Efficient computation of the Knowledge Gradient for Bayesian Optimization

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Abstract

Bayesian optimization is a powerful collection of methods for optimizing stochastic expensive black box functions. One key component of a Bayesian optimization algorithm is the acquisition function that determines which solution should be evaluated in every iteration. A popular and very effective choice is the Knowledge Gradient acquisition function, however there is no analytical way to compute it. Several different implementations make different approximations. In this paper, we review and compare the spectrum of Knowledge Gradient implementations and propose One-shot Hybrid KG, a new approach that combines several of the previously proposed ideas and is cheap to compute as well as powerful and efficient. We prove the new method preserves theoretical properties of previous methods and empirically show the drastically reduced computational overhead with equal or improved performance. All experiments are implemented in BOTorch and code is available on github.

1 Introduction

The problem of optimizing an expensive, stochastic, black box function appears in many domains, such as in simulation-based optimization \cite{1}, in machine learning hyperparameter tuning \cite{19}, or in engineering optimization \cite{24}. In such problems, the mapping between decision variables and outputs is not a simple mathematical expression but rather a complex computer simulation, a wet lab biological experiment or machine learning training pipeline, from the perspective of an optimization algorithm, they are black boxes. Formally, given a point in a low dimensional continuous space (typically $D \leq 10$), $x \in X \subset \mathbb{R}^D$, we aim to find the point with the highest expected output

$$x^* = \arg \max_{x \in X} \mathbb{E}[f(x)]$$

where $f : X \rightarrow \mathbb{R}$ is a stochastic black box function and the expectation is over the stochasticity in repeated calls to $f(x)$, e.g. multiple simulation runs with a different random number seed.

For such problems, Bayesian optimization (BO) methods have become a powerful and widely studied toolbox for finding the optimum using as few expensive black box evaluations as possible. BO methods consist of two main components, a Gaussian Process surrogate model, and an acquisition function. The surrogate model is trained to predict $f(x)$, outputting both a prediction and an uncertainty/confidence. The acquisition function, $\alpha(x)$, quantifies the exploration, exploitation trade-off for evaluating the black box at a new point $x$, and the new point with the highest acquisition value is then passed to the black box for evaluation.

There exist many acquisition functions, the arguably most commonly used method is Expected Improvement (EI) \cite{8} that measures the expected amount that a new output $y = f(x)$ improves over the current
best sampled output. [srinivas2010] proposes to optimize an optimistic upper-confidence bound (UCB) acquisition function where the benefit of a point $x$ is quantified using a quantile of the distribution $f(x)$. EI and UCB are quick any easy to implement because there is an analytical solution. Thompson sampling (TS) [20] corresponds to using the GP to sample a set of predicted objective function values at a finite set of locations, the point with largest sample realization is chosen for evaluation, one may think of the sampled function as a randomly generated acquisition function to be maximized. This acquisition function is simple to implement though scales cubically with discretization size and more involved tricks are required otherwise. In contrast with EI and UCB, there exist many acquisition functions with more sophisticated theoretical motivation that also comes with much greater implementation difficulty. entropy Search (ES) [6] considers an information-based acquisition function where a GP over outputs generates a distribution over the input domain that models the probability of any input being the maximizer. This acquisition criterion involves computing the expected entropy reduction of the global solution and may be used for noisy observations. Computing the distribution over the input domain and its entropy and the same distribution and entropy for each possible future outcome, an average of one step look ahead entropies, introduces extensive mathematical and implementation problems to be tackled. Predictive Entropy Search [7] proposed a quicker implementation however with more sophisticated approximations. Max Value entropy search [21] methods aim to reduce entropy of the predictive distribution of the output value and cheaper methods have been proposed.

Knowledge Gradient (KG) [5] is derived from Bayesian Decision theory and samples locations that provide the greatest increase in the peak of the GP posterior mean. However, as with entropy methods, numerical approximations are required and several implementations using different approximations have been proposed in the literature varying in their complexity, accuracy and computational cost, we provide a detailed review of these methods in Section 3. Some are simple to implement and find optimal points in simple convenient cases while struggling in more challenging problems. Other KG implementations are more involved to implement (open source versions are recommended) and also perform very well across a broad range of use cases but incur a larger computational overhead.

With this work, we aim to take steps towards an algorithm that has both well founded theoretical motivation (like KG and entropy methods) while also being easy to implement and cheap to compute (like EI and UCB methods). We in particular focus on KG methods. In this manuscript, we give a detailed review of the major technical milestones in the development of KG implementations and then merge these enhancements to provide an implementation of KG that is simple and cheap to compute, yet also practical and performing well across a broad range of problems.

We hope this can make KG a far more accessible Bayesian Optimization acquisition function for the average user and newcomers to the field, and due to its computational efficiency also broaden the scope of problems for which KG is a preferred choice.

In Sections 2 and 3 we provide the mathematical background on BO and the major milestones of KG implementation. In Section 4 we describe a natural novel implementation, One-Shot-Hybrid KG, and discuss it’s complexity, theoretical properties and practical implementation. In Section 5 we present numerical ablation studies across the methods comparing time and opportunity cost and finally conclude in Section 6.

2 Bayesian Optimization

Bayesian optimization sequentially collects data from the black box function and builds a surrogate model, most often a Gaussian process (GP) model. Let the $n$ collected inputs be denoted $X^n = (x_1, x_2, \ldots, x_n) \subset X$ with outputs $Y^n \in \mathbb{R}^n$ and $D^n$ the dataset of pairs. A Gaussian process is specified by prior mean, $\mu^0(x)$ that is typically constant $\mu^0(x) = \text{mean}(Y^n)$, and prior kernel $k(x, x') \in \mathbb{R}$ that gives the covariance (expected similarity) between the output values at $x$ and $x'$. Common choices of kernel are the Squared Exponential
Gradient (KG) quantifies the value of a new hypothetical observation in Section 4. We aim to create a simple, easy to use Knowledge Gradient implementation. In the following, we provide a blackbox objective.

\[
r_i^2 = \sum_{i=1}^{D} \frac{(x_i - x'_i)^2}{\ell_i^2},
\]

\[
k_{RBF}(x, x'; \sigma_0, l) = \sigma_0 \exp \left( -\frac{r_i^2}{2} \right)
\]

\[
k_{Mat}(x, x'; \sigma_0, l) = \sigma_0 \left( 1 + \sqrt{5r_i} + 5r_i^2 / 3 \right) \exp \left( -\sqrt{5r_i} \right)
\]

where the \( \theta = \{\sigma_0, l_1, ..., l_D\} \) are hyperparameters estimated using maximum marginal likelihood [15]. In our experiments, we adopt the squared exponential kernel. After observing \( n \) points, the posterior mean and covariance functions are given by

\[
\mu^n(x) = k(x, X^n)(k(X^n, X^n) + \sigma^2I)^{-1}Y^n,
\]

\[
k^n(x, x') = k(x, x') - k(x, X^n)(k(X^n, X^n) + \sigma^2I)^{-1}k(X^n, x').
\]

For each BO iteration, the latest data is used to build a new model, then given a new candidate \( x^{n+1} \), an acquisition function \( \alpha(x^{n+1}, \mu(\cdot), k(\cdot, \cdot)) \) quantifies the expected benefit of evaluating the black box at \( x^{n+1} \), accounting for both exploration and exploitation. The acquisition function is optimized over \( X \) to find the most beneficial next point \( x^{n+1} = \arg \max_{x^{n+1}} \alpha(x^{n+1}, \cdot) \) which is then passed to the expensive black box function \( y^{n+1} = f(x^{n+1}) \). The dataset is updated, \( \mathcal{D}^{n+1} \), and the next iteration starts, see pseudocode in Algorithm 2. In this work, we focus exclusively on the Knowledge Gradient acquisition function and its many implementations.

**Algorithm 1** The Bayesian Optimization Algorithm. An initial dataset of \( n_0 \) points is collected over the domain \( X \). Then new points are sequentially determined and evaluated for the rest of the budget \( N \). In each round, a Gaussian process regression model is fit to the current dataset and the acquisition function is optimized to find the next point to evaluate. Finally, the best predicted point is returned.

**Require**: blackbox objective \( f : X \rightarrow \mathbb{R} \), budget \( N \), initialisation budget \( n_0 \), GP kernel \( k(x, x'|\theta) \), acquisition function \( \alpha(x, \mu(\cdot), k(\cdot, \cdot)) \)

\[ X^{n_0} \leftarrow \text{LHC}(X, n_0) \]

\[ \mathcal{D}^{n_0} \leftarrow \{(x^i, f(x^i)) | x^i \in X^{n_0}\} \]

\[ \text{for } n = n_0, ..., N-1 \text{ do} \]

\[ \mu^n(\cdot), k^n(\cdot, \cdot) \leftarrow \mathcal{GP}(\mathcal{D}^n, k(\cdot, \cdot)) \]

\[ x^{n+1} \leftarrow \arg \max_{x^{n+1}} \alpha(x^{n+1}, \mu^n(\cdot), k^n(\cdot, \cdot)) \]

\[ y^{n+1} \leftarrow f(x^{n+1}) \]

\[ \mathcal{D}^{n+1} \leftarrow \mathcal{D}^n \cup \{(x^{n+1}, y^{n+1})\} \]

\[ \text{end for} \]

\[ \mu^N(\cdot), k^N(\cdot, \cdot) \leftarrow \mathcal{GP}(\mathcal{D}^N, k(\cdot, \cdot)) \]

**return** \( x^* = \arg \max_x \mu^N(x) \)

3 A Tour of Knowledge Gradient Implementations

We aim to create a simple, easy to use Knowledge Gradient implementation. In the following, we provide a mathematical review of existing methods after which we present our new method as the natural next step in Section 4.

Given a set of past observations \( \mathcal{D}^n \) and a proposed new sampling point location \( x^{n+1} \), Knowledge Gradient (KG) quantifies the value of a new hypothetical observation \( y^{n+1} = f(x^{n+1}) \) by the expected increase in the peak of the posterior mean

\[
\text{KG}(x^{n+1}) = \mathbb{E}_{y^{n+1}} \left[ \max_{x} \mu^{n+1}(x) | x^{n+1} \right] - \max_{x'' \in X} \mu^n(x'').
\]
where we suppress arguments \( \mu^n(\cdot), k^n(\cdot, \cdot) \) and \( D^n \) for brevity. Unfortunately, \( \max_{x' \in X} \mu^{n+1}(x') \) and the enclosing expectation has no explicit formula and approximations are required. We here emphasize, **accurate approximation is the central challenge in implementing Knowledge Gradient methods** and has been the focus of many prior works. These methods rely on the following “reparameterization trick”: at time \( n \), the new posterior mean is an unknown random function, however, it may be written as

\[
\mu^{n+1}(x) = \mu^n(x) + \tilde{\sigma}(x; x^{n+1}) Z
\]

(4)

where \( \tilde{\sigma} : X \times X \rightarrow \mathbb{R} \) is a deterministic scalar valued function and the scalar random variable \( Z \sim \mathcal{N}(0, 1) \) captures the posterior predictive randomness of the yet unobserved \( y^{n+1} \), see Appendix A. Hence one may also write

\[
\text{KG}(x^{n+1}) = \mathbb{E}_Z \left[ \max_{x'} \mu^n(x') + \tilde{\sigma}(x'; x^{n+1}) Z \right] - \max_{x'' \in X} \mu^n(x'').
\]

(5)

Moreover, by Jensen’s inequality and the convexity of the \( \max() \), it is easily shown that \( \text{KG}(x^{n+1}) \geq 0 \), there is never an *expected* disadvantage to collecting more data.

### 3.1 Discrete Knowledge Gradient

The early KG methods for continuous spaces, \([3, 17]\), approximated \( \text{KG}(x^{n+1}) \) by replacing the domain of the inner maximization from the continuous space \( X \) to a finite discretization of \( d \) points, \( X_d \subset X \). \( X_d \) may simply be a latin hypercube design over \( X \), or the past sampled points \( X^n \) or both. Denoting vectors \( \bar{\mu} = \mu^n(X_d) \in \mathbb{R}^d \) and \( \bar{\sigma}(x^{n+1}) = \tilde{\sigma}(X_d; x^{n+1}) \in \mathbb{R}^d \), then

\[
\text{KG}_d(x^{n+1}, X_d) = \mathbb{E}_Z \left[ \max \{ \bar{\mu} + \bar{\sigma}(x^{n+1}) Z \} \right] - \max \bar{\mu}.
\]

The \( \max \{ \bar{\mu} + \bar{\sigma}(x^{n+1}) Z \} \) is a piece-wise linear function of \( Z \), thus the expectation over Gaussian \( Z \), and therefore \( \text{KG}_d(\cdot) \), is analytically tractable, the algorithm has been proposed in \([4]\) and is provided in Appendix B for completeness. If the current best predicted point is in the discretization, \( \arg \max \mu^n(x) \in X_d \), the discrete Knowledge Gradient is a *lower bound* of the true Knowledge Gradient

\[
0 \leq \text{KG}_d(x^{n+1}, X_d) \leq \text{KG}(x^{n+1})
\]

and increasing the density of points in \( X_d \) such that \( X_d \rightarrow X \) tightens the bound. The REVI \([11]\) and the MiSo \([14]\) algorithms used \( \text{KG}_d(\cdot) \) with 3000 uniformly random distributed points. While this method provides an analytic lower bound, it suffers the curse of dimensionality. To be space filling, the number of points in \( X_d \) must grow exponentially with input dimension \( D \). Further, a totally random discretization is highly likely to contain many useless points in uneventful regions of the space \( X \) resulting in wasted computation, a sparse \( X_d \) results in a loose ineffective lower bound, see Figure 2 centre-left plot.

### 3.2 Monte-Carlo Knowledge Gradient

To avoid the curse of dimensionality, the expectation over \( Z \) in Equation 5 may be stochastically approximated by Monte-Carlo sampling \([22, 23]\). Given \( x^{n+1} \), the method samples \( n_z \) standard Gaussian values, \( Z_{MC} \in \mathbb{R}^{n_z} \). For each sample, \( Z_j \in Z_{MC} \), it constructs a corresponding posterior mean realisation, \( \mu_j^{n+1}(x) = \mu^n(x) + \tilde{\sigma}(x; x^{n+1}) Z_j \), and finds the maximum with a continuous numerical \texttt{Optimizer()} like L-BFGS \([10]\) or conjugate gradient \([18]\) with multiple restarts. We use \texttt{Optimizer()} to denote a functional taking an arbitrary function \( g : X \rightarrow \mathbb{R} \) as input and returning maxima from all \( Z_j \) as follows

\[
\text{KG}_{MC}(x^{n+1}, Z_{MC}) = \frac{1}{n_z} \sum_j \text{Optimizer}(\mu_j^{n+1}(x')) - \text{Optimizer}(\mu^n(x'')).
\]

4
Assuming \( \text{Optimizer}() \) converges, the result is an unbiased, consistent stochastic estimate of true Knowledge Gradient. Slightly abusing \( Z_{MC} \) notation, we have

\[
\mathbb{E}_{Z_{MC}|n_z}[\text{KG}_{MC}(x^{n+1}, Z_{MC})] = \text{KG}(x^{n+1}),
\]

\[
\lim_{n_z \to \infty} \text{KG}_{MC}(x^{n+1}, Z_{MC}) = \text{KG}(x^{n+1}).
\]  

(6)  

(7)

For larger input dimension \( D \), the \( \text{Optimizer}() \) over \( X \subset \mathbb{R}^D \) may simply be run for more steps (linear in \( D \)) to converge thus avoiding the curse of dimensionality. Compared with discrete KG that discretizes optimization over \( X \) and continuously integrates over (1 dimensional) \( Z \), Monte-Carlo KG instead continuously optimizes over \( X \) and discretely integrates over \( Z \) with Monte Carlo samples, see Figure 2 centre right. However, for a good estimate, \( n_z \) must be large, e.g. \( n_z = 1000 \), and many \( \text{Optimizer}() \) calls are required. Furthermore, if \( Z_j \approx Z'_j \), the optimal value may be near identical and need not be called twice. Finally to optimize \( \text{KG}_{MC}(x^{n+1}, Z_{MC}) \) over \( x^{n+1} \), a stochastic gradient ascent optimizer is required, e.g. Adam \( 9 \), and must be set up correctly to ensure convergence. A small choice of \( n_z \) or poor inner \( \text{Optimizer}() \) increases bias and variance in the KG estimate. Further, repeated calls to \( \text{KG}_{MC}() \) for different values of \( x^{n+1} \) can be expensive as all the \( Z_{MC} \) values are resampled and the \( \text{Optimizer}() \) calls must be executed from scratch.

### 3.3 Hybrid Knowledge Gradient

The Hybrid Knowledge Gradient first proposed in \( 12 \) aims to combine the best of both Discrete KG (analytic tractability, speed) and Monte-Carlo KG (scalability to higher input dimensions). Given \( x^{n+1} \), a set of \( n_z = 5 \) unique, deterministic \( Z \) values is constructed from uniformly spaced Gaussian quantiles

\[
Z_h = \{\Phi^{-1}(0.1), \Phi^{-1}(0.3), \Phi^{-1}(0.5), \Phi^{-1}(0.7), \Phi^{-1}(0.9)\} \subset \mathbb{R}
\]

where \( \Phi^{-1} : [0, 1] \to \mathbb{R} \) is the inverse Gaussian cumulative distribution function. Following Monte-Carlo KG, for each \( Z_j \in Z_h \), the posterior mean realisation is constructed, \( \mu_j^{n+1}(x) \), and optimized with \( \text{Optimizer}() \) however the resulting optimal input \( x^*_j \) is stored in a set \( X_{MC} \),

\[
X_{MC} = \{x^*_j | \mu_j^{n+1}(x^*_j) = \text{Optimizer}(\mu_j^{n+1}(x)), j = 1, \ldots, n_z \}.  
\]  

(8)

Finally, following Discrete Knowledge Gradient, the optimal inputs \( X_{MC} \) form the discretization used in Hybrid KG, i.e.,

\[
\text{KG}_h(x^{n+1}) = \text{KG}_d(x^{n+1}, X_{MC}).
\]  

(9)

Thus Hybrid Knowledge Gradient is a deterministic, analytic, maximized lower bound to the true Knowledge Gradient. Hybrid KG scales to higher dimensional inputs like Monte-Carlo KG, while reducing computation using only \( n_z = 5 \). Similar to Monte-Carlo KG, repeated calls to \( \text{KG}_h(x^{n+1}) \) for different \( x^{n+1} \) still require executing all the \( \text{Optimizer}() \) calls from scratch.

### 3.4 One-Shot Knowledge Gradient

With the goal of reducing the computation of Monte-Carlo KG, with a few changes, we next show how to derive One Shot KG \( 2 \). If we assume we are given a set of \( Z_{MC} \) each with corresponding optimal points \( X_{MC} \), each \( Z_j \in Z_{MC} \) is paired with a \( x^*_j \in X_{MC} \), the One-Shot estimate of KG is as follows,

\[
\text{KG}_{OS}(x^{n+1}, Z_{MC}, X_{MC}) = \frac{1}{n_z} \sum_j \mu_j^{n+1}(x^*_j) - \max_{x'} \mu^n(x').
\]

(10)

\( \text{KG}_{OS} \) would be a very poor under estimate if \( x^*_j \in X_{MC} \) points are random, and when the points are all optimized it recovers \( \text{KG}_{MC} \). In One-Shot KG, the random samples \( Z_{MC} \) are fixed for each BO iteration.
hence KG\textsubscript{OS} is deterministic. Next, in the search for \(x^{n+1}\), we may simultaneously search over \(X_{MC}\) hence the KG\textsubscript{OS} estimate improves over the course of the search for the next candidate point \(x^{n+1}\),

\[
x^{n+1*} = \arg\max_{x^{n+1}} \max_{X_{MC}} \text{KG\textsubscript{OS}}(x^{n+1}, X_{MC}, Z_{MC}). \tag{11}
\]

equivalently, this acquisition function may be optimized with the same deterministic optimizer

\[
\text{Optimizer}_{x^{n+1}, X_{MC}}(\text{KG\textsubscript{OS}}(x^{n+1}, X_{MC}, Z_{MC})), \tag{12}
\]

where \(Z_{MC}\) are frozen constant values and all the \(x\) points are optimized over the same domain \(X\), the final optimal \(x^{n+1*}\) is used as the next sample (the final optimized \(X_{MC}\) is no longer explicitly required). In Monte-Carlo KG and Hybrid KG, one optimizer searches for \(x^{n+1}\), and at each candidate \(x^{n+1}\), nested optimizers are applied to find \(X_{MC}\), even if subsequent \(x^{n+1}\) are very close and optimization of \(X_{MC}\) may be largely repeated. One-Shot KG optimizes both \(x^{n+1}\) and \(X_{MC}\) at the same time in a single optimizer, significantly reducing computational effort to find \(X_{MC}\). However, freezing \(Z_{MC}\) and not ensuring \(X_{MC}\) is fully converged introduces bias.

### 4 One Shot Hybrid Knowledge Gradient

In this work we propose a simple unification of the aforementioned innovations. We take discrete KG and and make the discretization an explicit variable to be optimized along with the next sample point, that is

\[
x^{n+1*} = \arg\max_{x^{n+1}} \max_{X_d} \text{KG\textsubscript{OSH}}(x^{n+1}, X_d) \tag{13}
\]
Figure 2: Methods for computing $\text{KG}(x^{n+1})$ at $x^{n+1} = \bar{x}$. Left: $\mu^n(x)$ and samples of $\mu^n(x^{n+1})$ determined by a scalar $Z \sim N(0,1)$. Centre-left: $\text{KG}_M$ replaces $X$ with up to 3000 points $x_i \in X_d$ and $\mu^n(x^{n+1}(x))$ is linear in $Z$. Centre-right: $\text{KG}_{MC}$ samples up to 1000 functions $\mu^n(x^{n+1}(x))$ functions and maximizes each of them numerically. Right: $\text{KG}_h$ samples up to 5 functions $\mu^n(x^{n+1}(x))$ and maximizes them numerically, the arg max points $x_1^*, ..., x_5^*$ are used as $X_d$ in $\text{KG}_d$.

where $\text{KG}_{OSH}(\cdot) = \text{KG}_d(\cdot)$ but we use separate notation for clarity here. The optimization is performed over the joint domain $(x^{n+1}, X_d) \in X^{n+1+n_d}$. Note that neither $Z_h$ or $Z_{MC}$ are required. This method may be viewed as Discrete KG and One-Shot KG where both tricks have been applied simultaneously, the hybrid trick: enabling $n_z = |X_d| = 5$ and a tight lower bound estimate of true KG, and the one-shot trick: simultaneous optimization drastically reducing execution time. As discrete KG is analytically tractable, the gradients with respect to both arguments are also analytically tractable and hence may be optimized with any deterministic gradient ascent algorithm.

For a given discretization size, the One-Shot Hybrid KG has almost exactly the same computational cost as discrete KG. Both methods compute $\text{KG}_d(\cdot)$ and $\nabla_{x^{n+1}} \text{KG}_d(\cdot)$ for gradient ascent over $x^{n+1}$. However, One-Shot Hybrid KG also computes $\nabla_{X_d} \text{KG}_d(\cdot)$ for gradient ascent over $X_d$. In practice we use PyTorch that supports automatic differentiation via the back-propagation algorithm and GPU acceleration.

### 4.1 Theoretical Properties

As Hybrid One-Shot KG is simply an extension of Discrete KG, it inherits the theoretical properties of Discrete KG in continuous spaces previously proven in [16]. The algorithm converges in the limit of infinite budget, with infinitely many BO iterations and calls to the expensive black box, the true optimal input will be found. We only require that $\text{KG}_d(x^{n+1}, X_d) \geq 0$ for all $x^{n+1} \in X$, which is trivially satisfied by enforcing that $x^*_n = \arg \max \mu^n(x)$ is included in the set $X_{MC}$ and thus

$$
\max_{X_d} \text{KG}_d(x^{n+1}, X_d) = \max_{X_d} \mathbb{E}_Z \left[ \max_{X_d \cup \{x_n^*\}} \mu^n(x) + Z \tilde{\sigma}(x^{n+1}, X_d \cup \{x_n^*\}) \right] - \max \mu^n(x) \quad (14)
$$

$$
\geq \mathbb{E}_Z \left[ \mu^n(x_n^*) + Z \tilde{\sigma}(x^{n+1}, x_n^*) \right] - \max \mu^n(x) \quad (15)
$$

$$
= \mu^n(x_n^*) + \mathbb{E}[Z|\tilde{\sigma}(x^{n+1}, x_n^*) - \max \mu^n(x) \quad (16)
$$

$$
= 0. \quad (17)
$$

The equality holds when $k^n(x^{n+1}, x) = c$ (typically $c = 0$), and there is no benefit in sampling $x^{n+1}$, if this equality holds for all $x^{n+1} \in X$, it can be shown that the true optimal input is known. Further details can be found in [14], [13].

Also inherited from Discrete KG is the consistency of the One Shot Hybrid KG estimator as the discretization size increases to infinity, increasing discretization size increases accuracy of the KG estimate. Let $X_d^k = \{x_i | x_i \sim U(X), i = 1, ..., d\}$ be the uniformly randomly generated discretization over $X$ with $d$ points, then we have that

$$
\lim_{d \to \infty} \text{KG}_{OSH}(x^{n+1}, X_d) = \lim_{d \to \infty} \text{KG}_d(x^{n+1}, X_d) = \text{KG}(x^{n+1}). \quad (18)
$$

While the result may be clear, the practical implication of this is two fold. Firstly, $d$ is an algorithm hyperparameter. One may choose to increase $d$ and improve the accuracy (and cost) of each $\text{KG}_{OSH}(\cdot)$. 


Figure 3: Illustration of the One-Shot Hybrid KG acquisition function optimization. (a) shows an initial sample $x^{n+1}$ (red) and set $X_{MC}$ over a black-box function landscape, with brighter colors indicating higher function values. (d) shows the surface of the maximum posterior over the set $X_{MC}$ for $Z$. The One-Shot Hybrid KG aims to maximize the expectation of the piece-wise linear function (red). (b) shows the resulting $x^{n+1}$ and $X_{MC}$ after applying Optimizer() to Discrete KG where both, $x^{n+1}$ and $X_{MC}$ are optimized at the same time in the optimizer. (c) shows the final $x^{n+1}$ and $X_{MC}$ achieved by the optimizer with an optimized epigraph (f).
call or alternatively, one may run Optimizer() for more iterations so that even for small \( d \) the sparse \( X_d \) converges towards an optimum. In contrast, for one-shot KG where the first call to KGOS() with random \( X_{MC} \) is a poor estimate of true KG regardless of \( n_z \), increasing the hyperparameter will not increase KG estimate accuracy, the algorithm requires Optimizer() to be run for multiple iterations for the KG estimate to become more accurate. Hence One Shot hybrid KG may be somewhat less sensitive to hyperparameter settings. In our experiments, we run the methods for a range of hyper parameter settings comparing final performance however creating a strictly controlled experiment for comparison is a non trivial task which we leave to future work.

5 Numerical Experiments

In this section we compare all KG implementations under the following acquisition function parameters:

- Discrete Knowledge Gradient (DISC): We test this approach under 3, 10, and 1000 quasi-random uniformly distributed points.
- Monte-Carlo Knowledge Gradient (MC): We generate \( n_z = 3 \) and 10 quasi-random standard Gaussian values.
- Hybrid Knowledge Gradient (HYBRID): We generate \( n_z = 3 \) and 10 uniformly spaced Gaussian quantiles.
- One-Shot Knowledge Gradient (ONESHOT): We generate \( n_z = 3, 10, 128, \) and 500 quasi-random standard Gaussian values.
- One-Shot Hybrid Knowledge Gradient (ONESHOT-HYBRID): We optimize over a discretization size of 3 and 10.

For each method that depends on quasi-random samples, we fix the samples at each BO iteration. The resulting acquisition function is an entirely deterministic optimization problem and may be optimized using a deterministic optimizer. For One-Shot Knowledge Gradient, we used implementations available in BOTorch [2]. The remaining algorithms have been implemented from scratch.

5.1 GP-Generated Experiments

We consider a 100 test functions generated from a Gaussian process with a squared exponential kernel and hyper-parameters \( l_X = 0.1, \sigma^2 = 1 \). All functions are generated on a continuous space \( X = [0, 1]^D \) with dimensionality \( D = \{2, 6\} \), and without observation noise. The total budget of evaluations is set to \( B = 100 \) and the results over the 100 test functions are aggregated to obtain confidence intervals (CI). To obtain the wall clock time, we measure the acquisition function evaluation time of each generated test function immediately after the initial design is evaluated.

We initially train the Gaussian process model to a set of \( 2(D + 1) \) initial black-box evaluations from the overall budget using a Latin hypercube (LHS) ‘space-filling’ experimental design. Furthermore, we assume that the hyper-parameters are known throughout the whole run of the algorithm to avoid the issue of model mismatch.

Fig. 4 shows the Opportunity cost (OC) once the budget, \( B \), is depleted and the evaluation time in logarithmic scale. In both figures, DISC presents a performance close to random sampling when sparse discretizations are employed. Compared to other methods, a moderately high discretization size (1000) must be used to obtain competitive results. Notably, MC avoids the curse of dimensionality and drastically reduces the discretization size required compared to DISC. However, a small discretization size (\( n_z = 3 \)) produces high variance estimates of KG which reduces its performance. Furthermore, optimizing the discretization requires solving \( n_z \) sequential inner optimization problems at each acquisition function call which drastically increases the wall-clock time.
The HYBRID approximation improves over MC by generating a low variance approximation of KG which results in a superior performance when a low discretization is considered. However, HYBRID shows a similar evaluation time given by solving all inner optimization problems sequentially. On the other hand, ONESHOT avoids this problem by jointly optimizing the discretization space and the new solution. This results in a considerable decrease of the acquisition evaluation time, however, similar to DISC, ONESHOT relies on a moderately high discretization size to achieve competitive results. Lastly, the newly proposed ONESHOT-HYBRID achieves a computational time comparable with DISC with competitive performance for low a higher discretization sizes.

6 Conclusion

In this paper we considered the problem of implementing a fast and accurate approximation of KG. We proposed One-Shot Hybrid Knowledge Gradient, a fast method to compute KG that scales to higher dimensions. We empirically demonstrate the effectiveness of the proposed approach where One-Shot Hybrid Knowledge Gradient is both fast to compute and preserves its performance even under low discretization sizes in higher dimensions.

As future work, we also plan to extend the algorithm to be able to handle constraints, and for batch acquisition, i.e., where several solutions are to be selected in every iteration.

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A One Step Look-Ahead Posterior Mean Derivation

At iteration $n$ during optimization, let the training inputs be $X^n = (x^1, ..., x^n)$ and the training outputs $Y^n = (y^1, ..., y^n)$. Given a prior mean and kernels functions, $\mu^0(x) : X \rightarrow \mathbb{R}$ and $k^0(x, x') : X \times X \rightarrow \mathbb{R}$. Finally let the new sample point be $x^{n+1}$. Updating the mean function with data from the $0^{th}$ step to $n^{th}$ step is given by

$$
\mu^n(x) = \mu^0(x) + k^0(x, X^n) K^{-1} \left( Y^n - \mu^0(X^n) \right)
$$

where $K = k^0(X^n, X^n) + \sigma^2 I$.

A simple change of indices from $0 \rightarrow n$ and $n \rightarrow n + 1$, yields the one-step updated posterior mean

$$
\mu^{n+1}(x) = \mu^n(x) + \frac{k^n(x, x^{n+1})}{k^n(x^{n+1}, x^{n+1}) + \sigma^2} \left( y^{n+1} - \mu^n(x^{n+1}) \right).
$$

which contains the random $y^{n+1}$ which has a predictive distribution

$$
P[y^{n+1}|x^{n+1}, X^n, Y^n] = N(\mu^n(x^{n+1}), k^n(x^{n+1}, x^{n+1}) + \sigma^2).
$$

hence we may take factorise the one-step look head posterior mean expression as follows

$$
\mu^{n+1}(s, x) = \mu^n(s, x) + k^n(x, x^{n+1}) \frac{1}{\sqrt{k^n(x^{n+1}, x^{n+1}) + \sigma^2}} \frac{y^{n+1} - \mu^n(x^{n+1})}{\sqrt{k^n(x^{n+1}, x^{n+1}) + \sigma^2}}
$$

where the left factor is a deterministic and the right factor is the (at time $n$) stochastic Z-score of the new $y^{n+1}$ value. One may simply sample $Z \sim N(0, 1)$ values and compute Equation 23 to generate posterior mean functions.

B Discrete KG Algorithm
Algorithm 2 Knowledge Gradient by discretization. This algorithm takes as input a set of linear functions parameterised by a vector of intercepts $\mu$ and a vector of gradients $\sigma$. It then computes the intersections of the piece-wise linear epigraph (ceiling) of the functions and the expectation of the output of the function given Gaussian input. Vector indices are assumed to start from 0.

Require: $\mu, \sigma \in \mathbb{R}^n$

$O \leftarrow \text{order}(\sigma)$  \hspace{1cm} $\triangleright$ get sorting indices of increasing $\sigma$

$\mu \leftarrow \mu[O], \sigma \leftarrow \sigma[O]$  \hspace{1cm} $\triangleright$ arrange elements

$I \leftarrow [0, 1]$  \hspace{1cm} $\triangleright$ indices of elements in the epigraph

$\tilde{Z} \leftarrow [-\infty, \frac{\mu_0 - \mu_i}{\sigma_i - \sigma_j}]$  \hspace{1cm} $\triangleright$ z-scores of intersections on the epigraph

for $i = 2 \text{ to } n_z - 1$ do

($\star$)

$j \leftarrow \text{last}(I)$

$z \leftarrow \frac{\mu_i - \mu_j}{\sigma_j - \sigma_i}$

if $z < \text{last}(\tilde{Z})$ then

Delete last element of $I$ and of $\tilde{Z}$

Return to ($\star$)

end if

Add $i$ to end of $I$ and $z$ to $\tilde{Z}$

end for

$\tilde{Z} \leftarrow [\tilde{Z}, \infty]$  \hspace{1cm} $\triangleright$ assuming python indexing

$A \leftarrow \phi(\tilde{Z}[1:]) - \phi(\tilde{Z}[:1])$

$B \leftarrow \Phi(\tilde{Z}[1:]) - \Phi(\tilde{Z}[:1])$

$\text{KG} \leftarrow B^T \mu[I] - A^T \sigma[I] - \max \mu$  \hspace{1cm} $\triangleright$ compute expectation

return $\text{KG}$