Bayesian optimization (BO) is a powerful method for optimizing complex black-box functions that are costly to evaluate directly. Although useful out of the box, complexities arise when the domain exhibits non-smooth structure, noise, or greater than five dimensions. Extending BO for these issues is non-trivial, which is why we suggest casting BO methods into the probabilistic programming paradigm. These systems (PPS) enable users to encode model structure and naturally reason about uncertainties, which can be leveraged towards improved BO methods. Here we present a probabilistic domain-specific language where BO is native, showing the Bayesian approach to optimization is more naturally expressed in a PPS, and better equipped to address the above issues. We validate the approach on standard optimization benchmarks, while demonstrating the utility of programmable structure to address the inner-optimization problem of BO. Importantly, we also show that the framework enables the user to more readily use advanced techniques such as unscented BO and noisy expected improvement.

Keywords: Probabilistic programming; Bayesian optimization; Gaussian process

1 Introduction

It is often the case in machine learning and data science problems that we wish to optimize an objective function that is expensive to evaluate, noisy or uncertain, and/or lacks structure and derivatives. Bayesian optimization (BO) is a powerful approach, with applications from drug design [1] to robotics [2, 3], A/B testing [4] to environment monitoring [5]. Yet BO encounters issues in medium-sized parameter spaces (5-10 dimensions), and in complex structured domains where expert knowledge could be useful. In practice experimenting with BO techniques can be cumbersome – there’s often a complexity vs. per-iteration performance tradeoff – and advanced methods are non-trivial to implement.

Probabilistic programming would appear to be a natural paradigm for BO, offering a structured approach to probabilistic modeling and reasoning under uncertainty. Probabilistic programming languages (PPL) aim to simplify probabilistic modeling and inference by providing language constructs for defining probabilistic generative models and inference algorithms [6, 7, 8, 9]. A core philosophy is decoupling modeling and inference: a model program implicitly defines a distribution on random variables whilst the system back-end implements general-purpose inference methods. Many PPL exist, but none explicitly designed for BO; [10] provides a vanilla BO wrapper for PPL models. Here we present a novel probabilistic program-embedding of Bayesian optimization.

Our specific contributions are:

1. Proposal of a probabilistic domain-specific language (DSL) for Bayesian optimization. We include custom formulations of Gaussian process models and optimization algorithms that behoove the use of probabilistic programmed Bayesian optimization in practice. The language notably features inference metaprogramming [7].
2. A prototype implementation of our PPL (embedded in C++): Gaussian process probabilistic programming and optimization (G3PO) [2].
3. Empirical validation on benchmark optimization problems, while demonstrating the utility of probabilistic programming to improve Bayesian optimization, specifically incorporating domain knowledge via model program structure.
4. Demonstration that the implementation of advanced Bayesian optimization methods becomes trivial in G3PO, which we illustrate with several Bayesian optimization methods used in industry. In similar vein, the ease of developing in G3PO enables the user to more readily experiment and iterate over their modeling choices, a driving aim of the probabilistic programming field.
The prior work \cite{11} introduced the concept (and Gaussian process modeling) towards data-efficient robotics methods. We build significantly on that design proposal here.

2 Background

2.1 Probabilistic Programming

Probabilistic programming systems (PPS) represent probabilistic generative models as programs written in a specialized language that provides syntax for the definition and conditioning of random variables \cite{6,7,8,9}. Specifically, a PPS implements two required constructs: the ability to draw values at random from distributions, and the ability to condition values of variables (which allow data from real world observations to be incorporated into a probabilistic program) \cite{12} - typically with \texttt{sample} and \texttt{observe} primitives, respectively. Importantly, the set of random variables is dynamically typed such that programs may differ from execution to execution.

Core to PPS design is the decoupling of modeling and inference; model code is generally concise and modular, and inference algorithms are capable of operating on arbitrary programs. Inference methods run by the system back-end (referred to as an “inference engine”) are typically implemented as forward-simulation sampling methods (namely SMC and particle MCMC \cite{13}) or variational inference.

A model program specifies a joint distribution $p(y, x)$ over data $y$ and variables $x$. Inference is over the space of possible program execution traces, where an execution trace is a map from random choices to their specific values. Formally the probability of an execution trace can be defined as

$$p(y, x) = \prod_{n=1}^{N} p(y_n|g_n, x_n)p(x_n|x_{n-1})$$

where $y_n$ is the $n$-th \texttt{observe}'d data point, $p(y_n|g_n)$ is its normalized likelihood, $g_n(x_n)$ is the program argument with random procedures $g_n(x_n)$, $x_n$ is the ordered set of all random choices with $p(x_n|x_{n-1})$ its normalized prior probability, and $x$ and $y$ are the sets of all latent and observing random procedures, respectively \cite{8}.

For more detailed derivation and further information on probabilistic programming we refer the reader to the recent tutorial \cite{14}.

2.2 Bayesian Optimization

**Algorithm 1 Bayesian optimization**

**Inputs:** data $D$, surrogate model $\hat{f}$, acquisition function $\alpha$

**Outputs:** performance pairs $\{\theta_t, y_t\}_{t=1:T}$

1: for $t \leq 1$, while $t < T$, ++t do
2: Train the model $f$ from $D$
3: Find $\theta^*$ that minimizes the acquisition surface $\alpha(\theta)$
4: Evaluate $y_t = \hat{f}(\theta^*)$ on the real system
5: Update $D \leftarrow D \cup \{(\theta^*_t, y_t)\}$
6: return $\{\theta_t, y_t\}_{t=1:T}$

Given an arbitrary objective function $f : \varnothing \rightarrow \mathbb{R}$ that can be evaluated for a point $\theta \in \varnothing$ to produce potentially noisy outputs, the aim of BO is to find the global maximum $\theta^* = \arg \max_{\theta \in \varnothing} f(\theta)$.

BO relies on both a probabilistic surrogate model $\hat{f}$ and an acquisition function $\alpha$ to define a strategy for efficiently maximizing $f$. That is, from $\hat{f}$ we can estimate the expected value and uncertainty in $f(\theta)$ for all possible parameterizations $\theta \in \varnothing$, and $\alpha : \varnothing \rightarrow \mathbb{R}$ guides the parameter search by assigning an expected utility of evaluating $f$ at a given $\theta$. This process is shown in Alg. 1 where we accumulate a dataset $D$ from evaluating parameter sets on the true objective, and $T$ specifies our “evaluation budget” for doing so.

The most common probabilistic model used in BO, and the one we consider in this article, is a Gaussian process (GP) \cite{15}. Crucially, the GP’s ability to express model uncertainty allows us to tradeoff exploration and exploitation for

\footnote{https://tinyurl.com/LavinMansinghkaPP18}

\footnote{Note we use probabilistic programming system (PPS) and language (PPL) somewhat interchangeably.}
efficient optimization. Nonetheless, other probabilistic models are possible such as random forests \cite{16} and Bayesian neural networks \cite{17}.

Acquisition functions aim to maximize “utility”, defined in terms of expectations over the surrogate model posterior; in Algorithm 1 utility guides the search over the acquisition surface $\alpha$. Commonly used choices include expected improvement (EI) \cite{18}, upper confidence bound (UCB) \cite{19}, and predictive entropy search \cite{20}. The acquisition function balances exploration vs. exploitation, and can be critical to the performance of Bayesian optimization, thus making up a significant portion of the Bayesian optimization literature. Here we focus on EI, as it generally shows favorable results in practice and has several useful extensions in literature. For further information on BO we refer the reader to the recent review \cite{21}.

3 Bayesian Program Optimization

Here we develop the probabilistic program embedding of Bayesian optimization from the conceptual design in \cite{11}. We refer to the implemented domain-specific language as “G3PO: Gaussian process probabilistic programming and optimization”, and include more description in Appendix A. The modeling structure we define in G3PO allows the user to define the set of optimization parameters and corresponding constraints, as shown in the code listing in Appendix B.

Given a program defining the joint density $p(Y, X, \theta)$ with fixed $Y$, our aim is to optimize w.r.t the subset of variables $\theta$ while marginalizing out latent variables $X$.

$$\theta^* = \arg \max_{\theta \in \vartheta} p(\theta | Y) = \arg \max_{\theta \in \vartheta} p(Y, \theta) = \arg \max_{\theta \in \vartheta} \int p(Y, X, \theta) dX$$

The target function for our BO scheme is $\log p(Y, \theta)$. The posterior of Gaussian process surrogate models (i.e. particles) is used to define the acquisition function $\alpha$, for which we take a Monte Carlo estimate of the integrated expected improvement (EI):

$$\alpha_{EI}(\theta) = \sum_{i=1}^{N} \left( \mu_{m}(\theta) - \hat{u}_{m}^* \right) \Phi \left( \gamma_{i}^m(\theta) \right) + \sigma_{m}(\theta) \phi \left( \gamma_{i}^m(\theta) \right)$$

with $\sigma_{m}(\theta) = \sqrt{k_{m}(\theta, \theta)}$ and $\gamma_{i}^m(\theta) = \frac{\mu_{i}^m(\theta)-\hat{u}_{m}^*}{\sigma_{m}(\theta)}$ as in \cite{10}, where $\phi$ and $\Phi$ represent the PDF and CDF of a unit normal distribution, respectively.

Importantly, the GP mean and variance is propagated, giving an implicit uncertainty quantification. As noted in \cite{11}, quantifying the specific uncertainties in G3PO is trivial; we can sample model programs for aleatoric (system stochasticity such as observation and process noise) and epistemic (subjective uncertainty due to limited data) uncertainty measures.

4 Results

4.1 Benchmark experiments

To show the efficacy of the PP-BO approach we demonstrate the “inner-optimization” problem. The inner-optimization problem is a known issue in BO, specifically because direct numerical optimization of the expected improvement struggles to converge \cite{22}; this occurs at the $\min(\alpha)$ in Alg. 1 seeking the optimal query $\theta^*$. One reason is the response surface is often highly multi-modal, and several concentrated evaluations (perhaps near a local optimum) make the surface jagged and difficult to navigate. Moreover, decomposing a task is a desirable tactic in high-dimension, but non-trivial when considering sub-optimizations. A good alternative is Thompson sampling \cite{23}, a randomized strategy which samples a reward function from the posterior and selects that yielding the highest simulated reward. Because we’re operating in the space of probabilistic programs we can take this one step further and optimize over Thompson samples drawn from the model source code. Shown in the example code of Appendix B the procedure executes as follows:

\footnote{Hence the article name, given the Bayesian approach implicit in both probabilistic programming and in the method for optimization}
1. Sample a model from the posterior distribution of models (particles).
2. Perform a numerical optimization to find the configuration with highest performance predicted by that particle; because we are optimizing a predicted performance, the objective function is both smooth and decomposable.
3. Compute the expected improvement of that configuration.
4. Repeat 1-3 until we have several promising configurations.
5. Select the configuration that yields the highest expected improvement.

In the results plots of Fig. 1, this approach is “source-sampling”, compared with standard BO (“vanilla”), “structured”, and “structured with source-sampling”. In this example of structured BO we define one GP for the first term of the Branin-Hoo equation and another GP for the second. With this trivial model structure the optimization converges significantly faster than vanilla BO. Our probabilistic programming formulation of BO enables the user to easily encode domain knowledge this way. See Appendix B for code snippets.

Figure 1: Results of four PP-BO variants (described in the text and shown as G3PO code in Appendix B) on the Branin-Hoo benchmark optimization task (http://www.sfu.ca/~ssurjano/optimization.html). All converge to the global optimum 3.98.

Beyond promising results on the benchmark BO problems, this approach has valuable implications for use in practice. First and foremost, computational efficiency: using a single model sample to evaluate the performance of a configuration is very inexpensive relative to averaging over the entire distribution. There is also an inherent robustness in running independent optimizations per particle, rather than a single numerical optimization that could get stuck in local minima. Third, ease of development: notice how simple it is in the source code for the developer to implement, experiment with, and introspect model-sampling within Bayesian optimization and acquisition functions. This is but one example of how the user can exploit the source code in PP-BO. Other approaches to structured BO include [24, 25, 26], but without the ability to exploit the program source code in the optimization. The recently proposed MC-integration approach of [22] is another sampling-based approach to the inner-optimization problem of BO. We leave it to future work to compare the methods.

4.2 Affordances

A main motivation of probabilistic programmed Bayesian optimization is the ability to implement advanced methods trivially. Here we show extensions to the expected improvement (EI) acquisition function that are particularly useful in practice for reasoning about noise in the optimization procedure.

To exacerbate the effect of noise on the optimization procedure, we use the RKHS function from [29], where the global maximum is at a narrow peak (representing a region of high risk) that may or may not be the ideal solution given significant input noise – see Fig. 2.
4.2.1 Unscented Bayesian Optimization

*Unscented Bayesian optimization* is able to perform sample efficient optimization while taking into consideration input noise to find safe optima, demonstrated to mitigate risk in robot grasping. The underlying mechanism is applying the *unscented transform* \[30\] to both the acquisition function and optimal incumbent, which propagates probability distributions through nonlinear functions. Thus rather than assuming deterministic queries of the system, UBO analyzes the transformed posterior distributions. From transforming the query distribution through the acquisition function we have the unscented expected improvement:

$$UEI(x) = \sum_{i=0}^{2d} \omega(i)EI(x(i)).$$

See [27] for details on the unscented transform’s sampling strategy to compute \(x\) and \(\omega\). Here we show that by formulating BO as native within a probabilistic DSL we can get UEI for free. See Fig. 2 for our results.

To reproduce the effect of input noise in [27], the authors generate Monte Carlo samples according the input noise distribution at each iteration, yielding the expected outcome and the instability. In probabilistic programming, not only do we is this additional sampling step unnecessary (as we already have the posterior over particles), but our posterior over particles is a more accurate representation of the true posterior because we run EI on the space of particles, sidestepping the need for UT’s approximate sampling phase.

Moreover, the unscented optimal incumbent strategy, \(UOI(x) = \sum_{i=0}^{2d} \omega(i) \sum_{j=1}^{m} \mu_j(x(i))\), is the default operation in PP-BO. Additionally, it’s noted that UBO is a more computationally efficient strategy to BO with input uncertainties than alternative approaches, so it follows that the computationally efficient approach to safe BO is easy out of the box with PP-BO.

5 Concluding Remarks

Powerful acquisition function strategies are often computationally intensive and algorithmically complicated [31]. Yet when cast in the space of probabilistic programs, advanced Bayesian optimization techniques can be rather trivial. We demonstrated this by reproducing state-of-art techniques designed for reasoning with uncertainties, in simple probabilistic programs. Additionally we showed a succinct approach to the inner-optimization problem of BO by utilizing programmed model structure.

\[\text{At time of posting we have results with unscented BO [27]. In-progress are “noisy EI” [28], BO with tree-structured dependencies [24], and multi-objective BO [3], to be completed for publication/presentation (along with open-sourced code).}\]
One direction of future work is to experiment with the more powerful class of acquisition functions “predictive entropy search” [20], where we hope to show the information-theoretic value afforded by probabilistic programming. We also anticipate using G3PO for experiments with probabilistic programming approaches to reinforcement learning and structured control [11].

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A Gaussian Process Probabilistic Programming & Optimization

The probabilistic DSL described here (and suggested in [11]) prominently features (i) programmable inference, (ii) modular and structured optimization, and (iii) explicit uncertainty quantification. The framework emphasizes Gaussian process (GP) models and Bayesian optimization (BO) methods, thus we refer to the prototype PPL as “G3PO: Gaussian process probabilistic programming and optimization”. Throughout this appendix are code samples, and the repository is to be open-sourced upon publication.

A.1 G3PO Language Design

The design and initial prototype G3PO is an embedded language that is implemented via C++ preprocessor macros that expand into calls against a runtime library. C++ is chosen as the host language mainly for computation efficiency over alternatives such as Python, and to utilize the built-in metaprogramming techniques, namely template metaprogramming and CRTP. We extend the language with macros to define the standard observe and sample stochastic primitives, which enable the passing of program flow between models and inference engines. A simple contrived example:

```cpp
// Sample the params for linear regression model:
LinearModel() {
    alpha = sample(Normal(0.0, 1.0));
    beta = sample(Normal(0.0, 1.0));
    noise = 2.0;
}
auto lm = LinearModel();
// Condition on data:
observe(lm, x_data, y_data);
```

Additionally, programmable inference is exposed to the user via InferenceEngine modules, which defines part of the computation graph to be executed by the desired inference algorithm. Broadly speaking this approach is referred to as “inference metaprogramming” [32], where the user manually defines inference and/or optimization subproblems to be fed to the backend engine. This enables the user to construct model programs of both static and dynamic components, and easily experiment with modular inference strategies. For example, one could run a particle Gibbs inference engine to sample from the model while running gradient updates or perhaps HMC inference over the differentiable parameters. Composable inference strategies are similarly available in Edward [33], Venture [7], and Turing.jl [34].

In G3PO the InferenceEngines are handled by the backend DAG execution trace structure. The trace runs inference by initializing a defined number of particle programs, and executing them via the user-defined ModelProgram::forward method. In ModelProgram::forward we define the program flow, usually a mix of deterministic operations and stochastic primitives; the function observe conditions variables on data, predict makes predictions in light of this data, and sample draws samples from the model.

Crucially, a ModelProgram is able to handle both parametric and nonparametric models: The parametric component learns a fixed number of parameters and allows the user to specify domain knowledge, while a nonparametric model, e.g. Gaussian process, learn an unbounded number of parameters that grows with the training data [35]. [26] also suggests semi-parametric models with probabilistic programming, but specific to their “auto-tuner.” For the time being we refer the reader to the poster of [11], which proposed this design towards model-based policy search: https://tinyurl.com/LavinMansinghkaPP18.

Sampling from the parametric components is simple: select one of the particles with probability weighted by its likelihood. For a nonparametric model we must sample one of its response surfaces, for which we use an efficient approach similar to Thompson sampling; the approach works well in practice and is theoretically grounded [36].

A.2 Gaussian Process Implementation

A known issue with Gaussian process models is poor scalability: for \( n \) data points there’s an \( O(n^3) \) computational complexity associated with inverting the covariance matrix. In practice we often receive incremental observations, and can thus take advantage of the previously computed Cholesky decomposition to reduce the complexity. Implementing

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7 https://en.wikipedia.org/wiki/Expression_templates

8 The curiously recursive template pattern (CRTP) is a technique to implement compile-time polymorphism; using a pure virtual method you are solving the inheritance at runtime instead of compile time, whereas CRTP solves this at compile time so the execution will be faster.

---
the incremental version of Cholesky decomposition yields $O(n^2)$ complexity, which applies to both training (i.e. `observe` statements) and inference.

To further address the high computational complexity of Gaussian processes we implement a variation of the treed-GP [37]. Treed GPs train multiple GPs on different subsets of the data, akin to decision trees used by random forests for regression. We implement this approach in the probabilistic programming framework by expressing a distribution over trees, constructed by iteratively building a decision tree with GPs at the leaves. When a threshold for number of data points is reached, GPs recursively split across the input dimension of maximal variance. The result is each particle uses a decision tree to make predictions, and an overall prediction is produced by averaging over all particles. In the case of the threshold larger than the number of measurements, the single leaf never gets split, and we have traditional GP regression.

We implement adaptive domain scaling, where the user defines hyperpriors to be placed on the GP hyperparameters within a `ModelProgram`. Then to initialize scaling for the input variables we sample directly from the generative model defined by the program. The result is an affine scaling to a $[-1, 1]$ hypercube for both the inputs and outputs of the GP, similar to that of [10].

Note the implementation includes standard classes of kernels and supports kernel composition, as well as automatic relevance determination [38]. While the squared exponential kernel is typically used, it is too smooth for many real-world problems (e.g. robotics models with environment interactions [2]). We thus prefer the Matérn-5/2 kernel in our experiments. By initializing a GP within a `ModelProgram` as `SMCEngine<GPModel>` we instruct the backend engine to learn the kernel hyperparameters with Hamiltonian Monte Carlo (HMC) steps. We refer the reader to [11] for example probabilistic programs that implement inference metaprogramming over multiple GPs. We also note a recent project on GP-focused probabilistic programming by [39].

## B Bayesian Optimization Example Code

Below is G3PO source code implementing several flavors of Bayesian optimization, utilizing the probabilistic program model structure. See main text for descriptions.

```c++
/* Define a program with its parametric and GP components. */

class BHGP : Particle {
    // Constructor samples param values s.t. each particle is
    // initialized uniquely.
    // Note: backend maintains a global RNG
    alpha_ = sample(Normal(0.0, 20.0));
    beta_ = sample(Normal(0.0, 20.0));
    gp1_.mean = sample(Normal(0.0, 10.0));
    gp1_.stddev = sample(Normal(0.0, 200.0));
    gp1_.linear_scales = {sample(Normal(0.0, 15.0)),
                         sample(Normal(0.0, 15.0))};
    // repeat for 'gp2_'
}

class BHModel : ModelProgram {
    BHModel() {
        eng_.set_num_particles(100);
    }
    void forward(const BHParams& p) {
        sample(eng_, p.x1_.value(), p.x2_.value());
    }
    SMCEngine<BHGP> eng_;  // spawns particles of given type
};

/* BO parameters for Branin–Hoo function. */

struct BHParams : OptParams{
    BHParams() : x1_(-5, 10), x2_(0, 15),
               max_num_iters_(1000), minimizer_(true)
};
```
ParameterConstraints<double> x1_;  
ParameterConstraints<double> x2_;  
double max_num_iters_;  
bool minimizer_;  
}  
*/  
  
/* Vanilla inner-optimization of EI in our framework */  
void maximize_ei(ModelProgram& m, OptParams& p, double incumbent) {  
  NLOpt opt(p);  // numerical optimizer  
  auto obj = [=]() {  
    double r = m.expected_improvement/incumbent, p);  
    return r;  
  };  
  opt.set_objective_function(obj);  
  opt.run_optimization();  
}  
*/  
  
/* Alternative 'nested' EI that samples from the model */  
double ei_with_samples(ModelProgram& m,  
OptParams& p, double incumbent) {  
  NLOpt opt(p);  
  auto objective = [=]() {  
    return m.sample_predict(p);  
  };  
  opt.set_objective_function(objective);  
  opt.run_optimization();  
}  
*/  
  
// Execution snippet:  
BO(BHParams()) bo;  
bo.SetObjective(real_world_func);  // i.e. Branin–Hoo  
bo.SetAcqFunc(maximize_ei);  
bo.SetAcqFunc(ei_with_samples);  
bo.RunOptimization();  
