Analogical-based Bayesian Optimization

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Abstract

Some real-world problems revolve to solve the optimization problem \( \max_{x \in X} f(x) \) where \( f(\cdot) \) is a black-box function and \( X \) might be the set of non-vectorial objects (e.g., distributions) where we can only define a symmetric and non-negative similarity score on it. This setting requires a novel view for the standard framework of Bayesian Optimization that generalizes the core insightful spirit of this framework. With this spirit, in this paper, we propose Analogical-based Bayesian Optimization that can maximize black-box function over a domain where only a similarity score can be defined. Our pathway is as follows: we first base on the geometric view of Gaussian Processes (GP) to define the concept of influence level that allows us to analytically represent predictive means and variances of GP posteriors and base on that view to enable replacing kernel similarity by a more genetic similarity score. Furthermore, we also propose two strategies to find a batch of query points that can efficiently handle high dimensional data.

Keywords: Bayesian Optimization, Analogical-based Bayesian Optimization.

1. Introduction

Bayesian optimization (BO) has emerged as a powerful solution for these varied design problems (Shahriari et al., 2016). BO has been widely applied to a mixed variety of real-world problems from interactive user interfaces (Brochu et al., 2010), robotics (Lizotte et al., 2007; Martinez-Cantin et al., 2007), environmental monitoring (Román and Fabio, 2012), information extraction (Wang et al., 2014), combinatorial optimization (Hutter et al., 2011; Wang et al., 2014), automatic machine learning (Bergstra et al., 2011; Hoffman et al., 2014; Snoek et al., 2012; Swersky et al., 2013), sensor networks (Srinivas et al., 2010), adaptive Monte Carlo (MC) (Mahendran et al., 2012), experimental design (Azimi et al., 2012), and reinforcement learning (Brochu et al., 2010b) to name a few.

Fundamentally, BO is a sequential model approach to solve the optimization \( \max_{x} f(x) \) with regard to a black-box function \( f(\cdot) \), wherein one is capable of querying the value of \( f(x) \) for any given \( x \). We initially place prior belief on the function \( f(\cdot) \) which could be a GP. Subsequently, this belief is updated using queried data points and their labels. To decide which point should be queried next, we recruit the acquisition which is closely related to the updated belief. A good acquisition function must balance the exploitation and exploration to guarantee suggesting points with high values in low density area.

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In this paper, we propose Analогical-based Bayesian Optimization that can optimize the black-box function \( f(x) \) on a domain \( \mathcal{X} \) where we can endow a non-negative and symmetric similarity score function \( S(\cdot, \cdot) \). Our pathway is as follows: we first base on the geometric view of Gaussian Processes (GP) to define the concept of influence level that allows us to analytically represent predictive means and variances of GP posteriors and base on that view to enable replacing kernel similarity by a more genetic similarity score. Furthermore, we also propose two strategies to find a batch of query points that can efficiently handle high dimensional data.

2. GP-based Bayesian Optimization

In this section, we present GP-based Bayesian Optimization. The objective is to minimize a black-box function: \( \max_{x \in \mathcal{X}} f(x) \) where the feasible set \( \mathcal{X} \subset \mathbb{R}^d \). At first, we have not any collected data, we hence assume that \( f \) is a random function drawn from a Gaussian Process \( \mathcal{GP}(0, K(\cdot, \cdot)) \) (i.e., \( f \sim \mathcal{GP}(0, K(\cdot, \cdot)) \)), where \( f: \mathcal{X} \rightarrow \mathbb{R} \) is the zero function (i.e., \( f(x) = 0, \forall x \in \mathcal{X} \)), \( K: \mathcal{X} \times \mathcal{X} \rightarrow \mathbb{R} \) is a p.s.d kernel. Later at time \( t \), assuming that we have collected the argument-and-value set \( \mathcal{D}_t = \{(x_1, y_1), \ldots, (x_{t-1}, y_{t-1})\} \) wherein each \( y_i = f(x_i) + \epsilon_i \) with \( \epsilon_i \sim \mathcal{N}(0, \sigma^2) \), we are in need of specifying the next point \( x_t \) to query.

Given the set \( \mathcal{D}_t \), the posterior \( f^{(t)} = f \mid \mathcal{D}_t \) is the \( \mathcal{GP}(\mu^{(t)}(x), K^{(t)}(\cdot, \cdot)) \) where \( \mu^{(t)} : \mathcal{X} \setminus \mathcal{D}_t \rightarrow \mathbb{R} \) and \( K^{(t)} : (\mathcal{X} \setminus \mathcal{D}_t) \times (\mathcal{X} \setminus \mathcal{D}_t) \rightarrow \mathbb{R} \) whose formulations are

\[
\mu^{(t)}(x) = K^{(t)}_x \left[ K^{(t)}_\sigma \right]^{-1} y^{(t)} = K^{(t)} \left( x, x' \right) - K^{(t)}_x \left[ K^{(t)}_\sigma \right]^{-1} \left( K^{(t)}_{x'} \right)^T \\
K^{(t)}_x = K^{(t)} \left[ K \left( x_i, x_j \right) \right]_{i,j=1}^{t-1}, K^{(t)}_\sigma = K^{(t)} + \sigma^2 I, \text{ and } y^{(t)} = \left[ y_i \right]_{i=1}^{t-1}.
\]

Therefore, given any \( x \in \mathcal{X} \setminus \mathcal{D}_t \), \( f^{(t)}(x) \) is a Gaussian random variable with the mean and the standard deviation as \( \mu^{(t)}(x) \) and \( \sigma^{(t)}(x) = V^{(t)}(x)^{1/2} = K^{(t)}(x, x)^{1/2} \), respectively. The principle to choose the next query point \( x_t \) is to balance the exploitation against the exploration. The exploitation level of the point \( x \) is expressed via the value of \( \mu^{(t)}(x) \) and its exploration level is represented through the value of \( \sigma^{(t)}(x) \). Therefore, the next query point \( x^{(t)} \) is evaluated as

\[
x^{(t)} = \arg\max_x \left( \mu^{(t)}(x) + \kappa \sigma^{(t)}(x) \right)
\]

The above expression implies that we wish to minimize the mean \( \mu^{(t)}(x) \) for the exploitation and simultaneously maximize the variance \( \sigma^{(t)}(x) \) for the exploration. The exploitation and exploration is trade-off since if we favor the exploration, the query point tends to stay close to the previous query points, hence having a small variance (i.e., the standard deviation); in contrast, if we favor the exploration, the query point tends to stay far away the previous query points for a high variance (i.e., the standard deviation), hence having a low mean value. Here we note that \( \kappa > 0 \) is used to trade-off the exploitation against the exploration.

To observe the geometric nature of GP-based Bayesian Optimization (BO), we now investigate the geometric view of GP-based BO. Since \( \tilde{K} \left( x, x' \right) = K \left( x, x' \right) + \sigma \| x - x' \| \) is a p.s.d kernel, there exists a feature map \( \tilde{\Phi} : \mathcal{X} \rightarrow \mathcal{H} \) (i.e., \( \mathcal{H} \) is a Reproducing Kernel Hilbert Space) such that \( \tilde{K} \left( x, x' \right) = \tilde{\Phi}(x)^T \tilde{\Phi}(x') \). We now denote \( \mathcal{L}^{(t)} = \text{span} \left\{ \tilde{\Phi}(x_1), \ldots, \tilde{\Phi}(x_{t-1}) \right\} \) by the linear span of \( \tilde{\Phi}(x_1), \ldots, \tilde{\Phi}(x_{t-1}) \) and further define the projection of a given vector \( \tilde{\Phi}(x) \) onto \( \mathcal{L}^{(t)} \) and the
rejection of $\tilde{\Phi}(x)$ from $\mathcal{L}^{(t)}$ as

$$P^{(t)}(x) = \sum_{i=1}^{t-1} p_i(x) \tilde{\Phi}(x_i)$$

$$R^{(t)}(x) = \tilde{\Phi}(x) - P^{(t)}(x)$$

**Theorem 1.** (Geometric view) We define the coefficient vector of the projection $P^{(t)}(x)$ as $p(x) = [p_1(x)]^{T}_{i=1,\ldots,t-1}$. We then have $p(x) = K^{(t)}_L \left[ K^{(t)}_\sigma \right]^{-1}$. In addition, the variance $V^{(t)}(x)$ is exactly $\|R^{(t)}(x)\| - \sigma$, where $\|R^{(t)}(x)\|$ is the Euclidean distance from $\tilde{\Phi}(x)$ to the linear span $\mathcal{L}^{(t)}$ and the mean $\mu^{(t)}(x)$ is exactly $\langle p(x), y^{(t)} \rangle = \sum_{i=1}^{t-1} p_i(x) y_i$.

We now restate the criterion to find the next query point as shown in Eq. (2) as

$$x_{t+1} = \arg\max_{x} \left( \sum_{i=1}^{t-1} p_i(x) y_i + \kappa \sqrt{\|R^{(t)}(x)\| - \sigma} \right)$$

This view supports us to think out of the GP-based Bayesian Optimization. In particular, we propose a novel Similarity-based Bayesian Optimization framework that still preserves the insightful spirit of the GP-based Bayesian Optimization.

3. Analogical-based Bayesian Optimization

3.1 Thinking Out of the Gaussian Process

The kernel function $K(\cdot, \cdot)$ can be thought as a similarity score which measures the similarity level between any two points. Leveraging this remark with the geometric view of GP-based Bayesian Optimization inspires us to think out of the Gaussian Process. In particular, we propose a Analogical-based Bayesian Optimization (ABO) for which the kernel similarity can be replaced by a more generic class of similarity scores. To motivate this idea, we observe that the predictive mean can be computed as follows

$$\mu^{(t)}(x) = \sum_{i=1}^{t-1} p_i(x) y_i$$

where each $p_i(x)$ stands for the coefficient of $\tilde{\Phi}(x_i)$ in the projection of $\tilde{\Phi}(x)$ onto $\mathcal{L}^{(t)} = \text{span}\left\{\tilde{\Phi}(x_1), \ldots, \tilde{\Phi}(x_{t-1})\right\}$.

The formula in Eq. (3) and the expressive meaning of $p_i(x)$ enables us to assign $p_i(x)$ as the influence level of $x_i$ to $x$ given $\mathcal{D}_t$, for which we denote as $I(x, x_i \mid \mathcal{D}_t)$. If this influence level is high (i.e., $\tilde{\Phi}(x_i)$ plays an important role in the formula of $P^{(t)}(x)$ or $\tilde{\Phi}(x)$), the collected value $y_i$ associating with $\tilde{\Phi}(x_i)$ highly affects to the predictive mean $\mu^{(t)}(x)$. With the notion of the influence level in hand, we can rewrite the formula for the predictive mean as

$$\mu^{(t)}(x) = \sum_{i=1}^{t-1} I(x, x_i \mid \mathcal{D}_t) y_i$$

We now turn to express the variance $V^{(t)}(x)$ (or the standard deviation $\sigma^{(t)}(x) = V^{(t)}(x)^{1/2}$) using the notion of the influence level. Using the formula in Eq. (1), we can rewrite the variance as

$$V^{(t)}(x) = \left| K(x, x) - \sum_{i=1}^{t-1} I(x, x_i \mid \mathcal{D}_t) K(x, x_i) \right|$$
The formula of the variance $V^{(t)}(x)$ in Eq. (5) discloses that if $x$ locates in the region highly affected by $x_i(s)$ and being close to $x_i(s)$, its variance would be low. In contrast, if $x$ tends to move further away $x_i(s)$, its variance tends to decrease. Therefore, in GP-based Bayesian Optimization, Gaussian Process allows us to place the uncertainty over the ground-truth function $f$ and also quantitatively characterize the uncertainty of this function evaluated at a point (i.e., $f(x)$) which is influenced by other queried points as in Eqs. (4).

### 3.2 Bayesian Optimization with a Generic Similarity Score

With the support of the above views and reasons, we propose to replace the kernel function $K(x, x')$ by a more generic similarity score $S(x, x')$ wherein $S: \mathcal{X} \times \mathcal{X} \to \mathbb{R}$ is non-negative and symmetric. The formulas for the predictive mean and variance as shown in Eqs. (4, 5) are rewritten as

$$
\mu^{(t)}(x) = \sum_{i=1}^{t-1} I(x, x_i | D_t) y_i
$$

$$
V^{(t)}(x) = \left| S(x, x) - \sum_{i=1}^{t-1} I(x, x_i | D_t) S(x, x_i) \right|
$$

where $I(x) = [I(x, x_i | D_t)]_{i=1,...,t-1}^T$ can be computed as $S_x^{(t)} \left[ S^{(tt)} + \sigma^2 \mathbb{I} \right]^{-1}$ (if available) with $S_x^{(t)} = [S(x, x_i)]_{i=1,...,t-1}$ and $S^{(tt)} = [S(x_i, x_j)]_{i,j=1}^{t-1}$.

However, for a generic similarity score $S(., .)$, the matrix $S^{(tt)} + \sigma^2 \mathbb{I}$ might be a singular matrix, hence making the computation infeasible. To address this issue, we note that $I(x) = S_x^{(t)} \left[ S^{(tt)} + \sigma^2 \mathbb{I} \right]^{-1}$ or equivalently $S_x^{(t)} = I(x) \times (S^{(tt)} + \sigma^2 \mathbb{I})$ and therefore propose to find $I(x)$ as

$$
I(x) = \text{argmin}_I \left\| S_x^{(t)} - I \left( S^{(tt)} + \sigma^2 \mathbb{I} \right) \right\|^2 \quad (6)
$$

To find optimal solution of the optimization problem in Eq. (5), we denote $r_t = \text{rank} \left( S^{(tt)} + \sigma^2 \mathbb{I} \right)$ and let $B^{(tt)}$ be the base matrix of the row space of the matrix $S^{(tt)} + \sigma^2 \mathbb{I}$. It is apparent that the size of $B^{(tt)}$ is $r_t \times (t - 1)$ which depends on the similarity score $S(., .)$. The following theorem states that instead of solving the optimization problem in Eq. (5) we can solve a similar optimization with a smaller size.

**Theorem 2.** (Equivalent problem) Let us denote $J(x) = \text{argmin}_J \left\| S_x^{(t)} - J B^{(tt)} \right\|^2 \in \mathbb{R}^{r_t}$. The following statements hold

i) The matrix $B^{(tt)} \left( B^{(tt)} \right)^T$ is invertible.

ii) $J(x) = S_x^{(t)} \left( B^{(tt)} \right)^T \left[ B^{(tt)} (B^{(tt)})^T \right]^{-1}$. $I(x)$ can be formed by augmenting $J(x)$ with the zero entries.

It is apparent that if the matrix $S^{(tt)} + \sigma^2 \mathbb{I}$ is invertible (i.e., $\text{rank} \left( S^{(tt)} + \sigma^2 \mathbb{I} \right) = t - 1$) and symmetric, we can gain the formulation being similar to GP-based OP as shown in the following corollary.

**Corollary 3.** Assuming that the matrix $S^{(tt)} + \sigma^2 \mathbb{I}$ is invertible (i.e., $\text{rank} \left( S^{(tt)} + \sigma^2 \mathbb{I} \right) = t - 1$) and symmetric, we then have $B^{(tt)} = S^{(tt)} + \sigma^2 \mathbb{I}$, and $I(x) = J(x) = S_x^{(t)} \left( S^{(tt)} + \sigma^2 \mathbb{I} \right)^{-1}$.

It is worth noting that $J(x)$ does not match with $y^{(t)}$ and $S_x^{(t)}$ in general. To make the computation tractable, we fill the missing values in $J(x)$ by 0. As a sequence, the calculations of $S_x^{(t)} D^{(tt)} y^{(t)}$ and $S_x^{(t)} D^{(tt)} \left( S_x^{(t)} \right)^T$ can be realized by eliminating the irrelevant entries in $y^{(t)}$ and $S_x^{(t)}$. 

4
In the sequel, we demonstrate that the influence vector evaluated as in Eq. \( \text{[8]} \) has the same geometric interpretation as that of GP-based Bayesian Optimization in Theorem \( \text{[1]} \). The only difference is that the empirical feature map is used instead of the feature map \( \Phi(\cdot) \). Given the collected training set \( D_{t-1} \), the empirical feature map is defined as

\[
\Phi_e(x) = \left[ S(x, x_i) + \sigma^2 \mathbb{I}(x, x_i) \right]_{i=1}^{t-1}
\]

The following theorem shows that the influence vector evaluated as in Eq. \( \text{[8]} \) is exactly the coefficients of the vectors \( \Phi_e(x_i)(s) \) in the projection of \( \Phi_e(x) \) onto the linear span of \( \{ \Phi_e(x_1), \ldots, \Phi_e(x_{t-1}) \} \).

**Theorem 4.** (Geometric view with empirical feature map) Let us denote the projection of \( \Phi_e(x) \) onto the linear span of \( \{ \Phi_e(x_1), \ldots, \Phi_e(x_{t-1}) \} \) by \( P_e(x) \). Let \( I_i(x) \) be the \( i \)-th component of the influence vector evaluated as in Eq. \( \text{[8]} \). We then have

\[
P_e(x) = \sum_{i=1}^{t-1} I_i(x) \Phi_e(x_i)
\]

Theorem \( \text{[8]} \) indicates that the influence vector evaluated as in Eq. \( \text{[8]} \) preserves the key spirit of the influence concept in GP-based Bayesian Optimization.

### 3.3 Acquisition Function and Strategy to Query

In this section, we present two kinds of acquisition function and the strategy to find a batch of query points. The maximization of the proposed acquisition functions is based on the fixed-point technique wherein each point in the current queried set has its own trajectory to gradually converge to an equilibrium point, which is also a local maxima of the current acquisition function. Two proposed acquisition functions are formulated as

\[
u_1^{(t)}(x) = S_x^{(t)} D^{(t)} y^{(t)}
\]

\[
u_2^{(t)}(x) = S_x^{(t)} D^{(t)} y^{(t)} + \kappa \left[ S(x, x) - S_x^{(t)} D^{(t)} \left( S_x^{(t)} \right)^\top \right]^{1/2}
\]

To maximize the above acquisition functions, we use the fixed point technique. In particular, we need to find an equilibrium point such that \( \nabla u(x^*) = 0 \) or \( \nabla u(x^*) + x^* = x^* \) where \( u(x) \) can be \( u_1^{(t)}(x) \) or \( u_2^{(t)}(x) \). To address it, we define \( g(x) = \nabla u(x) + x \) and start with an initial point \( x^{(0)} \), and then find the next point as \( x^{(t+1)} = g(x^{(t)}) \). This sequence will converge to an equilibrium point equi \( (x^{(0)}) \).

We now respectively debut with \( x_1, x_2, \ldots, x_{t-1} \) as initial points (i.e., \( x_i = x^{(0)}, i = 1, \ldots, t-1 \) respectively). The \( x_i \) (s) converge to the equilibrium points equi \( (x_i) \) (s) and some of them might be coincided. We now define the set of equilibrium points by \( EQ^{(t)} \) (i.e., \(|EQ^{(t)}| \leq t-1\)). Given a batch size \( n_b \), with the first strategy we choose the top \( n_b \) equilibrium points with highest predictive variance (i.e., \( \left| S(x, x) - S_x^{(t)} D^{(t)} \left( S_x^{(t)} \right)^\top \right| \)) and with the second strategy we choose the top \( n_b \) equilibrium points with highest objective value (i.e., \( u_2^{(t)}(x) \)). In addition, in the first strategy we propose the two-stage strategy wherein the first stage bases on exploitation and the second stage bases on exploration. The gradient (or subgradient) of \( u_1^{(t)}(x) \) and \( u_2^{(t)}(x) \) (or \( g(x) = \nabla u(x) + x \) can be conveniently computed as follows

\[
\nabla u_1^{(t)}(x) = \nabla S_x^{(t)} D^{(t)} y^{(t)}
\]

\[
\nabla u_2^{(t)}(x) = \nabla u_1^{(t)}(x) + \frac{\kappa \nabla S(x, x)}{2 V^{(t)}(x) \operatorname{sign}(V^{(t)}(x))} - \frac{\kappa \left( \nabla S_x^{(t)} D^{(t)} \left( S_x^{(t)} \right)^\top + S_x^{(t)} D^{(t)} \left( \nabla S_x^{(t)} \right)^\top \right)}{2 V^{(t)}(x) \operatorname{sign}(V^{(t)}(x))}
\]

ANALOGICAL-BASED BAYESIAN OPTIMIZATION
4. Application of Similarity-based Bayesian Optimization

In this section, we present a typical example optimization problem wherein the existing approaches are infeasible to accurately solve it whilst our proposed ABO can efficiently figure out its solution. Assuming that we are dealing with the following optimization problem:

\[ \max_x g(x) \triangleq \mathbb{E}_{p(\omega | x)} [f(\omega, x)] \]

In the above optimization problem, the formula of the function \( f(\omega, x) \) is clear, but the evaluation of the expectation is intractable. Therefore, we consider the function \( g(x) \) as a black box function. Given \( x \), we can use Monte Carlo (MC) estimation to evaluate \( g(x) \) using \( \omega_i(s) \) drawn from \( p(\omega | x) \).

Certainly, we are free to employ the traditional GP-based BO in this case. However, the Gaussian kernel function of this approach is based on the Euclidean (or Mahalanobis) distance, hence entailing unsatisfied solution. It is more appealing if we recruit the symmetric KL divergence to measure similarity score as between \( x, x' \) as follows

\[ S(x, x') = \text{const} - D_{SYM}(x, x') = \text{const} - \frac{D_{KL}(p(\cdot | x) || p(\cdot | x'))}{2} - \frac{D_{KL}(p(\cdot | x') || p(\cdot | x))}{2} \]

The derivative of \( S(x, x') \) w.r.t \( x \) is as follows

\[
\nabla_x S(x, x') = \int \nabla_x \log p(\cdot | x) p(\cdot | x') \, d\omega \\
- \int \nabla_x \log p(\cdot | x) \log \frac{\exp(1) p(\cdot | x)}{p(\cdot | x')} \, p(\cdot | x) \, d\omega
\]

(7)

It is obvious that in case that the evaluation of the derivative in Eq. (7) is intractable, we can estimate it using MC estimation. Therefore, in general the execution of ABO for the above Bayesian optimization problem is always feasible. To demonstrate the idea and simplify the problem, we assume that \( x = (\mu, \Sigma) \) and \( p(\omega | x) = \mathcal{N}(\omega | \mu, \Sigma) \) where \( \Sigma = \text{diag} \left( \left[ \sigma_i \right]_{i=1}^d \right) \). We then have

\[
S(x, x') = \text{const} - \frac{1}{4} \left( \text{tr} \left( \Sigma^{-1} \Sigma' \right) + \text{tr} \left( \Sigma \Sigma'^{-1} \right) \right) \\
- \frac{1}{4} (\mu - \mu')^T \left( \Sigma^{-1} + \Sigma'^{-1} \right) (\mu - \mu') \\
= \text{const} - \frac{1}{4} \sum_{i=1}^d \left( \frac{\sigma_i}{\sigma_i'} + \frac{\sigma_i'}{\sigma_i} \right) - \frac{1}{4} \sum_{i=1}^d (\mu_i - \mu_i')^2 \left( \frac{1}{\sigma_i} + \frac{1}{\sigma_i'} \right)
\]

where \( x' = (\mu', \Sigma') \) and \( \Sigma' = \text{diag} \left( \left[ \sigma_i' \right]_{i=1}^d \right) \).

The derivative is now tractable as follows

\[
\nabla S_{\mu_i} = -\frac{1}{2} (\mu_i - \mu_i') \left( \frac{1}{\sigma_i} + \frac{1}{\sigma_i'} \right) \\
\nabla S_{\sigma_i} = -\frac{1}{4} \left( \frac{1}{\sigma_i'} - \frac{\sigma_i'}{\sigma_i} \right) - \frac{1}{4} (\mu_i - \mu_i')^2 \frac{1}{\sigma_i^2}
\]

5. Experiment
References

Javad Azimi, Ali Jalali, and Xiaoli Fern. Hybrid batch bayesian optimization. *arXiv preprint arXiv:1202.5597*, 2012.

James S. Bergstra, Bardenet Rémi, Yoshua Bengio, and Balázs Kégl. Algorithms for hyper-parameter optimization. In *Advances in Neural Information Processing Systems 24*, pages 2546–2554, 2011.

Eric Brochu, Tyson Brochu, and Nando de Freitas. A bayesian interactive optimization approach to procedural animation design. In *Proceedings of the 2010 ACM SIGGRAPH/Eurographics Symposium on Computer Animation*, SCA '10, pages 103–112, 2010a.

Eric Brochu, Vlad M. Cora, and Nando de Freitas. A tutorial on bayesian optimization of expensive cost functions, with application to active user modeling and hierarchical reinforcement learning. *CoRR*, 2010b.

Matthew Hoffman, Bobak Shahriari, and Nando Freitas. On correlation and budget constraints in model-based bandit optimization with application to automatic machine learning. In Samuel Kaski and Jukka Corander, editors, *Proceedings of the Seventeenth International Conference on Artificial Intelligence and Statistics*, volume 33, pages 365–374, 2014.

Frank Hutter, Holger H. Hoos, and Kevin Leyton-Brown. Sequential model-based optimization for general algorithm configuration. In *Proceedings of the 5th International Conference on Learning and Intelligent Optimization*, pages 507–523, 2011.

Daniel J. Lizotte, Tao Wang, Michael H. Bowling, and Dale Schuurmans. Automatic gait optimization with gaussian process regression. In *IJCAI*, pages 944–949, 2007.

Nimalan Mahendran, Ziyu Wang, Firas Hamze, and Nando De Freitas. Adaptive mcmc with bayesian optimization. In *Proceedings of the Fifteenth International Conference on Artificial Intelligence and Statistics*, pages 751–760, 2012.

R. Martinez-Cantin, N. de Freitas, A. Doucet, and J. Castellanos. Active policy learning for robot planning and exploration under uncertainty. In *Proceedings of Robotics: Science and Systems*, Atlanta, GA, USA, June 2007.

Marchant Román and Ramos Fabio. Bayesian optimisation for intelligent environmental monitoring. In *2012 IEEE/RSJ International Conference on Intelligent Robots and Systems, IROS 2012, Vilamoura, Algarve, Portugal, October 7-12, 2012*, pages 2242–2249, 2012.

Bobak Shahriari, Kevin Swersky, Ziyu Wang, Ryan P Adams, and Nando de Freitas. Taking the human out of the loop: A review of bayesian optimization. *Proceedings of the IEEE*, 104(1): 148–175, 2016.

Jasper Snoek, Hugo Larochelle, and Ryan P Adams. Practical bayesian optimization of machine learning algorithms. In *Advances in Neural Information Processing Systems 25*, pages 2951–2959, 2012.

Niranjan Srinivas, Andreas Krause, Matthias Seeger, and Sham M. Kakade. Gaussian process optimization in the bandit setting: No regret and experimental design. In *Proceedings of the 27th International Conference on Machine Learning (ICML-10)*, pages 1015–1022. Omnipress, 2010.

Kevin Swersky, Jasper Snoek, and Ryan P Adams. Multi-task bayesian optimization. In C. J. C. Burges, L. Bottou, M. Welling, Z. Ghahramani, and K. Q. Weinberger, editors, *Advances in Neural Information Processing Systems 26*, pages 2004–2012. 2013.
Ziyu Wang, Masrour Zoghi, Frank Hutter, David Matheson, and Nando De Freitas. Bayesian optimization in high dimensions via random embeddings.

Ziyu Wang, Babak Shakibi, Lin Jin, and Nando Freitas. Bayesian Multi-Scale Optimistic Optimization. In Proceedings of the Seventeenth International Conference on Artificial Intelligence and Statistics, pages 1005–1014, 2014.
Appendix A. All Proofs

For comprehensibility, we first revise some definitions and notations used in the paper.

\[ \tilde{K} (x, x') = K (x, x') + \sigma I (x, x') \text{ and } \hat{K} (x, x') = \Phi (x) \trans \hat{\Phi} (x') \]

\[ \mathcal{L}^{(t)} = \text{span} \left\{ \hat{\Phi} (x_1), \ldots, \hat{\Phi} (x_{t-1}) \right\} \]

\[ p (x) = \sum_{i=1}^{t-1} p_i (x) \hat{\Phi} (x_i) \text{ and } \mathcal{R}^{(t)} (x) = \hat{\Phi} (x) - p (x) \]

**Theorem 5.** We define the coefficient vector of the projection \( p (x) = [p_i (x)]_{i=1}^{t-1} \). We then have

\[ p (x) = \left[ K_\sigma^{(tt)} \right]^{-1} (K_x^{(t)}) \trans \] where \( K_\sigma^{(tt)} = K^{(tt)} + \sigma^2 I \) with \( K^{(tt)} = [K (x_i, x_j)]_{i,j=1}^{t-1} \). In addition, the variance \( V^{(t)} (x) \) is exactly \( \| \mathcal{R}^{(t)} (x) \| - \sigma \), where \( \| \mathcal{R}^{(t)} (x) \| \) is the distance from \( \hat{\Phi} (x) \) to the linear span \( \mathcal{L}^{(t)} \) and the mean \( \mu^{(t)} (x) \) is exactly \( \langle p (x), y^{(t)} \rangle = \sum_{i=1}^{t-1} p_i (x) y_i \).

**Proof** It is apparent that

\[ p (x) = \arg \min_d J (d) \triangleq \left\| \hat{\Phi} (x) - \sum_{i=1}^{t-1} d_i \hat{\Phi} (x_i) \right\|^2 \]

We then have

\[ J (d) = \tilde{K} (x, x) - \sum_{i=1}^{t-1} \tilde{K} (x, x_i) d_i + \sum_{i=1}^{t-1} \sum_{j=1}^{t-1} d_i d_j \tilde{K} (x_i, x_j) \]

\[ = \tilde{K} (x, x) - \sum_{i=1}^{t-1} K (x, x_i) d_i + \sum_{i=1}^{t-1} \sum_{j=1}^{t-1} d_i d_j \tilde{K} (x_i, x_j) \text{ (since } x \neq x_i, \forall i) \]

\[ = \tilde{K} (x, x) - K_x^{(t)} d \trans + d \trans \left[ K^{(tt)} + \sigma^2 I \right] d \]

\[ = \tilde{K} (x, x) - K_x^{(t)} d \trans + d \trans K_\sigma^{(tt)} d \]

\[ \nabla J (d) = \left( K_x^{(t)} \right) \trans - K_\sigma^{(tt)} d \]

Setting the derivative to 0, we gain

\[ p (x) = d^* = \left[ K_\sigma^{(tt)} \right]^{-1} \left( K_x^{(t)} \right) \trans \]

We now remind the formula to compute the influence vector \( I (x) \)

\[ I (x) = \arg \min_I \left\| S_x^{(t)} - I \left( S^{(tt)} + \sigma^2 I \right) \right\|^2 \] (8)

**Theorem 6.** Let us denote \( J (x) = \arg \min_J \left\| S_x^{(t)} - J B^{(tt)} \right\|^2 \in \mathbb{R}^n \). The following statements hold

i) The matrix \( B^{(tt)} \left( B^{(tt)} \right)^\trans \) is invertible.

ii) \( J (x) = S_x^{(t)} \left( B^{(tt)} \right)^\trans \left[ B^{(tt)} \left( B^{(tt)} \right)^\trans \right]^{-1} \). \( I (x) \) can be formed by augmenting \( J (x) \) with the zero entries.
Proof. We sketch out the proof as follows.

i) \( \text{rank} \left( B^{(tt)} (B^{(tt)})^T \right) = \text{rank} (B^{(tt)}) = r_t. \) In addition, the size of the matrix \( B^{(tt)} (B^{(tt)})^T \) is \( r_t \times r_t. \) It follows that this matrix is invertible.

ii) Setting the derivative of the objective function w.r.t \( J \) to 0, we gain

\[
0 = 2 \left( J (x) B^{(tt)} - S^{(t)}_x \right) \left( B^{(tt)} \right)^T
\]

\[
J (x) = S^{(t)}_x \left( B^{(tt)} \right)^T \left[ B^{(tt)} (B^{(tt)})^T \right]^{-1}
\]

According to the definition of \( B^{(tt)} \), we gain

\[
\{ J B^{(tt)} : J \in \mathbb{R}^{r_t} \} = \left\{ I \left( S^{(tt)} + \sigma^2 \mathbb{I} \right) : I \in \mathbb{R}^{r_t} \right\} = C^{(t)}
\]

Therefore, we arrive at

\[
\| S^{(t)}_x - I (x) \left( S^{(tt)} + \sigma^2 \mathbb{I} \right) \| = \| S^{(t)}_x - J (x) B^{(tt)} \| = \max_{v \in C^{(t)}} \| S^{(t)}_x - v \|
\]

It concludes this proof since \( B^{(tt)} \) is a submatrix of \( S^{(tt)} + \sigma^2 \mathbb{I}. \) \( \square \)

Corollary 7. Assuming that the matrix \( S^{(tt)} + \sigma^2 \mathbb{I} \) is invertible (i.e., \( \text{rank} (S^{(tt)} + \sigma^2 \mathbb{I}) = t - 1 \)) and symmetric, we then have \( B^{(tt)} = S^{(tt)} + \sigma^2 \mathbb{I} \), and \( I (x) = J (x) = S^{(t)}_x (S^{(tt)} + \sigma^2 \mathbb{I})^{-1}. \)

Proof. We derive as

\[
I (x) = J (x) = S^{(t)}_x \left( B^{(tt)} \right)^T \left[ B^{(tt)} (B^{(tt)})^T \right]^{-1} = S^{(t)}_x B^{(tt)} \left[ B^{(tt)} B^{(tt)} \right]^{-1}
\]

\[
= S^{(t)}_x B^{(tt)} \left( B^{(tt)} \right)^{-1} \left( B^{(tt)} \right)^{-1} = S^{(t)}_x \left( B^{(tt)} \right)^{-1}
\]

\( \square \)

Theorem 8. Let us denote the projection of \( \Phi_e (x) \) onto the linear span of \( \{ \Phi_e (x_1), \ldots, \Phi_e (x_{t-1}) \} \) by \( \mathcal{P}_e (x) \). Let \( I_i (x) \) be the \( i \)-th component of the influence vector evaluated as in Eq. (8). We then have

\[
\mathcal{P}_e (x) = \sum_{i=1}^{t-1} I_i (x) \Phi_e (x_i)
\]

Proof. We have

\[
\mathcal{P}_e (x) = \sum_{i=1}^{t-1} I_i (x) \Phi_e (x_i)
\]

It is apparent that

\[
I (x) = \arg \min_I \left\| \Phi_e (x) - \sum_{i=1}^{t-1} I_i \Phi_e (x_i) \right\|^2
\]

We note that

\[
\Phi_e (x) = \left[ S (x, x_i) + \sigma^2 \mathbb{I} (x, x_i) \right]_{i=1}^{t-1} = \left[ S (x, x_i) \right]_{i=1}^{t-1} = S^{(t)}_x (\text{since } x \neq x_i, \forall i)
\]

\[
\sum_{i=1}^{t-1} I_i \Phi_e (x_i) = I \left[ \Phi_e (x_i) \right]_{i=1}^{t-1} = I \left[ \Phi_e (x_i) \right]_{i=1}^{t-1} = I \left( S^{(tt)} + \sigma^2 \mathbb{I} \right) (\text{since } \Phi_e (x_i)_{i=1}^{t-1} \text{ is symmetric})
\]
Therefore, we gain the conclusion.