Incorporating Expert Prior in Bayesian Optimisation via Space Warping

Anil Ramachandran*, Sunil Gupta, Santu Rana, Cheng Li, Svetha Venkatesh

Applied Artificial Intelligence Institute (A²I²), Deakin University, Australia

Abstract

Bayesian optimisation is a well-known sample-efficient method for the optimisation of expensive black-box functions. However, when dealing with big search spaces the algorithm goes through several low function value regions before reaching the optimum of the function. Since the function evaluations are expensive in terms of both money and time, it may be desirable to alleviate this problem. One approach to subside this cold start phase is to use prior knowledge that can accelerate the optimisation. In its standard form, Bayesian optimisation assumes the likelihood of any point in the search space being the optimum is equal. Therefore any prior knowledge that can provide information about the optimum of the function would elevate the optimisation performance. In this paper, we represent the prior knowledge about the function optimum through a prior distribution. The prior distribution is then used to warp the search space in such a way that space gets expanded around the high probability region of function optimum and shrinks around low probability region of optimum. We incorporate this prior directly in function model (Gaussian process), by redefining the kernel matrix, which allows this method to work with any acquisition function, i.e., acquisition agnostic approach. We show the superiority of our method over standard Bayesian optimisation method through optimisation of several benchmark functions and hyperparameter tuning of two algorithms: Support Vector Machine (SVM) and Random forest.

Keywords: Bayesian optimisation, Gaussian process, Black-box function, Probability integrity transform, Space warping

1. Introduction

Design of a product/process traditionally involves extensive number of parameters that highly influence the characteristics of the final outcome and can only be measured through random experiments. The product could be a physical product such as a new
super alloy with room temperature superconductivity or a highly tuned machine learning model with human-level object classification accuracy. Often the experiments, i.e. casting an alloy with a new composition or training a machine learning model with new hyperparameters can be costly both in terms of money and time. Hence it is necessary to reach the target goal with as few experiments as possible. The relationship between these tunable parameters and the output characteristics can be represented by a mathematical function. However, the underlying function behind many complex problems (e.g. casting an alloy) are not explicitly known (black-box) and expensive to evaluate. Therefore naive approaches like random or grid search become inefficient with increasing experimental complexity.

Bayesian optimisation has recently become an established and sample-efficient approach for the optimisation of such black-box functions and found several interesting applications in miscellaneous domains: such as reducing the extensive number of experiments that are usually required for a good material design [1], designing high-strength alloys [2], designing graphene thermoelectrics [3], optimisation of short polymer fiber synthesis [4], designing renewable energy systems and real-time control [5], optimisation of robot gait parameters [6, 7], environmental monitoring and sensor set selection [8] and hyperparameter tuning of machine learning models [9].

Bayesian optimisation is a sequential model based approach where it initially builds a prior over the unknown objective function and iteratively chooses the next function evaluation point by optimising a cheap surrogate function. The surrogate function selects the evaluation points by keeping a balance between exploiting the region where function value is expected to be optimal (exploitation) and exploring the region where the uncertainty about the function value is high (exploration). With minimum evaluation points, Bayesian optimisation can reach the global optimum of expensive black-box functions and this makes the Bayesian optimisation an ideal candidate for the optimisation of such unknown functions. However, when dealing with big search spaces, the algorithm visits low function value regions more often before reaching the optimum. The main reason for this is that Bayesian optimisation assumes that every point in the search space is equally likely to be optimum. We call this as cold start phase of Bayesian optimisation. For complex models with big search spaces and large amount of data, this cold start phase can be extremely expensive and wasteful of resources and it is desirable to shorten this cold start phase.

In order to shorten the cold start phase and thus to improve the optimisation efficiency, one can make use of any available prior knowledge about the solution. There are generally two types of prior knowledge which are used to construct several Bayesian optimisation frameworks in literature. (1) Prior knowledge of related function evaluation data from previous optimisations [10,11,12,13,14,15,16,17], (2) Prior knowledge about function itself. Since the former methods require data from similar function optimisations, they become infeasible for the optimisation of complex models. The latter approach can be further divided into two types. (i) The function may not be a complete black-box rather, we may know its behavior particularly e.g. we may know that the output is monotonically increasing or decreasing with respect to a particular variable or the output is uni-modal along certain variable etc, (ii) Experimenter are usually expert of their field and may have some intuition of “good” and “bad” regions. This knowledge can be used as a prior over the optimum location. Although there has
been research on developing methods to incorporate former type of prior knowledge [18, 19], there has been no work to incorporate the latter type of prior. Since the likelihood of searching the optimum is equally likely along the whole space, obtaining some expert prior information about the optimum location is, certainly, useful. For this reason, a Bayesian optimisation framework that can incorporate domain expert prior regarding the optimum location is still an open problem.

In this paper, we propose a new Bayesian optimisation framework that can incorporate prior knowledge about optima location and thus can accelerate the optimisation efficiency. To incorporate such knowledge, we represent the prior knowledge about the optimum location through a prior distribution. We then use this prior distribution to warp the search space. We use probability integrity transform to achieve the warping. The transformation of search space based on the prior assumption enables the Bayesian optimisation to encourage function evaluations to come from high likelihood regions as indicated by the prior. This is achieved through incorporating the warped space information directly into the Gaussian process by redefining the kernel matrix, which makes the method agnostic to any acquisition function. We prove that the new kernel (we call it as warped kernel) is a valid Mercer kernel. In addition, we also show that the convergence of new Bayesian optimisation framework is always guaranteed with any prior distribution even if it is misspecified as long as it has a non-zero likelihood for the true optimum. We validate our new Bayesian optimisation method through application to optimisation of several benchmark functions and hyperparameter tuning of two algorithms: Support Vector Machine (SVM) and Random Forest.

2. Background

Let \( f : \mathcal{X} \rightarrow \mathbb{R} \) be an expensive black-box (unknown) function defined over a compact set \( \mathcal{X} \subseteq \mathbb{R}^d \) and we need to find the maximum of this function. That is, we need to find a point \( \mathbf{x}_* \) in \( \mathcal{X} \) such that \( \mathbf{x}_* = \arg\max_{\mathbf{x} \in \mathcal{X} \subseteq \mathbb{R}^d} f(\mathbf{x}) \). Bayesian optimisation is a sample efficient solution for the optimisation of these type of expensive black-box functions. Next, we provide an overview of various components of Bayesian optimisation.

2.1. Gaussian Process

As the function \( f(\mathbf{x}) \) is an unknown, black-box function, Bayesian optimisation builds a surrogate model of the function, generally using Gaussian process (GP) [20], random forests [21] or Bayesian neural networks [22]. This paper focuses on GP modeling because the model is robust and at the same time it is easily analyzable. Let us say, we have some perturbed function evaluation data comprising of \( n \) observations \( \mathcal{D}_n = (x_i, y_i) \mid i = 1, 2, \ldots, n \) and need to make prediction at a new input \( \tilde{\mathbf{x}} \) which is not part of the data, \( \mathcal{D}_n \). In such a case, GP prior gives a probabilistic view for every possible functions using a mean function \( (\mu : \mathcal{X} \rightarrow \mathbb{R}) \) and a kernel function \( (k : \mathcal{X} \times \mathcal{X} \rightarrow \mathbb{R}) \) [20]. It is assumed that, the function \( f(\mathbf{x}) \) can be sampled as \( f(\mathbf{x}) \sim \text{GP}(\mu(\mathbf{x}), k(\mathbf{x}, \mathbf{x}')) \) where \( \mu(\mathbf{x}) \) is a mean function, and \( k(\mathbf{x}, \mathbf{x}') \) is a kernel function. Since the mean function can be set to zero without loss in generality, we assume it as a zero function for the simplicity of the modeling. Kernel function specifies the correlation between the function values at any two points \( \mathbf{x} \) and \( \mathbf{x}' \). There are many
kernel functions including squared exponential kernel, Matérn kernel and linear kernel. As an example, squared exponential kernel computes the covariance between function values at any two points \( x \) and \( x' \) as

\[
k(x, x') = \sigma_0^2 \exp\left(-\frac{1}{2l^2} \| x - x' \|^2 \right)
\]

where \( l \) is a length scale parameter related to the smoothness of the function and \( \sigma_0^2 \) is the function variance. The function values \( f(x_1), \ldots, f(x_n) \) follow a multivariate Gaussian distribution \( \mathcal{N}(0, K) \), where \( K(i, i') = k(x_i, x_{i'}) \) and the noisy function measurements (outputs), \( y_i = f(x_i) + \epsilon_i \) where \( \epsilon_i \sim \mathcal{N}(0, \sigma^2) \) being the measurement noise. Given a new query point \( \tilde{x} \), the function values \( f_{1:n} \) and \( f(\tilde{x}) \) are jointly Gaussian and can be written as

\[
\begin{bmatrix} f_{1:n} \\ f(\tilde{x}) \end{bmatrix} \sim \mathcal{N}\left( \begin{bmatrix} 0 \\ k(\tilde{x}, \tilde{x}) \end{bmatrix}, \begin{bmatrix} K & k \\ k^T & k(\tilde{x}, \tilde{x}) \end{bmatrix} \right)
\]

where \( k = \begin{bmatrix} k(\tilde{x}, x_1) \; k(\tilde{x}, x_2) \; \ldots \; k(\tilde{x}, x_n) \end{bmatrix} \). This leads to the predictive distribution as \( p(f(\tilde{x}) \mid D_{1:n}, \tilde{x}) = \mathcal{N}(\mu_{\tilde{x}}(\tilde{x}), \sigma_{\tilde{x}}^2(\tilde{x})) \), where the predictive mean and variance are respectively given by \( \mu_{\tilde{x}}(\tilde{x}) = k^T (K + \sigma^2 I)^{-1} f_{1:n} \) and \( \sigma_{\tilde{x}}^2(\tilde{x}) = k(\tilde{x}, \tilde{x}) - k^T (K + \sigma^2 I)^{-1} k \).

### 2.2. Acquisition functions

So far, we have discussed how to build a probabilistic model for a smooth function using a Gaussian process and how to update this prior after gathering new observations. Next, we will give a brief overview about another important component of Bayesian optimisation called acquisition function - used to recommend the next promising function evaluation point. The acquisition function is a cheap surrogate to the function \( f(x) \) and is constructed using the posterior information derived by combining the GP prior with observed data, \( D_n \). While recommending new query points, acquisition function keeps a trade-off between exploitation and exploration criteria which eventually guide towards the optimum of the objective function, i.e. for a function \( f(x) \), the next point is sampled as \( x_{n+1} = \arg\max_x \alpha(x \mid D_n) \). Popular choices of acquisition functions are Expected Improvement (EI) \(^{23}\), GP-UCB \(^{24}\) and Predictive Entropy Search (PES) \(^{25}\). Since predictive entropy search is computationally expensive, we perform experiments using EI and GP-UCB.

**Expected Improvement (EI)** maximizes the expected improvement over the current best observation. We can write the improvement function as \( I(x) = \max \{ 0, f_{n+1}(x) - f(x^+) \} \) where \( x^+ = \arg\max_{x \in \mathbb{X}} f(x) \). If the predicted value is greater than the current best value, \( I(x) \) is set to positive, else it is set to zero. Then the new evaluation point can be written as \( x = \arg\max_x E(I(x) \mid D_{1:n}) \). Analytic form of EI can be written as

\[
\alpha_n(x) = \begin{cases} 
(\mu_n(x) - f(x^+)) \Phi(z) + \sigma_n(x) \phi(z) & \text{if } \sigma_n(x) > 0 \\
0 & \text{if } \sigma_n(x) = 0
\end{cases}
\]

where \( \Phi, \phi \) are the cumulative and probability density functions of standard normal distribution, \( z = (\mu_n(x) - f(x^+)) / \sigma_n(x) \) and \( \mu_n(x) = k^T (K + \sigma^2 I)^{-1} y \).
where \( z = \frac{\mu_n(x) - f(x^*)}{\sigma_n(x)} \). \( \phi(.) \) and \( \Phi(.) \) are respectively the probability distribution function (pdf) and cumulative distribution function (cdf) of a standard normal distribution.

**GP-UCB** selects the next observation point based on an upper confidence bound of predictive distribution. GP-UCB selects the next function evaluation point by the following maximization

\[
\alpha_n(x) = \underset{x \in D}{\text{argmax}} \left( \frac{\mu_n(x)}{\gamma_n} + \sqrt{\frac{\gamma_n \sigma_n(x)}{2}} \right)
\]

where \( \gamma_n = 2 \log \left( \frac{2\pi}{n} \right) + 4d \log \left( \frac{dnbr}{\log (2da/\delta)} \right) \) is \( n \)-dependent weight derived in [24] to ensure global optimisation.

### 2.3. Related works

Standard Bayesian optimisation is a sequential approach where it assumes the likelihood of any point being the function optimum is equal along the search space. This may cause the algorithm to spend more evaluation budget near low function values and consequentially make the optimisation costly especially when dealing with big search spaces. One way to help the algorithm to jump quickly towards the optima location is to incorporate any available prior knowledge about the optimum. Such prior knowledge can be of two types:

1. Prior knowledge from related function evaluations which are already optimised.
2. Prior knowledge regarding the solution from domain experts.

There are several settings in literature which utilize the knowledge from previous function optimisations to boost the optimisation performance of the function (target), \( f(x) \). One crucial requirement while transferring the knowledge from previous function optimisations is the relatedness between source (previous data) and the target. Preliminary works in transfer learning for Bayesian optimisation assume that the source and target are related and transfer the knowledge without checking the relatedness [10, 11]. Another similar approach that made assumption regarding the source/target similarity and transfer the source information in a multi-task setting is presented in [17]. However, performance of these methods drastically reduce when an unrelated source is used. To avoid this performance degradation, alternate transfer learning methods that consider the source/target similarity are proposed in [13-15]. Later, Feurer et al. [12, 14] proposed meta-learning approaches that use meta-features to measure the source/target similarity. All the above methods assume function space similarity rather than a more aligned similarity based on the optima locations of the function. Recently, Ramachandran et al. [16] proposed a transfer learning approach, where similarity across a source and target is estimated based on their optima locations. This similarity is then used to bias the distribution of the target function optimum through a mixture distribution.

There are many practical situations in which the data from the previous related optimisations (source functions) may not be available. However, some useful prior knowledge about the function may still be available. This type of prior knowledge can be divided into two types.
(i) Relationship of the function with its variables (e.g. monotonicity). In a recent method, proposed by Li et al. [18] uses ‘experimenter hunches’ that defines the underlying behavior of the experimental system. That is, authors incorporated monotonic information about the variables using a two-stage Gaussian process modeling. First stage models the monotonic trend in the underlying property. Several points are sampled from this GP and then combined with existing target observations to build a new GP in second stage. Authors proved the theoretical consistency of this method by providing a regret bound. Another similar approach proposed by Vellanki et al. [19] incorporates the shape of the control function as a prior information by modeling it using a Bernstein polynomial basis. Instead of directly optimising this control function, authors optimise its Bernstein coefficients.

(ii) Knowledge about the optima region of the underlying function from domain knowledge. A domain expert often has a vague understanding of good and bad regions of the function. Such prior knowledge about the optima location can be directly used to cut down the search space away from the optima and thus helps to improve the convergence of the target function quickly. However, there has been no work to incorporate this type of prior knowledge and remains an open problem.

3. Proposed Method

Our goal is to propose a computationally feasible Bayesian optimisation method that can incorporate any available prior knowledge about the function optimum to improve the optimisation efficiency. We aim to develop a method that is agnostic to any acquisition function. Since Bayesian optimisation generally assumes that any point in the search space is equally likely to be the optimum, any informative prior knowledge about the optimum of \( f(x) \) is most likely to give a desirable boost for finding the optima of the function. A domain expert’s vague understanding of good and bad regions can be approximately represented by a prior distribution, \( p(x_*) \) that provides a likelihood of any point \( x \) being the optimum. This prior distribution can then be used to differentially warp the search space in a manner such that the regions more likely to contain the optimum are expanded while the regions less likely to contain the optimum are shrunk. We use a well known technique called probability integral transform for warping the search space. Next we provide a discussion about probability integral transform and how we can effectively incorporate the prior knowledge to improve the optimisation efficiency by warping the search space.

3.1. Probability Integral Transform

Probability integral transform, as the name suggests, transforms any continuous random variable to a random variable following uniform distribution. The following Lemma formally presents the probability integral transform.

**Lemma 1.** Let \( x \) be any real-valued random variable following a continuous distribution and \( \Phi_x \) be its cumulative distribution function (cdf), then any random variable \( u = \Phi_x(x) \) follows a uniform distribution \( U(0, 1) \) defined on \( (0, 1) \).
Proof. We have defined, for any random variable, $u = \Phi_x(x)$. Then

$$\Phi_u(u) = P(u \leq u) = P(\Phi_x(x) \leq u), \text{ for any } u \in (0, 1)$$

$$= P(x \leq \Phi^{-1}_x(u)) = \Phi_x(\Phi^{-1}_x(u)) = u$$

Taking derivative with respect to $u$, we obtain the probability distribution function (pdf) of $u$ as $p(u) = 1$, $u \in (0, 1)$ which is $\mathcal{U}(0, 1)$ with support $(0, 1)$.

Next we illustrate in Figure 1 how transforming a variable $x_m$ through the prior cdf $\Phi_m$ leads to expansion and shrinkage of the space along the variable. We note that based on the $p(x_{*m})$ constructed in Figure 1, region $[-1, 1]$ is high likelihood region while $[-3, 1] \cup [1, 3]$ are low likelihood regions. We can see that the region $[-1, 1]$ of $x_m$ gets transformed to space $[0.18, 0.82]$ which is nearly 64% of the space $[0, 1]$ (Expansion). On the contrary, the region $[-3, 1] \cup [1, 3]$ get transformed to $[0, 0.18] \cup [0.82, 1]$ which is nearly 36% of the space $[0, 1]$ (Shrinkage). Essentially, $\Phi_m(x_m)$ warps the space in such a way so that in the warped space the distribution of the optimum becomes uniform.

3.2. Bayesian Optimisation in the Warped Space

Next we will discuss how the optimisation performance improves while transforming the original search space into the warped space. For that, let us consider a two-dimensional Levy function and plot its function evaluation points as recommended by Bayesian optimisation using both search spaces (original and warped) as shown in Figure 2. In Figure 2b in warped space (blue), Bayesian optimisation is able to quickly identify the region near the function minima and recommend samples near that. On the other hand, in original space (red), Bayesian optimisation initially samples far from the minimum region. However, as iterations increase, it is able to recommend points near the minimum of the function. Therefore, Bayesian optimisation in warped space reaches the optimum faster when compared to working in the original space.
Figure 2: 60 sample points recommended by Bayesian optimisation using both original and warped space for the two-dimensional Levy function.

Next we describe how to use such warping into Bayesian optimisation. Particularly, we have two goal here. (i) how to incorporate warping into Bayesian optimisation efficiently and (ii) how to incorporate warping into Bayesian optimisation so that it is agnostic to the acquisition function. Our solution to the above requirement is to intervene into Gaussian process directly and amend its kernel. For that, let us define

\[ p(x_m) \triangleq p(f(x_m) \geq f(x_m')) \; ; \; x_m \neq x_m' \]

as prior distribution over \( x_m \). The new kernel (warped kernel), \( \tilde{k}_m(x_m, x_m') \) (can be extended to any kernel, but here we explain based on the squared exponential kernel) can be written as

\[
\tilde{k}_m(x_m, x_m') = (\sigma_0^2)^d \exp\left(-\frac{1}{2l^2} | \Phi_m(x_m) - \Phi_m(x_m') |^2 \right)
\]

\[
\tilde{k}(x, x') = \prod_{m=1}^d \tilde{k}_m(x_m, x_m')
\]

where \( d \) is the input space dimension and \( \Phi_m(x_m) \) and \( \Phi_m(x_m') \) be the cdf transformations of the points \( x_m \) and \( x_m' \) along dimension \( m \) respectively. In the following, we define a **Lemma 2** that formally proves the warped kernel, \( \tilde{k}(x, x') \) is a valid Mercer kernel, and therefore can be used in Gaussian process to model the covariance between two points.

**Lemma 2.** The warped kernel \( \tilde{k}(x, x') \) is a valid Mercer kernel.

**Proof.** Any kernel, is said to be valid Mercer kernel if it holds two properties. (i) The kernel function is symmetric and (ii) The kernel is positive semi-definite. Since warped kernel, \( \tilde{k}(x, x') \) use the distance \( | \Phi_m(x_m) - \Phi_m(x_m') |^2 \) between points \( x_m \) and \( x_m' \) along each dimension \( m \), it is invariant to the swapping between \( x_m \) and \( x_m' \), i.e. \( | \Phi_m(x_m) - \Phi_m(x_m') |^2 \) is same as \( | \Phi_m(x_m') - \Phi_m(x_m) |^2 \). Thus \( \tilde{k}(x, x') \) is symmetric (\( \tilde{k}(x, x') = \tilde{k}(x', x) \)). Then the function \( \tilde{k}(x, x') \) is positive semi-definite.
as a function of | if its associated quadratic form is non-negative, i.e. for all points \( x_1, x_2, \ldots, x_n \epsilon \mathcal{X} \) and real numbers \( a_1, a_2, \ldots, a_n \epsilon \mathbb{R} \)

\[
\sum_{j=1}^{n} \sum_{k=1}^{n} a_j a_k \tilde{k}(x_j, x_k) \geq 0
\]

First let us consider \( \tilde{k} \) along the dimension \( m \). Since \( \tilde{k}_m(x_m, x'_m) \) can be seen as a function of \( | \Phi_m(x_m) - \Phi_m(x'_m) | \), it is a stationary function. This allow us to apply Bochner’s theorem to \( \tilde{k}_m(x_m, x'_m) \), i.e. \( \tilde{k}_m(x_m, x'_m) = \mathbb{E} \left[ \exp \left( -iw^T(\Phi_m(x_m) - \Phi_m(x'_m)) \right) \right] \) where \( w \) is a random variable of length \( n \). Then for all the points we can write

\[
\sum_{j=1}^{n} \sum_{k=1}^{n} a_j a_k \tilde{k}_m(x_{mj}, x_{mk}) = \sum_{j=1}^{n} \sum_{k=1}^{n} a_j a_k \mathbb{E} \left[ \exp \left( -iw^T(\Phi_m(x_{mj}) - \Phi_m(x_{mk})) \right) \right] = \mathbb{E} \left[ \sum_{j=1}^{n} \sum_{k=1}^{n} a_j \exp \left( -iw^T \Phi_m(x_{mj}) \right) a_k \exp \left( iw^T \Phi_m(x_{mk}) \right) \right] = \mathbb{E} \left[ \sum_{j=1}^{n} a_j \exp \left( -iw^T \Phi_m(x_{mj}) \right) \right]^2 \geq 0
\]

That means, \( \tilde{k}_m(x_m, x'_m) \) is a positive semi-definite matrix. Then from Schur product theorem [28], we know that the element-wise product of any positive semi-definite matrices is also a positive semi-definite matrix, i.e. \( \tilde{k}(x, x') = \prod_{m=1}^{d} \tilde{k}_m(x_m, x'_m) \) is also positive semi-definite and thus it is a valid Mercer kernel.

The predictive mean and variance according to the new warped kernel, \( \tilde{k}(x, x') \) can be respectively written as \( \mu_{n}(\tilde{x}) = \tilde{k}^T \left[ \tilde{K} + \sigma^2 I \right]^{-1} f_{1:n} \) and \( \sigma^2_n(\tilde{x}) = \tilde{k}(\tilde{x}, \tilde{x}) - \tilde{k}^T \left[ \tilde{K} + \sigma^2 I \right]^{-1} \tilde{k} \) where \( \tilde{k} = \left[ \tilde{k}(\tilde{x}, x_1) \tilde{k}(\tilde{x}, x_2) \ldots \tilde{k}(\tilde{x}, x_n) \right] \) and \( \tilde{K}(i, i') = \tilde{k}(x_i, x'_{i'}) \). From Lemma 2, we proved that warped kernel, \( \tilde{k}(x, x') \) is a valid Mercer kernel and thus the function values \( f(x_1), \ldots, f(x_n) \) follow a multivariate Gaussian distribution \( \mathcal{N}(0, \tilde{K}) \). In the following we provide a discussion about the convergence guarantee of Bayesian optimisation after the incorporation of prior knowledge.

### 3.2.1. Discussion about Convergence Guarantee

To understand the convergence behavior of our proposed method, let us consider two prior distributions as shown in Figure 3. The two priors mainly differ in that the prior in Figure 3a has some regions \([-3, 1] \cup [1, 3]\) with zero likelihood of optimum whereas the prior in Figure 3b has nonzero likelihood of optimum at all points. For the first prior, any point in the region \([-3, -1]\) gets assigned to point 0 in cdf space. Similarly, any point in the region \([1, 3]\) gets assigned to point 1 in cdf space, i.e. the region \([-3, 1] \cup [1, 3]\) has zero likelihood for being the optima. Thus due to a misspecified
Figure 3: (a) When concentrated prior is used for warping the search space. (b) When widely distributed prior is used for warping the search space.

Algorithm 1 Bayesian Optimisation Algorithm using warped kernel.

1. **Input:** Initial observations $D_n = (x_i, y_i)_{i=1}^{n_0}$
2. **Output:** $\{x_n, y_n\}_{n=1}^{N}$
3. **for** $n = n_0, \ldots, N$ **do**
   
   (a) Compute the kernel matrix $\tilde{K}$ using all $\Phi(x_i)$’s.
   
   (b) Find $x_n$ by optimising the acquisition function using either eq. (3) or eq. (4).
   
   (c) Find the objective function: $y_n = f(x_n) + \epsilon_n$.
   
   (d) Augment to the data $D_{1:n} = D_{1:n-1} \cup (x_n, y_n)$ and update $\tilde{K}$.
4. **end for**

(or misleading) prior, if $x_*$ happens to be in the zero likelihood region, the optimiser will miss it. But, for the second prior in Figure 3b, which has nonzero likelihood of optimum at all points, even if the prior is misspecified, convergence to $x_*$ is always guaranteed as there is always a small probability of it being the optimum. Since in our algorithm we only use a prior of second type, our algorithm is guaranteed to converge as it borrows the convergence behaviour of the traditional Bayesian optimisation.

The proposed Bayesian optimisation method is explained in Algorithm 1.

3.2.2. Some Example Prior Distributions and the Corresponding Warping Functions

We assume expert has some knowledge about the optima, which can be used to construct a prior distribution $g(x_*)$. In the following we provide few transformations based on some standard parametric distributions that may be relevant to practical applications.

1. **Normal distribution:** Most common continuous distribution used for prior assumption is normal distribution as a domain expert may often be able to guess a good region for function values. Here we consider truncated normal distribution since the
search space in Bayesian optimisation is defined as a compact space. The cdf of truncated normal distribution with pdf, 
\[ f(x_*)|\mu, \sigma^2) = \frac{1}{\sqrt{2\pi \sigma^2}} \exp\left(-\frac{(x_*-\mu)^2}{2\sigma^2}\right) \] 
assuming \( a < x_* < b \) is given by
\[ \Phi(x_*|\mu, \sigma^2, a, b) = \frac{\Phi(x_*|\mu, \sigma^2) - \Phi(a|\mu, \sigma^2)}{\Phi(b|\mu, \sigma^2) - \Phi(a|\mu, \sigma^2)} \] (6)
where \( \Phi(x_*|\mu, \sigma^2) = \frac{1}{2} \left[ 1 + \text{erf} \left( \frac{x_*-\mu}{\sigma \sqrt{2}} \right) \right] \).

2. **Truncated gamma distribution:** In other experiments such as hyperparameter tuning of machine learning models, the value of many hyperparameters are constrained to be non-negative. In such cases, an appropriate continuous distribution for the prior is gamma distribution. Since, the gamma distribution is defined over \( x_* \epsilon (0, \infty) \), while we need to supply the prior on a compact space, we consider a truncated version of gamma distribution defined over \( x_* \epsilon (a, b) \). The closed form expression for the cdf of the truncated gamma distribution is as follows. Let the pdf of truncated gamma distribution be defined by 
\[ f(x_*; \alpha, \beta) = Cx_*^{\alpha-1}e^{-\beta x_*} \] where \( x_* \epsilon (a, b) \). By simple calculation, \( C \) can be estimated to be 
\[ C = \frac{\beta^\alpha}{\gamma(\alpha, \beta b) - \gamma(\alpha, \beta a)} \] where \( \gamma(\alpha, \beta b) \) and \( \gamma(\alpha, \beta a) \) are the lower incomplete gamma functions. Now for the truncated gamma distribution with pdf, \( f(x_*; \alpha, \beta) = Cx_*^{\alpha-1}e^{-\beta x_*} \) \( x_* \epsilon (a, x_*') \), its cdf can be written as
\[ \Phi(x_*'; \alpha, \beta) = \frac{\gamma(\alpha, \beta x_*') - \gamma(\alpha, \beta a)}{\gamma(\alpha, \beta b) - \gamma(\alpha, \beta a)} \] (7)

4. Experiments

We experiment the proposed Bayesian optimisation method on some benchmark functions as well as on various real data experiments. **Since in our experiments the aim is to find the global minima of the function, instead of \( f(x) \) we passed \( 1 - f(x) \) to the optimiser.** The experiments on benchmark functions are designed to illustrate the accelerated convergence of our method to reach the minimum of the function due to prior knowledge. In real data experiments, we tune the hyperparameters of two algorithms: Support Vector Machine (SVM) and Random Forest. For these algorithms, we use the prior knowledge gained by previous studies [29]. We demonstrate the superiority of our method by comparing it with following two baselines.

1. Standard BO - This baseline is the standard Bayesian optimisation algorithm.
2. Prior based Search - In this baseline, function evaluation points are randomly sampled from the prior (see section 3.2.2).

4.1. Experimental setting

In all the experiments, square-exponential kernel is used for Gaussian process modelling and maximum likelihood estimate is used for estimating Gaussian process kernel length scale. All the results are averaged over 10 runs with random initial values.
4.2. Benchmark functions

4.2.1. Gaussian function:

We generated a 3-dimensional Gaussian function with the following form

\[ f(x) = 1 - \exp \left( -\frac{1}{2} (x - \mu)(x - \mu)^T \right) \]

where \( \mu = [0.2, 0.2, 0.2] \). Here truncated normal distribution is selected as prior distribution. To demonstrate how optimisation performance changes with prior mean, we shift the mean of the prior by different amounts from the true minimum (0.2). In particular, we shift the prior mean from the true function minimum location by 5%, 10% and 20% of the search space. The standard deviation is set to 1 for all these cases to cover the full search space. Figure 4 shows the minimum value obtained with respect to iterations for each selected prior (using both Expected Improvement and GP-UCB acquisition functions). Each method starts with the same four random observations from \([-2, 2]\) along each dimension. The performance of proposed Bayesian optimisation method clearly outperforms the standard Bayesian optimisation method when the prior mean is close (5%/10% off) to the true minimum. When the prior mean moves away from the true minimum (20% off), the performance of the proposed method starts to degrade and becomes similar to standard Bayesian optimisation.

4.2.2. Branin function:

Next we try to find the minimum of Branin function defined on the region \( x_1 \in (-5, 10), x_2 \in (0, 15) \). Branin function can be mathematically written as

\[ f(x) = a \left( x_2 - bx_1^2 + cx_1 - r \right)^2 + s (1 - t) \cos (x_1) + s \]

where \( a = 1, b = 5.1/(4\pi^2), c = 5/\pi, r = 6, s = 10, t = 1/(8\pi) \). Here also we selected truncated normal distribution as prior distribution. Once again we analyze three cases: prior mean off by 5%, 10% and 20% of the search space. For the first case, we simulate a case with high confidence and thus set the prior standard deviation to 0.25. For the other two cases, we simulate medium confidence and thus set the standard deviation to 4. Minimum value obtained with respect to iterations using both EI and GP-UCB acquisition functions for all three prior means are shown in Figure 5. With good prior, our method is able to converge faster than the baselines. When the prior mean is moving away from the true minimum, the performance of the proposed method starts to degrade as expected.

4.3. Hyperparameter Tuning

The performance of various machine learning algorithms highly depend on good values of their hyperparameters. In [29], authors proposed a framework based on functional ANOVA [30] to determine the most important hyperparameters of various algorithms (including support vector machines and random forest) and deduce priors over which values of these hyperparameters yield good performance. The most important hyperparameters are inferred by experimenting functional ANOVA in 100 different datasets available on OpenML [31]. We use these priors over hyperparameters in our
Acquisition Function: EI

Acquisition Function: GP-UCB

Figure 4: Gaussian function: Minimum value reached vs optimisation iterations (using both Expected improvement and GP-UCB). (a) & (b) Prior mean is 5% off from the true minimum (0.2). (c) & (d) Prior mean is 10% off from the true minimum. (e) & (f) Prior mean is 20% off from the true minimum.
Figure 5: Branin function: Minimum value reached vs optimisation iterations (using both Expected improvement and GP-UCB). (a) & (b) Prior mean is 5% off from the true minimum. (c) & (d) Prior mean is 10% off from the true minimum. (e) & (f) Prior mean is 20% off from the true minimum.
Table 1: The values of shape parameter $\alpha$ and inverse scale parameter $\beta$ of the prior truncated gamma distribution used when tuning hyperparameters of SVM with RBF and sigmoid kernel on two different binary classification datasets - 'german numer' and 'four class'.

| kernel/dataset | 'german numer' | 'four class' |
|----------------|---------------|--------------|
| RBF            | $\alpha = 2$, $\beta = 0.5$ | $\alpha = 2$, $\beta = 0.5$ |
| sigmoid        | $\alpha = 2$, $\beta = 0.5$ | $\alpha = 1$, $\beta = 0.5$ |

Figure 6: Hyperparameter tuning (SVM with RBF kernel): 1 - AUC vs optimisation iterations. (a) & (b) dataset - 'german numer'. (c) & (d) dataset - 'four class'.

proposed Bayesian optimisation method. In our experiments, we tune the hyperparameters of two algorithms: (1) Support Vector Machine (SVM) with two different kernel types: (i) Radial Basis Function (RBF) and (ii) Sigmoid; (2) Random forest.

4.3.1. Support Vector Machine (SVM):

Radial Basis Function (RBF) and sigmoid are two types of kernels used in SVM. The hyperparameters to tune for RBF kernel, i.e. $k(\mathbf{x}, \mathbf{x}') = \exp \left( -\gamma \| \mathbf{x} - \mathbf{x}' \|^2 \right)$ are kernel parameter ($\gamma$) and cost parameter ($C$). We set the range for $\gamma$ as $[10^{-15}, 10^3]$ and for $C$ as $[10^{-5}, 10^{15}]$. Similarly for sigmoid kernel, i.e. $k(\mathbf{x}, \mathbf{x}') = \tanh \left( -\gamma \mathbf{x}^T \mathbf{x}' + C \right)$, we have kernel parameter ($\gamma$) and cost parameter ($C$). The range for $\gamma$ is set as $[10^{-15}, 10^3]$ and for $C$ is $[10^{-5}, 10^{15}]$ [29]. For both kernels, and for both hyperparameters, we work in exponent space. For both kernel types, we
perform experiments on two different binary classification datasets - ‘german numer’ and ‘four class’ from LibSVM repository [32]. For both experiments, we randomly choose 70% of the data and used for training the classifier. The rest 30% is used for validation. The validation performance of hyperparameter tuning (measured via AUC) is optimised as a function of hyperparameter values. For all experiments, we use truncated gamma distribution as prior with its shape parameter $\alpha$ and inverse scale parameter $\beta$ estimated from [29]. The shape and inverse scale parameter values used while performing the experiments are given in Table 1. Figures 6a and 6b shows 1 - AUC performance on a held-out validation set (using both EI and GP-UCB) while tuning hyperparameters of SVM with RBF kernel on ‘german numer’ dataset. Using the selected prior, our proposed method is able to outperform the other two baselines. Figures 6c and 6d shows 1 - AUC performance on a held-out validation set (using both EI and GP-UCB) while tuning hyperparameters of SVM with RBF kernel on ‘four class’ dataset. Here also our proposed Bayesian optimisation method is showing better performance than baselines using the selected prior. Similarly, the 1 - AUC performance on a held-out validation set using both EI and GP-UCB acquisition functions while tuning hyperparameters of SVM with sigmoid kernel on ‘german numer’ dataset and on ‘four class’ dataset are respectively shown in Figures 7a, 7b, 7c and 7d. With the selected prior, our method clearly shows superiority over other two baselines.
4.3.2. Random Forest:

The hyperparameters to tune for random forest are the ‘minimum samples per leaf’, ‘maximum number of features sampled per node’ and ‘number of trees’. The range for ‘minimum samples per leaf’ and ‘maximum number of features sampled per node’ are set as $[1, 20]$ and $[0.1, 0.9]$ respectively [29]. For both of these hyperparameters, we selected truncated gamma distribution as prior distribution. The range for the ‘number of trees’ is set as $[10, 300]$. Since there is no clear prior knowledge available for this hyperparameter, we do not warp the search space along this dimension. Here the model performance (measured via quantile error) is optimised as a function of hyperparameters values. We consider a regression dataset called ‘forest-fires’ - from UCI machine learning repository [33]. Here the goal is to predict the burned area of forest fires using some meteorological and other data. We train the random forest and returns the out-of-bag quantile error based on the median. For the prior distribution on ‘minimum samples per leaf’ and ‘maximum number of features sampled per node’, the shape parameter, $\alpha$ is set as 0.5 and inverse scale parameter, $\beta$ as 1. Figures 8a and 8b shows out-of-bag quantile error with respect to iterations for our method and the baselines. With the prior selected, the proposed method clearly outperforms the baselines. For this dataset, the baseline Prior based Search performs better than the baseline Standard BO. We also consider another dataset - ‘carsmall’ from Statistics and Machine Learning Toolbox. The goal is to predict the median fuel economy of a

Figure 8: Hyperparameter tuning (Random Forest): Out-of-bag quantile error with respect to iterations. (a) & (b) dataset - ‘forest-fires’. (c) & (d) dataset - ‘carsmall’. 

(a)

(b)

(c)

(d)
car given its various features. For the prior distribution on ‘minimum samples per leaf’ and ‘maximum number of features sampled per node’, the shape parameter, $\alpha$ is set as 1 and inverse scale parameter, $\beta$ as 0.5. Out-of-bag quantile error with respect to iterations is shown in Figure 8c. The proposed method shows better performance than other two baselines.

5. Conclusion

We proposed a novel Bayesian optimisation framework incorporating prior assumption regarding the optima location of the objective function. The knowledge about the optima location is represented through a prior distribution which is then used to warp the search space around the optima location in such a way that the regions around the optima are expanded and regions away from the optima are shrunk. We used a well-known approach called probability integrity transform for warping the search space. Warped information is incorporated directly into Gaussian process by redefining its kernel. This enabled the proposed method agnostic to any acquisition function. We also proved that the redefined (warped) kernel is a valid Mercer kernel and with this kernel the convergence of Bayesian optimisation is always guaranteed. Our experiments with diverse optimisation tasks illustrated the superiority of our proposed method over standard Bayesian optimisation method and prior based random search.

Acknowledgment

This research was partially funded by the Australian Government through the Australian Research Council (ARC). Prof Venkatesh is the recipient of an ARC Australian Laureate Fellowship (FL170100006).

References

[1] P. I. Frazier, J. Wang, Bayesian optimization for materials design, in: Information science for materials discovery and design, Springer, 2016, pp. 45–75.

[2] A. Vahid, S. Rana, S. Gupta, P. Vellanki, S. Venkatesh, T. Dorin, New Bayesian-optimization-based design of high-strength 7xxx-series alloys from recycled aluminum, JOM (2018) 1–6.

[3] M. Yamawaki, M. Ohnishi, S. Ju, J. Shiomi, Multifunctional structural design of graphene thermoelectrics by Bayesian optimization, Science Advances 4 (2018) eaar4192.

[4] C. Li, D. R. de Celis Leal, S. Rana, S. Gupta, A. Sutti, S. Greenhill, T. Slezkak, M. Height, S. Venkatesh, Rapid Bayesian optimisation for synthesis of short polymer fiber materials, Scientific reports 7 (2017) 5683.

[5] A. K. B. Irani, Real-time control and optimal plant design for renewable energy systems using Bayesian optimization, Ph.D. thesis, The University of North Carolina at Charlotte, 2018.
[6] D. J. Lizotte, T. Wang, M. H. Bowling, D. Schuurmans, Automatic gait optimization with Gaussian process regression., in: IJCAI, volume 7, 2007, pp. 944–949.

[7] R. Martinez-Cantin, N. de Freitas, E. Brochu, J. Castellanos, A. Doucet, A Bayesian exploration-exploitation approach for optimal online sensing and planning with a visually guided mobile robot, Autonomous Robots 27 (2009) 93–103.

[8] R. Garnett, M. A. Osborne, S. J. Roberts, Bayesian optimization for sensor set selection, in: Proceedings of the 9th ACM/IEEE international conference on information processing in sensor networks, ACM, 2010, pp. 209–219.

[9] J. Snoek, H. Larochelle, R. P. Adams, Practical Bayesian optimization of machine learning algorithms, in: F. Pereira, C. J. C. Burges, L. Bottou, K. Q. Weinberger (Eds.), Advances in Neural Information Processing Systems 25, Curran Associates, Inc., 2012, pp. 2951–2959.

[10] R. Bardenet, M. Brendel, B. Kégl, M. Sebag, Collaborative hyperparameter tuning., in: ICML (2), 2013, pp. 199–207.

[11] D. Yogatama, G. Mann, Efficient transfer learning method for automatic hyperparameter tuning, Transfer 1 (2014) 1.

[12] M. Feurer, J. T. Springenberg, F. Hutter, Initializing Bayesian hyperparameter optimization via meta-learning., in: AAAI, 2015, pp. 1128–1135.

[13] T. T. Joy, R. Santu, S. Gupta, S. Venkatesh, Flexible transfer learning framework for Bayesian optimisation, in: Pacific-Asia Conference on Knowledge Discovery and Data Mining, Springer, 2016, pp. 102–114.

[14] M. Feurer, B. Letham, E. Bakshy, Scalable meta-learning for Bayesian optimization using ranking-weighted Gaussian process ensembles, in: AutoML Workshop at International Conference on Machine Learning (ICML), 2018.

[15] A. Ramachandran, S. Gupta, S. Rana, S. Venkatesh, Selecting optimal source for transfer learning in Bayesian optimisation, in: Pacific Rim International Conference on Artificial Intelligence, Springer, 2018, pp. 42–56.

[16] A. Ramachandran, S. Gupta, S. Rana, S. Venkatesh, Information-theoretic transfer learning framework for Bayesian optimisation, in: Joint European Conference on Machine Learning and Knowledge Discovery in Databases, Springer, 2018, pp. 827–842.

[17] K. Swersky, J. Snoek, R. P. Adams, Multi-task Bayesian optimization, in: Advances in neural information processing systems, 2013, pp. 2004–2012.

[18] C. Li, R. Santu, S. Gupta, V. Nguyen, S. Venkatesh, A. Sutti, D. R. D. C. Leal, T. Slezk, M. Height, M. Mohammed, et al., Accelerating experimental design by incorporating experimenter hunches, in: 2018 IEEE International Conference on Data Mining (ICDM), IEEE, 2018, pp. 257–266.
[19] P. Vellanki, S. Rana, S. Gupta, D. R. de Celis Leal, A. Sutti, M. Height, S. Venkatesh, Bayesian functional optimisation with shape prior, in: Proceedings of the Association for the Advancement of Artificial Intelligence (AAAI) Conference on Artificial Intelligence, volume 33, 2019, pp. 1617–1624.

[20] C. Rasmussen, C. Williams, Gaussian processes for machine learning, Gaussian Processes for Machine Learning (2006).

[21] F. Hutter, H. H. Hoos, K. Leyton-Brown, Sequential model-based optimization for general algorithm configuration, in: International Conference on Learning and Intelligent Optimization, Springer, 2011, pp. 507–523.

[22] J. T. Springenberg, A. Klein, S. Falkner, F. Hutter, Bayesian optimization with robust Bayesian neural networks, in: Advances in Neural Information Processing Systems, 2016, pp. 4134–4142.

[23] J. Močkus, V. Tiesis, A. Žilinskas, Toward global optimization, volume 2, Elsevier, 1978, pp. 117–128.

[24] N. Srinivas, A. Krause, S. M. Kakade, M. W. Seeger, Information-theoretic regret bounds for Gaussian process optimization in the bandit setting, IEEE Transactions on Information Theory 58 (2012) 3250–3265.

[25] J. M. Hernández-Lobato, M. W. Hoffman, Z. Ghahramani, Predictive entropy search for efficient global optimization of black-box functions, in: Z. Ghahramani, M. Welling, C. Cortes, N. D. Lawrence, K. Q. Weinberger (Eds.), Advances in Neural Information Processing Systems 27, Curran Associates, Inc., 2014, pp. 918–926.

[26] A. Shilton, S. Gupta, S. Rana, S. Venkatesh, Regret bounds for transfer learning in Bayesian optimisation, in: Artificial Intelligence and Statistics, 2017, pp. 307–315.

[27] J. E. Angus, The probability integral transform and related results, SIAM review 36 (1994) 652–654.

[28] J. Schur, Bemerkungen zur Theorie der beschränkten Bilinearformen mit unendlich vielen Veränderlichen., Journal für die reine und Angewandte Mathematik 140 (1911) 1–28.

[29] J. N. van Rijn, F. Hutter, Hyperparameter importance across datasets, in: Proceedings of the 24th ACM SIGKDD International Conference on Knowledge Discovery & Data Mining, ACM, 2018, pp. 2367–2376.

[30] H. Hoos, U. B. C. Ca, K. Leyton-Brown, An efficient approach for assessing hyperparameter importance, in: International conference on machine learning, 2014, pp. 754–762.

[31] J. Vanschoren, J. N. Van Rijn, B. Bischl, L. Torgo, OpenML: networked science in machine learning, ACM SIGKDD Explorations Newsletter 15 (2014) 49–60.
[32] C.-C. Chang, C.-J. Lin, LIBSVM: a library for support vector machines. ACM transactions on intelligent systems and technology (TIST) 2 (2011) 27. URL: https://www.csie.ntu.edu.tw/~cjlin/libsvm.

[33] P. Cortez, A. d. J. R. Morais, A data mining approach to predict forest fires using meteorological data (2007).