Incorporating Expert Prior Knowledge into Experimental Design via Posterior Sampling

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Abstract. Scientific experiments are usually expensive due to complex experimental preparation and processing. Experimental design is therefore involved with the task of finding the optimal experimental input that results in the desirable output by using as few experiments as possible. Experimenters can often acquire the knowledge about the location of the global optimum. However, they do not know how to exploit this knowledge to accelerate experimental design. In this paper, we adopt the technique of Bayesian optimization for experimental design since Bayesian optimization has established itself as an efficient tool for optimizing expensive black-box functions. Again, it is unknown how to incorporate the expert prior knowledge about the global optimum into Bayesian optimization process. To address it, we represent the expert knowledge about the global optimum via placing a prior distribution on it and we then derive its...
posterior distribution. An efficient Bayesian optimization approach has been proposed via posterior sampling on the posterior distribution of the global optimum. We theoretically analyze the convergence of the proposed algorithm and discuss the robustness of incorporating expert prior. We evaluate the efficiency of our algorithm by optimizing synthetic functions and tuning hyperparameters of classifiers along with a real-world experiment on the synthesis of short polymer fiber. The results clearly demonstrate the advantages of our proposed method.

**Keywords** Experimental design · Bayesian optimization · Prior knowledge · Hyperparameter tuning · Thompson sampling

1 Introduction

Experimenting advances scientific progress. However, experimenters usually are annoyed by the allocation of time and resource before conducting experiments, or how to achieve experimental purposes rapidly and solidly. Experimental design is therefore involved with finding optimal experimental parameters, or experimental configurations that result in the best performance by using fewer experiments. In many cases, experimental design is in essence a black-box optimization problem as the form of the underlying function is unknown. With the underlying function \( f \), experimental design can be formulated as a maximization (or minimization) problem

\[
\mathbf{x}_* = \arg\max_{\mathbf{x} \in \mathcal{X}} f(\mathbf{x}),
\]

where \( \mathbf{x}_* \) is the global maximizer and \( \mathcal{X} \) is the search space of the design parameters or variables \( \mathbf{x} \). We assume an optimization setting where the evaluation of the function evaluation is expensive. This assumption holds fairly typically as performing experiments in most experimental design domains is costly in money and/or time. Due to this, we would like to optimize the function using as few evaluations as possible. Bayesian optimization (BO) is well known to be an efficient method for optimizing expensive black-box functions [5] and shows competitive performance in broad applications, such as material search [26], experimental design [5] and hyperparameter tuning for machine learning models [21].

Typical BO consists of two main steps. The first step models the function relating input variables \( \mathbf{x} \) to output \( y \) based on existing observations using a probabilistic model. Gaussian process (GP) is a popular choice used in BO since its posterior has a tractable analytical form [16]. The second step uses the posterior GP to construct an acquisition function which qualifies the information about the next evaluation and then acquires the maximizer of the acquisition function to be the next evaluation. The only prior knowledge in BO (using a GP) is that the unknown function \( f \) is smooth and can be modeled using a GP with an appropriate kernel. Some work has incorporated various forms of expert prior knowledge about \( f \) such as monotonicity [17,12] and unimodality [1]. However, in an optimization problem, the main goal is to reach
close-to-optimum solutions. Any expert prior knowledge about the optimum location would be extremely valuable. This kind of expert prior knowledge or hypothesis is indeed common in practice. For example, domain experts through their experience over time have some hunches about the region in the parameter space that yields good product quality (section 5.3). An experienced modeler also has some practical experience about potential model hyperparameters [18,6]. To the best of our knowledge, no work in the context of Bayesian optimization has incorporated expert prior knowledge about the location of the global optimum.

In this paper, we therefore aim to facilitate experimental design by leveraging expert prior knowledge about the location of the global optimum in Bayesian optimization. We propose to represent this expert prior knowledge through a vague probability distribution of a random variable $x^*$ i.e. $\pi(x^*)$, where $x^*$ is the estimation for $x_*$. Currently, there is no provision in BO algorithms to incorporate the expert prior $\pi(x^*)$. Some acquisition functions used in BO such as entropy search (ES) [8], predictive entropy search (PES) [9] and Thompson sampling (TS) [10] employ the samples from the posterior distribution $p(x^* | D_n)$ conditioning on the observations $D_n = \{x_i, y_i\}_{i=1}^n$, where $y_i$ is a noisy function value at $x_i$. In these cases, $p(x^* | D_n)$ is computed in the standard GP that implicitly includes a uniform expert prior on the global optimum. However, it is unknown how to obtain the posterior distribution of $x^*$ after introducing a non-uniform expert prior $\pi(x^*)$ on the global optimum. In this paper, we derive a simple yet efficient approach to compute the posterior distribution $p(x^* | D_n, \pi)$ and then adopt posterior sampling to suggest the next evaluation. The main contributions in this paper are:

- We propose an efficient approach to incorporate the expert prior knowledge about the global optimum into Bayesian optimization to facilitate experimental design;
- We theoretically analyze the convergence of the proposed algorithm and discuss the robustness of incorporating expert prior;
- We evaluate the efficiency of our algorithm by optimizing synthetic functions and several real-world applications including hyperparameter tuning and material design.

1.1 Related Work

Researchers and practitioners believe that their experience or understanding on optimization process can leverage Bayesian optimization (BO). The prior knowledge about the latent function shape such as monotonicity [12] and unimodality [11] has been considered into BO and demonstrated improvement over the standard BO without that kind of prior knowledge. Another line of related work is to obtain the knowledge from related tasks and then transfer them to the target task. One representative work is multi-task BO [24], which transfers the knowledge about the source function to the optimization of the target function via multi-task GP [4]. Similar ideas such as meta-learning [7]
and warm-start initialization [15] have also been applied to hyperparameter tuning. However, these methods are not capable to directly incorporate the available expert prior knowledge about the global optimum \( \pi(x^*) \), which is the focus of this paper. Further, our method can also use related source observations to construct \( \pi(x^*) \) and thus covers the problem territory traditionally addressed by existing transfer learning methods.

There are limited BO studies taking the prior knowledge about the optimum location into account. Siivola et al. [20] stated that the global optimum is unlikely to lie in the boundary of the search space and proposed to overcome the over-exploration on boundary by placing virtual derivative signs (‘+’ or ‘-’) on the boundary. The virtual derivative signs around the boundary are a weak form of prior knowledge for the GP model so that this method does not demonstrate any advantages in experiments if the region of placing derivative signs is not large enough. Our prior knowledge is straightforwardly related with the location of the global optimum and is a strong prior. Moreover, our method can support \( \pi(x^*) \) at any location instead of only the non-boundary region assumption as [20,13].

Someone may argue why not reduce the search space to align with the expert prior on the global optimum. The reason is that once the expert prior is much off from the true optimum location, then the reduced search space may not contain the global optimum and one has to restart the optimization. Our proposed method can still converge with a misleading prior (refer to section 4).

2 Bayesian Optimization

The goal of BO is to find the global maximizer \( x^* = \arg\max_{x \in X} f(x) \) in the domain: \( X \rightarrow \mathbb{R} \) by using as few evaluations as possible for an unknown and derivative-free function \( f(x) \). Recall that \( D_n = \{x_i, y_i\}_{i=1}^n \) denotes a set of \( n \) observations, where \( y_i \) is a noisy function value at \( x_i \), i.e. \( y_i = f(x_i) + \varepsilon_i \) with \( \varepsilon_i \sim \mathcal{N}(0, \sigma^2) \), and \( \sigma^2 \) is a noise variance. The first step of the BO is to model the latent function using Gaussian process (GP) [16]. A GP is a collection of random variables where the joint distribution of any finite subset of these variables is still a Gaussian distribution. It can be specified by the mean function \( \mu \) and the covariance function \( K \). Without the loss of generality, a zero-mean GP is often employed in BO, i.e. \( f \sim \mathcal{GP}(0, K) \). Then for a predicted point \( x' \), the mean and variance of its function value can be computed as

\[
\begin{align*}
\mu(x') &= k^T K^{-1} y_{1:n} \\
\sigma^2(x') &= k(x', x') - k^T K^{-1} k
\end{align*}
\]

where \( y_{1:n} = \{y_i\}_{i=1}^n \), \( k = [k(x', x_1) \cdots k(x', x_n)]^T \) and the Gram matrix \( K = [k(x_i, x_j)]_{i,j \in \{1, \ldots, n\}} + \sigma^2 I \). The \( k \) is a kernel function and some common choices for the GP include the square exponential (SE) kernel and the Matérn kernel [16]. The second step of BO is to construct an acquisition function
Algorithm 1 Thompson Sampling for BO

Input: observations \( D_0 = \{x_0, y_0\} \), the kernel \( k \)

1: for \( n = 1, 2, \ldots \) do
2: build the GP \( GP(\mu_n, K_n) \) conditioning on \( D_{n-1} \)
3: randomly sample a function \( f_n \sim GP(\mu_n, K_n) \) (section 3.1)
4: obtain the next evaluation \( x_n = \arg\max_{x \in X} f_n(x) \);
5: evaluate \( y_n = f(x_n) + \epsilon \);
6: augment the data \( D_n = D_{n-1} \cup \{x_n, y_n\} \);
7: end for

quantifying the information about the next evaluation based on the GP. The popular acquisition functions include expected improvement (EI), probability improvement (PI) and upper confidence bound (UCB) \([5]\).

Information-theoretic acquisition functions have recently emerged since they directly measure the uncertainty about the global optimum \( x^* \). Popular acquisition functions include entropy search (ES) \([8]\) and predictive entropy search (PES) \([9]\), which are defined respectively

\[
\alpha_{ES}(x) = H[p(x^* | D_n)] - E_{p(y|x, D_n)}[H[p(x^* | D_n \cup (x, y))]]
\]

\[
\alpha_{PES}(x) = H[p(y | D_n, x)] - E_{p(x^*|D_n)}[H[p(y | D_n, x, x^*)]].
\]

These two entropy-based methods often involve sophisticated approximations. The common term for them is the posterior distribution \( p(x^*|D_n) \). More specifically we can understand it as a conditional density function of the random variable \( x^* \) given \( D_n \). We can write it

\[
p(x^* | D_n) = \int p(x^* | f)p(f | D_n)df,
\]

where \( p(x^* | f) = p(f(x^*) = \max_{x \in X} f(x)) \). Eq.(5) implies the generative process of \( x^* \) in GP model: sampling a function from the posterior \( p(f | D_n) \) and then maximizing this function to obtain \( x^* \). This process is also known as Thompson sampling (TS). For BO, at step \( i \), we randomly sample a function from the posterior GP \( f_i \sim GP \) and obtain the next evaluation \( x_i = \arg\max_{x \in X} f_i(x) \). The sequential TS in BO is shown in Alg.1

3 Bayesian optimization via Posterior Sampling

Suppose that the expert knowledge about the location of the global optimum \( x_* \) is available in prior. Our goal is to accelerate experimental design by incorporating this kind of expert prior knowledge into BO.

Recall that \( x_* \) is the global optimum. Since it is unknown, we denote its estimation by \( x^* \). Formally, we represent the expert prior as a probability distribution of the random variable \( x^* \), denoted by \( \pi(x^*) \) or \( \pi \). We do not limit \( \pi \) in non-boundary regions \([20]\) while extending it to any region aligning with
Fig. 1: The graphical model for the optimum $x^*$ in the standard GP (a) and in the GP with the expert prior knowledge $\pi(x^*)$ (b). The shadow circle denotes observation and the plain circle denotes unobserved variable. $\mathcal{D}_n$ is the function observations and $\pi$ is the expert prior knowledge about $x^*$.

The transformation from Eq.(8) to (9) employs Eq.(5). The target posterior $p(x^* \mid \mathcal{D}_n, \pi)$, therefore, can be inferred

$$p(x^* \mid \mathcal{D}_n, \pi) \propto p(x^* \mid \mathcal{D}_n) \pi(x^*) \quad (10)$$

Subsequently, the next evaluation point can be suggested by randomly sampling from the target posterior above. Since the $p(x^* \mid \mathcal{D}_n)$ is intractable, we cannot directly sample from Eq.(10). In practice, we can sample $N$ maxima $\{x^*_i\}_{i=1}^N$ from $p(x^* \mid \mathcal{D}_n)$ (we show how to do it in section 3.1) and weight it by
Algorithm 2 BO via posterior sampling (PS)

Input: observations \( \mathcal{D}_0 = \{x_0, y_0\} \), the kernel \( k \), the prior distribution \( \pi(x^*) \)

1: for \( n = 1, 2, \cdots \) do
2: \hspace{1em} compute \( \mathcal{G}P(\mu_n, K_n) \) conditioning on \( \mathcal{D}_{n-1} \)
3: \hspace{1em} for \( i = 1, \cdots, N \) do
4: \hspace{2em} randomly sample a function \( f^i \sim \mathcal{G}P(\mu_n, K_n) \) and obtain the maximizer \( x^*_i \) (section 3.1)
5: \hspace{1em} end for
6: \hspace{1em} sample a new point \( x_n \) via Eq.(11)
7: \hspace{1em} evaluate \( y_n = f(x_n) + \epsilon \)
8: \hspace{1em} augment the data \( \mathcal{D}_n = \mathcal{D}_{n-1} \cup \{x_n, y_n\} \)
9: end for

using \( \pi \), or

\[
p(x^* = x^*_i \mid \mathcal{D}_n, \pi) \propto \frac{\pi(x^*_i)}{\sum_{i=1}^N \pi(x^*_i)}
\] (11)

Then a new point can be sampled from Eq.11. Our algorithm for a maximization problem is presented in Alg. 2. Our proposed method incorporating prior knowledge to update the GP posterior is straightforward to apply to PES (refer to Eq.(11)).

3.1 Sampling \( x^* \) from posterior GP

We can sample a function \( f \) from the posterior GP and return the global maximizer \( x^* \). However, evaluating such an \( f \) is very costly since it requires the complexity \( O(m^3) \), where \( m \) is the number of function evaluations necessary to find the optimum. In theory \( m \) is perhaps very huge. Following the method in [9, 25], we approximate a sampled function using the linear model \( f(x) \approx \phi(x)^T \theta \), where \( \phi \) is a set of random feature and \( \theta \) is the corresponding sampled weights from its posterior distribution.

Briefly, according to Bochner’s theorem [3], a shift-invariant kernel \( k \) can be rewritten as

\[
k(x, x') = 2\alpha \mathbb{E}_{p(w)}[\cos(w^T x + b) \cos(w^T x' + b)]
\] (12)

where \( b \sim \mathcal{U}[0, 2\pi] \), \( p(w) = \frac{s(w)}{\alpha} \) is the normalized density of the Fourier dual \( s(w) \) of the kernel \( k \) and \( \alpha = \int s(w)dw \). Further, the kernel can be approximated by \( k(x, x') \approx \phi(x)^T \phi(x') \), where \( \phi(x) = (F^i(x))_{i=1}^m \), \( F^i(x) = \sqrt{2\alpha/m} \cos(w_i^T x + b_i) \) is a pair sampled from \( p(w, b) \). For a Bayesian linear model, conditioning on observation \( \mathcal{D}_n \), the posterior distribution of the weights \( \theta \) is a Gaussian distribution \( \mathcal{N}(\mathbf{m}, \mathbf{v}) \) with

\[
\mathbf{m} = (\Phi^T \Phi + \sigma_w^2 I)^{-1} \Phi^T y_{1:t}
\] (13)

\[
\mathbf{v} = (\Phi^T \Phi + \sigma_w^2 I)^{-1} \sigma_w^2
\] (14)
Fig. 2: The top describes the Thompson samples (colored lines) from the GP given three observations and the returned minimizers (circles). The bottom is the density estimation $p(x^* \mid D_n)$ for minimizers shown in the top.

where $\Phi = [\phi(x_1), \ldots, \phi(x_t)]$.

Let $\phi^{(i)}(x)$ and $\theta^{(i)}$ denote a set of random features and a sample from the posterior distribution of $\theta$. The sampled function can be constructed subsequently by $f^{(i)}(x) = \phi^{(i)}(x)^T \theta^{(i)}$. We then can maximize this function to obtain $x^*_i = \arg\max_{x \in X} f^{(i)}(x)$. We demonstrate an example for a minimization problem in Figure 2.

4 Analysis and Discussion

In this section we would like to understand how the proposed algorithm with a non-uniform prior on $x^*$ behaves. We first make definition about an informative prior and demonstrate the robustness of our algorithm with different priors. We further provide regret insights. We denote posterior sampling with a non-uniform $\pi$ as $\text{PS-G}$.

**Definition 1** Let the search space be $[a, b]$. The distribution $\pi(x^*)$ is an informative prior if two conditions hold: (i) the probability density of the true optimum $x_*$ at the non-uniform prior should be higher than that at the uniform prior, i.e. $\pi(x_*) = \frac{1}{b-a} + r_1$ with $r_1 > 0$; (ii) pick $\delta \in (0, 1)$ then $\exists r_2$, with the probability greater than $1-\delta$, the distance between the true optimum $x_*$ and the best point in the prior is smaller than $r_2$, i.e. $p(||x_* - x^*|| \leq r_2) > 1-\delta$.

The first condition describes the probability of sampling the true optimum with the prior. The higher $r_1$ is, the more informative $\pi$ is. The second condition describes the probability mass around the true optimum. The lower $r_2$ is, the more informative $\pi$ is. We demonstrate a setting of prior in Figure 3.
Fig. 3: The illustration for different priors. \([a, b]\) is the support of the search space and \(x^*\) is the true prior. ‘U’ denotes a uniform prior. According Definition 1, \(\pi_1\) is not an informative prior, \(\pi_2\) and \(\pi_3\) are informative priors, and \(\pi_3\) is more preferable than \(\pi_2\).

Based on Eq.\((10)\), we can know that PS-G with an informative prior tends to sample evaluation points concentrated around the true optimum \(x^*\) because the prior makes a strong impact on the GP itself posterior \(p(x^*|D_n)\). Whilst PS-G with a non-informative (or misleading) prior first samples points by following the prior distribution. After sufficient information about \(f\) has been provided by previous points, PS-G also sample near-optimum points since the GP itself posterior begins to make more effect on the combined posterior. We observe TS and PS-G with different Gaussian priors in a 1D toy example. The results are shown in Figure 4. We can see that both TS and PS-G can converge. TS tends to explore while the PS-G with a prior \(\pi(x^*)\) close to the global minimizer tends to recommend points concentrating around the global minimizer. Note that the density estimate for \(x^*\) in this case is narrower than TS at the same iterations \((n = 6, 8)\), the advantage facilitating optimization. As we expect, PS-G with such a prior indeed takes more iterations for convergence. Of course, PS-G is vulnerable if with an extremely misleading prior.

Finally we analyze the regret of our algorithm with an informative prior. In BO, we are interested in the cumulative regret [22], which is defined as for a maximization problem

\[
R(n) = \sum_{i=1}^{n} \left[ f(x^*_i) - f(x_i) \right].
\] (15)

Since posterior sampling uses a random policy, we compute the expected cumulative regret, called Bayesian cumulative regret, i.e. \(BR(n) = \mathbb{E}[R(n)]\). The expectation in \(BR(n)\) is with respect to any randomness in the algorithm
(a) An example of using Thompson sampling (TS) on a toy 1D design problem. The top subfigure shows the the density estimation for \( x^* \). \( n \) is the number of observations. The bottom subfigure shows the next evaluation suggested by TS that randomly samples a point from the density estimation for \( x^* \) as the next evaluation. The global minimizer of the synthetic function is at \( x = 2 \). At \( n = 8 \), TS almost converges to the global minimizer.

(b) An example of using posterior sampling with a Gaussian prior \( \pi(x^*) \) close to the global minimizer. The top subfigure shows the the density estimation for \( x^* \) and the prior \( \pi(x^*) \) used in this example. The bottom subfigure shows the next evaluation suggested by PS-G. In this case, the PS-G sample points concentrating on the global minimizer and obtains the narrower density estimation of \( x^* \).

(c) An example of using posterior sampling with a Gaussian prior \( \pi(x^*) \) far from the global minimizer. The top subfigure shows the the density estimation for \( x^* \) and the prior \( \pi(x^*) \) used in this example. The bottom subfigure shows the next evaluation suggested by PS-G. In this case, the PS-G sample points aligning with the prior in the beginning and then will converge to the global minimizer since the gross prior becomes weak compared to the the density of \( x^* \).

Fig. 4: The illustration for the robustness of PS-G on a toy 1D design problem. \( n \) is the number of iterations. The global minimizer is at \( x_* = 2 \). The top subfigures show the the density estimation for \( x^* \) (blue) and the prior \( \pi(x^*) \) (green). The bottom subfigures show the next evaluation suggested by algorithms.
including prior on $f$ and noisy distribution. A algorithm is no-regret when
$$\lim_{n \to \infty} \frac{1}{n} BR(n) = 0.$$  

Let $D_n$ denote the collection of $n$ recommended points by PS-G and $D'_n$ denote the collection of $n$ recommended points by TS. $x$ and $\hat{x}$ are the realization of $D_n$ and $D'_n$ respectively. Then we have $E_{\hat{x}}[||x^* - \hat{x}||] \leq E_{\hat{x}'}[||x^* - \hat{x}'||]$ with a high probability. This is actually easy to obvious since PS-G with an informative prior can sample more concentrated points than TS we discuss before. Further, based on this equation, for a uni-modal function $f$, we can safely conclude that the upper bound of Bayes cumulative regret for PS-G is tighter than that of TS at a high probability. For a multi-modal function $f$, a point closer to the true optimum does not indicate its function value closer to $f(x^*)$. Give a small distance $d$ positively relevant with $r_2$ in condition (ii) of Definition 1, we can know that $||x^* - \hat{x}|| \leq d$ hold with a high probability. If $f$ is a Lipschitz-continuous function, then for any point in the support of $f$, we have $|f(x^*) - f(x)| \leq L||x^* - x||$. With a further assumption $|f(x^*) - f(x^*)| \geq Ld$, we can derive $f(x^*) \leq f(x^*) - Ld \leq f(\hat{x})$ with a high probability. It means that PS-G still can obtain the collection of evaluation points which have higher function values than the second global optimum with a high probability. Overall, PS-G can potentially sample near-optimum evaluation points.

Similar with the regret analysis for TS in [19,11], our PS-G is also a no-regret algorithm and thus has convergence guarantee.

5 Experiments

We show the performance of our method (PS) in various tasks. We use a truncated Gaussian $N(\mu, \Sigma)$ or Gamma prior $\Gamma(\alpha, \beta)$ because they exhibit different notions of tail decay and are widely used in machine learning. There does not exist a BO method which can directly incorporate the expert prior $\pi(x^*)$. The algorithms compared in this paper are:

- Our algorithm (PS or PS-G or PS-G-$\mu$-$\Sigma$)
- The non-boundary search method (DBO) [20]
- The standard BO methods without any expert prior (TS, PES and EI)
- The random search on the given prior (Prior-based Random search)

The prior-based Random search can measure the impact of $\pi(x^*)$. We use the SE kernel $k(x, x') = \gamma^2 \exp(-\Sigma_{i=1}^{D} \frac{1}{2l_i^2}(x_i - x'_i)^2)$ for GP modeling, where $\gamma^2$ is the function variance, $l_i$ is the lengthscale for the $i$th dimension, $D$ is the input dimension and we use $\sigma^2$ as the noise variance. For the DBO, virtual derivative sign observations are added if the next proposed point is within 5% of the length of the edge of the search space to any border. The code of our algorithm is shared in https://tini.to/PJJH.
Fig. 5: (a) The 2D objective function sampled from a known GP prior. The white '+' denotes the global minimizer. The red symbols denote the modes of Gaussian priors ‘π1’, ‘π2’ and ‘π3’. (b) optimizing the 2D synthetic function by PS-G with different number of Thompson samples. (c) optimizing the 2D synthetic function by PS-G with the priors of different means but the same covariance $1/16$. (d and e) optimizing the 2D synthetic function by PS-G with the priors of the same mean ($π1$ and $π3$) but the different covariance. (d) optimizing the 2D synthetic function by different algorithms.
5.1 Optimization for Synthetic Function

We generate a 2D objective function sampled from the GP prior with the fixed hyperparameters $\gamma^2 = 1$, $l_i = 0.1$ and $\sigma^2 = 10^{-6}$. The domain is $X = [0, 1]^2$. To generate the function, we first randomly initialize 10,000 locations in $X$. Next, we compute a covariance matrix using the GP prior mentioned above. This covariance matrix is then used to draw a random sample for function values from a 10,000-dimensional multi-variate normal distribution. Then we fit a GP using these 10,000 function observations and use the mean function of the GP as our synthetic function. We demonstrate this function in Figure 5 (a) and we are interested in the global minimizer $x^* = [0.64; 0.50]$. For the synthetic function optimization, we use the known hyperparameters mentioned above into the SE kernel. We started from 3 observations obtained by Latin hypercuber sampling in the domain and repeated experiments 20 times with different initializations. We reported the average and standard errors of simple regret (SR).

On the number of Thompson samples Since the Eq.(11) in our algorithm depends on the number of Thompson samples, we investigate how our algorithm performs with different number of samples. We use the Gaussian prior ‘π1’ in Figure 5 (a) with mean $\mu = [0.56; 0.60]$ and covariance matrix $\Sigma = 1/16I$ (make sure the search space belong to 97.5% confidence level of the prior), where $I$ is the identity matrix. We use different number of Thompson samples (100, 200 and 500) for PS-G. A comparison in terms of simple regret is shown in Figure 5 (b). The results show that PS-G outperforms TS and is little sensitive to the number of Thompson samples. However, we recommend to use $100 \times D$ Thompson samples for reliable estimation.

On different priors We investigate the behavior of the PS-G algorithm when using different priors on $x^*$. Especially we want to understand how our algorithm behaves with different beliefs on prior. We use three Gaussian priors with the modes denoted as ‘π1’, ‘π2’ and ‘π3’ in Figure 5 (a). As before, we use 200 Thompson samples in our algorithms.

- In the first experiment, we use the Gaussian priors with different means and the same covariance. The results in Figure 5 (c) show that PS-G significantly outperforms baseline algorithms and the PS-G with the prior ‘π1’ that is the closest to the global optimum performs the best.
- In the second experiment, we use the Gaussian priors with the same mean (π1) but with the different covariance. The results in Figure 5 (d) indicate that the stronger covariance belief the prior that is close to the global optimum, the better the PS-G.
- In the third experiment, we still use the Gaussian priors with the same mean (π3) but with the different covariance. Note that π3 is far away from the true minimizer. The results in Figure 5 (e) indicate that the weaker covariance belief the prior that is far from the global optimum, the better.
the PS-G. It is easy to understand since the prior will gradually approach to the uniform distribution with the covariance becomes broad.

- In the last experiment, we compare our PS-G algorithm with the comprised mean (π1) and covariance (1/16I) to baselines. The results in Figure 5 (f) show the advantages of the PS-G algorithm. Note that we also compare the PES with the expert prior on x∗ (PES-G) with the standard PES. The result further verifies the efficiency of our method computing the posterior distribution of x∗.

**Optimizing the Hartmann 6D** The global minimizer is $x_\star = [0.20169, 0.150011, 0.476874, 0.275332, 0.311652, 0.6573]$. Suppose we have the Gaussian prior with the mean $\mu = [0.3, 0.3, 0.6, 0.4, 0.4, 0.75]$ and the covariance matrix $\Sigma = 1/8I$. Since PES works slowly in high dimension, we only compare PS-G with EI, TS and prior-based Random Search. The experimental result in Figure 5 (d) shows the effectiveness of our method.

![Fig. 6: simple regret on optimizing Hartmann 6D](image)

**5.2 Hyperparameter Tuning for Classifiers**

In this experiment, we rely on a recent study by [18] who has concluded a good range for some hyperparameters for SVM, random forest and adaboost. For example, SVM can achieve better performance with low values for the gamma hyperparameter and random forest tends to perform well when using small values for minimal samples per leaf. We were inspired by that and constructed vague hyperparameter priors for our experiments via appropriate truncated gamma distributions.

We tune hyperparameters for three classifiers: SVM with RBF kernel (SVM-Rbf), SVM with Sigmoid kernel (SVM-Sigmoid) and random forest (RF).
SVM-Rbf and SVM-Sigmoid use two hyperparameters - complexity (regularization) and gamma. The range of complexity hyperparameter is \([2^{-5}, 2^{15}]\) and gamma is \([2^{-15}, 2^3]\) [18]. The RF includes two hyperparameters - ‘Fraction of random features sampled per node’ and ‘minimal samples per leaf’ and the corresponding range is \([0.1, 0.9]\) and \([1, 20]\). Other hyperparameters involved with these classifiers are set to their default values as in Scikit-learn [14]. We set the noise variance \(\sigma^2_n = 10^{-3}\) for all algorithms and measure the average F-measure over 10-fold cross validations. Since the optimal hyperparameters for these classifiers are expected to locate in the boundary, the non-boundary search methods such as D-BO [20] and BOCK [13] are not applicable. We used the datasets from openML100 [2] - a comprehensive benchmark suites of machine learning datasets. The prior distribution of hyperparameter gamma for both SVM-Rbf and SVM-Sigmoid is a truncated Gamma distribution \(\Gamma(2, 2)\), shown in Figure 7 (a), and the prior of other hyperparameters is a uniform distribution by default. We run the experiments for 10 times. Figure 7 (b,c) shows the differences in maximal validation accuracy during 30 iterations for SVM-Rbf between the PS-G and baselines: values greater than 0 indicate that sampling according to PS-G was better by this amount than the baseline, and vice versa. These differences are aggregated using a violinplot. We can see that PS-G with the Gamma prior works best in the experiments of SVM-Rbf. For the SVM-Sigmoid, PS-G again outperforms the baselines for the dataset credit-approval while all algorithms are close for the cylinder-bands.

For random forest, we used the truncated Gamma prior distribution on ‘minimal sample per leaf’ \(\Gamma(1, 3)\) in Figure 7 (f). The experimental results in Figure 7 (g,h) show the efficiency of the PS-G algorithm.

### 5.3 Maximizing the Desirable SPF

Short polymer fibers (SPF) are often used to coat natural fabrics to make them superior in many aspects e.g. more resistive to pilling, improved water repellence etc. Different types of fabrics generally require different sizes of the fibers for optimal results. The fibers are produced by injecting a polymer liquid through a high speed coagulant (e.g. butanol) flow inside a specially designed apparatus [23,12]. We aim to search for the sample with the maximal percentage fibers with length falling into the range of \([50, 150]\) microns. There are five parameters: geometric factors: channel width (mm), constriction angle (degree), and device position (mm); and, flow factors: butanol speed (cm/s), polymer concentration (ml/h) involved in the experimental device, which construct 162 discrete combinations totally. Random search is most straightforward. However, this experiment is very costly and each takes at least half day, including component preparation, experimental process and post analysis. BO becomes an ideal choice for this expensive experimental design.

Several material experts have offered expert prior knowledge that the optimal sample normally lies in the high value of butanol speed in this case. In this experiment, butanol speed is discrete including 43, 68 and 95. Based on this
Fig. 7: Hyperparameter tuning for SVM and Random forest. (a): the prior $\Gamma(2,2)$ used on the hyperparameter gamma (log-scale) in SVM-Rbf and SVM-Sigmoid. (b,c): the differences in maximal validation accuracy during 30 iterations for SVM-Rbf between PS-G and baselines. 'Diff1' denotes the comparison between PS-G and PES, 'Diff2' denotes the comparison between PS-G and TS, 'Diff3' denotes the comparison between PS-G and EI, and 'Diff4' denotes the comparison between PS-G and prior-based random search. (d,e): the differences in maximal validation accuracy for SVM-Sigmoid between PS-G and baselines. (f): the prior $\Gamma(1,3)$ used on the minimal sample per leaf in Random forest. (g,h): the differences in maximal validation accuracy for RF between PS-G and baselines.
weak prior knowledge, we have designed a truncated Gaussian on the butanol speed (Figure 5.1(a)) so that we can incorporate this knowledge to accelerate adaptive experimental design through our developed framework. Since the search space is discrete, we can directly compute the posterior for each combination based on Eq. (10) and then re-sample to suggest the next evaluation point. We run algorithms for 5 times with different 3 initial samples. Figure 5.1 (b) show the maximal value we achieved at each iteration. The results indicate that the prior knowledge is effective on posterior sampling for experimental design. We also demonstrate the optimal sample we have obtained in 5.1 (c), which has satisfied short polymer fiber experts.

6 Conclusion

We are the first to present how to incorporate arbitrarily expert prior knowledge about the global optimum location $x^*$ to facilitate experimental design. We have used BO to perform sequential experimental design. There are two difficulties to hinder this work to be fully explored before: a) it is not clear how to represent the prior knowledge about the optimum location in a tractable form although the human can perceive, b) it is not clear how to incorporate it into BO either in practice or theory. In this paper, we have addressed both challenges. We have represented the prior knowledge about the optimum location via a vague probability density function $\pi(x^*)$. We infer the updated posterior conditioned on the prior $\pi(x^*)$. Posterior sampling is then employed to suggest the next evaluation. We demonstrate the efficiency of the proposed approach in several optimization tasks. Choosing a proper prior $\pi(x^*)$ is non-trivial but our algorithm can also converge with a gross prior. It is interesting to develop algorithms to detect the misleading prior quickly in future. We ex-
pect our work can provide insight towards incorporating some perceived expert knowledge into experimental design or Bayesian optimization.

Descriptions

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Conflicts of interest/Competing interests

The authors declare that they have no conflict of interest.

Availability of data and material

Most of data is public in this paper.

Code availability

https://tini.to/PJJH.

Authors’ contributions

All authors contributed to manuscript writing. Problem formulation, algorithm development were performed by Cheng Li, Sunil Gupta, Santu Rana and Svetha Venkatesh. Experimental running and software coding were performed by Cheng Li. The experimental results were discussed by all authors.

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