x \in Q} a_N(x) \right] \leq E^\pi \left[ \sup_{x \in Q} a_{N-1}(x) \right] +$$

$$\int_{z_1, \ldots, z_N} \sup_{x \in Q} \frac{L_{N-1}(x, x_N, w_N)}{\Sigma_{N-1}(x_N, w_N, x_N, w_N) + \lambda_{(x_N, w_N)}} \Pi_{i=1}^{N-1} \phi_i(z_i) | z_N | \phi_N(z_N) dz_1 \cdots dz_N$$

$$\leq E^\pi \left[ \sup_{x \in Q} a_{N-1}(x) \right] +$$

$$\int_{z_1, \ldots, z_{N-1}} \sup_{x \in Q} \frac{L_{N-1}(x, x_N, w_N)}{\Sigma_{N-1}(x_N, w_N, x_N, w_N) + \lambda_{(x_N, w_N)}} \Pi_{i=1}^{N-1} \phi_i(z_i) dz_1 \cdots dz_{N-1}$$

$$\leq E^\pi \left[ \sup_{x \in Q} a_{N-1}(x) \right] +$$

$$\sqrt{\frac{2}{\pi}} \int_{z_1, \ldots, z_{N-1}} \sup_{x \in Q} \frac{L_{N-1}(x, x_N, w_N)}{\sqrt{\Sigma_{N-1}(x_N, w_N, x_N, w_N) + \lambda_{(x_N, w_N)}}} \Pi_{i=1}^{N-1} \phi_i(z_i) dz_1 \cdots dz_{N-1}$$

$$\leq E^\pi \left[ \sup_{x \in Q} a_{N-1}(x) \right] +$$

$$\sqrt{\frac{2}{\pi}} \int_{z_1, \ldots, z_{N-1}} \sup_{x \in Q, w \in W} \sqrt{\Sigma_{N-1}(x, w, x, w)} \Pi_{i=1}^{N-1} \phi_i(z_i) dz_1 \cdots dz_{N-1}$$

$$\leq E^\pi \left[ \sup_{x \in Q} a_{N-1}(x) \right] +$$

$$\sqrt{\frac{2}{\pi}} \sqrt{\sup_{x \in Q, w \in W} \Sigma_0(x, w, x, w)}$$

$$\vdots$$

$$\leq \sup_{x \in Q} a_0(x) + N \sqrt{\frac{2}{\pi}} \sqrt{\sup_{x \in Q, w \in W} \Sigma_0(x, w, x, w)},$$

where $L_n(x, y, z) = \int \Sigma_n(x, w, y, z) dp(w)$. This shows that $E^\pi \left[ \sup_{x \in Q} a_N(x) \right] < \infty$. \hfill \Box

Theorem 6. Let $Q$ be a finite set of $A$. Suppose that $|W| < \infty$, and $s \in A$. We have that

$$\lim_{N \to \infty} \sup_{\pi} E^\pi \left[ \max_{x \in Q} a_N(x) \mid S^0 = s \right] = \lim_{N \to \infty} E^{QBO} \left[ \max_{x \in Q} a_N(x) \mid S^0 = s \right]$$

Proof. We first note that the limit of $S^0_Q$ exists a.s. by Lemma 13 and we denote it by $S^0_Q$. By Lemma 15 under the BQO policy $V^N_Q \left( S^\infty_Q \right) = U_Q \left( S^\infty_Q \right)$ a.s. Furthermore, $V^{BQO,0}_Q(s; N)$ is non-decreasing in $N$ and bounded above by Lemma 7 and so by Fatou’s lemma we have that $\lim_{N \to \infty} V^{BQO,0}_Q(s; N) = V^{BQO,0}(s; \infty)$. Thus, for
any $N > 0$,

$$V_Q^{BQO,0}(s; \infty) = E^{BQO}[V_Q^N(S_Q^0) \mid S^0 = s]$$

$$= E^{BQO}[U_Q(S_Q^0) \mid S^0 = s]$$

$$= E^{BQO}[E[\max_{x \in Q}G(x) \mid S^0 = S_Q^0] \mid S^0 = s]$$

$$= E[\max_{x \in Q}G(x) \mid S^0 = s]$$

$$= U_Q(s)$$

and $U_Q(s) \geq V_Q^0(s; \infty)$ by Lemma [7]. This ends the proof because $V_Q^0(s; \infty) \geq V_Q^{BQO,0}(s; \infty)$.

**Lemma 12.** Let $\mathcal{H}$ be the Reproducing Kernel Hilbert Space (RKHS) associated to any isotropic kernel $\Sigma_0$ defined in $(\mathbb{R}^d \times W) \times (\mathbb{R}^d \times W)$, where $|W| < \infty$, we have the following:

1. Consider the operator $\bar{P}_{1:n} : \mathcal{H} \to \text{span} \{\Sigma_0(x_i, w_1, \cdot, \cdot)\} \subset \mathcal{H}$ defined by

$$\bar{P}_{1:n}h := \Sigma_0(\cdot, (x, w)_{1:n}) A_n^{-1} \langle \Sigma_0(\cdot, (x, w)_{1:n}), h \rangle$$

where $\Sigma_0(\cdot, (x, w)_{1:n}) = (\Sigma_0(\cdot, x_1, w_1), \ldots, \Sigma_0(\cdot, x_n, w_n))$, $A_n := [\Sigma_0(x_i, w_i, x_j, w_j)]_{i,j=1:n}$ and

$$\langle \Sigma_0(\cdot, (x, w)_{1:n}), h \rangle := \begin{bmatrix} h(x_1, w_1) \\ \vdots \\ h(x_n, w_n) \end{bmatrix}.$$ 

We have that $\|\bar{P}_{1:n}\| \leq 1$, and $\|1 - \bar{P}_{1:n}\| \leq 1$

2. Suppose that $\Sigma_{w,w'}(x, y) := \Sigma_0(x, w, y, w')$ is continuous for any $w, w' \in W$. Consider the operator $P_{1:n} : \mathcal{H} \to \text{span} \{\Sigma_0(x_i, w_1, \cdot)\} \subset \mathcal{H}$ defined by

$$P_{1:n}h := \Sigma_0(\cdot, (x, w)_{1:n}) A_n^{-1} \langle \Sigma_0(\cdot, (x, w)_{1:n}), h \rangle$$

where $\Sigma_0(\cdot, (x, w)_{1:n}) = (\Sigma_0(\cdot, x_1, w_1), \ldots, \Sigma_0(\cdot, x_n, w_n))$, $A_n := [\Sigma_0(x_i, w_i, x_j, w_j) + 1_{\{x_i, w_i \neq x_j, w_j\}} \lambda(x_i, w_i)]_{i,j=1:n}$ and

$$\langle \Sigma_0(\cdot, (x, w)_{1:n}), h \rangle := \begin{bmatrix} h(x_1, w_1) \\ \vdots \\ h(x_n, w_n) \end{bmatrix}.$$ 

We have that $\|P_{1:n}\Sigma_0(x', w', \cdot)\| \leq \sup_{x \in A, w \in W} \Sigma_0(x, w, x, w) + \lambda(x, w)$, and $\|(1 - P_{1:n}) \Sigma_0(x', w', \cdot)\| \leq \sup_{x \in A, w \in W} \Sigma_0(x, w, x, w) + \sup_{x \in A, w \in W} \Sigma_0(x, w, x, w)$ for all $x', w'$.

3. $\Sigma_n(\cdot, y, w) = \Sigma_0(\cdot, y, w) - P_{1:n}h_{y,w}$ where $h_{y,w}(z, w') := \Sigma_0(z, w', y, w)$

4. $\Sigma_n(x, w, x, w) = \langle \Sigma_0(x, w, \cdot), (1 - P_{1:n}) \Sigma_0(x, w, \cdot) \rangle$

5. $|\nabla_x P_{1:n}h(x, w)|^2 \leq d \|P_{1:n}h\|^2_H \left(\sup_{r \leq d+1} \frac{\partial^2}{\partial x_i \partial w_j} \Sigma_0(x, w, r, w) \mid x=r \right)$ for any $h \in H$ if $\Sigma_0(\cdot, w, \cdot, w)$ is in $C^1$.

**Proof.** 1. Define $V = [\Sigma_0(x_1, w_1, \cdot), \ldots, \Sigma_0(x_n, w_n, \cdot)] \in \mathcal{H}^n$. It is easy to see that:

$$\bar{P}_{1:n} = V (VTV)^{-1}VT.$$ 

Furthermore, it is well known that in that case $\bar{P}_{1:n}$ is a projection onto the space generated by

$$\{\Sigma_0(x_1, w_1, \cdot), \ldots, \Sigma_0(x_n, w_n, \cdot)\},$$

consequently we have that $\|\bar{P}_{1:n}\| \leq 1$. Similarly, we can see that $\|1 - \bar{P}_{1:n}\| \leq 1$. 44
2. Define the kernel \( k(x, w, y, w') = \sum_0 (x, w, y, w') + \lambda_{(x, w)} 1_{\{x = y, w = w'\}} \) for \( \lambda_{(x, w)} > 0 \), and let \( \tilde{H} \) be its RKHS. Define

\[
\tilde{P}_{1:n} h = k(\cdot, (x, w)_{1:n})A_n^{-1} \langle k(\cdot, (x, w)_{1:n}), h \rangle_H
\]

\[
P_{1:n} h_1 = \sum_0 (\cdot, (x, w)_{1:n})A_n^{-1} \langle \sum_0 (\cdot, (x, w)_{1:n}), h_1 \rangle_H
\]

where \( h \in \tilde{H}, h_1 \in H \) and \( A_n := [k(x_i, w_i, x_j, w_j)]_{i,j=1:n} \).

Observe that if \( h_1 = \sum_0 (x, w, \cdot) + \lambda_{(x, w)} 1_{\{x = y, w = w_1\}} \), \( h = \sum_0 (x, w, \cdot) \) and \( (x, w) \neq (x_i, w_i) \) for all \( i \), we have that

\[
\|P_{1:n} h\|^2_H = \langle P_{1:n} h, P_{1:n} h \rangle_H
\]

\[
= \sum_{i,j=1}^n a_i a_j \sum_0 (x_i, w_i, x_j, w_j)
\]

\[
\leq \sum_{i,j=1}^n a_i a_j \left( \sum_0 (x_i, w_i, x_j, w_j) + \lambda_{(x, w)} 1_{\{x = y, w = w_1\}} \right)
\]

\[
= \langle \tilde{P}_{1:n} h_1, \tilde{P}_{1:n} h_1 \rangle_H
\]

\[
\leq \|h_1\|^2_H, \text{ by (1)}
\]

\[
= \sum_0 (x, w, x, w) + \lambda_{(x, w)}
\]

where \( a_i \) is the \( i \)th entry of \( A_n^{-1} [h(x_1, w_1), \ldots, h(x_n, w_n)]' \).

Now take \( (x, w) = (x_i, w_i) \) for some \( i \), and \( h = \sum_0 (x, w, \cdot) \). Consider a sequence of points \( \{ (y_m, w) \} \subset A \times W \rightarrow (x_i, w) \) such that \( y_m \neq x_j \) for all \( j \). Let \( a_i^m \) be the \( k \)th entry of \( A_n^{-1} [\sum_0 (y_m, w, x_1, w_1), \ldots, h(y_m, w, x_n, w_n)]' \).

Thus, we have that \( a_i^m \rightarrow a_k \) where \( a_k \) is the \( k \)th entry of \( A_n^{-1} [\sum_0 (x_i, w_i, x_1, w_1), \ldots, \sum_0 (x_i, w_i, x_n, w_n)]' \). By the previous result for all \( m \),

\[
\sum_{i,j=1}^n a_i^m a_j^m \sum_0 (x_i, w_i, x_j, w_j) \leq \sup_{x \in A, w \in W} \left[ \sum_0 (x, w, x, w) + \lambda_{(x, w)} \right]
\]

and so

\[
\|P_{1:n} h\|^2_H = \sum_{i,j=1}^n a_i a_j \sum_0 (x_i, w_i, x_j, w_j) \leq \sup_{x \in A, w \in W} \left[ \sum_0 (x, w, x, w) + \lambda_{(x, w)} \right] .
\]

Now observe that by the previous equation and using that \( A_n \) is positive definite,

\[
\| (1 - P_{1:n}) h \|^2_H = \sum_0 (x, w, x, w) - 2P_{1:n} h(x, w) + \|P_{1:n} h\|^2_H
\]

\[
\leq \sum_0 (x, w, x, w) + \sup_{x \in A, w \in W} \left[ \sum_0 (x, w, x, w) + \lambda_{(x, w)} \right]
\]

\[
\leq \sup_{x \in A, w \in W} \left[ \sum_0 (x, w, x, w) + \lambda_{(x, w)} \right] + \sup_{x \in A, w \in W} \sum_0 (x, w, x, w) ,
\]

as we wanted to prove.

3. The proof is a simple consequence of the definition of \( P_{1:n} h \).

4. We have that

\[
\langle \sum_0 (x, w, \cdot), (1 - P_{1:n}) \sum_0 (x, w, \cdot) \rangle = \sum_0 (x, w, x, w) - \langle \sum_0 (x, w, \cdot), P_{1:n} \sum_0 (x, w, \cdot) \rangle
\]

\[
= \sum_0 (x, w, x, w) - P_{1:n} \sum_0 (x, w, \cdot) (x, w)
\]

\[
= \sum_0 (x, w, x, w) .
\]
5. It follows from the proof of Corollary 4.36 of Ingo and Christmann (2008).

 Lemma 13. Suppose that $|W| < \infty$. Given a finite set $Q \subset A$. Consider any $s = (\mu, \Sigma) \in \mathcal{H}_1$, and policy $\pi$. We have that the following happens almost surely:

1. $(S'_Q)$ converges to $S'_Q = (\mu_\infty, \Sigma_\infty) \in \mathcal{H}$, and $\mu_\infty (x, w) = \lim_n \mu_n (x, w)$ for all $x \in A \cap \mathbb{Q}^d \cup Q$, $w \in W$. Furthermore, $\Sigma_\infty (x, x', w') = \lim_n \Sigma_n (x, w, x', w')$ for all $x, x' \in A$, and $w, w' \in W$.

2. The convergence of $\{\Sigma_n\}$ is uniform.

3. Let $w, w' \in W$, and define $g_{w,w'} (x, x') := \Sigma_\infty (x, w, x', w')$. We have that $g_{w,w'}$ is continuous.

4. $E_\infty [F (x, w)] = \mu_\infty (x, w)$ exists for all $x \in A, w \in W$.

5. The limit of $E_n (F^2 (x, w))$ exists for all $x \in A \cap \mathbb{Q}^d \cup Q$, $w \in W$, and it is equal to $\mu_\infty (x, w)^2 := E_\infty (F^2 (x, w))$. Furthermore, $\Sigma_\infty (x, w, x, w) = \mu_\infty (x, w)^2 - \mu_\infty^2 (x, w)$ for all $x, w$.

Proof. By the convergence of conditional expectations property implied by the Doob’s martingale convergence theorem and the fact that $F (x, w)$ has second moments, we must have that for any points $x, x', w, w'$, it happens almost surely that $\mu_n (x, w) \to E [F (x, w) | \mathcal{F}_\infty]$, $\Sigma_n (x, x', w') \to \text{cov} (F (x, w), F (x', w')) | \mathcal{F}_\infty$ and $\Sigma_n (x, w, x, w) \to \text{var} (F (x, w) | \mathcal{F}_\infty)$.

Consequently, $\Sigma_n (x, x', w') \to \Sigma_\infty (x, x', w')$, $\mu_n (x, w) \to \mu_\infty (x, w)$ for all $x, x' \in \mathbb{Q}^d \cap A \cup Q$, $w, w' \in W$ a.s. (the previous affirmation is true because for any points $x, x' \in \mathbb{Q}^d \cap A \cup Q$, $w, w' \in W$ the event $\{\Sigma_n (x, x', w') \to \Sigma_\infty (x, x', w') \}$ is false with probability zero, and so the event

$$\bigcup_{x,x' \in \mathbb{Q}^d \cap A \cup Q : w,w' \in W} \{\Sigma_n (x, w, x', w') \to \Sigma_\infty (x, w, x', w') \}, \mu_n (x, w) \to \mu_\infty (x, w)\}$$

has probability zero.

Let’s now prove that the sequence $\Sigma_n$ is equicontinuous. Fix any $x \in A, w \in W$, observe that for any $x, y' \in A$, by the Mean Value Theorem and Lemma 12, we have that if $h = \Sigma_0 (x, w, y', \cdot)$,

$$|\Sigma_n (x, w, x', w) - \Sigma_n (x, w, y', w)| \leq \sup_{r \in A} |\nabla_r (1 - P_{1:n}) h (r, w)| |x' - y'|$$

$$\leq |x' - y'| d \|(1 - P_{1:n}) h\|| \sup_{r \in A} \sup_{i < n + 1} \frac{\partial}{\partial r_i} \Sigma_0 (x, w, r, w) |_{x=r}$$

$$= |x' - y'| d \left( \sup_{x \in A, w \in W} \left[ \Sigma_0 (x, w, x, w) + \lambda_{x, w} + \sup_{x \in A, w \in W} \Sigma_0 (x, w, x, w) \right] \right)$$

$$\times \left( \sup_{r \in A, w \in W} \sup_{i < n + 1} \frac{\partial}{\partial x_i} \frac{\partial}{\partial r_i} \Sigma_0 (x, w, r, w) |_{x=r} \right)$$

so $\{\Sigma_n (x, w, y', \cdot)\}_n$ is equicontinuous for all $x, w$.

Now, let $\epsilon > 0$ and $\delta < \epsilon$ such that if $|(x, w) - (y, z)| < \delta$, then $z = w$, and $|a - \Sigma_0 (y, z, x, z)| < \epsilon$ where $a = \Sigma_0 (x, w, x, w) = \Sigma_0 (y, z, x, z)$. Observe that by Lemma 12

$$|\Sigma_n (x, w, x, w) - \Sigma_n (y, w, y, w)| \leq |\Sigma_0 (x, w, x, w) - \Sigma_0 (y, w, y, w)|$$

$$\leq \left[ |\Sigma_0 (x, w, x, w) - \Sigma_0 (y, w, w)| + \left| \left( \Sigma_0 (x, w, \cdot), P_{1:n} \Sigma_0 (x, w, \cdot) \right) - \left( \Sigma_0 (y, w, \cdot), P_{1:n} \Sigma_0 (y, w, \cdot) \right) \right| \right]$$

$$\leq \epsilon + \left| \left( \Sigma_0 (x, w, \cdot) - \Sigma_0 (y, w, \cdot), P_{1:n} \Sigma_0 (x, w, \cdot) \right) \right|$$

$$\leq \epsilon + \left( \sqrt{\Sigma_0 (x, w, x, w) + \Sigma_0 (y, w, y, w) - 2 \Sigma_0 (x, w, y, w)} \right)$$

$$\leq \epsilon + 2 \sqrt{2} \epsilon \left( \sup_{x \in A, w \in W} \left[ \Sigma_0 (x, w, x, w) + \lambda_{(x, w)} \right] \right)$$
thus, \( \{\Sigma_n(\cdot, \cdot, \cdot, \cdot)\} \) is equicontinuous.

Now, take any \( x, x' \in A, w, w' \in W \). Let \( \delta > 0 \) and \( q, q' \in \mathbb{Q}^d \cap A \) such that \( |q - x| < \delta, |q' - x'| < \delta \). Thus,

\[
|\Sigma_n(x, w, x', w') - \Sigma_m(x, w, x', w')| \leq |\Sigma_n(x, w, x', w') - \Sigma_n(q, w, q', w')| + |\Sigma_n(q, w, q', w') - \Sigma_m(q, w, q', w')| + |\Sigma_m(q, w, q', w') - \Sigma_m(x, w, x', w')|,
\]

which implies that \( \{\Sigma_n(x, w, x', w')\} \) is a Cauchy sequence if \( \{\Sigma_n(q, w, q', w')\} \) converges, and thus \( \{\Sigma_n(x, w, x', w')\} \) converges too. Consequently, \( \Sigma_n(x, w, x', w') \to \Sigma_\infty(x, w, x', w') \) for all \( x, x' \in A, w, w' \in W \). Furthermore, the convergent is uniform because \( \{\Sigma_n\} \) is equicontinuous, which implies that \( \Sigma_\infty \) is continuous. Observe, that since \( \Sigma_\infty(x, w, x, w) \) exists for all \( x, w \), we must have that \( \mu_\infty(x, w) \) exists for all \( x, w \). Observe that the limit of kernels is a kernel, and so \( \Sigma_\infty \) is a kernel. This proves (1), (2), (3) and (4). Similarly, we can prove (5).

\[ \square \]

**Lemma 14.** Suppose that \(|W| < \infty\). Given \( s_0 \in \mathcal{H}_1 \), \( Q \) a finite set of \( A \cap \mathbb{Q}^d \), then \( R_Q^{N-1}(S^n; x, w) \) converges uniformly to \( R_Q^{N-1}(S^\infty; x, w) \) a.s.

**Proof.** By Lemma 13 we have that \( \Sigma_n(x, w, r, w') \) converges uniformly to \( \Sigma_\infty(x, w, r, w') \) for all \( x, r, w, w' \) a.s. Since we assume that the noise is bounded, we have that

\[
\Sigma_0(x, w, x, w) + K_\lambda \geq \Sigma_n(x, w, x, w) + \lambda(x, w) \geq k_\lambda
\]

where \( K_\lambda, k_\lambda > 0 \) are the bounds of the variance of the noise. Thus, for all \( x, w \)

\[
\frac{1}{\Sigma_n(x, w, x, w) + \lambda(x, w)} \Rightarrow \frac{1}{\Sigma_\infty(x, w, x, w) + \lambda(x, w)} \quad \text{a.s.}
\]

Now,

\[
\left| R_Q^{N-1}(S^n; x, w) - R_Q^{N-1}(S^\infty; x, w) \right| = \left| E \left[ \max_{z \in Q} [a_n(z) + \tilde{\sigma}_n(z, x, w) Z] - E \left[ \max_{z \in Q} [a_\infty(z) + \tilde{\sigma}_\infty(z, x, w) Z] \right] \right] \right|
\]

\[
\leq E \left[ \max_{z \in Q} \left| [a_n(z) + \tilde{\sigma}_n(z, x, w) Z] - a_\infty(z) - \tilde{\sigma}_\infty(z, x, w) Z \right| \right]
\]

thus it is clear that \( R_Q^{N-1}(S^n; x, w) \Rightarrow R_Q^{N-1}(S^\infty; x, w) \) for all \( x, w \) a.s., because \( a_n(z) \to a_\infty(a), \tilde{\sigma}_n(z, x, w) \Rightarrow \tilde{\sigma}_\infty(z, x, w) \) a.s., and \( Q \) is finite.

\[ \square \]

**Lemma 15.** Suppose that \(|W| < \infty\). Under the BQO policy, for any finite set \( Q \) of \( A \cap \mathbb{Q}^d \), if \( s = (\mu_0, \Sigma_0) \in \mathcal{H}_1 \), then \( V^n_Q(S^\infty_Q) = U_Q(S^\infty_Q) \) a.s. where \( S^\infty_Q \) is the limit of \( \left( S^n_Q \right) \), and

\[
V^n_Q(s) = \sup_{\pi \in \Pi} E^{\pi} \left[ \max_{x \in Q} \mu_N(x) \mid S^n = s \right]
\]

\[
U_Q(s) = E \left[ \max_{x \in Q} G(x) \mid S^0 = s \right]
\]

**Proof.** By Lemma 14 and Lemma 17, there exists a measurable set \( F \) of probability one, such that if \( \omega \in F \), \( R_Q^{N-1}(S^n; x, w) \) converges uniformly to \( R_Q^{N-1}(S^\infty; x, w) \), and the statement of the Lemma 17 is true. Fix a \( \omega \in F \).

Let \( \varepsilon > 0 \). By Lemma 14, \( R_Q^{N-1}(S^\infty; x, w) \) is continuous, and so it is uniformly continuous because \( A \) is compact. Consequently, there exists \( \delta > 0 \) such that if \( \|(x, w) - (y, w')\| < \delta \), then \( w = w' \) and

\[
\left| R_Q^{N-1}(S^\infty; x, w) - R_Q^{N-1}(S^\infty; y, w') \right| < \varepsilon.
\]

(22)
By Lemma \[17\] the same \(\delta > 0\) can be chosen such that that if the policy chooses an infinite number of points in \(B_{\delta}(x) \times \{w\}\), thus \(\left| R_{Q}^{N-1}(S^{\infty};x,w) - V_{Q}^{N}(S^{\infty}) \right| < \varepsilon \).

In order to simplify the notation, we assume that \(A = [0,1]\). We build a collection of finite sets of number of rationals \(Q_{n}\) such that \(\bigcup_{n} Q_{n} = A \cap \mathbb{Q}\) (for example, see proof of Theorem \[5\]). We order the elements of \(Q_{n} = \{q_{m}\}_{n \geq m \geq 1}\) such that \(q_{m} \leq q_{m+1}\). We define the intervals \(I_{m} = [q_{m}, q_{m+1})\) if \(m < n - 1\), and \(I_{n-1} = [q_{n-1}, q_{n}]\). By Lemma \[16\] we know that there exists \(Q_{n}\) such that \(\sup_{m} |q_{m} - q_{m+1}| < \delta\).

Take any finite set \(Q = A \cap \mathbb{Q}^{d}\). Let \(I = \{1, \ldots, n - 1\}\). Let \(B' := \bigcup_{w \in W} B_{w} \times \{w\}\) where \(B_{w} \subset I\) for all \(w\), and \(B_{w}\) satisfies that there exists \(x_{w} \in I_{i}\) for all \(i \in B_{w}\), \(w \in W\), and define \(\varepsilon' := R_{Q}^{N-1}(S_{Q}^{\infty};x_{w},w) - V_{Q}^{N}(S_{Q}^{\infty})\) for all \((x,w)\) such that \(x \in I_{i}\) for all \(i \notin B_{w}\) and \(w \in W\). Observe that by Proposition \[1\] \(R_{Q}^{N-1}(s;x,w) \geq V_{Q}^{N}(s)\) for all \((x,w)\).

Assume that \(B' \neq \emptyset\). By Lemma \[17\] there exists \(N\) such that if \(n > N\), \((x,w)\) is not chosen if \(x \in I_{i}\) where \(i \in B_{w}\) and \(w \in W\). Take any \((x_{w},w)\), such that \(x_{w} \in I_{i}\) for some \(i \in B_{w}\), \(w \in W\), and define \(\varepsilon' := R_{Q}^{N-1}(S_{Q}^{\infty};x_{w},w) - V_{Q}^{N}(S_{Q}^{\infty})\) for all \((x,w)\) such that \(x \in I_{i}\) where \(i \notin B_{w}\) and \(w \in W\). Observe that \(\varepsilon' \leq R_{Q}^{N-1}(S_{Q}^{\infty};x_{w},w) - R_{Q}^{N-1}(S_{Q}^{\infty};y,w')\). Define \(\varepsilon_{1} := \varepsilon'/2\). Since \(R_{Q}^{N-1}(S_{Q}^{\infty};x_{w},w)\) converges uniformly to \(R_{Q}^{N-1}(S_{Q}^{\infty};x,w)\), we have that there exists \(n > N\) such that

\[
R_{Q}^{N-1}(S_{Q}^{\infty};x_{w},w) > R_{Q}^{N-1}(S_{Q}^{\infty};x_{w},w) - \varepsilon_{1} \\
\geq R_{Q}^{N-1}(S_{Q}^{\infty};y,w') + \varepsilon_{1} \\
> R_{Q}^{N-1}(S_{Q}^{\infty};y,w')
\]

which contradicts that we would not choose a point \((x,w)\) if \(x \in I_{i}\), \(w \in W\), \(i \in B_{w}\) and \(n > N\). Consequently, \(B'\) is the empty set.

Thus, we have that for all \((x,w)\) and \(\varepsilon > 0\), \(R_{Q}^{N-1}(S_{Q}^{\infty};x,w) \leq \varepsilon + V_{Q}^{N}(S_{Q}^{\infty})\), and so \(R_{Q}^{N-1}(S_{Q}^{\infty};x,w) = V_{Q}^{N}(S_{Q}^{\infty})\). Finally, Lemma \[18\] implies the result.

\[\square\]

**Lemma 16.** Let \(Q_{m} = \bigcup_{n=1}^{m} \bigcup_{i=0}^{n} \{\frac{i}{n}\}\) for \(m \geq 1\). If \(\varepsilon > 0\), we have that there exists \(M\) such that if \(m \geq M\), and the elements of \(Q_{m}\) are sorted such that \(q_{k} \leq q_{k+1}\), then \(|q_{k+1} - q_{k}| < \varepsilon\) for all \(k\).

**Proof.** The proof is trivial.

\[\square\]

**Lemma 17.** Suppose that \(|W| < \infty\). Let \(s = (\mu, \Sigma) \in \mathcal{H}_{1}\). It almost surely happens that: for every \(\varepsilon > 0\) and \(w \in W\), there exists \(\delta_{0} > 0\) such that if the policy \(\pi\) measures an infinite number of alternatives in \(B_{\delta}(x) \times \{w\}\) for \(\delta < \delta_{0}\), where \(B_{\delta}(x)\) is the open ball of radius \(\delta\) with center \(x\), and \(x \in A\), we then have that

\[
\left| R_{Q}^{N-1}(S_{Q}^{\infty};x,w) - V_{Q}^{N}(S_{Q}^{\infty}) \right| < \varepsilon.
\]

**Proof.** We can assume without loss of generality that the Gaussian process is separable, because the probability space is complete and so there exists a separable version of every stochastic process defined in \(A\) (Neveu \[1965\] Pollard, D. \[2016\]). Let \(x \in A\) and \(w \in W\). We define \(f(y) := F(y, w)\). Since \(\Sigma_{0}(.; w, \cdot, w)\) is Lipschitz continuous, thus \(f\) is continuous a.s., and so by Adler and Taylor \[2007\], we have that for all \(a > 0\)

\[
\int_{0}^{a} H^{1/2}(u) \, du < \infty
\]
where $H$ is the log-entropy function for $A$. By Lemma 1.3.1 and the fact that $f$ is continuous a.s., there exists a measurable set $F$ of probability one, such that if $\omega \in F$, the limits of the parameters of the GP exist and $f$ is continuous. Fix a $\omega \in F$. Let $\varepsilon > 0$. We then have that
\[
\lim_{a \to 0} \int_0^a H^{1/2}(u) \, du = 0,
\]
thus there exists $\delta' > 0$ such that $\varepsilon > \delta'$, and if $a \leq \delta'$, then $0 \leq \int_0^a H^{1/2}(u) \, du < \varepsilon$.

A simple extension of Lemma 1.3.1 of Chapter 1 of Adler and Taylor (2007) shows that the canonical metric $d(s,t) = \left\{ \left( E \left( \left| (f(s) - f(t))^2 \right| \right) \right)^{1/2} \right\}$ satisfies that there exists $\delta$ such that $d(x,y) < \delta'$ if $|y - x| < \delta$. Define $\epsilon(\delta) := \sup_{|y-x|<\delta} |f(x) - f(y)|$, which is finite because $f$ is bounded ($f$ is continuous in a compact set).

Observe that for all $n$
\[
d^2(x,y \mid \mathcal{F}_n) = E \left[ (f(x) - \mu_n(x,w) - f(y) + \mu_n(y,w))^2 \mid \mathcal{F}_n \right] = \Sigma_n(x,w,x,w) + \Sigma_n(y,w,y,w) - 2\Sigma_n(x,w,y,w)
\]
\[
= \Sigma_{n-1}(x,w,x,w) + \Sigma_{n-1}(y,w,y,w) - 2\Sigma_{n-1}(x,w,y,w) - 2\Sigma_{n-1}(y,w,x,w) + 2\Sigma_{n-1}(x,w,x,w)\Sigma_{n-1}(y,w,x,w, w_n) = \Sigma_{n-1}(x_n, w_n, x_n, w_n) + \lambda_{x_n, w_n}
\]
\[
= \Sigma_{n-1}(x_n, w_n, x_n, w_n) + \Sigma_{n-1}(y,w,y,w) - 2\Sigma_{n-1}(x,w,y,w) - (\Sigma_{n-1}(x, w, x_n, w_n) - \Sigma_{n-1}(y, w, x_n, w_n))^2
\]
\[
\leq d^2(x,y \mid \mathcal{F}_{n-1})
\]
\[
\vdots
\]
\[
\leq d^2(x,y).
\]

Now, we will show that for all $n$, $H_n(u) \leq H(u)$ where $H_n$ is the log-entropy function for $A$ associated to the Gaussian process on $f$ given $\mathcal{F}_n$, and $u > 0$. Let $\{B_j(x_j;u)\}_{j=1}^{N(u)}$ be a cover of $A$, where $B_j(x_j;u)$ is the ball with center $x_j$ and radius $u$ using the metric $d$. Define the sequence of balls $\{B_j^u(x_j;u)\}_{j=1}^{N(u)}$, where $B_j^u(x_j;u)$ is the ball with center $x_j$ and radius $u$ using the metric $d(x,y \mid \mathcal{F}_n) \leq d^2(x,y)$, we have that $\{B_j^u(x_j;u)\}_{j=1}^{N(u)}$ is a cover of $A$, and thus $H_n(u) \leq H(u)$. So, for all $n$, we have that $\int_0^a H_n^{1/2}(u) \, du < \varepsilon$ if $a \leq \delta'$.

Define $\epsilon_n(\delta) := \sup_{|y-x|<\delta} |f(x) - \mu_n(x,w) - f(y) + \mu_n(y,w)|$. We will prove by induction on $n$ that for all $n$, $\Sigma_n(x,w,x,w) > 0$. The result is true when $n = 0$. Suppose that it is true if $m < n$. Thus,
\[
\Sigma_n(x,w,x,w) = \Sigma_{n-1}(x,w,x,w) - \Sigma_{n-1}(x_n, w_n, x_n, w_n) + \lambda_{x_n, w_n},
\]
and $\Sigma_{n-1}(x_n, w_n, x_n, w_n) \geq \Sigma_{n-1}(x_n, w_n, x_n, w_n) + \lambda_{x_n, w_n}$, consequently,
\[
\Sigma_{n-1}(x, w, x, w) (\Sigma_{n-1}(x_n, w_n, x_n, w_n) + \lambda_{x_n, w_n}) \geq \Sigma_{n-1}(x, w, x, w) \Sigma_{n-1}(x_n, w_n, x_n, w_n) + \lambda_{x_n, w_n} \lambda_{x_n, w_n} > \Sigma_{n-1}(x, w, x, w),
\]
and then $\Sigma_n(x,w,x,w) > 0$. By induction we have that $\Sigma_n(x,w,x,w) > 0$ for all $n$. Fix $n$, we then have that the GP on $f$ given $\mathcal{F}_n$ is nondegenerate, and so by Theorem 1.5.4 and Corollary 1.3.4 of Adler and Taylor (2007), we have that there exists $K$ such that
\[
E[\epsilon_n(\delta) \mid \mathcal{F}_n] \leq K \int_{\delta'}^{\delta'} H_n^{1/2}(\varepsilon) \, d\varepsilon < K\varepsilon.
\]
Furthermore, in the proof of Theorem 1.3.3 of [Adler and Taylor (2007)], it is shown that for all \( u > 1 \),

\[
P \left[ \sup_{d_n(y,x) \leq \delta'} (f(y) - \mu_n(y,w) + \mu_n(x,w) - f(x)) \geq uS \, | \mathcal{F}_n \right] \leq 2^{1-u^2}
\]

where \( S \) is a constant such that \( 0 \leq S \leq \int_0^{\delta'} H_n^{1/2} (\varepsilon) \, d\varepsilon \), and \( d_n(\cdot, \cdot) := d(\cdot, \cdot \mid \mathcal{F}_n) \). Consequently,

\[
E \left[ (\varepsilon_n(\delta))^2 \mid \mathcal{F}_n \right] = \int_0^\infty P \left[ \sup_{d_n(y,x) \leq \delta'} (f(y) - \mu_n(y,w) + \mu_n(x,w) - f(x))^2 \geq u \mid \mathcal{F}_n \right] \, du
\]

\[
= \int_0^\infty P \left[ \sup_{d_n(y,x) \leq \delta'} (f(y) - \mu_n(y,w) + \mu_n(x,w) - f(x)) \geq \sqrt{u} \mid \mathcal{F}_n \right] \, du
\]

\[
= 2S^2 \int_0^\infty P \left[ \sup_{d_n(y,x) \leq \delta'} (f(y) - \mu_n(y,w) + \mu_n(x,w) - f(x)) \geq tS \mid \mathcal{F}_n \right] \, dt
\]

\[
\leq 2S^2 + 2S^2 \int_1^\infty 2^{1-u^2} \, du
\]

\[
= S^2 \left[ 2 + 2 \int_1^\infty 2^{1-u^2} \, du \right]
\]

\[
\leq \left( \int_0^{\delta'} H_n^{1/2} (\varepsilon) \, d\varepsilon \right)^2 \left[ 2 + 2 \int_1^\infty 2^{1-u^2} \, du \right]
\]

\[
\leq \varepsilon^2 K'
\]

where \( K' := 2 + 2 \int_1^\infty 2^{1-u^2} \, du \geq 0 \). In particular, \( \varepsilon^2(\delta) \) is in \( L^1 \), and so we must have that \( E[\varepsilon^2(\delta) \mid \mathcal{F}_n] \rightarrow E[\varepsilon^2(\delta) \mid \mathcal{F}_\infty] \), and \( E \left[ \sup_{|y-x| < \delta} |f(y) - f(x)| \mid \mathcal{F}_n \right] \rightarrow E \left[ \sup_{|y-x| < \delta} |f(y) - f(x)| \mid \mathcal{F}_\infty \right] \) a.s.

Note that,

\[
\varepsilon(\delta) \leq \varepsilon'(\delta) + \sup_{|y-x| < \delta} |\mu_n(x,w) - \mu_n(y,w)|
\]

where \( \varepsilon'(\delta) = \sup_{d(x,y) < \delta} |f(x) - \mu_n(x,w) - f(y) + \mu_n(y,w)| \). Consequently,

\[
E[\varepsilon^2(\delta) \mid \mathcal{F}_n] \leq E[\varepsilon_n^2(\delta) \mid \mathcal{F}_n] + \left( \sup_{|y-x| < \delta} (\mu_n(y,w) - \mu_n(x,w)) \right)^2
\]

\[
+ 2E[\varepsilon_n(\delta) \mid \mathcal{F}_n] \left( \sup_{|y-x| < \delta} (\mu_n(y,w) - \mu_n(x,w)) \right)
\]

\[
\leq \varepsilon^2 K' + \left( E \left[ \sup_{|y-x| < \delta} (f(y) - f(x)) \mid \mathcal{F}_n \right] \right)^2 + 2K\varepsilon E \left[ \sup_{|y-x| < \delta} (f(y) - f(x)) \mid \mathcal{F}_n \right]
\]

and so

\[
E[\varepsilon^2(\delta) \mid \mathcal{F}_\infty] \leq \varepsilon^2 K' + \left( E \left[ \sup_{|y-x| < \delta} (f(y) - f(x)) \mid \mathcal{F}_\infty \right] \right)^2 + 2K\varepsilon E \left[ \sup_{|y-x| < \delta} (f(y) - f(x)) \mid \mathcal{F}_\infty \right]
\]

a.s. Similarly,

\[
E[\varepsilon(\delta) \mid \mathcal{F}_\infty] \leq K\varepsilon + E \left[ \sup_{|y-x| < \delta} (f(y) - f(x)) \mid \mathcal{F}_\infty \right] \) a.s.
\]

We will prove that \( \sup_{|y-x| < \delta} |\mu_\infty(x,w) - \mu_\infty(y,w)| < \infty \) a.s. Suppose that \( \sup_{|y-x| < \delta} |\mu_\infty(x,w) - \mu_\infty(y,w)| = \infty \) in a set \( B \subset \Omega \) such that \( P[B] > 0 \). We then have that

\[
\infty = E \left[ \sup_{|y-x| < \delta} |\mu_\infty(x,w) - \mu_\infty(y,w)| \right]
\]

\[
= E \left[ \sup_{|y-x| < \delta} E[f(y) - f(x) \mid \mathcal{F}_\infty] \right]
\]

\[
\leq E \left[ E \left[ \sup_{|y-x| < \delta} f(y) - f(x) \mid \mathcal{F}_\infty \right] \right]
\]

\[
= E \left[ \sup_{|y-x| < \delta} f(y) - f(x) \right].
\]
However, \( E \left[ \sup_{|y-x|<\delta} f(y) - f(x) \right] < \infty \), which is a contradiction. Consequently, the event
\[
\sup_{|y-x|<\delta} |\mu(x,w) - \mu_{\infty}(x,w)| < \infty
\]
occur a.s. Similarly, \( E \left[ \sup_{|y-x|<\delta} (f(y) - f(x)) \right| \mathcal{F}_w < \infty \) a.s.

By using a similar argument than the previous one and the fact that \( F \) is bounded a.s., we can then see that \( \sup_{x \in A} |\mu(x,w)| < \infty \) a.s.

Now observe that if \( E \left[ \sup_{|y-x|<\delta} (f(y) - f(x)) \right| \mathcal{F}_w < \infty \), we then have that
\[
0 \leq E \left[ \lim_{\delta \to 0^+} \sup_{|y-x|<\delta} E [(f(y) - f(x)) \mid \mathcal{F}_w] \right] = \lim_{\delta \to 0^+} E \left[ \sup_{|y-x|<\delta} E [(f(y) - f(x)) \mid \mathcal{F}_w] \right] \text{ by the dominated convergence theorem,}
\leq \lim_{\delta \to 0^+} E \left[ \sup_{|y-x|<\delta} (f(y) - f(x)) \right]
\leq \lim_{\delta \to 0^+} K \int_0^{\delta'} H^{1/2}(r) \, dr = 0
\]
and thus \( \lim_{\delta \to 0^+} E \left[ \sup_{|y-x|<\delta} (f(y) - f(x)) \right| \mathcal{F}_w = 0 \) a.s.

Observe that there exists a sequence i.i.d. standard normal random variables \( \{\varepsilon_k\}_k \) such that we observe \( F(x_i, w_i) + \sqrt{\lambda(x_i, w_i)} \varepsilon_i \) the \( i \)-th time that \( F \) is queried. By the strong law of large numbers, there exists a measurable set \( F_1 \) of probability one, such that \( \frac{1}{n} \sum_{j=1}^n \varepsilon_j \) converges to the zero random variable.

Fix a \( \omega \in F \cap F_1 \), and take \( \delta_0 < \delta \) such that
\[
E \left[ \sup_{|y-x|<\delta} (f(y) - f(x)) \right| \mathcal{F}_w < \varepsilon / \max (\sup_{x \in A} |\mu(x,w)| + L, 1),
\]
and \( \int_0^{\delta'} H^{1/2}(r) \, dr < \varepsilon / \max (\sup_{x \in A} |\mu_{\infty}(x,w)| + L, 1) \) where \( \delta' = \sup_{|y-x|<\delta_0} d(x,y) \) and \( L \) is an upper bound of \( |f| \) (e.g. \( L \geq |f(x)| \) for all \( x \in A \)).

Suppose that the policy \( \pi \) measures an infinite number of alternatives in \( B_{\delta_0}(x) \times w \). Consider the collection \( C = \{y_n\}_{i \geq 1} \) where \( y_n = f(x_n) + \lambda(x_n, w) \varepsilon_n \) and \( x_n \in B_{\delta_0}(x) \). We know that \( \frac{1}{m} \sum_{j=1}^m \varepsilon_n \) converges to zero. Furthermore, \( \lambda(x, w) \) is bounded for all \( x, w \), and so \( \frac{1}{m} \sum_{j=1}^m \lambda(x_n, w) \varepsilon_n \) is bounded for \( m \) large, and converges to zero. Thus for \( m \) large
\[
\left| \frac{1}{m} \sum_{i=1}^m y_n \right| \leq \frac{1}{m} \sum_{i=1}^m |f(x_n)| + \frac{1}{m} \sum_{i=1}^m \sqrt{\lambda(x_n, w)} \varepsilon_i
\leq L + \frac{1}{m} \sum_{i=1}^m \sqrt{\lambda(x_n, w)} \varepsilon_i
\]
where \( L \geq |f(x_n)| \) (\( f \) is bounded because \( \omega \in F \cap F_1 \), and thus \( \frac{1}{m} \sum_{i=1}^m y_n \) is bounded for \( m \) large, and then there exists a convergent subsequence of \( \{ \frac{1}{m} \sum_{i=1}^m y_n \} \). Denote this convergent subsequence by \( y_n \), and its limit by \( Z_{\delta_0} \). Observe that,
\[
z_m - \varepsilon(\delta_0) \leq f(x) + \frac{1}{m} \sum_{i=1}^m \sqrt{\lambda(x_n, w)} \varepsilon_i \leq z_m + \varepsilon(\delta_0)
\]
and thus
\[
Z_{\delta_0} - \varepsilon(\delta_0) \leq f(x) \leq Z_{\delta_0} + \varepsilon(\delta_0).
\]
Now, by Lemma 5 (remember that $\omega \in F \cap F_1$), we have that
\[
\Sigma_\infty (x, w; x, w) = E \left[ (f(x) - \mu_\infty (x, w))^2 \mid \mathcal{F}_\infty \right] 
\leq E \left[ e^2 (\delta_0) + |Z_{\delta_0}|^2 + 2e (\delta_0) |Z_{\delta_0}| \mid \mathcal{F}_\infty \right] - \mu_\infty^2 (x, w) 
\leq E \left[ e^2 (\delta_0) \mid \mathcal{F}_\infty \right] + 2E [e (\delta_0) \mid \mathcal{F}_\infty] L + E [e (\delta_0) \mid \mathcal{F}_\infty] (L + |\mu_\infty (x, w)|) 
\leq \hat{e} := e^2 K' + e^2 + 2K e^2 + 2(K e + e) + (K e + e)
\]

Since $Q$ and $W$ are finite, $|\Sigma_{w'} p(w') [\Sigma_\infty (z, w', x, w)]| < \hat{e}_2 := |W| \sup_w p(w) \sqrt{\hat{e}} \sup_{x, w} \sqrt{\Sigma_\infty (x, w, x, w)}$ for all $z \in Q$.

Now observe that,
\[
\left| R_Q^{-1} (S^\infty; x, w) - V_Q^N (S^\infty) \right| = E \left[ \max_{z \in Q} [a_{\infty + 1} (z) \mid \mathcal{F}_\infty] - V_Q^N (S^\infty) \right] 
\leq E \left[ \max_{z \in Q} \left[ \frac{\sum_{w'} p(w') [\Sigma_\infty (z, w', x, w)]}{\sqrt{\Sigma_\infty (x, w, x, w) + \lambda_{x, w}}} \right] \mid \mathcal{F}_\infty \right] 
\leq \sqrt{2/\pi} \frac{1}{\sqrt{k_\lambda}} \hat{e}_2
\]

where $Z \sim N (0, 1)$. This ends the proof. $\Box$

**Lemma 18.** Suppose that $|W| < \infty$. Let $Q$ be a finite set of $A$. If $R_Q^{-1} (S^\infty; x, w) = V_Q^N (S^\infty)$ for all $(x, w)$ a.s., then $V_Q^N (S^\infty) = U_Q (S^\infty)$ a.s.

**Proof.** It is essentially the same proof than the proof of Lemma 9. $\Box$

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