Abstract

While Bayesian Optimization (BO) is a very popular method for optimizing expensive black-box functions, it fails to leverage the experience of domain experts. This causes BO to waste function evaluations on commonly known bad regions of design choices, e.g., hyperparameters of a machine learning algorithm. To address this issue, we introduce Prior-guided Bayesian Optimization (PrBO). PrBO allows users to inject their knowledge into the optimization process in the form of priors about which parts of the input space will yield the best performance, rather than BO’s standard priors over functions which are much less intuitive for users. PrBO then combines these priors with BO’s standard probabilistic model to yield a posterior. We show that PrBO is more sample efficient than state-of-the-art methods without user priors and 10,000× faster than random search, on a common suite of benchmarks and a real-world hardware design application. We also show that PrBO converges faster even if the user priors are not entirely accurate and that it robustly recovers from misleading priors.

1 Introduction

Bayesian Optimization (BO) is a data efficient method for the joint optimization of design choices that gained great popularity in recent years. It is impacting a wide range of areas, including hyperparameter optimization (Snoek et al., 2012b; Falkner et al., 2018), AutoML (Feurer et al., 2015a; Hutter et al., 2018), robotics (Calandra et al., 2016), computer vision (Nardi et al., 2017; Bodin et al., 2016), environmental monitoring (Marchant & Ramos, 2012), combinatorial optimization (Hutter et al., 2011), experimental design (Azimi et al., 2012), RL (Brochu et al., 2010), Computer Go (Chen et al., 2018), hardware design (Koepfinger et al., 2018; Nardi et al., 2019) and many others. It promises greater automation so as to increase both product quality and human productivity. As a result, BO is also established in many large tech companies, e.g., with Google Vizier (Golovin et al., 2017) and Facebook BoTorch (Balandat et al., 2019).

Nevertheless domain experts often have substantial prior knowledge that standard BO cannot incorporate. Users could incorporate prior knowledge by narrowing the search space; however, this type of hard prior can lead to poor performance by missing important regions. BO also supports a prior
over functions \( p(f) \), e.g., via a kernel function. However, this is not the prior experts have: users often know which ranges of hyperparameters tend to work best, and are able to specify a probability distribution \( p_{\text{best}}(x) \) to quantify these priors. E.g., many users of the Adam optimizer (Kingma & Ba, 2015) know that its best learning rate is often in the vicinity of 1e-3, and yet not know the best value for a new application of Adam. Similarly, Navruzyan et al. (2019) derived neural network hyperparameter priors for image datasets based on their experience with five datasets. In these cases, users know potentially good values for a new application, but cannot be certain about them.

As a result, many competent users instead revert to manual search, which can fully incorporate their prior knowledge. A recent survey showed that most NeurIPS 2019 and ICLR 2020 papers that reported having tuned hyperparameters used manual search, with only a very small fraction using BO (Bouthillier & Varoquaux, 2020). In order for BO to be adopted widely, and help facilitate faster progress in the ML community by tuning hyperparameters faster and better, it is therefore crucial to devise a method that fully incorporates priors into BO. This is precisely the main contribution of this paper. The individual steps we make towards this main contribution are as follows:

1. Introduce PrBO, a novel BO variant that combines prior knowledge about the locality of the optimum with a probabilistic model of the observations made.
2. Demonstrate on a comprehensive set of real-world applications and synthetic benchmarks that accurate prior knowledge help PrBO to dramatically outperform standard BO and 10 000 \( \times \) random search respectively.
3. Demonstrate that PrBO is able to overcome misleading prior knowledge and still finds well-performing configurations.

PrBO is publicly available as part of the HyperMapper optimization framework.\(^1\)

2 Background

2.1 Bayesian Optimization

Bayesian Optimization (BO) is an approach for optimizing an unknown function \( f \) that is expensive to evaluate over an input space \( \mathcal{X} \). In this paper, we assume that we always want to minimize \( f \), thus, the goal is to approximate the minimum of a continuous function \( f : \mathcal{X} \to \mathbb{R} \), \( x^* \in \arg\min_{x\in\mathcal{X}} f(x) \).

BO approximates \( x^* \) with an optimal sequence of evaluations \( x_1, x_2, \ldots \in \mathcal{X} \), with each new \( x_{n+1} \) depending on the previous function values \( y_1, y_2, \ldots, y_n \) at \( x_1, \ldots, x_n \). BO achieves this by building a posterior on \( f \) based on the set of evaluated points. At each BO iteration, a new point is selected and evaluated based on the posterior and the posterior is updated to include the new point \( (x_{n+1}, y_{n+1}) \).

The points explored by BO are dictated by the acquisition function, which attributes a value to each \( x \in \mathcal{X} \) by balancing the predicted value and uncertainty of the prediction for each \( x \). In this work, as the acquisition function we choose Expected Improvement (EI) (Mockus et al., 1978), which quantifies the expected improvement over the best function value found so far: \( EI_{f_{\text{inc}}}(x) := \int_{y_n}^{\infty} \max(f_{\text{inc}} - y, 0)p(y|x)dy \), where \( f_{\text{inc}} \) is the incumbent function value, i.e., the best objective function value found so far, and \( p(y|x) \) is a probabilistic model, e.g., a Gaussian Process. Alternatives to EI would be Probability of Improvement (PI) (Jones, 2001), upper-confidence bounds (UCB) (Srinivas et al., 2010), and entropy-based methods (e.g., Hernández-Lobato et al. (2014)).

2.2 Gaussian Process Regression

A Gaussian process (GP) can be described as a regression model that defines a distribution over functions (Williams & Rasmussen, 2006). This is a non-parametric, data-driven model, however we do still make some assumptions about the shape of the final approximated function – in particular, we assume a correlation model can fit the data, with the similarity between points as a function of a distance measure between them. GPs are defined entirely by their mean and covariance function; the predictive distribution of a GP with kernel \( K \) and kernel parameters \( \theta \) is a Gaussian with posterior mean \( \hat{\mu} = K(\theta, x, X)K(\theta, X, X)^{-1}y \) and variance \( \hat{\sigma}^2 = K(\theta, x, x) - K(\theta, x, X)K(\theta, X, X)^{-1}K(\theta, x, X)^\top \).

\(^1\)https://github.com/luinardi/hypermapper/wiki/prior-injection
3 Bayesian Optimization with Priors

We propose a BO approach dubbed PrBO that allows field experts to inject user prior knowledge into the optimization. PrBO uses a Bayesian approach to combine a user-defined prior with a probabilistic model that captures the likelihood of the observed data \((x_i, y_i)_{i=1}^n\). PrBO is independent from the probabilistic model being used, e.g., GPs, Random Forests or Bayesian Neural Networks.

3.1 Priors

PrBO allows users to inject prior knowledge into BO. This is done via a prior distribution that informs where in the input space \(\mathcal{X}\) we expect to find good \(f(x)\) values. A point is considered “good” if it leads to low function values. We denote the prior distribution \(P_g(x)\), where \(g\) denotes that this is a prior on good points and \(x \in \mathcal{X}\) is a given point. In the same way, we define a distribution on where in the input space we expect to have “bad” points: \(P_b(x) = 1 - P_g(x)\)

In practice \(x\) contains several dimensions but it is difficult for domain experts to provide a multivariate distribution \(P_g(x)\). Users can easily specify, e.g., draw, a univariate or bivariate probability distribution for continuous dimensions or provide a list of probabilities for discrete dimensions. In PrBO, users are free to define a complex multi-variate distribution, but we expect the standard use case to be that users only want to specify univariate distributions, implicitly assuming a prior that factors as \(P_g(x) = \prod_{i=1}^{D} P_g(x_i)\), where \(D\) is the number of dimensions in \(\mathcal{X}\), \(x_i\) is the \(i\)-th input dimension of \(\mathcal{X}\), and \(g\) denotes that this is a prior on good points. While a non-factorized prior can of course be more powerful, throughout our experiments, we use this factorized prior to mimic what we expect standard users to be able to provide. We study the effect of factorized priors in Appendix F.

3.2 Model

Whereas the standard probabilistic model in BO, e.g., a GP, quantifies \(p(y|x)\) directly, that model is hard to combine with the user-defined prior \(P_g(x)\). We therefore now introduce a method to translate our standard probabilistic model \(p(y|x)\) into a model that is easier to combine with this prior. Similar to the TPE work in Bergstra et al. (2011), we model \(p(x|y)\) and \(p(y)\) instead of \(p(y|x)\).

The essential computation we perform for this translation is to quantify the probability that a given input \(x\) is “good” under our standard probabilistic model \(p(y|x)\). We define settings as “good” if their observed \(y\)-value is below a certain quantile \(\gamma\) of the observed function values (so that \(p(y < f_\gamma) = \gamma\), as in TPE. We in addition exploit the fact that our standard probabilistic model \(p(y|x)\) has a Gaussian form, and under this Gaussian prediction we can compute the probability \(M_g(x)\) of the function value lying below a certain quantile using the standard closed-form formula for PI (Kushner 1964):

\[
M_g(x) = p(f(x) < f_\gamma|x) = \Phi \left( \frac{f_\gamma - \mu_x}{\sigma_x} \right),
\]

where \(\mu_x\) and \(\sigma_x\) are the mean and standard deviation of the probabilistic model at \(x\), and \(\Phi\) is the standard normal CDF, see Figure 1. Likewise, we compute a probability \(M_b(x)\) of \(x\) being bad.

3.3 Posterior

PrBO combines the prior in Section 3.1 and the model in Eq. (1) into a posterior on “good” points. This posterior represents the updated beliefs on where we can find good points, based on the prior and data that has been observed. The posterior is computed as the product of the prior and the model:

\[
g(x) \propto P_g(x)M_g(x)^\frac{t}{\beta},
\]

where \(t\) is the current optimization iteration, \(\beta\) is an optimization hyperparameter, and \(P_g(x)\) and \(M_g(x)\) are defined in Section 3.1 and Eq. (1) respectively. We note that this posterior is not normalized, but this suffices for PrBO as the normalization constant cancels out (c.f. Section 3.5).

The \(t/\beta\) fraction in Eq. (2) controls how much weight is given to the model. As the optimization progresses, more weight is given to the model over the prior. Intuitively, we put more emphasis on the model as it observes more data and becomes more accurate. We do this under the assumption that the
We note that, since our posterior is not normalized, computing it directly as in Equation (2) can lead with higher \( \beta \) (bottom) on the right and left of the global optimum in light green crosses. After 20 iterations, see

This section visualizes the prior \( P(x) \) and \( P_b(x) \), quantile \( \gamma \) and BO budget \( B \).

Algorithm 1 PrBO Algorithm. \( D \) keeps track of all function evaluations so far: \( \{x_i, y_i\}_{i=1}^\beta \).

\[
\begin{align*}
1: & \quad \text{Input: Input space } X, \text{ user-defined prior distributions } P_y(x) \text{ and } P_b(x), \text{ quantile } \gamma \text{ and BO budget } B. \\
2: & \quad \text{Output: Optimized point } x_{\text{inc}}. \\
3: & \quad D \leftarrow \text{Initialize}(X). \\
4: & \quad \text{for } t = 1 \text{ to } B \text{ do} \\
5: & \quad \quad M_g(x) \leftarrow \text{fit\_model\_good}(D) \\
6: & \quad \quad M_b(x) \leftarrow \text{fit\_model\_bad}(D) \\
7: & \quad \quad g(x) \leftarrow P_y(x) \cdot M_g(x)\cdot t \beta \\
8: & \quad \quad b(x) \leftarrow P_b(x) \cdot M_b(x)\cdot t \beta \\
9: & \quad \quad x_t \in \arg \max_{x \in X} EI_f(x) \\
10: & \quad \quad y_t \leftarrow f(x_t) \\
11: & \quad \quad D = D \cup (x_t, y_t) \\
12: & \quad \text{end for} \\
13: & \quad x_{\text{inc}} \leftarrow \text{ComputeBest}(D) \\
14: & \quad \text{return } x_{\text{inc}}
\end{align*}
\]

The model will eventually be better than the user at predicting where to find good points. This also allows to recover from "bad" priors as we show in Section 4.2; as in any good Bayesian model, the data ultimately washes out the prior. The \( \beta \) hyperparameter defines the balance between prior and model, with higher \( \beta \) values giving more importance to the prior to numerical issues. Namely, the posterior can reach extremely low values if the prior and model probabilities are low, especially as the \( t/\beta \) exponent grows. To prevent this, in practice, PrBO uses the logarithm of the posterior instead: \( \log(g(x)) \propto \log(P_y(x)) + \frac{t}{\beta} \cdot \log(M_g(x)) \).

Once again, we also define a posterior distribution on bad \( x \), \( b(x) \), with a similar approach. We then use these quantities to compute a density model \( p(x|y) \) as follows:

\[
p(x|y) \propto \begin{cases} 
  g(x) & \text{ if } f(x) < f_\gamma \\
  b(x) & \text{ if } f(x) \geq f_\gamma.
\end{cases}
\]  

(3)

3.4 Model and Posterior Visualization

This section visualizes the prior \( P_y(x) \), the model \( M_g(x) \), and the posterior \( g(x) \) for a 1-dimensional Branin function and their evolution over the optimization iterations. We define this function by setting the second dimension of the Branin function to the global optimum \( x_2 = 2.275 \) and optimizing the first dimension. We perform an initial design of \( D + 1 = 2 \) random points sampled from the prior and use a GP as predictive model. We use a Beta distribution prior \( P_b(x) = B(3, 3) \) which resembles a truncated Gaussian centered close to the global optimum and compute the model \( M_g(x) \) and posterior \( g(x) \) following Eq. (1) and (2) respectively. Figure 2 shows the optimization at different stages.

Figure 2a shows the initialization phase (bottom) and the Beta prior (top). After 5 BO iterations, in Figure 2b (top), the posterior is high near the global minimum, around \( x = \pi \), where both the prior and the model agree there are good points. After 10 BO iterations in Figure 2c (top), there are three regions with high posterior. The middle region, where PrBO is exploiting until the optimum is found, and two regions to the right and left, which will lead to future exploration as shown in Figure 2d (bottom) on the right and left of the global optimum in light green crosses. After 20 iterations, see Figure 2e (top), the posterior vanishes where the model is certain there will be no improvement, but is high wherever there is uncertainty in the GP. Note that the influence of the prior after 20 iterations is weaker, because of \( t/\beta \) in Eq. (2).
We adopt the EI formulation used in \cite{Bergstra2011} by replacing their Adaptive Parzen
Algorithm 1 shows the PrBO algorithm, based on the components defined in the previous sections. In
As defined in Section 3.2,
3.5 Acquisition Function
Then \( p(y < f_{\gamma}) = \gamma \) and \( \gamma \) is a quantile of the observed objective values \( \{y^{(i)}\} \).
and computes the posteriors \( g(x) \) and \( b(x) \) (lines 7 and 8 respectively). The EI acquisition function
so that finally
\[
EI_{f_{\gamma}}(x) = \frac{\gamma f_{\gamma} \gamma g(x) - g(x) \int_{-\infty}^{f_{\gamma}} yp(y) dy}{\gamma g(x) + (1 - \gamma) b(x)} \propto \left( \gamma + \frac{b(x)}{g(x) (1 - \gamma)} \right)^{-1}.
\] (6)
Eq. (6) shows that to maximize improvement we would like points \( x \) with high probability under
low probability under \( b(x) \), i.e., minimizing the ratio \( b(x)/g(x) \). We note that the point
that maximizes the ratio for our unnormalized posteriors will be the same that maximizes the ratio for
normalized posterior and, thus, the computation of the normalized posteriors is unnecessary.

3.6 Putting It All Together
Algorithm 1 shows the PrBO algorithm, based on the components defined in the previous sections. In
Line 3, PrBO starts with a design of experiments (DoE) phase, where it randomly samples a number
of points from the user-defined prior \( P_{y}(x) \). After initialization, the BO loop starts at Line 4. In each
loop iteration, PrBO fits the probabilistic model on the previously evaluated points (lines 5 and 6)
and evaluates the posteriors \( g(x) \) and \( b(x) \) (lines 7 and 8 respectively). The EI acquisition function
is computed next, using the posteriors, and the point that maximizes EI is selected as the next point
to evaluate at line 9. The black-box function evaluation is performed at Line 10. This BO loop is
repeated for a pre-defined number of iterations, according to the user-defined budget \( B \).
Extending PrBO to Multi-Objective Optimization. PrBO can also be used in a multi-objective setting, by using random scalarizations [Paria et al., 2019]. Details can be found in the Appendix B.

4 Experiments

We implement both GPs and Random Forests (RF) as predictive models and use GPs in our experiments unless stated otherwise. We set the model weight $\beta = 10$ and the model quantile to $\gamma = 0.05$, see our sensitivity hyperparameter study in Appendices A and B. Before starting the main BO loop, we randomly sample $D + 1$ points consistently on all benchmarks. We optimize our EI acquisition function using a multi-start local search, similar to the one used in SMAC (Hutter et al., 2011). We start with four synthetic benchmarks: Branin, SVM, FC-NET and XGBoost, which are 2, 2, 6 and 8 dimensional respectively. The last three are part of the Profet benchmarks (Klein et al., 2019), generated by a generative model built using performance data on OpenML or UCI datasets. See Appendix C for more details on the experimental setup. SVM from Profet has similar results to the other benchmarks, we report them in Appendix D.

4.1 Prior Selection

In this section we study the effect of choosing a prior. How does prior selection affect the performance of PrBO? A suitable property of the prior is that, by selecting a tighter prior around an optimum, we would expect sampling from the prior to have an increased performance. To the limit, if the prior is composed by only one point which is one of the global optima, then the first sample (and all of them) from the prior will hit the optimum. To have a sanity check of this property, we build an artificial prior in a controlled way. We rely on an automated computation of the prior by computing a univariate Kernel Density Estimation (KDE) using a Gaussian kernel on the synthetic benchmarks introduced above. We note that the goal of these synthetic priors is to have an unbiased prior for our experiments, whereas manual priors would be biased by our own expertise of these benchmarks. In practice, users will manually define these priors without needing additional experiments. We refer an interested reader to Appendix F for multivariate KDE prior experiments.

We experiment with an array of varying quality priors. We select a constant $10D$ points in each prior and vary the size of the random sample dataset so that we can make the priors more sharply peaked around the optima in a controlled environment. We use the best performing $10D$ samples to create the prior from a random sample dataset size of $10D^{100}$; we refer to this prior as $x\%$ in Figure 4. As an example the XGBoost benchmark has $d = 8$, so, $100\%$ means we sample 80 points and use all 80 to create the prior, $10\%$ means we sample 800 points and use the best performing 80 to create the prior, $1\%$ means we sample 8000 and use the best 80 to create the prior, and so on.
Figure 4 shows the performance of purely sampling from the prior and running PrBO respectively after 10D function evaluations with different priors. A bigger random sample dataset and a smaller percentage leads to a tighter prior around the optimum, making the argument for a stronger prior. This is confirmed by Figure 4, where a sharply peaked prior (right side of the figure) leads to a better performance in both scenarios. In addition we observe that in contrast to sampling from the prior, PrBO achieves a smaller regret by being able to evolve from the initial prior and making independent steps towards better values of the objective function. More extensive experiments with a similar trend, including the rest of the benchmarks, are in Appendix I.

4.2 Prior Forgetting

In this section, we show that PrBO can recover from a wrong prior, thanks to our predictive model and the $t/\beta$ parameter in the posterior computation Eq. 2. As BO progresses, the predictive model becomes more accurate and receives more weight, guiding optimization away from the wrong prior and towards better values of the objective function. Figure 3 shows PrBO on the 1D Branin function with an exponential prior. Columns (b), (c), and (d) show PrBO after $D + 1 = 2$ initial samples and 0, 10, 20 BO iterations respectively. After initialization, as shown in column (b), the posterior is nearly identical to the exponential prior and guides PrBO towards the region of the space on the right, which is towards the local optimum. This happens until the predictive model becomes certain there will be no more improvement from sampling that region (columns (c) and (d)). After that, the predictive model guides the posterior towards exploring regions with high uncertainty. Once the global minimum region is found, the posterior starts balancing exploiting the global minimum and exploring regions with high uncertainty, as shown in (d) (bottom). Notably, the posterior after $x > 4$ falls to 0 in (b) (top), as the predictive model is certain there will be no improvement from sampling that region of the local optimum. Additional examples of forgetting are provided in Appendix A, while a comparison of PrBO with wrong priors, no prior, and correct priors is provided in Appendix C.

4.3 Comparison Against Strong Baselines

Figure 5 compares PrBO to other optimization methods using the log simple regret on five runs (mean and std error reported) on the synthetic benchmarks. We compare the results of PrBO with and without priors (both weak and strong) to 10,000x random search (RS, i.e., for each BO sample we draw 10,000 random samples) sampling from the strong prior only, and Spearmint (Snoek et al., 2012a) which is a well-adopted BO approach using GPs and the EI acquisition function.

PrBO Prior beats 10,000x RS on all benchmarks while this is not always the case for other optimization methods, including Spearmint. It performs better than PrBO with a weak prior as expected. It also either outperforms or matches the performance of sampling from the prior; this is expected because prior sampling cannot recover from a non-ideal prior. The two methods are identical up to the initialization phase because they both sample from the same prior in that phase.

PrBO Prior is more sample efficient and finds better or equal results than Spearmint on three out of the four benchmarks. On XGBoost, PrBO leads the performance until 139 BO iterations, where
Spearmint catches up. However, even if Spearmint performs better than PrBO after 139 iterations, the difference on the objective function values at the end of the optimization is small, about 8.986 for Spearmint and 9.026 for PrBO respectively. Although Spearmint is able to better fine-tune on one of the benchmarks, namely XGBoost, PrBO with a good prior consistently shows tremendous speedups in the early phases of the optimization process and can still overcome the limitations of the prior by achieving better results than prior sampling. Thus in comparison to Spearmint and other traditional BO approaches, PrBO makes use of the best of both worlds, leveraging prior knowledge and efficient optimization based on BO.

4.4 The Spatial Use-case

We next apply PrBO to the Spatial [Koeplinger et al., 2018] real-world application. Spatial is a programming language and corresponding compiler for the design of application accelerators, i.e., FPGAs. We apply PrBO to three Spatial benchmarks, namely, 7D shallow and deep CNNs, and 10D molecular dynamics grid application. We compare the performance of PrBO to RS, manual optimization, and HyperMapper [Nardi et al., 2019], the current state-of-the-art BO solution for Spatial. For a fair comparison both PrBO and HyperMapper use RFs as predictive probabilistic model. The manual optimization and the prior for PrBO were provided by an unbiased Spatial developer, who is not an author of this paper. The priors were provided once and kept unchanged for the whole project. More details on the setup, including the priors used, are presented in Appendix E.

Figure 6 shows the log regret on the Spatial benchmarks. PrBO vastly outperforms RS in all benchmarks, notably, RS does not improve over the default configuration in MD Grid. PrBO also outperforms HyperMapper in the MD Grid benchmark (1.28× speedup). In the CNN benchmarks, PrBO and HyperMapper find similar minima, however PrBO converges faster (1.58× and 1.4× faster for shallow and deep respectively). At last, we note that PrBO is able to leverage the expert’s prior and outperform the expert’s configuration in all benchmarks (2.68×, 1.06×, and 10.4× speedup for shallow CNN, deep CNN, and MD Grid, respectively), though the difference is small in Deep CNN, where the expert’s configuration was already close to the optimum. Thus, PrBO leverages the best of both worlds (the expert prior and BO) to provide a new performance SOTA for Spatial.

5 Related Work

TPE by Bergstra et al. [2011] in HyperOpt [Bergstra et al., 2013] supports limited hand-designed priors in the form of normal or log-normal distributions. We generalize over this approach by allowing more flexible priors, proposing a model-agnostic approach (i.e., PrBO is not limited to the TPE model), and a fully Bayesian treatment where we give more importance to the model as iterations progress. In addition, we show that PrBO outperforms TPE in Appendix E. In parallel work, Li et al. [2020] allow users to specify priors via a probability distribution, similarly to our approach. Their two-level approach first samples a number of configurations by maximizing Thompson samples from

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2We believe PrBO performs worse on this benchmark due to its local search approach no longer finding the optimum of the acquisition function after approximately 90 BO iterations. In future work, we will explore this hypothesis further.
a GP posterior and then chooses the configuration that has the highest prior as the next to evaluate. In contrast, our method leverages the information from the prior better by using a fully Bayesian approach.

Similarly, black-box optimization tools, such as SMAC \cite{Hutter2011} or iRace \cite{Lopez-Ibanez2016} also support simple hand-designed priors, e.g. log-transformations. However, these are not properly reflected in the predictive models and both cannot explicitly recover from bad priors. The same applies to the works of Oh et al. \cite{Oh2018} and Siivola et al. \cite{Siivola2018}.

Our work also relates to meta-learning for BO \cite{Vanschoren2019}, where BO is applied to many similar optimization problems in a sequence such that knowledge about the general problem structure can be exploited in future optimization problems. In contrast to meta-learning, PrBO is the first method that allows human experts to explicitly specify their priors. Further differences to many meta-learning methods for BO are that PrBO does not depend on any meta-features \cite{Feurer2015} and only incorporates a single prior instead of many priors from different experiments \cite{Lindauer2018}.

6 Conclusions and Future Work

We introduce PrBO, a Bayesian Optimization framework that allows users to inject their expert knowledge into the optimization in the form of priors about which parts of the input space will yield the best performance. These are different than standard priors over functions which are much less intuitive for users. BO failed so far to leverage the experience of domain experts, not only causing inefficiency but also getting users away from applying of BO approaches because they could not exploit their years of knowledge in optimizing their black-box functions. PrBO addresses this issue and will nudge new users to adopt BO. We showed that PrBO is more sample efficient than state-of-the-art methods, and 10,000× faster than random search, on synthetic and real-world benchmarks. We also showed that PrBO converges faster and that it robustly recovers from misleading priors.

In future work, we will study how our approach can be used to leverage prior knowledge from meta-learning. Bringing these two worlds together and to automatically get the best of them will likely boost the performance of BO even further.

7 Broader Impact

Our work proposes a novel Bayesian Optimization approach that combines users’ prior knowledge with Bayesian Optimization’s probabilistic model. Our work is foundational and thus will not directly bring societal or ethical consequences. However, PrBO will likely be used in the development of applications for a wide range of areas and, thus, indirectly contribute to their impacts in society. In particular, we envision that PrBO will impact a multitude of fields by allowing ML experts to inject their priors into Bayesian Optimization. We recall that only a small fraction of recent ML research has used Bayesian Optimization for hyperparameter tuning, often favoring manual tuning \cite{Bouthiller2020}. PrBO has the potential to bridge this gap and increase the adoption of Bayesian Optimization, helping experts fine-tune solutions faster and better, using less computational resources. As such, PrBO will contribute to the sustainability of AI.

We also envision that PrBO will have an impact in the democratization of ML. Currently, ML models require expert knowledge in order to fine-tune models and achieve good performance in new applications. The effectiveness of Bayesian Optimization in AutoML \cite{Feurer2015, Hutter2018} and hyperparameter tuning \cite{Snoek2012, Falkner2018} has already been demonstrated. We believe PrBO will bolster this impact. Though non-ML experts may not have priors of their own, they still can leverage the priors established by experts. In the future, we envision that experts might even provide defaults for these priors together with public implementations of their new algorithms.

At last, we note that PrBO will also have a broader impact in optimizing non-ML design decisions for new applications. For instance, Bayesian Optimization has already been demonstrated in computer vision, strengthening applications in simultaneous location and mapping (SLAM) \cite{Nardi2017, Bodin2016} and object detection \cite{Zhang2015}. We argue that enabling users to inject their expertise in the application field in the form of priors will also lead to better and faster results.
We confirm this with our results with Spatial, where PrBO achieves state-of-the-art performance with priors provided by a Spatial expert.

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A  Prior Forgetting Supplementary Experiments

In this section, we show additional evidence that PrBO can recover from wrongly defined priors so to complement section 4.2. Figure 7 shows PrBO on the 1D Branin function as in Figure 3 but with a decay prior. Column (a) of Figure 7 shows the decay prior and the 1D Branin function. This prior emphasize the wrong belief that the optimum is likely located on the left side around \( x = -5 \) while the optimum is located at the orange dashed line. Columns (b), (c), and (d) of Figure 7 show PrBO on the 1D Branin after \( D + 1 = 2 \) initial samples and 0, 10, and 20 BO iterations, respectively. In the beginning of BO, as shown in column (b), the posterior is nearly identical to the prior and guides PrBO towards the left region of the space. As more points are sampled, the model becomes more accurate and starts guiding the posterior away from the wrong prior (column (c)). Notably, the posterior before \( x = 0 \) falls to 0, as the predictive model is certain there will be no improvement from sampling this region. After 20 iterations, PrBO finds the optimum region, despite the poor start (column (d)). The peak in the posterior in column (d) shows PrBO will continue to exploit the optimum region as it is not certain if the exact optimum has been found. The posterior is also high in the high uncertainty region after \( x = 4 \), showing PrBO will explore that region after it finds the optimum.

Figure 8 shows PrBO on the standard 2D Branin function. We use exponential priors for both dimensions, which guides optimization towards a region with only poor performing high function values. Figure 8a shows the prior and Figure 8b shows optimization results after \( D + 1 = 3 \) initialization samples and 50 BO iterations. Note that, once again, optimization begins near the region incentivized by the prior, but moves away from the prior and towards the optima as BO progresses. After 50 BO iterations, PrBO finds all three optima regions of the Branin.

B  PrBO for Multi-objective Optimization

PrBO can also be used in a multi-objective setting, by using random scalarizations (Paria et al., 2019) on the posterior in Eq. 2. The scalarization approach uses a set of weights and a scalarizing function to convert multiple objective values into a single objective. Formally, given a weight distribution \( \mathcal{L} \) defined on the simplex \( \sum_{k=1}^{K} \lambda_k = 1, \lambda_k \geq 0 \), a scalarization function is defined as \( s(\lambda, x) \) where \( \lambda \sim \mathcal{L} \) and \( s : \mathbb{R}^K \times \mathcal{X} \rightarrow \mathbb{R} \) is a function producing scalar values defined over \( \mathcal{X} \) and the support of \( \mathcal{L} \). The scalarization function \( s \) is constructed such that optimizing the function with respect to \( x \) for a given set of weights \( \lambda \) yields a point in the Pareto front, with different \( \lambda \) yielding different points in the Pareto front.

![Figure 7: PrBO on the 1D Branin function with a decay prior. The leftmost column shows the log posterior before any samples are evaluated, in this case, the posterior is equal to the decay prior. The other columns show the model and posterior after 0 (only random samples), 10, and 20 BO iterations. 2 random samples are used to initialize the GP model.](image-url)
For multi-objective applications, we consider separate priors and models for each objective. For the priors, the user provides one probability distribution per variable \( i \) and per objective \( k \). We then construct the prior for each objective \( k \) by multiplying the probability distributions for that objective, as in Section 3.1. Similarly, for the model, we fit a separate GP for each objective \( k \) and compute a probabilistic model for each objective following Eq. (1).

At last, we use the prior and model for each objective to define one posterior \( g_k(x) \) for each objective \( k \). In order to scalarize the posteriors, we then randomly sample a set of weights \( \lambda \) and multiply the weighted posteriors:

\[
g(x) = \prod_{k=1}^{K} g_k(x)^{\lambda_k},
\]

where \( K \) is the number of objectives and \( \lambda_k \) is the weight given to objective \( k \). The same equation is used to scalarize the bad posteriors \( b(x) \), only using \( b_k(x) \) instead of \( g_k(x) \). Once again, we use the logarithm of the scalarized posterior in practice, to improve numerical stability, computed with:

\[
\log(g(x)) = \sum_{k=1}^{K} \lambda_k \cdot \log(g_k(x)).
\]

Our multi-objective PrBO algorithm is shown in Algorithm 2. This algorithm is implemented in the open-source implementation of PrBO.

C Experimental Setup

We use a combination of publicly available implementations for our predictive models. For our Gaussian Process (GP) model, we use GPy’s (since 2012) GP implementation with the Matérn5/2 kernel. We use different length-scales for each input dimensions, learned via Automatic Relevance Determination (ARD) (Neal, 2012). For our Random Forests (RF), we use scikit-learn’s RF implementation (Pedregosa et al., 2011). We set the fraction of features per split to 0.5, the minimum number of samples for a split to 5 and disable bagging. We also adapt our RF implementation to use the same split selection approach as Hutter et al. (2014).

For our constrained Bayesian Optimization (cBO) approach, we use scikit-learn’s RF classifier, trained on previously explored configurations, to predict the probability of a configuration being feasible. We then weight our EI acquisition function by this probability of feasibility, as proposed.
The Branin function has two input dimensions and three global minima.

We use four synthetic benchmarks in our experiments.

We optimize our EI acquisition function using a multi-start local search, similar to the one used by Gardner et al. (2014). We normalize our EI acquisition function before considering the probability of feasibility, to ensure both values are in the same range. This cBO implementation is used in the Spatial use-case as in Nardi et al. (2019).

For all experiments, we set the model weight hyperparameter to \( \beta = 10 \) and the model quantile to \( \gamma = 0.05 \), see Appendices K and L. Before starting the main BO loop, PrBO is initialized by random sampling \( D + 1 \) points from the prior, where \( D \) is the number of input variables. We use the public implementation of Spearminit, which by default uses 2 random samples for initialization.

We set the bandwidth of our KDE priors to \( 100n^{-\frac{2}{3}} \), where \( D \) is the number of input dimensions, see Appendix F. We normalize our KDE priors before computing the posterior, to ensure they are in the same range as our model. We also implement interleaving which randomly samples a point to explore during BO with a 10% chance.

We optimize our EI acquisition function using a multi-start local search, similar to the one used in SMAC (Hutter et al., 2011). Namely, we start local searches on the 10 best points evaluated in previous BO iterations, on the 10 best performing points from a set of 10,000 random samples and on the 10 best performing points from 10,000 random samples drawn from the prior. To compute the neighbors of each of these 30 total points, we normalize the range of each objective to \([0, 1] \) and randomly sample four neighbors from a truncated Gaussian centered at the original value and with standard deviation \( \sigma = 0.2 \).

We use four synthetic benchmarks in our experiments.

**Branin.** The Branin function is a well-known synthetic benchmark for optimization problems (Dixon, 1978). The Branin function has two input dimensions and three global minima.

**SVM.** is a hyperparameter-optimization benchmark in 2D based on Profet (Klein et al., 2019). This benchmark is generated by a generative meta-model built using a set of SVM classification models trained on 16 OpenML tasks. The benchmark has two input parameters, corresponding to SVM hyperparameters.

**FC-Net.** is a hyperparameter and architecture optimization benchmark in 6D based on Profet. The FC-Net benchmark is generated by a generative meta-model built using a set of feed-forward neural networks trained on the same 16 OpenML tasks as the SVM benchmark. The benchmark has six input parameters corresponding to network hyperparameters.

**XGBoost.** is a hyperparameter-optimization benchmark in 8D based on Profet. The XGBoost benchmark is generated by a generative meta-model built using a set of XGBoost regression models in 11

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**Algorithm 2 Multi-objective PrBO.** \( D \) keeps track of all function evaluations so far: \((x_i, y_i)_{i=1}^b, M^k_g(x) \) and \( M^k_b(x) \) are the models per objective \( k \).

1. **Input:** Input space \( \mathcal{X} \), user-defined prior distributions \( P^k_g(x) \) and \( P^k_b(x) \), weight distribution \( \mathcal{L} \) and budget \( B \).
2. **Output:** Optimized Pareto points \( \mathcal{X}_{inc} \).
3. \( D \leftarrow \text{Initialize}(\mathcal{X}) \)
4. for \( t = 1 \) to \( B \) do
5. Sample \( \mathcal{X}^t \sim \mathcal{L} \)
6. \( M^k_g(x) \leftarrow \text{fit_model_good}(D) \) \( \forall k \leq K \)
7. \( M^k_b(x) \leftarrow \text{fit_model_bad}(D) \) \( \forall k \leq K \)
8. \( g(x) \leftarrow \prod_{k=1}^{K} (P^k_g(x) \cdot M^k_g(x)^{\frac{1}{K}})^{\lambda_k} \)
9. \( b(x) \leftarrow \prod_{k=1}^{K} (P^k_b(x) \cdot M^k_b(x)^{\frac{1}{K}})^{\lambda_k} \)
10. \( x_t \in \arg \max_{x \in \mathcal{X}} EI_{f_t}(x) \)
11. \( y_t \leftarrow f(x_t) \)
12. \( D = D \cup (x_t, y_t) \)
end for
14. \( \mathcal{X}_{inc} \leftarrow \text{ComputePareto}(D) \)
15. **return** \( \mathcal{X}_{inc} \)

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by Gardner et al. (2014). We normalize our EI acquisition function before considering the probability of feasibility, to ensure both values are in the same range. This cBO implementation is used in the Spatial use-case as in Nardi et al. (2019).

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3https://github.com/HIPS/Spearmint
Table 1: Search spaces for our synthetic benchmarks. For the Profet benchmarks, we report the original ranges and whether or not a log scale was used.

| Benchmark | Parameter | Parameter values | Log scale |
|-----------|-----------|------------------|-----------|
| Branin    | $x_1$     | $[-5, 10]$       | -         |
|           | $x_2$     | $[0, 15]$        | -         |
| SVM       | $C$       | $e^{-10}, e^{10}$ | ✓         |
|           | $\gamma$  | $e^{-10}, e^{10}$ | ✓         |
| FCNet     | learning rate | $10^{-6}, 10^{-1}$ | ✓         |
|           | batch size | $[8, 128]$       | ✓         |
|           | units layer 1 | $16, 512$       | ✓         |
|           | units layer 2 | $16, 512$       | ✓         |
|           | dropout rate l1 | $[0.0, 0.99]$   | -         |
|           | dropout rate l2 | $[0.0, 0.99]$   | -         |
| XGBoost   | learning rate | $10^{-6}, 10^{-1}$ | ✓         |
|           | gamma      | $[0, 2]$         | -         |
|           | L1 regularization | $10^{-5}, 10^{3}$ | ✓         |
|           | L2 regularization | $10^{-5}, 10^{3}$ | ✓         |
|           | number of estimators | $10, 500$   | -         |
|           | subsampling | $[0.1, 1]$       | -         |
|           | maximum depth | $[1, 15]$       | -         |
|           | minimum child weight | $[0, 20]$   | -         |

Figure 9: Log regret comparison of PrBO with and without priors, $10,000 \times$ RS, and Spearmint (mean +/- one std on 5 repetitions). We run the benchmark for 200 iterations.

UCI datasets. The benchmark has eight input parameters, corresponding to XGBoost hyperparameters.

The search spaces for each benchmark are summarized in Table 1. For the Profet benchmarks, we report the original ranges and whether or not a log scale was used. However, in practice, Profet’s generative model transforms the range of all hyperparameters to a linear $[0, 1]$ range. We use Emukit’s public implementation for these benchmarks (Palayı et al., 2019).

D SVM Regret Comparison

In addition to the experiments in Section 4.3, we show the performance of PrBO on the SVM benchmark. Figure 9 shows a log regret comparison of PrBO, Spearmint, Prior Sampling and $10,000 \times$ RS. We note that the results are similar to the other benchmarks in Figure 5. Namely, PrBO with a strong prior outperforms RS and spearmint. PrBO also outperforms Spearmint with a weak prior and even with a uniform prior.
E Spatial Real-world Application

Spatial (Koeplinger et al., 2018) is a programming language and corresponding compiler for the design of application accelerators on reconfigurable architectures, e.g. field-programmable gate arrays (FPGAs). These reconfigurable architectures are a type of logic chip that can be reconfigured via software to implement different applications. Spatial provides users with a high-level of abstraction for hardware design, so that they can easily design their own applications on FPGAs. It allows users to specify parameters that do not change the behavior of the application, but impact the runtime and resource-usage (e.g. logic units) of the final design. During compilation, the Spatial compiler estimates the ranges of these parameters and estimates the resource-usage and runtime of the application for different parameter values. These parameters can then be optimized during compilation in order to achieve the design with the fastest runtime. We fully integrate PrBO as a pass in Spatial’s compiler, so that Spatial can automatically use PrBO for the optimization during compilation. This enables Spatial to seamlessly call PrBO during the compilation of any new application to guide the search towards the best design on an application-specific basis.

In our experiments, we introduce for the first time the automatic optimization of three Spatial real-world applications, namely, 7D shallow and deep CNNs, and a 10D molecular dynamics grid application. Previous work by Nardi et al. (2019) had applied automatic optimization of Spatial parameters on a set of benchmarks but in our work we focus on real-world applications raising the bar of state-of-the-art automated hardware design optimization. PrBO is used to optimize the parameters to find a design that leads to the fastest runtime. The search space for these three applications is based on ordinal and categorical parameters; to handle these discrete parameters in the best way we implement and use a Random Forest surrogate instead of a Gaussian Process one as explained in Appendix C. These parameters are application specific and control how much of the FPGAs’
Table 3: Search space, priors, and expert configuration for the Shallow CNN application. The default value for each parameter is shown in bold.

| Parameter name | Type    | Values          | Expert | Prior                      |
|----------------|---------|-----------------|--------|----------------------------|
| LP             | Ordinal | [1, 4, 8, 16, 32] | 16     | [0.4, 0.065, 0.07, 0.065, 0.4] |
| P1             | Ordinal | [1, 2, 3, 4]    | 1      | [0.1, 0.3, 0.3, 0.3]        |
| SP             | Ordinal | [1, 4, 8, 16, 32] | 16     | [0.4, 0.065, 0.07, 0.065, 0.4] |
| P2             | Ordinal | [1, 2, 3, 4]    | 4      | [0.1, 0.3, 0.3, 0.3]        |
| P3             | Ordinal | [1, 2, ..., 31, 32] | 1      | [0.01, 0.021, 0.021, 0.021, 0.021, 0.021, 0.021, 0.021, 0.021, 0.021, 0.021, 0.021] |
| x276           | Categorical | [false, true] | true  | [0.1, 0.9] |

Table 4: Search space, priors, and expert configuration for the Deep CNN application. The default value for each parameter is shown in bold.

| Parameter name | Type    | Values          | Expert | Prior                      |
|----------------|---------|-----------------|--------|----------------------------|
| LP             | Ordinal | [1, 4, 8, 16, 32] | 8      | [0.4, 0.065, 0.07, 0.065, 0.4] |
| P1             | Ordinal | [1, 2, 3, 4]    | 1      | [0.1, 0.3, 0.3, 0.3]        |
| SP             | Ordinal | [1, 4, 8, 16, 32] | 8      | [0.4, 0.065, 0.07, 0.065, 0.4] |
| P2             | Ordinal | [1, 2, 3, 4]    | 2      | [0.1, 0.3, 0.3, 0.3]        |
| P3             | Ordinal | [1, 2, ..., 31, 32] | 1      | [0.01, 0.021, 0.021, 0.021, 0.021, 0.021, 0.021, 0.021, 0.021, 0.021, 0.021, 0.021, 0.021, 0.021] |
| x276           | Categorical | [false, true] | true  | [0.1, 0.9] |
resources we want to use to parallelize each step of the application’s computation. The goal here is to find which steps are more important to parallelize in the final design, in order to achieve the fastest runtime. Some parameters also control whether we want to enable pipeline scheduling or not, which consumes resources but accelerates runtime. We refer to Koeplinger et al. (2018) and Nardi et al. (2019) for more details on Spatial’s parameters.

The three Spatial benchmarks also have feasibility constraints in the search space, meaning that some parameter configurations are infeasible. A configuration is considered infeasible if the final design requires more logic resources than what the FPGA provides, i.e., it is not possible to perform FPGA synthesis because the design does not fit in the FPGA. To handle these constraints, we use our cBO implementation (Appendix C). Our goal is thus to find the design with the fastest runtime under the constraint that the design fits the FPGA resource budget.

The priors for these Spatial applications take the form of a list of probabilities, containing the probability of each ordinal or categorical value being good. Each benchmark also has a default configuration, which ensures all methods start with at least one feasible configuration. The priors and the default configuration for these benchmarks were provided once by an unbiased Spatial developer, who is not an author of this paper, and kept unchanged during the entire project. The search space, priors, and the expert configuration used in our experiments for each application are presented in Tables 2, 3, and 4.

### F Multivariate Prior Comparison

Figure 10 shows a log regret comparison of PrBO with univariate and multivariate KDE priors. We show results for univariate and multivariate versions of our weak and strong KDE priors. We use the best $10D$ points out of $1,000D$ and $10,000,000D$ randomly sampled points to create our weak and strong priors, respectively. We use the same points to create the univariate and multivariate priors. We recall that the goal of these synthetic priors is to have an unbiased prior for our experiments,
Figure 11: Log regret comparison of PrBO with varying prior quality. The line and shaded regions show the mean and standard deviation of the log simple regret after 5 runs. All methods were initialized with $D + 1$ random samples, where $D$ is the number of input dimensions, indicated by the vertical dashed line. We run the benchmarks for $100D$ iterations, capped at 300.

whereas manual priors would be biased by our own expertise of these benchmarks. In practice, users will manually define these priors without needing additional experiments.

We note that in all cases PrBO achieves similar performance with univariate and multivariate priors. For the Branin and SVM benchmarks, the weak multivariate prior leads to slightly better results than the weak univariate prior. However, we note that the difference is small, in the order of $10^{-4}$ and $10^{-6}$, respectively.

Surprisingly, for the XGBoost benchmark, the univariate version for both the weak and strong priors lead to better results than their respective multivariate counterparts, though, once again, the difference in performance is small, around 0.2 and 0.03 for the weak and strong prior, respectively, whereas the XGBoost benchmark can reach values as high as $f(x) = 600$. Our hypothesis is that this difference comes from the bandwidth estimator $(100n^{-\pi})$, which leads to larger bandwidths, consequently, smoother priors, when a multivariate prior is constructed.

G Misleading Prior Comparison

Figure 11 shows the effect of injecting a misleading prior in PrBO. We compare PrBO with a wrong prior, no prior, a weak prior, and a strong prior. To create the misleading prior, we use a univariate KDE prior built with the worst $10D$ out of $10,000,000D$ random samples. For all benchmarks, we note that the misleading prior slows down convergence, as expected, since it pushes the optimization away from the optima in the initial phase. However, PrBO is still able to forget the misleading prior and achieve similar regret to PrBO without a prior.
Figure 12: Log regret comparison of PrBO and TPE. The line and shaded regions show the mean and standard deviation of the log simple regret after 5 runs. PrBO was initialized with $D + 1$ random samples, where $D$ is the number of input dimensions, indicated by the vertical dashed line. We run the benchmarks for 100$D$ iterations, capped at 300.

**H Comparison to TPE**

We compare PrBO to the TPE approach of Bergstra et al. (2011) on our four synthetic benchmarks. We use Hyperopt’s implementation of TPE, which defines priors as one of a list of supported distributions, including Uniform, Normal, and Lognormal distributions. Since it is not possible to input the KDE priors introduced in Section 4.1 into the TPE algorithm, we instead use manually defined priors in the format supported by the Hyperopt implementation. We note that this is straightforward in PrBO, as PrBO supports any form of probability distribution as a prior. We are then able to perform a fair comparison between the two approaches that use the same exact prior.

We define the prior for each input parameter as a Gaussian distribution with mean at the optimum and with standard deviation equal to half of the parameters range. For the Branin prior, we arbitrarily choose one of the optima, i.e., the $(\pi, 2.275)$ optimum. For the Profet benchmarks, we use the minimum out of $10,000,000D$ random samples as an approximation of the optimum. We note that using Hyperopt’s Gaussian priors leads to an unbounded search space, which sometimes leads TPE to suggest parameter configurations outside the allowed parameter range. To prevent these values from being evaluated, we convert values outside the parameter range to be equal to the upper or lower range limit, depending on which limit was exceeded.

Figure 12 shows a log regret comparison between PrBO and TPE on our four synthetic benchmarks. PrBO outperforms TPE in three out of four benchmarks, namely, Branin, SVM, and FCNet. We note, however, that the good performance of TPE on XGBoost may be an artifact of the approach of clipping values to its maximal or minimal values as mentioned above. In fact, the clipping nudges TPE towards promising configurations in this case, since XGBoost has low function value near the edges of the search space. Overall, the better performance of PrBO is expected, since PrBO is able to combine prior knowledge with more sample-efficient surrogates, which leads to better performance.

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4https://github.com/hyperopt/hyperopt
Figure 13: Simple regret of sampling from the prior with different priors for our synthetic benchmarks. We provide 5 repetitions for each experiment and mean +/- one std error bars. A more informative prior gives better results in all benchmarks.

1 Prior Bandwidth Selection

We show the effect of different bandwidth sizes on the univariate KDE prior. For that, we compare the performance of sampling from the prior and PrBO with different bandwidth sizes. We use scipy’s Gaussian KDE implementation and modify its bandwidth size with four variations of Scott’s Rule $\hat{a} = \frac{3.54}{n^{\frac{1}{10}}}$, we refer to this prior as $x$; we experiment with $a = 1, b = 4$ (scipy’s default); $a = 1, b = 0$; $a = 10, b = 0$; and $a = 100, b = 0$. Note that larger values for $a$ and smaller values for $b$ lead to smaller bandwidths. For each bandwidth size, we show results for an array of varying quality priors. We select a constant $10D$ points in each prior and vary the size of the random sample dataset. We follow the following rule: we use the best performing $10D$ samples to create the prior from a random sample dataset size of $10D\frac{1}{100}$; we refer to this prior as $x\%$. We experiment with dataset sizes varying from $10D$ to $10^7D$.

Figure 13 shows the performance of purely sampling from the prior. We note that, in most cases, using a larger dataset leads to better results. This is expected, sampling more points means we find more points near the optima and, therefore, the prior will be built with points closer to the optima. Likewise, we note that smaller bandwidths often lead to better results, especially as more points are sampled. This is also expected, since a smaller bandwidth means the prior distribution will be more peaked around the optima. However, there are a couple of exceptions to these trends. First, for the Branin, sampling more points does not lead to a better prior when we use $a = 1, b = 4$, this is likely because the multiple minima of the Branin and the bigger bandwidth lead the prior to be

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(a) $a = 1, b = 4$  
(b) $a = 1, b = 0$  
(c) $a = 10, b = 0$  
(d) $a = 100, b = 0$
Also, the prior are better to explore and also recovering from misleading priors. There are two exceptions
different dataset sizes. PrBO performs better for nearly all dataset sizes and benchmarks. This is
results, we use a

Figure 15 shows a performance comparison between PrBO and sampling from the prior. For these
leads to the best results in all benchmarks, as expected.

The effects of these misleading priors can be especially noticed for the 100% random samples dataset. Based on these results, we set our KDE
priors to $100n^{-\frac{2}{
}}$, where $D$ is the number of input dimensions.

Figure 14 shows the performance of PrBO for different priors. The same observations from Figure 13 hold here. Namely, sampling more points and using smaller bandwidths lead to better performance. Also, the 100% dataset once again leads to inconsistent results, since it is a misleading prior for PrBO. Based on these results, we use the smallest bandwidth and largest dataset in our experiments, i.e. $a = 100$, $b = 0$, and 0.0001%. Intuitively, this is a reasonable choice, since these priors will be our closest approximation to an ideal prior that is centered exactly at the optima, where sampling from the prior always leads to the optimum. Our results in Figures 13 and 14 shows that this combination leads to the best results in all benchmarks, as expected.

Figure 15 shows a performance comparison between PrBO and sampling from the prior. For these results, we use $a = 100$, $b = 0$ and compare the regret of PrBO and sampling from the prior for different dataset sizes. PrBO performs better for nearly all dataset sizes and benchmarks. This is expected as PrBO complements the prior with its probabilistic model, learning which regions within the prior are better to explore and also recovering from misleading priors. There are two exceptions

Figure 14: Simple regret of PrBO with different priors for our synthetic benchmarks. We provide 5 repetitions for each experiment and mean +/- one std error bars. A more informative prior gives better results in all benchmarks.
We show the effect of the $\beta$ hyperparameter introduced in Section 3.2 for the quantile identifying the points considered to be good. To show this, we compare the performance of PrBO with a weak KDE prior and different $\gamma$ values. We use our weak prior as it leads to greater variation in performance, which helps to visualize better the impact of the $\gamma$ hyperparameter. For all experiments, we initialize PrBO with $D + 1$ random samples and then run PrBO until it reaches $10D$ function evaluations. For each $\gamma$ value, we run PrBO five times and report mean and standard deviation.

Figure 16 shows the results of our comparison. We first note that values near the lower and higher extremes lead to degraded performance, this is expected, since these values will lead to an excess of either exploitation or exploration. Further, we note that PrBO achieves similar performance for all values of $\gamma$, however, $\gamma = 0.03$ and $\gamma = 0.05$ consistently lead to better performance, with $\gamma = 0.05$ usually leading to lower deviation.

### J $\gamma$-Sensitivity Study

We show the effect of the $\gamma$ hyperparameter introduced in Section 3.2 for the quantile identifying the points considered to be good. To show this, we compare the performance of PrBO with a weak KDE prior and different $\gamma$ values. We use our weak prior as it leads to greater variation in performance, which helps to visualize better the impact of the $\gamma$ hyperparameter. For all experiments, we initialize PrBO with $D + 1$ random samples and then run PrBO until it reaches $10D$ function evaluations. For each $\gamma$ value, we run PrBO five times and report mean and standard deviation.

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### K $\beta$-Sensitivity Study

We show the effect of the $\beta$ hyperparameter introduced in Section 3.3 for controlling the influence of the prior over time. To show the effects of $\beta$, we compare the performance of PrBO with a weak KDE prior and different $\beta$ values on our four synthetic benchmarks. We use our weak prior as it leads to greater variation in performance, which helps to visualize better the impact of the $\beta$ hyperparameter. For all experiments, we initialize PrBO with $D + 1$ random samples and then run PrBO until it reaches $10D$ function evaluations. For each $\beta$ value, we run PrBO five times and report mean and standard deviation.

Figure 17 shows the results of our comparison. We note that values of $\beta$ that are too low (near 0.01) or too high (near 1000) lead to lower performance. This shows that putting too much emphasis on the model or the prior will lead to degraded performance, as expected. Further, we note that $\beta = 10$
Figure 17: Comparison of PrBO with a weak KDE prior and different values for the $\beta$ hyperparameter on our four synthetic benchmarks. We run PrBO with a budget of $10D$ function evaluations, including $D + 1$ randomly sampled DoE configurations.

lead to the best performance in three out of our four benchmarks. This result is reasonable, as $\beta = 10$ means PrBO will put more emphasis on the prior in early iterations, when the predictive model is still not accurate, and slowly shift towards putting more emphasis on the model as the model sees more data and becomes more accurate.