PRACTICAL BAYESIAN OPTIMIZATION OF MACHINE LEARNING ALGORITHMS

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Machine learning algorithms frequently require careful tuning of model hyperparameters, regularization terms, and optimization parameters. Unfortunately, this tuning is often a "black art" that requires expert experience, unwritten rules of thumb, or sometimes brute-force search. Much more appealing is the idea of developing automatic approaches which can optimize the performance of a given learning algorithm to the task at hand. In this work, we consider the automatic tuning problem within the framework of Bayesian optimization, in which a learning algorithm's generalization performance is modeled as a sample from a Gaussian process (GP). The tractable posterior distribution induced by the GP leads to efficient use of the information gathered by previous experiments, enabling optimal choices about what parameters to try next. Here we show how the effects of the Gaussian process prior and the associated inference procedure can have a large impact on the success or failure of Bayesian optimization. We show that thoughtful choices can lead to results that exceed expert-level performance in tuning machine learning algorithms. We also describe new algorithms that take into account the variable cost (duration) of learning experiments and that can leverage the presence of multiple cores for parallel experimentation. We show that these proposed algorithms improve on previous automatic procedures and can reach or *surpass* human expert-level optimization on a diverse set of contemporary algorithms including latent Dirichlet allocation, structured SVMs and convolutional neural networks.

1. Introduction. Machine learning algorithms are rarely parameter-free; whether via the properties of a regularizer, the hyperprior of a generative model, or the step size of a gradient-based optimization, learning procedures almost always require a set of high-level choices that significantly impact generalization performance. As a practitioner, one is usually able to specify the general framework of an inductive bias much more easily than the particular weighting that it should have relative to training data. As a result, these high-level parameters are often considered a nuisance, making it desirable to develop algorithms with as few of these "knobs" as possible.

Another, more flexible take on this issue is to view the optimization of high-level parameters as a procedure to be automated. Specifically, we could view such tuning as the optimization of an unknown black-box function that reflects generalization performance and invoke algorithms developed for such problems. These optimization problems have a somewhat different flavor than the low-level objectives one often encounters as part of a training procedure: here function evaluations are very expensive, as they involve running the primary machine learning algorithm to completion. In this setting where function evaluations are expensive, it is desirable to spend computational time making better choices about where to seek the best parameters. Bayesian optimization (Mockus et al., 1978) provides an elegant approach and has been shown to outperform other state of the art global optimization algorithms on a number of challenging optimization benchmark functions (Jones, 2001). For continuous functions, Bayesian optimization typically works by assuming the unknown function was sampled from a

Gaussian process (GP) and maintains a posterior distribution for this function as observations are made. In our case, these observations are the measure of generalization performance under different settings of the hyperparameters we wish to optimize. To pick the hyperparameters of the next experiment, one can optimize the expected improvement (EI) (Mockus et al., 1978) over the current best result or the Gaussian process upper confidence bound (UCB)(Srinivas et al., 2010). EI and UCB have been shown to be efficient in the number of function evaluations required to find the global optimum of many multimodal black-box functions (Srinivas et al., 2010; Bull, 2011).

Machine learning algorithms, however, have certain characteristics that distinguish them from other black-box optimization problems. First, each function evaluation can require a variable amount of time: training a small neural network with 10 hidden units will take less time than a bigger network with 1000 hidden units. Even without considering duration, the advent of cloud computing makes it possible to quantify economically the cost of requiring large-memory machines for learning, changing the actual cost in dollars of an experiment with a different number of hidden units. It is desirable to understand how to include a concept of cost into the optimization procedure. Second, machine learning experiments are often run in parallel, on multiple cores or machines. We would like to build Bayesian optimization procedures that can take advantage of this parallelism to reach better solutions more quickly.

In this work, our first contribution is the identification of good practices for Bayesian optimization of machine learning algorithms. In particular, we argue that a fully Bayesian treatment of the GP kernel parameters is of critical importance to robust results, in contrast to the more standard procedure of optimizing hyperparameters (e.g. Bergstra et al. (2011)). We also examine the impact of the kernel itself and examine whether the default choice of the squared-exponential covariance function is appropriate. Our second contribution is the description of a new algorithm that accounts for cost in experiments. Finally, we also propose an algorithm that can take advantage of multiple cores to run machine learning experiments in parallel.

2. Bayesian Optimization with Gaussian Process Priors. As in other kinds of optimization, in Bayesian optimization we are interested in finding the minimum of a function $f(\mathbf{x})$ on some bounded set $\mathcal{X}$, which we will take to be a subset of $\mathbb{R}^D$. What makes Bayesian optimization different from other procedures is that it constructs a probabilistic model for $f(\mathbf{x})$ and then exploits this model to make decisions about where in $\mathcal{X}$ to next evaluate the function, while integrating out uncertainty. The essential philosophy is to use *all* of the information available from previous evaluations of $f(\mathbf{x})$ and not simply rely on local gradient and Hessian approximations. This results in a procedure that can find the minimum of difficult non-convex functions with relatively few evaluations, at the cost of performing more computation to determine the next point to try. When evaluations of $f(\mathbf{x})$ are expensive to perform — as is the case when it requires training a machine learning algorithm — it is easy to justify some extra computation to make better decisions. For an overview of the Bayesian optimization formalism, see, e.g., Brochu et al. (2010). In this section we briefly review the general Bayesian optimization approach, before discussing our novel contributions in Section 3.

There are two major choices that must be made when performing Bayesian optimization. First, one must select a prior over functions that will express assumptions about the function being optimized. For this we choose the Gaussian process prior, due to its flexibility and tractability. Second, we must choose an *acquisition function*, which is used to construct a utility function from the model posterior, allowing us to determine the next point to evaluate.

2.1. *Gaussian Processes.* The Gaussian process (GP) is a convenient and powerful prior distribution on functions, which we will take here to be of the form $f : \mathcal{X} \to \mathbb{R}$. The GP is defined by the property that any finite set of N points $\{\mathbf{x}_n \in \mathcal{X}\}_{n=1}^N$ induces a multivariate Gaussian distribution on $\mathbb{R}^N$. The nth of these points is taken to be the function value $f(\mathbf{x}_n)$, and the elegant marginalization properties of the Gaussian distribution allow us to compute marginals and conditionals in closed form. The support and properties of the resulting distribution on functions are determined by a mean function $m : \mathcal{X} \to \mathbb{R}$ and a positive definite covariance function $K : \mathcal{X} \times \mathcal{X} \to \mathbb{R}$. We will discuss the impact of covariance functions in Section 3.1. For an overview of Gaussian processes, see Rasmussen and Williams (2006).

2.2. *Acquisition Functions for Bayesian Optimization.* We assume that the function $f(\mathbf{x})$ is drawn from a Gaussian process prior and that our observations are of the form $\{\mathbf{x}_n, y_n\}_{n=1}^N$, where $y_n \sim \mathcal{N}(f(\mathbf{x}_n), \nu)$ and ν is the variance of noise introduced into the function observations. This prior and these data induce a posterior over functions; the acquisition function, which we denote by $a : \mathcal{X} \to \mathbb{R}^+$, determines what point in $\mathcal{X}$ should be evaluated next via a proxy optimization $\mathbf{x}_{\mathsf{next}} = \operatorname{argmax}_{\mathbf{x}} a(\mathbf{x})$, where several different functions have been proposed. In general, these acquisition functions depend on the previous observations, as well as the GP hyperparameters; we denote this dependence as $a(\mathbf{x}\,;\,\{\mathbf{x}_n, y_n\}, \theta)$. There are several popular choices of acquisition function. Under the Gaussian process prior, these functions depend on the model solely through its predictive mean function $\mu(\mathbf{x}\,;\,\{\mathbf{x}_n, y_n\}, \theta)$ and predictive variance function $\sigma^2(\mathbf{x}\,;\,\{\mathbf{x}_n, y_n\}, \theta)$. In the proceeding, we will denote the best current value as $\mathbf{x}_{\mathsf{best}} = \operatorname{argmin}_{\mathbf{x}_n} f(\mathbf{x}_n)$, $\Phi(\cdot)$ will denote the cumulative distribution function of the standard normal, and $\phi(\cdot)$ will denote the standard normal density function.

Probability of Improvement. One intuitive strategy is to maximize the probability of improving over the best current value (Kushner, 1964). Under the GP this can be computed analytically as

$$a_{\mathsf{PI}}(\mathbf{x}\,;\,\{\mathbf{x}_n, y_n\}, \theta) = \Phi(\gamma(\mathbf{x})) \qquad \gamma(\mathbf{x}) = \frac{f(\mathbf{x}_{\mathsf{best}}) - \mu(\mathbf{x}\,;\,\{\mathbf{x}_n, y_n\}, \theta)}{\sigma(\mathbf{x}\,;\,\{\mathbf{x}_n, y_n\}, \theta)}. \tag{1}$$

Expected Improvement. Alternatively, one could choose to maximize the expected improvement (EI) over the current best. This also has closed form under the Gaussian process:

$$a_{\mathsf{EI}}(\mathbf{x}\,;\,\{\mathbf{x}_n, y_n\}, \theta) = \sigma(\mathbf{x}\,;\,\{\mathbf{x}_n, y_n\}, \theta)\,(\gamma(\mathbf{x})\,\Phi(\gamma(\mathbf{x})) + \mathcal{N}(\gamma(\mathbf{x})\,;\,0, 1)) \tag{2}$$

GP Upper Confidence Bound. A more recent development is the idea of exploiting lower confidence bounds (upper, when considering maximization) to construct acquisition functions that minimize regret over the course of their optimization (Srinivas et al., 2010). These acquisition functions have the form

$$a_{\mathsf{LCB}}(\mathbf{x}\,;\,\{\mathbf{x}_n, y_n\}, \theta) = \mu(\mathbf{x}\,;\,\{\mathbf{x}_n, y_n\}, \theta) - \kappa\,\sigma(\mathbf{x}\,;\,\{\mathbf{x}_n, y_n\}, \theta), \tag{3}$$

with a tunable κ to balance exploitation against exploration.

In this work we will focus on the expected improvement criterion, as it has been shown to be better-behaved than probability of improvement, but unlike the method of GP upper confidence bounds (GP-UCB), it does not require its own tuning parameter. We have found expected improvement to perform well in minimization problems, but wish to note that the regret formalization is more appropriate for many settings. We perform a direct comparison between our EI-based approach and GP-UCB in Section 4.1.

3. Practical Considerations for Bayesian Optimization of Hyperparameters. Although an elegant framework for optimizing expensive functions, there are several limitations that have prevented it from becoming a widely-used technique for optimizing hyperparameters in machine learning problems. First, it is unclear for practical problems what an appropriate choice is for the covariance function and its associated hyperparameters. Second, as the function evaluation itself may involve a time-consuming optimization procedure, problems may vary significantly in duration and this should be taken into account. Third, optimization algorithms should take advantage of multi-core parallelism in order to map well onto modern computational environments. In this section, we propose solutions to each of these issues.

3.1. *Covariance Functions and Treatment of Covariance Hyperparameters.* The power of the Gaussian process to express a rich distribution on functions rests solely on the shoulders of the covariance function. While non-degenerate covariance functions correspond to infinite bases, they nevertheless can correspond to strong assumptions regarding likely functions. In particular, the automatic relevance determination (ARD) *squared exponential* kernel

$$K_{\mathsf{SE}}(\mathbf{x}, \mathbf{x}') = \theta_0 \exp\left\{-\frac{1}{2}r^2(\mathbf{x}, \mathbf{x}')\right\} \qquad r^2(\mathbf{x}, \mathbf{x}') = \sum_{d=1}^{D}(x_d - x'_d)^2/\theta_d^2. \tag{4}$$

is often a default choice for Gaussian process regression. However, sample functions with this covariance function are unrealistically smooth for practical optimization problems. We instead propose the use of the ARD Matérn 5/2 kernel:

$$K_{\mathsf{M52}}(\mathbf{x}, \mathbf{x}') = \theta_0 \left(1 + \sqrt{5r^2(\mathbf{x}, \mathbf{x}')} + \frac{5}{3}r^2(\mathbf{x}, \mathbf{x}')\right) \exp\left\{-\sqrt{5r^2(\mathbf{x}, \mathbf{x}')}\right\}. \tag{5}$$

This covariance function results in sample functions which are twice differentiable, an assumption that corresponds to those made by, e.g., quasi-Newton methods, but without requiring the smoothness of the squared exponential.

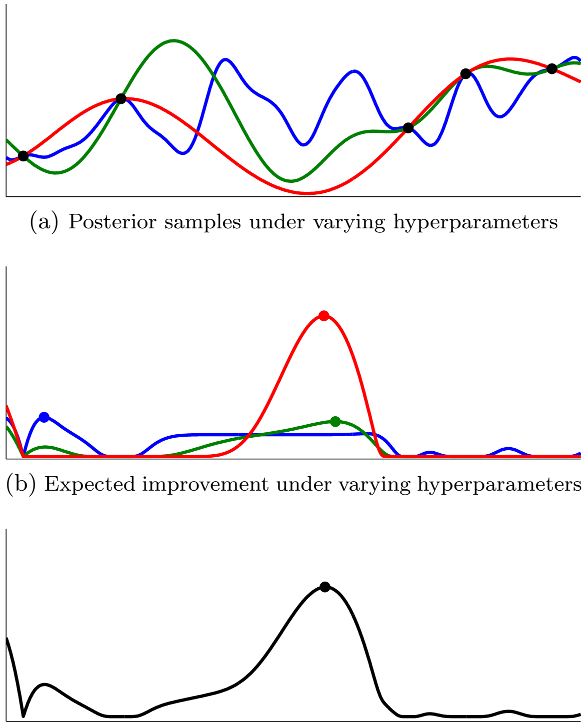
After choosing the form of the covariance, we must also manage the hyperparameters that govern its behavior (Note that these "hyperparameters" are different than the ones which are being subjected to the overall Bayesian optimization.), as well as that of the mean function. For our problems of interest, typically we would have $D+3$ Gaussian process hyperparameters: D length scales $\theta_{1:D}$, the covariance amplitude θ_0, the observation noise ν, and a constant mean m. The most commonly advocated approach is to use a point estimate of these parameters by optimizing the marginal likelihood under the Gaussian process

$$p(\mathbf{y} \,|\, \{\mathbf{x}_n\}_{n=1}^N, \theta, \nu, m) = \mathcal{N}(\mathbf{y} \,|\, m\mathbf{1}, \mathbf{\Sigma}_\theta + \nu\mathbf{I}),$$

where $\mathbf{y} = [y_1, y_2, \cdots, y_n]^{\mathsf{T}}$, and $\mathbf{\Sigma}_\theta$ is the covariance matrix resulting from the N input points under the hyperparameters θ.

However, for a fully-Bayesian treatment of hyperparameters (summarized here by θ alone), it is desirable to marginalize over hyperparameters and compute the *integrated acquisition function*:

$$\hat{a}(\mathbf{x}\,;\, \{\mathbf{x}_n, y_n\}) = \int a(\mathbf{x}\,;\, \{\mathbf{x}_n, y_n\}, \theta)\, p(\theta \,|\, \{\mathbf{x}_n, y_n\}_{n=1}^N)\, \mathrm{d}\theta, \tag{6}$$

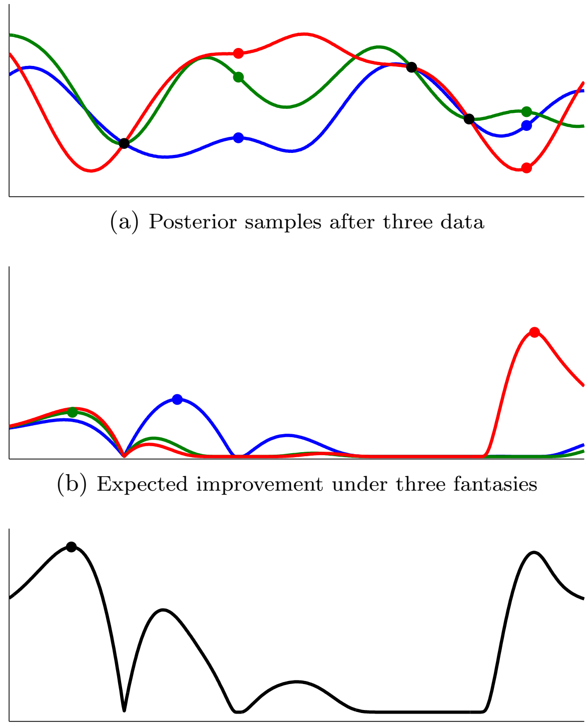


(a) Posterior samples under varying hyperparameters

(b) Expected improvement under varying hyperparameters

(c) Integrated expected improvement

Fig 1: Illustration of integrated expected improvement. (a) Three posterior samples are shown, each with different length scales, after the same five observations. (b) Three expected improvement acquisition functions, with the same data and hyperparameters. The maximum of each is shown. (c) The integrated expected improvement, with its maximum shown.



(a) Posterior samples after three data

(b) Expected improvement under three fantasies

(c) Expected improvement across fantasies

Fig 2: Illustration of the acquisition with pending evaluations. (a) Three data have been observed and three posterior functions are shown, with "fantasies" for three pending evaluations. (b) Expected improvement, conditioned on the each joint fantasy of the pending outcome. (c) Expected improvement after integrating over the fantasy outcomes.

where $a(\mathbf{x})$ depends on θ and all of the observations. For probability of improvement and expected improvement, this expectation is the correct generalization to account for uncertainty in hyperparameters. We can therefore blend acquisition functions arising from samples from the posterior over GP hyperparameters and have a Monte Carlo estimate of the integrated expected improvement. These samples can be acquired efficiently using slice sampling, as described in Murray and Adams (2010). As both optimization and Markov chain Monte Carlo are computationally dominated by the cubic cost of solving an N-dimensional linear system (and our function evaluations are assumed to be much more expensive anyway), the fully-Bayesian treatment is sensible and our empirical evaluations bear this out. Figure 1 shows how the integrated expected improvement changes the acquistion function.

3.2. *Modeling Costs.* Ultimately, the objective of Bayesian optimization is to find a good setting of our hyperparameters as quickly as possible. Greedy acquisition procedures such as expected improvement try to make the best progress possible in the next function evaluation. From a practial point of view, however, we are not so concerned with function evaluations as with wallclock time. Different regions of the parameter space may result in vastly different execution times, due to varying regularization, learning rates, etc. To improve our performance in terms of wallclock time, we propose optimizing with the *expected improvement per second*, which prefers to acquire points that are not only likely to be good, but that are also likely to be evaluated quickly. This notion of cost can be naturally generalized to other budgeted resources, such as reagents or money.

Just as we do not know the true objective function $f(\mathbf{x})$, we also do not know the *duration function* $c(\mathbf{x}) : \mathcal{X} \to \mathbb{R}^+$. We can nevertheless employ our Gaussian process machinery to model $\ln c(\mathbf{x})$ alongside $f(\mathbf{x})$. In this work, we assume that these functions are independent of each other, although their coupling may be usefully captured using GP variants of multi-task learning (e.g., Teh et al. (2005); Bonilla et al. (2008)). Under the independence assumption, we can easily compute the predicted expected inverse duration and use it to compute the expected improvement per second as a function of $\mathbf{x}$.

3.3. *Monte Carlo Acquisition for Parallelizing Bayesian Optimization.* With the advent of multi-core computing, it is natural to ask how we can parallelize our Bayesian optimization procedures. More generally than simply batch parallelism, however, we would like to be able to decide what $\mathbf{x}$ should be evaluated next, even while a set of points are being evaluated. Clearly, we cannot use the same acquisition function again, or we will repeat one of the pending experiments. We would ideally perform a roll-out of our acquisition policy, to choose a point that appropriately balanced information gain and exploitation. However, such roll-outs are generally intractable. Instead we propose a sequential strategy that takes advantage of the tractable inference properties of the Gaussian process to compute Monte Carlo estimates of the acquisiton function under different possible results from pending function evaluations.

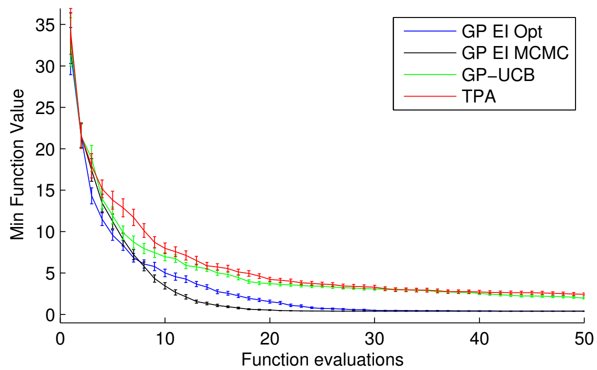
Consider the situation in which N evaluations have completed, yielding data $\{\mathbf{x}_n, y_n\}_{n=1}^N$, and in which J evaluations are pending at locations $\{\mathbf{x}_j\}_{j=1}^J$. Ideally, we would choose a new point based on the expected acquisition function under all possible outcomes of these pending evaluations:

$$\hat{a}(\mathbf{x}\,;\{\mathbf{x}_n, y_n\}, \theta, \{\mathbf{x}_j\}) = \int_{\mathbb{R}^J} a(\mathbf{x}\,;\{\mathbf{x}_n, y_n\}, \theta, \{\mathbf{x}_j, y_j\})\, p(\{y_j\}_{j=1}^J \,|\, \{\mathbf{x}_j\}_{j=1}^J, \{\mathbf{x}_n, y_n\}_{n=1}^N)\, \mathrm{d}y_1 \cdots \mathrm{d}y_J. \tag{7}$$

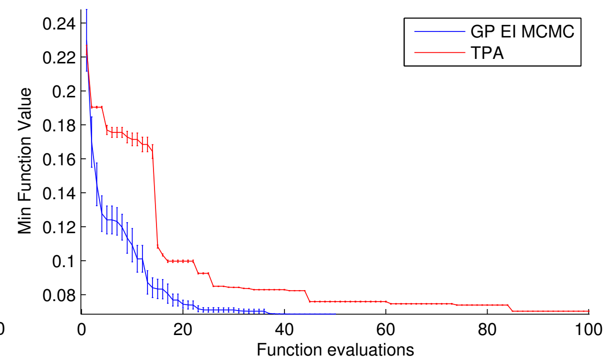
This is simply the expectation of $a(\mathbf{x})$ under a J-dimensional Gaussian distribution, whose mean and covariance can easily be computed. As in the covariance hyperparameter case, it is straightforward to use samples from this distribution to compute the expected acquisition and use this to select the next point. Figure 2 shows how this procedure would operate with queued evaluations. We note that a similar approach is touched upon briefly by Ginsbourger and Riche (2010), but they view it as too intractable to warrant attention. We have found our Monte Carlo estimation procedure to be highly effective in practice, however, as will be discussed in Section 4.

4. Empirical Analyses. In this section, we empirically analyse[1] the algorithms introduced in this paper and compare to existing strategies and human performance on a number of challenging machine learning problems. We refer to our method of expected improvement while marginalizing GP hyperparameters as "GP EI MCMC", optimizing hyperparameters as "GP EI Opt", EI per second as "GP EI per Second", and N times parallelized GP EI MCMC as "Nx GP EI MCMC".

[1] All experiments were conducted on identical machines using the Amazon EC2 service.



(a)



(b)

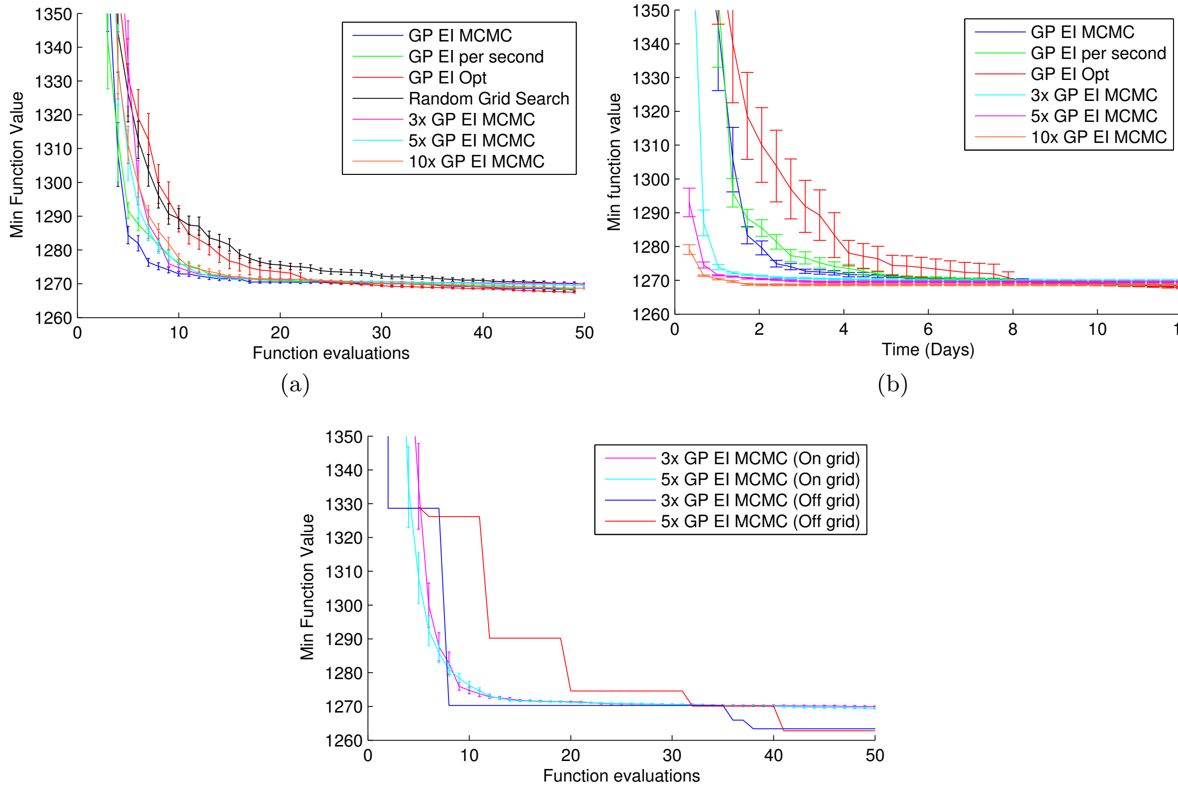
Fig 3: A comparison of standard approaches compared to our GP EI MCMC approach on the Branin-Hoo function (3a) and training logistic regression on the MNIST data (3b).

4.1. *Branin-Hoo and Logistic Regression.* We first compare to standard approaches and the recent Tree Parzen Algorithm[2] (TPA) of Bergstra et al. (2011) on two standard problems. The Branin-Hoo function is a common benchmark for Bayesian optimization techniques (Jones, 2001) that is defined over $x \in \mathbb{R}^2$ where $0 \leq x_1 \leq 15$ and $-5 \leq x_2 \leq 15$. We also compare to TPA on a logistic regression classification task on the popular MNIST data. The algorithm requires choosing four hyperparameters, the learning rate for stochastic gradient descent, on a log scale from 0 to 1, the ℓ_2 regularization parameter, between 0 and 1, the mini batch size, from 20 to 2000 and the number of learning epochs, from 5 to 2000. Each algorithm was run on the Branin-Hoo and logistic regression problems 100 and 10 times respectively and mean and standard error are reported. The results of these analyses are presented in Figures 3a and 3b in terms of the number of times the function is evaluated. On Branin-Hoo, integrating over hyperparameters is superior to using a point estimate and the GP EI significantly outperforms TPA, finding the minimum in fewer than half as many evaluations, in both cases.

4.2. *Online LDA.* Latent Dirichlet allocation (LDA) is a directed graphical model for documents in which words are generated from a mixture of multinomial "topic" distributions. Variational Bayes is a popular paradigm for learning and, recently, Hoffman et al. (2010) proposed an online learning approach in that context. Online LDA requires two learning parameters, τ_0 and κ, that control the learning rate $\rho_t = (\tau_0 + t)^{-\kappa}$ used to update the variational parameters of LDA based on the t^{th} minibatch of document word count vectors. The size of the minibatch is also a third parameter that must be chosen. Hoffman et al. (2010) relied on an exhaustive grid search of size $6 \times 6 \times 8$, for a total of 288 hyperparameter configurations.

We used the code made publically available by Hoffman et al. (2010) to run experiments with online LDA on a collection of Wikipedia articles. We downloaded a random set of 249,560 articles, split into training, validation and test sets of size 200,000, 24,560 and 25,000 respectively. The documents are represented as vectors of word counts from a vocabulary of 7,702 words. As reported in Hoffman et al. (2010), we used a lower bound on the per word perplexity of the validation set documents as the performance measure. One must also specify the number of topics and the hyperparameters η for the symmetric Dirichlet prior over the topic

[2]Using the publicly available code from `https://github.com/jaberg/hyperopt/wiki`



(a) (b)

(c)

Fig 4: Different strategies of optimization on the Online LDA problem compared in terms of function evaluations (4a), walltime (4b) and constrained to a grid or not (4c).

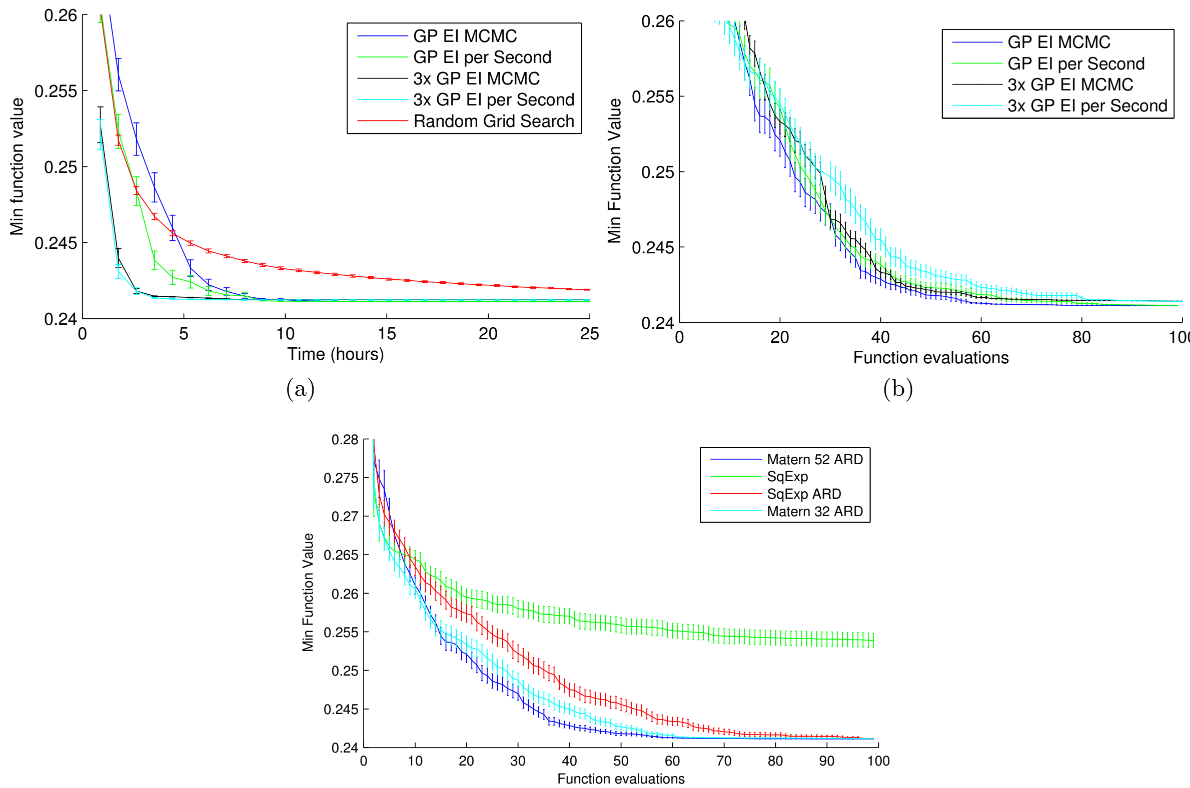
distributions and α for the symmetric Dirichlet prior over the per document topic mixing weights. We followed Hoffman et al. (2010) and used 100 topics and $\eta = \alpha = 0.01$ in our experiments in order to emulate their analysis and repeated exactly the grid search reported in the paper[3]. Each online LDA evaluation generally took between five to ten hours to converge, thus the grid search requires approximately 60 to 120 processor days to complete.

In Figures 4a and 4b we compare our various strategies of optimization over the same grid on this expensive problem. That is, the algorithms were restricted to only the exact parameter settings as evaluated by the grid search. Each optimization was then repeated one hundred times (each time picking two different random experiments to initialize the optimization with) and the mean and standard error are reported. Figures 4a and 4b respectively show the average minimum loss (perplexity) achieved by each strategy compared to the number of times online LDA is evaluated with new parameter settings and the duration of the optimization in days. Figure 4c shows the average loss of 3 and 5 times parallelized GP EI MCMC which are restricted to the same grid as compared to a single run of the same algorithms where the algorithm can flexibly choose new parameter settings within the same range by optimizing the expected improvement.

In this case, integrating over hyperparameters is superior to using a point estimate. While

[3]i.e. the only difference was the randomly sampled collection of articles in the data set and the choice of the vocabulary. We ran each evaluation for 10 hours or until convergence.

GP EI MCMC is the most efficient in terms of function evaluations, we see that parallelized GP EI MCMC finds the best parameters in significantly less time. Finally, in Figure 4c we see that the parallelized GP EI MCMC algorithms find a significantly better minimum value than was found in the grid search used by Hoffman et al. (2010) while running a fraction of the number of experiments.



(a) (b) (c)

Fig 5: A comparison of various strategies for optimizing the hyperparameters of M3E models on the protein motif finding task in terms of wallclock time (5a), function evaluations (5b) and different covariance functions(5c).

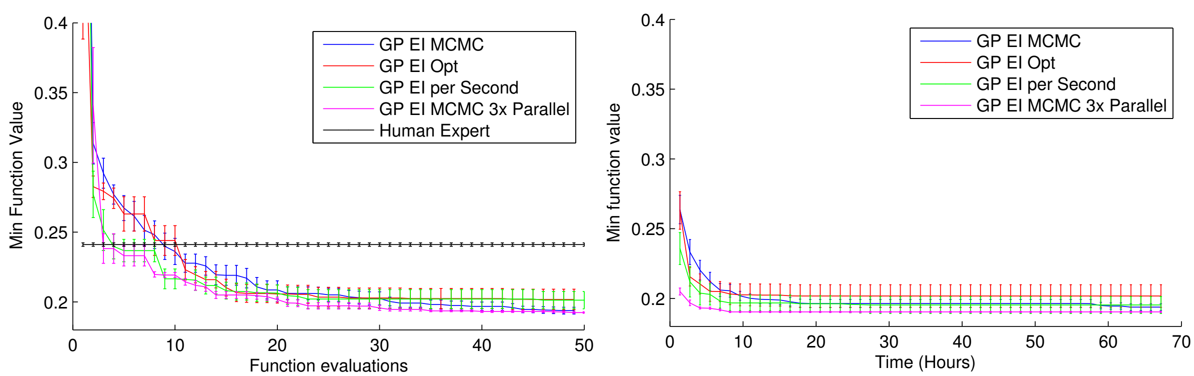
4.3. *Motif Finding with Structured Support Vector Machines.* In this example, we consider optimizing the learning parameters of Max-Margin Min-Entropy (M3E) Models (Miller et al., 2012), which include Latent Structured Support Vector Machines (Yu and Joachims, 2009) as a special case. Latent structured SVMs outperform SVMs on problems where they can explicitly model problem-dependent hidden variables. A popular example task is the binary classification of protein DNA sequences (Miller et al., 2012; Yu and Joachims, 2009; Kumar et al., 2010). The hidden variable to be modeled is the unknown location of particular subsequences, or *motifs*, that are indicators of positive sequences.

Setting the hyperparameters, such as the regularisation term, C, of structured SVMs remains a challenge and these are typically set through a time consuming grid search procedure as is done in Miller et al. (2012) and Yu and Joachims (2009). Indeed, Kumar et al. (2010) report that hyperparameter selection was avoided for the motif finding task due to being too computationally expensive. However, Miller et al. (2012) demonstrate that classification results depend highly on the setting of the parameters, which differ for each protein.

M3E models introduce an entropy term, parameterized by α, which enables the model to significantly outperform latent structured SVMs. This additional performance, however, comes at the expense of an additional problem-dependent hyperparameter. We emulate the experiments of Miller et al. (2012) for one protein with approximately 40,000 sequences. We explore 25 settings of the parameter C, on a log scale from 10^{-1} to 10^{6}, 14 settings of α, on a log scale from 0.1 to 5 and the model convergence tolerance, $\epsilon \in \{10^{-4}, 10^{-3}, 10^{-2}, 10^{-1}\}$. We ran a grid search over the 1,400 possible combinations of these parameters, evaluating each over 5 random 50-50 training and test splits.

In Figures 5a and 5b, we compare the randomized grid search to GP EI MCMC, GP EI per Second and their 3x parallelized versions, all constrained to the same points on the grid, in terms of minimum validation error vs wallclock time and function evaluations. Each algorithm was repeated 100 times and the mean and standard error are shown. We observe that the Bayesian optimization strategies are considerably more efficient than grid search which is the status quo. In this case, GP EI MCMC is superior to GP EI per Second in terms of function evaluations but GP EI per Second finds better parameters faster than GP EI MCMC as it learns to use a less strict convergence tolerance early on while exploring the other parameters. Indeed, 3x GP EI per second is the least efficient in terms of function evaluations but finds better parameters faster than all the other algorithms.

Figure 5c compares the use of various covariance functions in GP EI MCMC optimization on this problem. The optimization was repeated for each covariance 100 times and the mean and standard error are shown. It is clear that the selection of an appropriate covariance significantly affects performance and the estimation of length scale parameters is critical. The assumption of the infinite differentiability of the underlying function as imposed by the commonly used squared exponential is too restrictive for this problem.



(a) (b)

Fig 6: Validation error on the CIFAR-10 data for different optimization strategies.

4.4. *Convolutional Networks on CIFAR-10.* Neural networks and deep learning methods notoriously require careful tuning of numerous hyperparameters. Multi-layer convolutional neural networks are an example of such a model for which a thorough exploration of architechtures and hyperparameters is beneficial, as demonstrated in Saxe et al. (2011), but often computationally prohibitive. While Saxe et al. (2011) demonstrate a methodology for efficiently exploring model architechtures, numerous hyperparameters, such as regularisation parameters, remain. In this empirical analysis, we tune nine hyperparameters of a three-layer convolutional network, described in Krizhevsky (2009) on the CIFAR-10 benchmark dataset using the code provided[4]. This model has been carefully tuned by a human expert (Krizhevsky, 2009) to achieve a highly competitive result of 18% test error, which matches the published state of the art[5] result (Coates and Ng, 2011) on CIFAR-10. The parameters we explore include the number of epochs to run the model, the learning rate, four weight costs (one for each layer and the softmax output weights), and the width, scale and power of the response normalization on the pooling layers of the network.

We optimize over the nine parameters for each strategy on a withheld validation set and report the mean validation error and standard error over five separate randomly initialized runs. Results are presented in Figure 6 and contrasted with the average results achieved using the best parameters found by the expert. The best hyperparameters[6] found by the GP EI MCMC approach achieve an error on the *test set* of 14.98%, which is over 3% better than the expert and the state of the art on CIFAR-10.

5. Conclusion. In this paper we presented methods for performing Bayesian optimization of hyperparameters associated with general machine learning algorithms. We introduced a fully Bayesian treatment for expected improvement, and algorithms for dealing with variable time regimes and parallelized experiments. Our empirical analysis demonstrates the effectiveness of our approaches on three challenging recently published problems spanning different areas of machine learning. The code used will be made publicly available. The resulting Bayesian optimization finds better hyperparameters significantly faster than the approaches used by the authors. Indeed our algorithms *surpassed* a human expert at selecting hyperparameters on the competitive CIFAR-10 dataset and as a result beat the state of the art by over 3%.

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[4]Available at: `http://code.google.com/p/cuda-convnet/` using the architechture defined in `http://code.google.com/p/cuda-convnet/source/browse/trunk/example-layers/layers-18pct.cfg`

[5]Without augmenting the training data.

[6]The optimized parameters deviate interestingly from the expert-determined settings; e.g., the optimal weight costs are asymmetric (the weight cost of the second layer is approximately an order of magnitude smaller than the first layer), a learning rate two orders of magnitude smaller, a slightly wider response normalization, larger scale and much smaller power.

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