ProBO: a Framework for Using Probabilistic Programming in Bayesian Optimization

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Abstract
Optimizing an expensive-to-query function is a common task in science and engineering, where it is beneficial to keep the number of queries to a minimum. A popular strategy is Bayesian optimization (BO), which leverages probabilistic models for this task. Most BO today uses Gaussian processes (GPs), or a few other surrogate models. However, there is a broad set of Bayesian modeling techniques that we may want to use to capture complex systems and reduce the number of queries. Probabilistic programs (PPs) are modern tools that allow for flexible model composition, incorporation of prior information, and automatic inference. In this paper, we develop ProBO, a framework for BO using only standard operations common to most PPs. This allows a user to drop in an arbitrary PP implementation and use it directly in BO. To do this, we describe black box versions of popular acquisition functions that can be used in our framework automatically, without model-specific derivation, and show how to optimize these functions. We also introduce a model, which we term the Bayesian Product of Experts, that integrates into ProBO and can be used to combine information from multiple models implemented with different PPs. We show empirical results using multiple PP implementations, and compare against standard BO methods.

1. Introduction
The task of optimization is widespread in science and engineering. For example, one may want to find a material composition that most expresses some desired property, or choose control settings for a process that best achieve certain outcomes. Often, each iteration of an optimization procedure, referred to as a query or experiment, is expensive and costs a great deal of resources including money, time, or human effort. To reduce the cost of expensive optimization, it is paramount to develop methods that are data efficient and yield optimal designs in a minimal number of iterations.

One popular method for efficient optimization given expensive queries is known as Bayesian optimization (BO) (Shahriari et al., 2016; Snoek et al., 2012). In BO, a Bayesian model is used to model an experiment, and then is leveraged to choose subsequent designs $x$ to query. Specifically, one optimizes an acquisition function, which is defined with respect to the model, to choose each $x$.

The most common model used in BO today is the Gaussian Process (GP). This nonparametric Bayesian model makes few assumptions about outcomes $y$, and is particularly useful for black box optimization. There exist many popular acquisition functions that have been derived for GPs. There has also been some work deriving BO procedures for other flexible models including random forests (Hutter et al., 2011) and neural networks (Snoek et al., 2015).

However, to accurately model complex systems, we may want to choose from a broader library of Bayesian models and techniques. We may, for example, want to compose models—e.g. GPs, latent factor (e.g. mixture) models, deep bayesian networks, hierarchical regression models—in various ways, and use them in BO.

Recently developed probabilistic programming languages (PPLs) provide a general way to model structure, problem intuition, and prior knowledge in a Bayesian model (or, more generally, in a probabilistic program (PP)). They allow for easy model specification and composition, quick deployment, and automatic inference, often in the form of samples from an approximate posterior distribution.

PPLs give us a language and framework for building complex models and performing automatic inference, but it is not immediately clear how to make them compatible with standard acquisition functions, for use in a typical BO algorithm. In this paper, we aim to help bridge this gap, and provide a way for any PP or Bayesian model (and inference) implementation to be immediately plugged into a BO loop. Similar to how PPs run inference automatically, we aim to
perform BO automatically, given any user-specified PP and choice of acquisition strategy.

Specifically, we develop a framework (ProBO) for using an arbitrary probabilistic program within a Bayesian optimization procedure. We aim to achieve the following criteria:

1. One can plug in any PP that returns posterior samples, including those with differentiable inference (e.g. Hamiltonian Monte Carlo (HMC), black-box variational inference (BBVI)), exact inference (message passing, GPs), deep PPs (Bayesian neural networks), and universal PPs (simulator models).

2. One can use a variety of acquisition strategies, including Thompson sampling (TS), probability of improvement (PI), expected improvement (EI), upper confidence bound (UCB), and others.

A BO procedure that works automatically with any PP can provide various modeling advantages that benefit BO. For instance, we often have prior knowledge, expert insight, contextual information, or additional observations, all of which may be modeled. These can bias or constrain the optimization routine and improve query predictions, which can increase sample efficiency and greatly reduce the number of iterations needed for BO. A few examples are when:

- Inputs x yield experimental outcomes y according to a known family of functions (e.g. (Li et al., 2018), and our phase shift model in Fig. 2).
- There is an expected feature in the optimization landscape (e.g. (Andersen et al., 2017), (Neiswanger and Xing, 2017), and our basin model in Sec. 4.2).
- There is some latent structure, and inferences about it can yield better decisions on which points to query (e.g. corrupt BO and our denoising GP in Sec. 4.1).
- There exists a simulator that can approximate the experimental process (e.g. discussion in Sec. 5).

In summary, this paper provides the following contributions: We develop a BO framework that is compatible with arbitrary PPs. We describe how a variety of acquisition functions can be implemented approximately using basic PP operators, and how to efficiently optimize these acquisition functions. We give strategies for using PPs within BO in practice, including ensembling models and making the procedure robust to misspecification. Finally, we provide an empirical comparison with standard BO methods, showing that our framework can reduce the number of iterations in BO. Our python implementation of ProBO is available at https://github.com/willieneis/ProBO.

2. Framework

In this section, we first describe a general abstraction for PPs for use within our framework, then use this abstraction to develop black box versions of common acquisition functions that are compatible with arbitrary PPs, and finally show how to efficiently optimize these black box acquisition functions with a multi-fidelity optimization strategy.

2.1. Formalism for Probabilistic Programs

We describe a general formalism for discriminative probabilistic programs for use in BO. Suppose we are modeling a system which, given an input x ∈ X, yields observations y, written y ∼ System(x). We assume that y ∈ R × Y, i.e. the first dimension y0 ∈ R. Observing the system n times at different inputs yields a dataset \( D_n = \{(x_i, y_i)\}_{i=1}^n \). Let there exist a Bayesian model for data \( D_n \), with likelihood \( p(D_n | z) = \prod_{i=1}^n p(y_i | z; x_i) \), where z ∈ Z are latent variables. Let \( p(z) \) denote the PDF of the prior on z. We define the joint model PDF to be \( p(D_n, z) = p(z) p(D_n | z) \). The posterior (conditional) PDF can then be written \( p(z | D_n) = \frac{p(D_n, z)}{p(D_n)} \).

In our formalism, we assume only two basic PP operations:

1. Sample from the data conditional: given an input parameter x and latent variable z, draw from the generative distribution over data p(y | z; x). We write this \( y \leftarrow \text{pp.gen}(x, z) \).

2. Sample from the posterior conditional: given a dataset \( D_n = \{(x_i, y_i)\}_{i=1}^n \), draw S samples from the posterior distribution over latent variables. We write this \( z^S \leftarrow \text{pp.inf}(D_n, S) \).

Using PPs assumed to have only these two operations, we will carry out BO tasks such as constructing and optimizing acquisition functions.

Scope. This formalism encompasses a broad array of PPs, including those making use of Markov chain Monte Carlo (MCMC), most variational or exact inference methods (e.g. GPs and deep PPs (Tran et al., 2017)), and forward simulation methods (e.g. universal PPs (Le et al., 2016)), amortized inference (Ritchie et al., 2016), and ABC methods (Csilléry et al., 2010)).

For example, our formalism is compatible with popular PPL frameworks such as Stan (Carpenter et al., 2015), Edward (Tran et al., 2016), PyMC3 (Salvatier et al., 2016), Pyro (Bingham et al., 2018), GPy (GPy, 2012), Infer.NET (Minka, 2012), Venture (Mansinghka et al., 2014), Anglican (Wood et al., 2014), TensorFlow Probability (Dillon et al., 2017), ProbTorch (Siddharth et al., 2017), and others.

2.2. ProBO Framework

We give the ProBO framework in Alg. 1. Each iteration consists of four steps: draw posterior samples via pp_inf, select an input x by optimizing a black box acquisition function
using \texttt{pp.gen}, observe the system at \(x\), and add the new data to the dataset.

Algorithm 1 ProBO(D\(_n\))

1: for \(n = 1, \ldots, N\) do
2: \(z^S \leftarrow \text{pp.inf}(D_{n-1}, S)\) \(\triangleright\) Posterior sample
3: \(x_n \leftarrow \text{argmin}_{x \in X} \hat{a}(x, z^S, M)\) \(\triangleright\) Optimize \(\hat{a}\)
4: \(y_n \sim \text{System}(x_n)\) \(\triangleright\) Observe system at \(x_n\)
5: \(D_n \leftarrow D_{n-1} \cup (x_n, y_n)\) \(\triangleright\) Add data
6: Return \(D_N\).

Note that a special case of this framework is BO using GP models, where inference can be done exactly (step 1), there is a closed-form expression for the acquisition function \(a(x)\) (step 2), and observing \(\text{System}(x)\) means querying a function at \(x\) and getting a scalar output \(y \in \mathbb{R}\) (step 3).

However, for many Bayesian models and PPs, inference cannot be done exactly, and there does not exist an exact expression for \(a(x)\). Furthermore, many systems may have complex inputs \(x\) and extra observations \(y \in \mathcal{Y}\) (in addition to the value \(y^i \in \mathbb{R}\) to be optimized) (Wu et al., 2017; Astudillo and Frazier, 2017; Śwerski et al., 2013). We’d like to take any PP that models the available information, run any applicable approximate inference method, and use this automatically in BO.

In the following sections, using the two general PP operations defined in Sec. 2.1, we develop approximate acquisition functions \(\hat{a}(x)\) that can be applied broadly, and show how to efficiently optimize these functions. We refer to these as \textit{black box acquisition functions} since they are computed automatically via these two operations, without any model specific derivation.

2.3. Black Box Acquisition Functions

In the ProBO framework (Alg. 1), we denote the black box acquisition function with \(\hat{a}(x, z^S, M)\), where \(z^S\) are \(S\) latent variable posterior samples given by \texttt{pp.inf}. We also include a parameter \(M\), which represents the approximation quality of \(\hat{a}\). We will describe an adaptive method for choosing \(M\) during acquisition optimization in Sec. 2.4. We will make frequent use of the posterior predictive distribution, which is defined to be \(p(y|D_n; x) = \mathbb{E}_{p(z|D_n)}[p(y|z; x)]\).

There are a number of popular acquisition functions used commonly in Bayesian optimization, such as expected improvement (EI) (Močkus, 1975), probability of improvement (PI) (Kushner, 1964), GP upper confidence bound (UCB) (Srinivas et al., 2009), and Thompson sampling (TS) (Thompson, 1933). Special cases of sample-based (Monte Carlo) estimates of certain acquisition functions have been described in prior work (Snoek et al., 2012; Wilson et al., 2018; Hernández-Lobato et al., 2015). However, these focus on GP models where there are Gaussian assumptions for \(p(y|D_n; x)\).

Here, we propose a few simple acquisition estimates for arbitrary PPs that can be computed with \texttt{pp.inf} and \texttt{pp.gen}. Specifically, we give algorithms below for EI, PI, UCB, and TS acquisition strategies, though similar algorithms could be used for other acquisitions involving expectations or statistics of \(p(y|D_n; x)\) or \(p(y|z; x)\).

The popular EI acquisition function returns the expected improvement that querying at \(x\) will have over the minimal value observed so far. For \(y \in \mathbb{R}\), this can be written

\[
a_{\text{EI}}(x) = \int \mathbb{I} \{y \leq y_{\text{min}}\} \left(y_{\text{min}} - y\right) p(y|D_n; x) dy
\]

where \(y_{\text{min}} = \min_{y' \in D_n} y'\). We construct a nonparametric estimate for this in the black box EI (BB-EI) acquisition \(\hat{a}_{\text{EI}}(x)\) in Alg. 2, and illustrate BB-EI in Fig 1(a) for \(M \in \{50, 500\}\).

The PI acquisition function is similar to EI, but returns the probability that querying at \(x\) will improve upon the minimal value observed so far. PI can be written

\[
a_{\text{PI}}(x) = \int \mathbb{I} \left\{y \leq \min_{y' \in D_n} y'\right\} p(y|D_n; x) dy.
\]

We give the black box PI (BB-PI) acquisition function \(\hat{a}_{\text{PI}}(x)\) in Alg. 3, and visualize it in Fig 1(b).

The UCB acquisition function at a point \(x\) returns a lower confidence bound for \(p(y|D_n; x)\) (note that we use a lower
We give the black box UCB (BB-UCB) acquisition.

Algorithm 4 involves an estimate LCB

Algorithm 3 involves an estimate LCB

Algorithm 4

Algorithm 3

Algorithm 5

Algorithm 2

2.4. Multi-fidelity Optimization of Black Box Acquisition Functions

In the ProBO framework, we must optimize over the acquisition estimates defined in the previous section, i.e. compute

where \( M \) denotes the number of times pp.gen is called in an evaluation of \( \hat a \). However, in some probabilistic programs, the pp.gen operation can be costly, and we'd like to minimize the number of times it is called. As seen in Fig. 1, a small \( M \) will return a noisy estimate of \( a(x) \), while a large \( M \) will return a more-accurate estimate.

This is a special case of a multi-fidelity optimization problem (Forrester et al., 2007), with fidelity parameter \( M \). Unlike typical multi-fidelity settings, our goal is to reduce the number of calls to pp.gen for a single \( x \) only, via modifying the black box acquisition function \( \hat a(x, z^S, M) \). This way, the new \( \hat a \) can be dropped into any arbitrary global optimization routine which operates by making calls to \( \hat a \). Concretely, suppose we have \( F \) fidelities ranging from a small number of samples \( M_{\text{min}} \) to a large number \( M_{\text{max}} \), i.e.

\[
M_{\text{min}} = M_1 < \ldots < M_F = M_{\text{max}}.
\]

Intuitively, when calling \( \hat a(x, z^S, M) \) on a given \( x \), we'd like to use a small \( M \) if \( a(x) \) is far from the minimal value \( a(x^*) \), and a larger \( M \) if \( a(x) \) is close to \( a(x^*) \).

We propose the following procedure: Suppose \( a_{\text{min}} \) is the minimum value of \( \hat a \) seen so far during optimization (for any \( x \)). For a given fidelity \( M_f \) (starting with \( f=1 \)), we compute a lower confidence bound (LCB) for the sampling distribution of \( \hat a(x, z^S, M_f) \). We can do this via the bootstrap method (Efron, 1992) along with the LCB estimates described in Sec. 2.3. If this LCB is below \( a_{\text{min}} \), it remains plausible that the acquisition function minimum is at \( x \), and we repeat these steps at fidelity \( M_{f+1} \). After reaching a fidelity \( f^* \) where the LCB is above \( a_{\text{min}} \) (or upon reaching the highest fidelity \( f^* = F \)), we return the estimate \( \hat a(x, z^S, M_{f^*}) \). We give this procedure in detail in Alg. 6.

As a simple case, we could run a two-fidelity algorithm, with \( M \in \{M_{\text{min}} = M_1, M_{\text{max}} = M_2 \} \), where \( M_1 < M_2 \). For a given \( x \), the multi-fidelity acquisition method would first draw \( M_1 \) samples from pp.gen, and compute the LCB with the bootstrap. If the LCB is greater than \( a_{\text{min}} \), the method would return \( \hat a(x, z^S, M_1) \); if not, it would return \( \hat a(x, z^S, M_2) \). Near optima, this will call pp.gen \( M_1 + M_2 \) times, and will call it \( M_1 \) times otherwise. Hence, this method will reduce calls to pp.gen when \( M_1 \ll M_2 \), (dependent on the choice of LCB estimate).

One can apply any derivative-free (query-based) global optimization procedure that iteratively calls \( \hat a_{\text{min}} \). In general, we can replace the optimization step in ProBO with...
We may have multiple models that capture different aspects with latent variables. As an example, we show an ensemble of two PP models, where the prior on $M$ is given by, for instance, a parametric PP (e.g. a model with a logistic space). For our procedure constructs a model similar to a product of experts model, using only our two PP operations. Our procedure combines the posterior predictive densities of multiple PP models. Here, we develop a method to combine the posterior predictive densities of multiple PP models. The GP posterior predictive may be used with a deep Bayesian neural network written in Pyro (Bingham et al., 2014; Wang et al., 2015) to develop an algorithm that generates samples from the posterior predictive of the ensemble model $M_e$ and uses these in a black box acquisition function. We give this procedure in Alg. 7, where we’ve used Combine$(y_1, y_2)$ to denote a combination algorithm, which we detail in appendix Sec. B.

Algorithm 6 \( \hat{a}_{MF}(x, z^S, M_{1:f}) \) ▶ Multi-fidelity $\hat{a}$

1: $a_{\text{min}} \leftarrow \text{Min value of } \hat{a} \text{ seen so far}$
2: $\ell = -\infty, f = 1$
3: while $\ell \leq a_{\text{min}}$
4: \hspace{1em} $y_{1:M_f} \leftarrow \text{Call } pp \gen \text{ times}$
5: \hspace{1em} for $j = 1, \ldots, B$ do ▶ B bootstrap samples
6: \hspace{2em} $y_j \leftarrow \text{Resample}(y_{1:M_f})$ with replacement
7: \hspace{1em} $a_j \leftarrow \lambda(y_{1:M_f})$ ▶ Defined in a given $\hat{a}$
8: \hspace{1em} $\ell \leftarrow \text{LCB}(a_{1:B})$
9: \hspace{1em} $f \leftarrow f + 1$
10: Return $\hat{a}(x, z^S, M_f)$

Algorithm 7 $pp.\text{ens}(x, pp1.\gen, pp2.\gen, z_1^S, z_2^S)$ ▶ PP ensemble with BPoE

1: for $m = 1, \ldots, M$ do
2: \hspace{1em} $s_1, s_2 \sim \text{Unif}\{\{1, \ldots, S\}\}$
3: \hspace{1em} $y_{1,m} \leftarrow pp1.\gen(x, z_1, s_1, 1)$
4: \hspace{1em} $y_{2,m} \leftarrow pp2.\gen(x, z_2, s_2, 1)$
5: $y_{1:M} \leftarrow \text{Combine}(y_{1:M}, y_{2:M})$
6: Return $y_{1:M}$.

We can swap the $pp.\text{ens}$ operation in for the $pp.\gen$ operation in Algs. 2-5.

Note that the BPoE allows us to easily ensemble PPs written in different PPLs. For example, a hierarchical regression model written in Stan (Carpenter et al., 2015) using Hamiltonian Monte Carlo for inference could be combined with a deep Bayesian neural network written in Pyro (Bingham et al., 2018) using variational inference and with a GP written in GPy (GPy, 2012) using exact inference.

Example: Combining Phase-Shift and GP Models.

We describe an example and illustrate it in Fig. 2. Suppose we expect a few phase shifts in our input space $\mathcal{X}$, which partition $\mathcal{X}$ into regions with uniform output. We can model this system with $y \sim \mathcal{N}(y; \sum_{k=1}^{K} \text{logistic}(x; m_k, s_k, \mu_k) + b_k, \sigma^2)$, where latent variables $m_{1:K}, s_{1:K}, \mu_{1:K}$, and $b_{1:K}$ are assigned appropriate priors, and where logistic$(x; m, s, \mu) = \frac{m}{1+\exp(-s(x-\mu))}$. This model may accurately describe general trends in the system, but it may be ultimately misspecified, and underfit as the number of observations $n$ grows.

Alternatively, we could model this system as a black box using a Gaussian process. The GP posterior predictive may
converge to the correct landscape given enough data, but it is nonparametric, and does not encode our assumptions.

We can use the BPoE model to combine both the phase shift and GP models. We see in Fig. 2 that when \( n = 2 \) (first row), the BPoE model resembles the phase shift model, but when \( n = 50 \) (second row), it more closely resembles the true landscape modeled by the GP.

4. Empirical Results

The main goal of our empirical work is to show that we can directly plug models implemented with various PPL implementations into ProBO, and that these PPs can improve BO performance (i.e. increase the data efficiency and reduce the number of iterations) when compared with standard methods and models. We also aim to verify that our black box acquisition functions and extensions (e.g. multi-fidelity \( \text{aMF} \) and BPoE ensemble) perform well in practice.

We show experimental results on two tasks. The first is the task of corrupt BO, where we assume experimental observations \( y \) are corrupted (i.e. drawn from some corruption distribution) according to some probability. To perform accurate BO in this setting, models need to infer when to ignore or use subsets of the data.

The second experiment is a model selection task in neural networks that involves finding the optimal number of hidden units at each layer in a network (i.e. a basic type of neural architecture search (Zoph and Le, 2016; Kandasamy et al., 2018a)). To reduce the number of iterations needed in BO, we design a basin model that captures the relationship of validation error (i.e. classification error on a validation data set) with model complexity, and combine it with a GP in a BPoE ensemble (Sec. 3).

**Implementation Details.** For all GP implementations in the following experiments, we use the GPy library (GPy, 2012). We implement other PPs in Edward (Tran et al., 2016), where we use black box variational inference algorithms, and in Stan (Carpenter et al., 2015), where we use the No U-Turn Sampler (Hoffman and Gelman, 2011), a form of Hamiltonian Monte Carlo.

4.1. Corrupt BO

Consider the setting where, each time we conduct an experiment, we observe a “corrupt” output \( y \in \mathcal{Y} \) with probability \( p \), which is drawn according to some corruption distribution. We call this task corrupt BO. The corrupt distribution may have some dependence on input \( \mathcal{X} \) (e.g. \( p \) may be greater in a window around the optimum value \( x^* \)).

We develop a denoising PP model for this setting. Given a PP system model \( p_s \), and corruption model \( p_c \), we write our model as \( y \sim w_s p_s(z_s;x) + w_c p_c(z_c;x) \), where \( z_s, z_c \sim \text{Prior}(\cdot) \), and \( w_s, w_c \sim \text{Prior}(\cdot|x) \). This is a two component mixture of the system and a corruption model where weights \( (w_s, w_c) \) can also depend on input \( x \).

As a special case of this, we implement a denoising GP model, which we illustrate in Fig. 3. Here, we let the system model \( p_s \) be a GP, and the corruption model \( p_c \) be the \( \text{Unif}([-10, 10]) \) uniform distribution.

We show experimental results for ProBO using denoising GPs in the following synthetic corrupt BO task. For an \( x \in \mathbb{R}^d \), with probability \( 1 - p \) we query the function \( f(x) = \|x\|^2 - \frac{1}{d} \sum_{i=1}^{d} \cos(x_i) \), which has a minimum value of \( f(x^*) = -1 \) at \( x^* = 0 \), and with probability \( p \), we receive a corrupt value with distribution \( f(x) \sim \text{Unif}([f_{\text{max}}/10, f_{\text{max}}]) \), where \( f_{\text{max}} \) is \( \max_{x \in \mathcal{X}} f(x) \). Note that we use this corruption distribution (where corruption output is greater or equal to the minimum \( f(x^*) \)) so that

![Figure 2: Visualization of the Bayesian product of experts (BPoE) ensemble model (column 3) of a phase shift (PS) model (column 1), defined in Sec. 3, and a GP (column two). In the first row (\( n = 2 \)), when \( n \) is small, the BPoE ensemble more closely resembles the PS model. In the second row (\( n = 50 \)), when \( n \) is larger, the BPoE ensemble more closely resembles the GP model, and both accurately reflect the true landscape (red dashed line). In all figures, the posterior predictive is shown in gray.](image-url)
**Figure 3:** Visualization of the denoising model (Sec. 4.1) applied to GPs, for use in corrupt BO. When \( n = 20 \), the GP (a) is negatively affected by corrupt data (orange points), while the denoising GP (b) more accurately reflects the system data (blue points). When \( n = 50 \), the GP (c) remains biased by the corrupt data, while the denoising GP (d) converges to the true system (red dashed line). In all figures, the corruption probability is \( p = \frac{1}{2} \), and the model posterior predictive is shown in gray.

**Figure 4:** Results on corrupt BO experiments (Sec. 4.1). For low corruption \( (p = 1/100) \), ProBO with black box acquisition functions on denoising GPs is competitive with standard BO using exact acquisition functions on GP models (a-b). For higher corruption \( (p = 1/3) \), ProBO with denoising GPs converges to the optimal value, while standard BO with GPs does not, even as \( n \) grows large (c-d). Under high corruptions, standard BO with GPs can fare worse than RAND (blue dotted line) (c-d). All methods are averaged over 10 runs, and error bars represent one standard error.

**Figure 5:** Results on neural architecture tuning experiments (Sec. 4.2). We visualize the basin model (a) vs GP (b) on data from a four layer MLP (fixing all layers to same width to plot \( x \) in 1D). For low \( n \), the basin model more accurately captures the shape of the function (red dashed line). In (c) and (d) we show results of ProBO using a BPoE basin ensemble vs standard BO with GPs. Here, the ProBO methods outperform standard BO. All methods are averaged over 10 runs, and error bars represent one standard error.

**Figure 6:** Results on the multi-fidelity black box acquisition function experiments (Sec. 4.3), showing ProBO using the multi-fidelity \( \hat{a}_{\text{MF}} \) (Alg. 6) vs using a fixed high-fidelity \( \hat{a} \) \((M = 1000)\) and a fixed low-fidelity \( \hat{a} \) \((M = 10)\). Results for \( \hat{a}_{\text{EI}} \) (BB-EI) are in (a), and \( \hat{a}_{\text{UCB}} \) (BB-UCB) in (b). Here, \( \hat{a}_{\text{MF}} \) performs competitively with the high-fidelity \( \hat{a} \), while low fidelity \( \hat{a} \) performs worse. All methods are averaged over 10 runs, and error bars represent one standard error. In (c) we show the average number of \( \text{pp} \_\text{gen} \) calls per evaluation of \( \hat{a} \), and see that the multi-fidelity method maintains similar performance as the high fidelity method while reducing the number of calls.

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we are consistent with our stated goal to minimize $y^0_n$, the observed value of the system in $\mathbb{R}$ at iteration $n$, instead of operating in a more general design of experiments setting (Kandasamy et al., 2018b).

For this task we compare ProBO using denoising GPs and black box acquisition functions with standard BO using GPs and exact acquisition functions. We first show results for a low corruption setting ($p = 1/100$), in Fig. 4(a-b), where we plot the minimal found value $y_{\text{min}} = \min_{t \leq n} y^0_t$ vs iteration $n$. All methods are averaged over 10 runs, and error bars represent one standard error. Here, both models converge to a near-optimal value and perform similarly.

We then show results for a high corruption setting ($p = 1/3$), in Fig. 4(c-d). Here, ProBO with denoising GPs converges to a near-optimal value, while standard BO with GPs does not. For large $n$, BO with GPs fares worse than random sampling (RAND).

4.2. Tuning Neural Architectures

A popular application of BO is hyperparameter tuning of machine learning models. A recently popular task in this domain is known as neural architecture search (NAS). In this experiment we show that domain knowledge of features of a function landscape can be incorporated in ProBO via a BPoE ensemble (Sec. 3) to provide better sample efficiency (reduced iterations) for BO, in a basic NAS task.

When modeling datasets of moderate size, there are often two distinct phases as model complexity grows: a phase where the model underfits, where increasing modeling complexity reduces error on a held-out validation set; and a phase where the model overfits, where validation error increases with respect to model complexity. We design a model for this trend, which we refer to as a basin model:

$$y \sim \mathcal{N}(R(x) - \mu; a, b) + c, \sigma^2),$$

(5)

where $R(x; a, b) = a^T \text{ReLU}(x) + b^T \text{ReLU}(-x)$, and we’ve placed priors on parameters $\mu \in \mathbb{R}^d$, $a, b \in \mathbb{R}^d$, $c \in \mathbb{R}$, and $\sigma^2 > 0$. This model captures the inflection point with variable $\mu$, and uses variables $a$ and $b$ to model the slope of the optimization landscape above and below (respectively) $\mu$. We show a one dimensional view of validation error data from this system, and illustrate the basin model, in Fig. 5(a-b).

In this experiment, we optimize over the number of units (i.e. layer width) of the hidden layers in a four layer multilayer perceptron (MLP) neural network (Rosenblatt, 1961), trained on the Wisconsin Breast Cancer Diagnosis dataset (Blake and Merz, 1998). We compare ProBO using a BPoE ensemble (Sec. 3) of a basin model and a GP, with standard BO using a GP. We see in Fig 5(c-d) that ProBO with the BPoE ensemble can significantly outperform standard BO with GPs. In this optimization task, the landscape around the inflection point (of under to over fitting) can be very steep, which may hurt the performance of standard BO with GPs. In contrast, the basin model can capture this shape and quickly identify the inflection point via inferences about $\mu$.

4.3. Multi-fidelity Acquisition Optimization

Here, we empirically assess our multi-fidelity acquisition function optimization algorithm (Sec. 2.4). Our goal is to demonstrate that increasing the fidelity $M$ in black box acquisitions can yield better performance in ProBO, and that our multi-fidelity method (Alg. 6) maintains the performance of the high-fidelity acquisitions while reducing the number of calls to $\text{pp}. \text{gen}$.

We perform an experiment in a two-fidelity setting, where $M \in \{10, 1000\}$, and we apply our multi-fidelity method to BB-EI and BB-UCB, using a GP model and the synthetic BO task described in Sec. 4.1. Results are shown in Fig. 6, where we compare high-fidelity $\hat{a} (M = 1000)$, low-fidelity $\hat{a} (M = 10)$, and multi-fidelity $\hat{a}_\text{MF}$, for BB-EI (a) and BB-UCB (b). For both black box acquisition functions, the high-fidelity and multi-fidelity methods show comparable performance, while the low-fidelity method performs worse. We also see in (c) that the multi-fidelity method reduces the number of calls to $\text{pp}. \text{gen}$ by a factor of 3 on average, relative to the high fidelity method. It is worth noting that the low-fidelity method performs well, given its low cost, and may be the most applicable method depending on the PP noise, cost of calling $\text{pp}. \text{gen}$, and desired accuracy.

5. Conclusion

In this paper we presented ProBO, a framework for performing Bayesian optimization automatically using an arbitrary probabilistic program model. We developed black box acquisition functions, which do not require model-specific derivations, and showed how to efficiently optimize these functions. We developed a new model, the Bayesian product of experts (BPoE), which integrates nicely with our framework, and allows for combining information from multiple PPs, and performing BO with PP ensembles. Finally, we demonstrated promising empirical results on a corrupt BO task, and a neural network architecture tuning task, where we were able to drop in and use various existing PP implementations.

While not the focus of this paper, universal PPs (Le et al., 2016; Mansinghka et al., 2014; Wood et al., 2014) allow for models defined by arbitrary forward simulators, and aim to provide automatic inference for these models. They comprise a very broad class of models, and have the potential to incorporate sophisticated custom-built simulations of a broad array of systems. We think there may be the potential to incorporate sophisticated custom-built simulations of a broad array of systems. We think there may be the potential for running ProBO with models involving complex simulators of real world phenomena, and that this simulation-guided BO is an interesting avenue for future work.
References

Michael Riis Andersen, Eero Siivola, and Aki Vehtari. Bayesian optimization of unimodal functions. 2017.

Raul Astudillo and P Frazier. Multi-attribute bayesian optimization under utility uncertainty. In Proceedings of the NIPS Workshop on Bayesian Optimization, 2017.

Eli Bingham, Jonathan P. Chen, Martin Jankowiak, Fritz Obermeyer, Neeraj Pradhan, Theofanis Karaletsos, Rohit Singh, Paul Szerlip, Paul Horsfall, and Noah D. Goodman. Pyro: Deep Universal Probabilistic Programming. Journal of Machine Learning Research, 2018.

CL Blake and CJ Merz. Uci repository of machine learning databases. Irvine, ca: University of california, department of information and computer science, 1998.

Bob Carpenter, Andrew Gelman, Matt Hoffman, Daniel Lee, Ben Goodrich, Michael Betancourt, Marcus A Brubaker, Jiqiang Guo, Peter Li, and Allen Riddell. Stan: a probabilistic programming language. Journal of Statistical Software, 2015.

Katalin Csilléry, Michael GB Blum, Oscar E Gaggiotti, and Olivier François. Approximate bayesian computation (abc) in practice. Trends in ecology & evolution, 25(7):410–418, 2010.

Joshua V Dillon, Ian Langmore, Dustin Tran, Eugene Brevdo, Srinivas Vasudevan, Dave Moore, Brian Patton, Alex Alemi, Matt Hoffman, and Rif A Saurous. Tensorflow distributions. arXiv preprint arXiv:1711.10604, 2017.

Bradley Efron. Bootstrap methods: another look at the jackknife. In Breakthroughs in statistics, pages 569–593. Springer, 1992.

Alexander IJ Forrester, András Sóbester, and Andy J Keane. Multi-fidelity optimization via surrogate modelling. In Proceedings of the royal society of london a: mathematical, physical and engineering sciences, volume 463, pages 3251–3269. The Royal Society, 2007.

GPy. GPy: A gaussian process framework in python. http://github.com/SheffieldML/GPy, 2012.

José Miguel Hernández-Lobato, Michael A Gelbart, Matthew W Hoffman, Ryan P Adams, and Zoubin Ghahramani. Predictive entropy search for bayesian optimization with unknown constraints. 2015.

Geoffrey E Hinton. Training products of experts by minimizing contrastive divergence. Neural computation, 14 (8):1771–1800, 2002.

Matthew D Hoffman and Andrew Gelman. The no-u-turn sampler: Adaptively setting path lengths in hamiltonian monte carlo. arXiv preprint arXiv:1111.4246, 2011.

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

Kirthevasan Kandasamy, Willie Neiswanger, Jeff Schneider, Barnabas Poczos, and Eric Xing. Neural architecture search with bayesian optimisation and optimal transport. arXiv preprint arXiv:1802.07191, 2018a.

Kirthevasan Kandasamy, Willie Neiswanger, Reed Zhang, Akshay Krishnamurthy, Jeff Schneider, and Barnabas Poczos. Myopic bayesian design of experiments via posterior sampling and probabilistic programming. arXiv preprint arXiv:1805.09964, 2018b.

Harold J Kushner. A new method of locating the maximum point of an arbitrary multipeak curve in the presence of noise. Journal of Basic Engineering, 86(1):97–106, 1964.

Tuan Anh Le, Atılım Gunes Baydin, and Frank Wood. Inference compilation and universal probabilistic programming. arXiv preprint arXiv:1610.09900, 2016.

Cheng Li, Rana Santu, Sunil Gupta, Vu Nguyen, Svetla Venkatesh, Alessandra Sutti, David Rubin De Celis Leal, Teo Slezak, Murray Height, Mazher Mohammed, et al. Accelerating experimental design by incorporating experimenter hunches. In 2018 IEEE International Conference on Data Mining (ICDM), pages 257–266. IEEE, 2018.

Vikash Mansinghka, Daniel Selsam, and Yura Perov. Venture: a higher-order probabilistic programming platform with programmable inference. arXiv preprint arXiv:1404.0099, 2014.

Tom Minka. Infer. net 2.5. http://research. microsoft. com/infernet, 2012.

Jonas Mockus. On bayesian methods for seeking the extremum. In Optimization Techniques IFIP Technical Conference, pages 400–404. Springer, 1975.

Willie Neiswanger and Eric Xing. Post-inference prior swapping. In Proceedings of the 34th International Conference on Machine Learning-Volume 70, pages 2594–2602. JMLR. org, 2017.

Willie Neiswanger, Chong Wang, and Eric Xing. Asymptotically exact, embarrassingly parallel mcmc. In Proceedings of the 30th Conference on Uncertainty in Artificial Intelligence (UAI 2014), 2014.
Daniel Ritchie, Paul Horsfall, and Noah D Goodman. Deep amortized inference for probabilistic programs. *arXiv preprint arXiv:1610.05735*, 2016.

Frank Rosenblatt. Principles of neurodynamics, perceptrons and the theory of brain mechanisms. Technical report, Cornell Aeronautical Lab, Buffalo, NY, 1961.

John Salvatier, Thomas V Wiecki, and Christopher Fonnesbeck. Probabilistic programming in python using pymc3. *PeerJ Computer Science*, 2:e55, 2016.

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

N. Siddharth, Brooks Paige, Jan-Willem van de Meent, Alban Desmaison, Noah D. Goodman, Pushmeet Kohli, Frank Wood, and Philip Torr. Learning disentangled representations with semi-supervised deep generative models. In I. Guyon, U. V. Luxburg, S. Bengio, H. Wallach, R. Fergus, S. Vishwanathan, and R. Garnett, editors, *Advances in Neural Information Processing Systems 30*, pages 5927–5937, 2017.

Jasper Snoek, Hugo Larochelle, and Ryan P Adams. Practical bayesian optimization of machine learning algorithms. In *Advances in neural information processing systems*, pages 2951–2959, 2012.

Jasper Snoek, Oren Rippel, Kevin Swersky, Ryan Kiros, Nadathur Satish, Narayanan Sundaram, Mostofa Patwary, Mr Prabhat, and Ryan Adams. Scalable bayesian optimization using deep neural networks. In *International Conference on Machine Learning*, pages 2171–2180, 2015.

Niranjan Srinivas, Andreas Krause, Sham M Kakade, and Matthias Seeger. Gaussian process optimization in the bandit setting: No regret and experimental design. *arXiv preprint arXiv:0912.3995*, 2009.

Kevin Swersky, Jasper Snoek, and Ryan P Adams. Multi-task bayesian optimization. In *Advances in neural information processing systems*, pages 2004–2012, 2013.

William R Thompson. On the likelihood that one unknown probability exceeds another in view of the evidence of two samples. *Biometrika*, 25(3/4):285–294, 1933.

Dustin Tran, Alp Kucukelbir, Adji B. Dieng, Maja Rudolph, Dawen Liang, and David M. Blei. Edward: A library for probabilistic modeling, inference, and criticism. *arXiv preprint arXiv:1610.09787*, 2016.
A. The Bayesian Product of Experts (BPoE) Posterior Predictive Distribution

Here we characterize the posterior predictive PDF for the Bayesian product of experts model defined in Sec. 3. For convenience, we will provide our derivation for ensemble of two models. However, we can extend these results to an ensemble of an arbitrary number of models.

Suppose we are modeling a system which, given an input $x \in \mathcal{X}$, yields observations $y$, written $y \sim \text{System}(x)$, where $y \in \mathcal{Y}$. Observing the system at $n$ inputs yields a dataset $\mathcal{D}_n = \{(x_i, y_i)\}_{i=1}^n$.

Consider two Bayesian models $\mathcal{M}_1$ and $\mathcal{M}_2$, both for data $\mathcal{D}_n$.

Let $\mathcal{M}_1$ have likelihood $p_1(\mathcal{D}_n | z_1) = \prod_{i=1}^n p_1(y_i | z_1; x_i)$, where $z_1 \in \mathcal{Z}_1$ are latent variables with prior $p_1(z_1)$. We define the joint model PDF for $\mathcal{M}_1$ to be $p_1(\mathcal{D}_n, z_1) = p_1(z_1) \prod_{i=1}^n p_1(y_i | z_1; x_i)$. The posterior (conditional) PDF for $\mathcal{M}_1$ can then be written $p_1(z_1 | \mathcal{D}_n) = p_1(\mathcal{D}_n, z_1) / p_1(\mathcal{D}_n)$. We can write the posterior predictive PDF for $\mathcal{M}_1$ as

$$ p_1(y | \mathcal{D}_n; x) = \mathbb{E}_{p_1(z_1 | \mathcal{D}_n)} [p_1(y | z_1; x)]. \quad (6) $$

Similarly, let $\mathcal{M}_2$ have likelihood $p_2(\mathcal{D}_n | z_2) = \prod_{i=1}^n p_2(y_i | z_2; x_i)$, where $z_2 \in \mathcal{Z}_2$ are latent variables with prior PDF $p_2(z_2)$. We define the joint model PDF for $\mathcal{M}_2$ to be $p_2(\mathcal{D}_n, z_2) = p_2(z_2) \prod_{i=1}^n p_2(y_i | z_2; x_i)$, the posterior (conditional) PDF to be $p_2(z_2 | \mathcal{D}_n) = p_2(\mathcal{D}_n, z_2) / p_2(\mathcal{D}_n)$, and the posterior predictive PDF to be

$$ p_2(y | \mathcal{D}_n; x) = \mathbb{E}_{p_2(z_2 | \mathcal{D}_n)} [p_2(y | z_2; x)]. \quad (7) $$

Note that $z_1 \in \mathcal{Z}_1$ and $z_2 \in \mathcal{Z}_2$ need not be in the same space nor related.

Given models $\mathcal{M}_1$ and $\mathcal{M}_2$, we define the following Bayesian Product of Experts (BPoE) ensemble model, $\mathcal{M}_e$, with latent variables $z = (z_1, z_2) \in \mathcal{Z}_1 \times \mathcal{Z}_2$:

Prior PDF: $p(z) = p_1(z_1)p_2(z_2)$

Likelihood function: $p(\mathcal{D}_n | z) \propto p_1(\mathcal{D}_n | z_1)p_2(\mathcal{D}_n | z_2)$

$$ = \prod_{i=1}^n p_1(y_i | z_1; x_i)p_2(y_i | z_2; x_i) \quad (10) $$

Joint PDF: $p(\mathcal{D}_n, z) = p(\mathcal{D}_n | z)p(z)$

$$ \propto p_1(z_1)p_2(z_2)p_1(\mathcal{D}_n | z_1)p_2(\mathcal{D}_n | z_2) \quad (11) $$

We can write the posterior PDF for the BPoE ensemble model $\mathcal{M}_e$ as

$$ p(z | \mathcal{D}_n) \propto p(\mathcal{D}_n, z) = p_1(z_1)p_2(z_2)p_1(\mathcal{D}_n | z_1)p_2(\mathcal{D}_n | z_2) \quad (13) $$

$$ = p_1(z_1)p_1(\mathcal{D}_n | z_1)p_2(z_2)p_2(\mathcal{D}_n | z_2) \quad (14) $$

$$ = p_1(\mathcal{D}_n, z_1)p_2(\mathcal{D}_n, z_2) \quad (15) $$

$$ \propto p_1(z_1 | \mathcal{D}_n)p_2(z_2 | \mathcal{D}_n) \quad (16) $$
We can thus write the **posterior predictive PDF** for the BPoE ensemble model $M_e$ as

\[
p(y|D_n; x) = E_{p(z|D_n)} \left[ p(y|z; x) \right] = \int p(z|D_n)p(y|z; x)dz
\]

\[
= \int C_1 p_1(z_1|D_n)p_2(z_2|D_n)p_1(y|z_1; x)p_2(y|z_2; x)dz_1dz_2
\]

\[
= \int C_1 p_1(z_1|D_n)p_1(y|z_1; x)p_2(z_2|D_n)p_2(y|z_2; x)dz_1dz_2
\]

\[
= C_1 \int p_1(z_1|D_n)p_1(y|z_1; x)dz_1 \int p_2(z_2|D_n)p_2(y|z_2; x)dz_2
\]

\[
= C_1E_{p_1(z_1|D_n)} \left[ p_1(y|z_1; x) \right] E_{p_2(z_2|D_n)} \left[ p_2(y|z_2; x) \right]
\]

\[
= C_1 p_1(y|D_n; x)p_2(y|D_n; x)
\]

Therefore, we have the result, which we use in Sec. 3, that the posterior predictive PDF for the BPoE ensemble model $M_e$ is proportional to the product of the posterior predictive PDFs of the constituent models $M_1$ and $M_2$, i.e.

\[
p(y|D_n; x) \propto p_1(y|D_n; x)p_2(y|D_n; x).
\]

Via a similar argument we can also say that, for a BPoE ensemble model $M_e$ consisting of $K$ models $M_1, \ldots, M_K$, the posterior predictive PDF for $M_e$, $p(y|D_n; x)$, has the property

\[
p(y|D_n; x) \propto \prod_{i=1}^{K} p_i(y|D_n; x),
\]

where $p_i(y|D_n; x)$ is the posterior predictive PDF for constituent model $M_i$ in the ensemble.

### B. Combination Algorithms for the \texttt{pp.ens} Operation (Alg. 7)

In Sec. 3, we make use of combination algorithms from the embarrassingly parallel MCMC literature (Neiswanger et al., 2014; Wang et al., 2015), to define the \texttt{pp.ens} operation (Alg. 7) for use in applying the ProBO framework to a BPoE model. We describe these combination algorithms here in more detail.

For convenience, we describe these methods for two Bayesian models, $M_1$ and $M_2$, though these methods apply similarly to an arbitrarily large set of models.

The goal of these combination methods is to combine a set of $M$ samples

\[
y_{1,1:M} \sim p_1(y|D_n; x),
\]

from the posterior predictive distribution of a model $M_1$, with a disjoint set of $M$ samples

\[
y_{2,1:M} \sim p_2(y|D_n; x),
\]

from the posterior predictive distribution of a model $M_2$, to produce samples

\[
y_{3,1:M} \sim p(y|D_n; x)
\]

\[
\propto p_1(y|D_n; x)p_2(y|D_n; x),
\]

where $p(y|D_n; x)$ denotes the posterior predictive distribution of a BPoE ensemble model $M_e$, with constituent models $M_1$ and $M_2$.\[**\]}
We use the notation \( \text{Combine}(y_{1,1:M}, y_{2,1:M}) \) to denote a combination algorithm. We give a combination algorithm in Alg. 8 for our setting inspired by a combination algorithm presented in (Neiswanger et al., 2014).

**Algorithm 8** \( \text{Combine}(y_{1,1:M}, y_{2,1:M}) \)  
\[ 1: t_1, t_2 \overset{\text{id}}{\sim} \text{Unif}\left(\{1, \ldots, M\}\right) \\
2: \text{for } i = 1, \ldots, M \text{ do} \\
3: \quad c_1, c_2 \overset{\text{id}}{\sim} \text{Unif}\left(\{1, \ldots, M\}\right) \\
4: \quad u \sim \text{Unif}\left([0, 1]\right) \\
5: \quad \text{if } u > \frac{w(c_1, c_2)}{w(t_1, t_2)} \text{ then} \\
6: \quad \quad t_1 \leftarrow c_1 \\
7: \quad \quad t_2 \leftarrow c_2 \\
8: \quad y_{3,i} \sim \mathcal{N}\left(\bar{y}_{(t_1, t_2)}, \frac{i^{-1/2}}{2}\right) \\
9: \text{Return } y_{3,1:M}. \]

Where we must define a couple of terms used in Alg. 8. The mean output \( \bar{y}_{(t_1, t_2)} \), for indices \( t_1, t_2 \in \{1, \ldots, M\} \), is defined to be

\[
\bar{y}_{(t_1, t_2)} = \frac{1}{2} (y_{1,t_1} + y_{2,t_2}),
\]

and weights \( w_{(t_1, t_2)} \) (alternatively, \( w_{(c_1, c_2)} \)), for indices \( t_1, t_2 \in \{1, \ldots, M\} \), are defined to be

\[
w_{(t_1, t_2)} = \mathcal{N}\left(y_{1,t_1} \mid \bar{y}_{(t_1, t_2)}, i^{-1/2}\right) \mathcal{N}\left(y_{2,t_2} \mid \bar{y}_{(t_1, t_2)}, i^{-1/2}\right).
\]

Note that this \( \text{Combine}(y_{1,1:M}, y_{2,1:M}) \) algorithm (Alg. 8) holds for sample sets from two arbitrary posterior predictive distributions \( p_1(y \mid D_n; x) \) and \( p_2(y \mid D_n; x) \), without any parametric assumptions such as Gaussianity.