Abstract

The success of deep (reinforcement) learning systems crucially depends on the correct choice of hyperparameters which are notoriously sensitive and expensive to evaluate. Training these systems typically requires running iterative processes over multiple epochs or episodes. Traditional approaches only consider final performance of a hyperparameter although intermediate information from the learning curve is readily available. In this paper, we present a Bayesian optimization approach which exploits the iterative structure of learning algorithms for efficient hyperparameter tuning. First, we transform each training curve into numeric scores. Second, we selectively augment the data using the information from the curve. This augmentation step enables modeling efficiency while preventing the ill-conditioned issue of Gaussian process covariance matrix if augmenting the whole curve. We demonstrate the efficiency of our algorithm by tuning hyperparameters for the training of deep reinforcement learning agents and convolutional neural networks. Our algorithm outperforms all existing baselines in identifying optimal hyperparameters in minimal time.

1 Introduction

Deep learning (DL) and deep reinforcement learning (DRL) have lead to impressive breakthroughs in a broad range of applications such as game play (Mnih et al., 2013, Silver et al., 2016), motor control (Todorov et al., 2012), and image recognition (Krizhevsky et al., 2012). To maintain general applicability, these algorithms expose sets of hyperparameters to adapt their behavior to any particular task at hand. This flexibility comes at the price of having to tune an additional set of parameters as, particularly in DL and DRL, poor settings lead to drastic performance losses or divergence (Sprague, 2015, Smith, 2018, Henderson et al., 2018). On top of being notoriously sensitive to these choices, deep (reinforcement) learning systems often have high training costs in terms of computational resources and time. For example, a single training iteration on the Atari Breakout game took approximately 75 hours on a GPU cluster (Mnih et al., 2013). Tuning DRL parameters is further complicated as only noisy evaluations of an agent’s final performance are obtainable.

Bayesian optimization (BO) (Brochu et al., 2010, Hennig and Schuler, 2012, Shahriari et al., 2016) has recently achieved considerable success in optimizing these hyperparameters. This approach casts the tuning process as a global optimization problem based on noisy evaluations of a black-box function \( f \). BO constructs a surrogate model typically using a Gaussian process (Rasmussen, 2006) over this unknown function. This GP surrogate is used to build an acquisition function (Snoek et al., 2012, Hernández-Lobato et al., 2014, Wang and Jegelka, 2017) which suggests the next hyperparameter to evaluate.

In modern machine learning (ML) algorithms (Jordan and Mitchell, 2015), the training process is typically conducted in an iterative manner. A natural example is given by deep learning where training is often based on stochastic gradient descent and other iterative procedures. Similarly, the training of reinforcement learning agent is mostly carried out using multiple episodes. The knowledge accumulated during these training iterations can be useful to inform Bayesian optimization. However, most of the existing BO approaches (Snoek et al., 2012, Shahriari et al., 2016) define the objective function as the average performance over the final training iterations. In doing so, they ignore the useful information contained in the preceding training steps.

In this paper, we present a Bayesian optimization approach for tuning systems learning iteratively -- the cases of deep learning and deep reinforcement learning. First, we consider the joint space of input hyperparameters and number of training iterations to capture the learning progress at different time steps in the training process. We then
propose to transform the whole training curve into a numeric score according to user preference. To learn across the joint space efficiently, we introduce a data augmentation technique leveraging intermediate information from the iterative process. By exploiting the iterative structure of training procedures, we encourage our algorithm to consider running a larger number of cheap (but high utility) experiments, when cost-ignorant algorithms would only be able to run a few expensive ones. We demonstrate the efficiency of our algorithm on training DRL agents on several well-known benchmarks as well as the training of convolutional neural networks. In particular, our algorithm outperforms existing baselines in finding the best hyperparameter terms in wall-clock time. Our main contributions are summarized as

- the novel approach to optimizing the learning curve of a ML algorithm by using the training curve compression instead of averaged final performance,
- joint modeling of hyperparameter and iterations with data augmentation for increased sample-efficiency while preventing GP covariance conditioning issues,
- demonstration on tuning DRL and CNNs.

2 Related Work

In the following, we review a number of approaches that aim to minimize the number of training iterations needed to identify the optimal hyperparameters.

The first category employs stopping criteria to terminate some training runs early and instead allocate resources towards more promising settings. These criteria typically evolve around projecting a final score using earlier training stages. Freezethaw BO (Swersky et al., 2014) models the training loss over time using a GP regressor under the assumption that the training loss roughly follows an exponential decay. Based on this projection training resources are allocated to the most promising settings. Hyperband (Li and Jamieson, 2018; Falkner et al., 2018) dynamically allocates the computational resources (e.g., training epochs or dataset size) through random sampling and eliminates under-performing hyperparameter settings by successive halving. In addition, attempts have also been made to improve the epoch efficiency of other hyperparameter optimization algorithms, including Baker et al. (2017), Domhan et al. (2015), Klein et al. (2017a), and (Dat et al., 2019) which predict the final learning outcome based on partially trained learning curves to identify hyperparameter settings that are predicted to under-perform and early-stop their model learning. In the context of DRL, however, these stopping criteria may not be applicable due to the unpredictable fluctuations of DRL reward curves. In the supplement, we illustrate the noisiness of DRL training.

The second category [Swersky et al., 2013; Klein et al., 2017a; Kandasamy et al., 2017] aims to reduce the resource consumption of BO by utilizing low-fidelity functions which can be obtained by using a subset of the training data or by training the ML model for a small number of iterations. Multi-task BO (Swersky et al., 2013) requires the user to define a division of the dataset into pre-defined and discrete subtasks. Multi-fidelity BO with continuous approximation (BOCA) (Kandasamy et al., 2017) extends this idea to continuous settings. Specifically, BOCA first selects the hyperparameter input and then the corresponding fidelity to be evaluated at. The fidelity in this context refers to the use of different number of learning iterations. Analogous to BOCA’s consideration of continuous fidelities, Fabolas (Klein et al., 2017a) proposes to model the joint space of input hyperparameter and dataset size. Then, Fabolas optimizes them jointly to select the optimal input and dataset size.

The above approaches typically identify performance of hyperparameters via the average (either training or validation) loss of the last learning iterations. Thereby, they do not account for potential noise in the learning process (e.g., they might select unstable settings that jump to high performance in the last couple of iterations).

3 Bayesian Optimization for Iterative Learning (BOIL)

We present an efficient hyperparameter optimization algorithm for a machine learning system with iterative learning.

3.1 Problem setting

We consider a machine learning algorithm, which given a $d$-dimensional hyperparameter $x \in \mathcal{X} \subset \mathbb{R}^d$, is trained for $t$ iterations. This process has a training time cost $c(x,t)$ and produces training evaluations $r(x,t)$ for $t$ iterations, $t \in [T_{\text{min}}, T_{\text{max}}]$. These could be episode rewards in DRL or training accuracies in DL. An important property of iterative training is that we observe the whole curve at preceding steps $r(x,t'), \forall t' \leq t$. We consider the black-box function $f(x,t)$ mapping from the hyperparameter $x$ to the score associated with training curve $r(x,t)$. Formally, we aim to optimize $x^* = \arg \max_{x \in \mathcal{X}} f(x,t)$ at the same time we want to keep the overall training time $\sum_{i=1}^{N} c(x_i, t_i)$ of evaluated settings $[x_i, t_i]$ as low as possible.

3.2 Joint modeling of hyperparameter and iterations

We model the black-box function $f(x,t)$ as a joint GP where we assume that the objective function at $t$ is a slice of $f$ at $t$. As a consequence, this GP captures correlations in hyperparameter input and training iteration

$$f(x,t) \sim GP\{0, K([x,t],[x',t'])\}$$
Based on the above surrogate function, we can estimate the predictive mean and uncertainty of a Gaussian process for any input $z = [x, t]$, as the training time and build an additional GP surrogate model for the expected training cost (time) as a function of hyperparameter-iteration pairs $[x, t] \in \mathcal{X} \times \mathcal{R}$. The analytical formula for this GP is similar to Eq. (1) and Eq. (2), except the output $y$ is now the training time $c(x, t)$.

### Surrogate cost model

We consider the cost function $\tau(x, t)$, where the cost observation is denoted as $c(x, t)$, as the training time and build an additional GP surrogate model for the expected training cost (time) as a function of hyperparameter-iteration pairs $[x, t] \in \mathcal{X} \times \mathcal{R}$. The analytical formula for this GP is similar to Eq. (1) and Eq. (2), except the output $y$ is now the training time $c(x, t)$.

#### 3.3 Training curve compression

Existing BO approaches [Chen et al. 2018; Li and Jameson 2018] typically define the objective function as an average loss over the final learning episodes. However, this does not take into consideration how stable performance is or the training stage at which it has been achieved. In our model, averaging learning losses is likely to be misleading due to the noise of our observations -- particularly during the early stages of training. We suggest to compress the whole learning curve into a numeric score via a preference function representing the user’s desired training curve -- in the following we use the Sigmoid function. Given the training curve, we compute the utility score as

$$y = \sum_{i=1}^{t} r(i) \times l(i)$$

$$l(x) = \frac{1}{1 + \exp(-x)}$$

Note that more generally, $l(i)$ can depend on the length $t$ of the training curve and for appropriate choices, i.e. $l(i) = \frac{1}{t}$, we recover the averaging described above. The Sigmoid preference has a number of desirable properties. As the early weights are small, less credit is given to fluctuations at the initial stages, making it less likely for our surrogate to be biased towards randomly well performing settings. However, as weights monotonically increase, hyperparameters enabling learning (and therefore improved performance) are preferred. As weights saturate over time, stable, high performing configurations is preferred over short "performance spikes" characteristic of unstable training.
Figure 2: The condition number of GP covariance matrix goes badly if we add noisy observations closely each other. The large condition number measures the nearness to singularity. This happens when we add the whole curve of points into a GP.

Lastly, this utility score assigns higher values to the same performance if it is being maintained over more episodes. We illustrate the reward transformation using the Sigmoid function in Fig. 1. In Fig. 10 in the appendix, we further demonstrate that our model is robust with different preference choices.

3.4 Augmenting data with intermediate observations

When evaluating a configuration \( x \) for a number of iterations \( t \), we obtain not only a final score but also all reward sequences \( r(\mathbf{x}, t') \), \( \forall t' = 1, \ldots, t \). The auxiliary information from the curve can bring useful information for Bayesian optimization. Therefore, we propose to augment the sample set of our GP model using the information from the curve. This prevents the algorithm from reselecting the same input \( x \) at the lower fidelity (e.g., lower training iteration) \( t' < t \) by reducing uncertainty around these locations. This uncertainty reduction lowers the value of the acquisition function and encourages exploration elsewhere.

Ill-conditioned issue with augmenting a full curve. A naive approach for augmentation is to add a full curve of points \( \{[\mathbf{x}, j], y_j\}_{j=1}^t \) where \( y_j \) is computed from \( r(\mathbf{x}, j) \) using Eq. 4. However, this approach imposes serious issues in conditioning of the GP covariance matrix. As we cluster more evaluations closely, the conditioning of the GP covariance degrades further, as discussed in (McLeod et al., 2018). This conditioning issue is especially serious in our DRL noisy curve fluctuating widely. We highlight this negative effect in Fig. 2 where the log of condition number goes above 25 if we augment the whole curve. Then, we illustrate the effect on GP estimation in Fig. 3 wherein the GP mean estimation goes off significantly large and small in the bottom row due to the undesirable effect of the GP covariance condition number.

Therefore, it is essential to selectively augment the observations from the learning curve. While it is not trivial to intervene the condition number of the GP covariance, we can mitigate such conditioning issue by discouraging adding similar points closely each other, as shown in (McLeod et al., 2018). Among the existing active learning approaches (Osborne et al., 2012; Contal et al., 2013; Gal et al., 2017), we utilize a determinantal point process (Kulesza et al., 2012) which will relax to maximizing a GP variance under a greedy setting.

k-DPP for selecting most informative points. By an abuse of notation, we use \( M \)-DPP to represent \( k \)-DPP since \( k \) is the kernel in our context. Given a training curve \( r(\mathbf{x}, t) \) and conditioning on the inclusion of an existing observations \( D_n \), we want to find a diverse set \( [t_1, \ldots, t_M]\), \( \forall t_m \leq t \) to augmented into \( \mathbf{x} \) to form additional observations \( Z = [z_1, \ldots, z_M] \) where each \( z_m = [\mathbf{x}, t_m] \).

\[
p^M(D \cup Z \mid D) \propto \det(K_Z - K_D K_D^{-1} K_D Z). \tag{6}
\]

While the discrete-DPP sampler formally extends to the
Bayes Opt with Iterative Learning (BOIL)

Input: #iter $N$, initial data $D_0$, define $z = [x,t]$

1: for $n = 1,...,N$ do
2: Fit a GP and acquisition function $\alpha(x,t)$ from the joint space of parameter-iteration
3: Fit a surrogate model for cost function $\tau(x,t)$
4: Select $z_n = \text{arg max}_x \alpha(x,t) / \tau(x,t)$
5: Observe $r_n, c_n = f(z_n)$ #$r_n$ is a training curve, $c_n$ is a cost (i.e., training time)
6: Compute $y_n$ from the curve $r_n$ using Eq. (4)
7: Augment observations $z_{n,m}, y_{n,m}, c_{n,m}, \forall m \leq M$ given $r_n$ and $D_1$ in Alg. 1
8: $D_n = D_{n-1} \cup (z_n,y_n,c_n) \cup (z_{n,m},y_{n,m},c_{n,m})$
9: end for

Output: optimal $x^*$ and $y^* = \text{max}_{y \in D_N} y$

### 3.5 Algorithm

To enforce non-negativity and numerical stability in the utility $\alpha$ and cost functions $\tau$, we make use of the transformations $\alpha = \log(1 + \exp(\alpha))$ and $\tau = \log(1 + \exp(\tau))$.

At each iteration $n$, we query the input parameter $x_n$ and the number of iteration $t_n$:

$$z_n = [x_n, t_n] = \text{argmax}_{x,t} \alpha(x,t) / \tau(x,t). \quad (8)$$

By evaluating the black-box function, we obtain the training curve $r_n$ and the training time $c_n$. Using this information, we generate up to $M$ augmented observations $z_{n,m}, y_{n,m}, c_{n,m}, \forall m \leq M$ from the new point $z_n$ and add them into our dataset $D_n$. We summarize our approach in Alg. 2.

### 4 Experiments

We demonstrate our proposed model by tuning hyperparameters for several deep reinforcement learning agents and convolutional neural networks (CNN). We provide additional illustrations and experiments in the supplement.

#### 4.1 Experimental setup and baselines

All experimental results described below are averaged over 20 independently performed runs with different random seeds. Unless otherwise indicated, final performance is estimated by evaluating the chosen hyperparameter over the maximum number of iterations. All experiments are executed on a NVIDIA 1080 GTX GPU using the tensorflow-gpu Python package. The DRL environments are available through the OpenAI gym (Brockman et al., 2016) and MuJoCo (Todorov et al., 2012). Our DRL implementations are based on the open source from Open AI Baselines (Dhariwal et al., 2017). We will release all source codes and packages in the final version.

We use square-exponential kernels for the GPs in our model and estimate their parameters using maximum marginal likelihood (Rasmussen, 2006). In Alg. 1, we set maximum the number of augmented points $M = 15$ and a threshold for log of GP covariance condition number is $\delta = 20$. We note that the optimization overhead is much less than the function evaluation time. In particular, the data augmentation step takes only $1\%$ of the time used for each DRL evaluation.

We select to compare with Hyperband (Li and Jamieson, 2018) which demonstrates empirical successes in tuning deep learning applications in an iteration-efficient manner. We extend the discrete (Swersky et al., 2013) to the continuous multi-task BO (or CMTBO) -- which can be seen as our BOIL without augmentation. We do not compare with Fabolas (Klein et al., 2017) because Fabolas is designed for varying dataset sizes, not iteration axis. We omit to compare with BOCA (Kandasamy et al., 2017) because the source code is not available and the algorithm specification is not trivial to re-implement. We also expect the performance of (Kandasamy et al., 2017) to be close (if not inferior) to CMTBO. This is because CMTBO jointly optimizes the fidelity and input while BOCA first selects the...
Figure 4: Illustration of model behavior in two consecutive evaluations on a 2-dimensional optimization task of tuning DDQN on CartPole. Our model selects a point (black square) by balancing the cost function and the value function.

We next examine the count of augmented observations generated per iteration in Fig. 5. Although this number is fluctuating, it tends to reduce over time. BOIL does not add more augmented observations at the later stage when we have gained sufficient information and GP covariance conditioning falls below our threshold δ.

4.3 Tuning deep reinforcement learning and CNN

We now optimize hyperparameters for deep reinforcement learning algorithms; in fact, this application motivated the development of BOIL. The combinations of hyperparameters to be tuned, target DRL algorithm and environment are detailed below. Additional information about these settings including parameter ranges can be found in the supplement.

**Task descriptions.** We consider three DRL settings to demonstrate BOIL’s ability to optimize highly noisy objectives. In the first, we optimize learning rate $\alpha$ and discount factor $\gamma$ of a Dueling DQN (DDQN) (Wang et al., 2016) agent in the CartPole-v0 environment. In the last two, we optimize actor learning rate $\alpha_1$, critic learning rate $\alpha_2$ and discount factor $\gamma$ of Advantage Actor Critic (A2C) (Mnih et al., 2016) agents in the InvertedPendulum-v2 and Reacher-v2 environments. In all cases, the learning rates are part of Adam optimizers (Kingma and Ba, 2014) and we use the standard length of 200 steps per episode. Due to space considerations, we present the plots of the DDQN-Cartpole setting in the supplement and also refer to the supplement for further experimental details.

In addition to the DRL applications, we tune 6 hyperparameters for training a convolutional neural network (LeC...
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The information gathered here is then used to inform later fast assessments of a multitude of hyperparameters. The plots show that BO-L and BOIL reliably identify parameters leading to stable training. BOIL takes only half total time to find this optimal curve. Without considering the whole curve, BO can only identify sub-optimal hyperparameters.

Cun et al. [1998] on the SVHN dataset (Netzer et al., 2011) as summarized in Table 1c in the supplement. We use two CNN layers, two fully connected layers and RMSProp (Hinton et al., 2012) as the main optimizer. The dataset is divided into 10,000 training images and a held-out test set of 10,000 images for evaluation. Optimizing 6 hyperparameters demonstrates the scalability of our approach.

Comparison of final learning curves. We first demonstrate the improvement in stability gained by using the proposed learning curve compression. For this, we examine the learning curves of the best hyperparameters identified by BO, BO-L and BOIL. Fig. 6 shows the learning progress over $T_{\text{max}}$ episodes for each of these. The curves are smoothed by averaging over 100 consecutive episodes for increased clarity. We first note, that all three algorithms eventually obtain similar performance at the end of learning. However, since BO-L and BOIL take into account the preceding learning steps, they achieve higher performance more quickly. Furthermore, they achieve this more reliably as evidenced by the smaller error bars (shaded regions).

Performance comparisons across iterations and real-time. Fig. 7 plots the performance of different algorithms against the number of iterations as well as real-time. The performance is the utility score of the best hyperparameters identified by the baselines. Across all three tasks, BOIL identifies optimal hyperparameters using significantly less computation time than other approaches.

The plots show that other approaches such as BO and BO-L can identify well-performing hyperparameters in fewer iterations than BOIL. However, they do so only considering costly, high-fidelity evaluations resulting in significantly higher evaluation times. In contrast to this behavior, BOIL accounts for the evaluation costs and chooses to initially evaluate low-fidelity settings consuming less time. This allows fast assessments of a multitude of hyperparameters. The information gathered here is then used to inform later point acquisitions. Hereby, the inclusion of augmented observations is crucial as it prevents the algorithm to reselect the input parameter $x$ at lower fidelity $t'$ if $x$ has been evaluated at higher fidelity $t > t'$. In addition, this augmentation is essential to prevent from the GP kernel issue instead of adding the full curve of points into our GP model.

Hyperband [Li and Jamieson, 2018] exhibits similar behavior in that it uses low fidelity (small $t$) evaluations to reduce a pool of randomly sampled configurations before evaluating at high fidelity (large $t$). To hedge against noisy evaluations and other effects, this process is repeated several times. This puts Hyperband at a disadvantage particularly in the noisy DRL tasks. Since early performance fluctuates hugely, Hyperband can be misled in where to allocate evaluation effort. It is then incapable of revising these choices until an entirely pool of hyperparameters is sampled and evaluated from scratch. In contrast to this, BOIL is more flexible than Hyperband in that it can freely explore-exploit the whole joint space. The GP surrogate hereby allows BOIL to generalize across hyperparameters and propagate information through the joint space.

5 Conclusion and Future work

Our framework complements the existing BO toolbox for hyperparameter tuning with iterative learning. We present a way of leveraging our understanding that later stages of the training process are informed by progress made in earlier ones. This results in a more iteration-efficient hyperparameter tuning algorithm that is applicable to a broad range of machine learning systems. We evaluate its performance on a set of diverse benchmarks. The results demonstrate that our model can surpass the performance of well-established alternatives while consuming significantly fewer resources. Finally, we would like to note that our approach is not necessarily specific to machine learning algorithms but more generally applies to any process exhibiting an iterative structure to be exploited.
Figure 7: Comparison of performance over BO evaluations (Left) and real-time (Right). Given the same time budget, CMTBO, Hyperband and BOIL can take more evaluations than vanilla BO, BO-L and Rand. BOIL outperforms other competitors in finding the optimal parameters in an iteration-efficient manner. BOIL exploits the knowledge about the training curve by selectively augmenting the data for GP with informative observations. CMTBO is less efficient comparing to BOIL. CMTBO does not augment the observations from the curve that CMTBO requires more evaluations and it can unnecessarily reselect parameters at lower fidelity.
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Appendix

We provide the readers further insights into our design choices and a deeper understanding of the algorithms properties. First, we give a brief overview of Bayesian optimization with Gaussian processes. We then illustrate our models behavior on a two dimensional problem. Last, we give further details of our experiments for reproducibility purposes.

A Bayesian Optimization Preliminaries

Bayesian optimization is a sequential approach to global optimization of black-box functions without making use of derivatives. It uses two components: a learned surrogate model of the objective function and an acquisition function derived from the surrogate for selecting new points to inform the surrogate with. In-depth discussions beyond our brief overview can be found in recent surveys (Brochu et al., 2010; Shahriari et al., 2016; Frazier, 2018).

A.1 Gaussian processes

The most common choice of surrogate models is the Gaussian process (GP) (Rasmussen, 2006). A GP defines a probability distribution over functions \( f \) under the assumption that any subset of point \( \{ (x_i, f(x_i)) \} \) is normally distributed. Formally, this is denoted as:

\[
    f(x) \sim \text{GP} (m(x), k(x, x'))
\]

where \( m(x) \) and \( k(x, x') \) are the mean and covariance functions, given by \( m(x) = \mathbb{E}[f(x)] \) and \( k(x, x') = \mathbb{E}[(f(x) - m(x))(f(x') - m(x'))] \). Typically, the mean of GP is assumed to be zero everywhere. The kernel \( k(x, x') \) can be thought of as a similarity measure relating \( f(x) \) and \( f(x') \). Numerous kernels encoding different prior beliefs about \( f(x) \) have been proposed. A popular choice is given by the square exponential kernel \( k(x, x') = \sigma_f^2 \exp\left(-\frac{(x-x')^2}{2\sigma_x^2}\right) \). The length-scale \( \sigma_x^2 \) regulates the maximal covariance between two points and can be estimated using maximum marginal likelihood. The SE kernel encodes the belief that nearby points are highly correlated as it is maximized at \( k(x, x') = \sigma_f^2 \) and decays the further \( x \) and \( x' \) are separated.

For prediction at a new data point \( x_\star \), let denote \( f_\star = f(x_\star) \) we have

\[
    \begin{bmatrix} f \\ f_\star \end{bmatrix} \sim \mathcal{N} \left( \begin{bmatrix} 0 \\ k_s \end{bmatrix}, \begin{bmatrix} K & k_\star' \\ k_s & k_{ss} \end{bmatrix} \right) \tag{9}
\]

where \( k_{ss} = k(x_\star, x_\star), \ k_s = k(x_\star, x) \) for \( \forall i \leq N \) and \( K = [k(x_i, x_j)]_{i,j \leq N} \). The conditional probability of \( p(f_\star | f) \) follows a univariate Gaussian distribution as \( p(f_\star | f) \sim \mathcal{N}(\mu(x_\star), \sigma^2(x_\star)) \). Its mean and variance are given by

\[
    \mu(x_\star) = k_s [K + \sigma^2 \delta_{ij}]^{-1} y
\]

\[
    \sigma^2(x_\star) = k_{ss} - k_s [K + \sigma^2 \delta_{ij}]^{-1} k_\star'
\]

where \( \sigma^2 \) is the output noise variance. As GPs give full uncertainty information with any prediction, they provide a flexible non-parametric prior for Bayesian optimization. We refer the interested readers to (Rasmussen, 2006) for further details in Gaussian process.

A.2 Acquisition function

Bayesian optimization is typically applied in settings in which the objective function is expensive to evaluate. To minimize interactions with that objective, an acquisition function is defined to reason about the selection of the next evaluation point \( x_{t+1} = \arg \max_{x \in \mathcal{X}} \alpha(x) \). The acquisition function is constructed from the predictive mean and variance of the surrogate to be easy to evaluate and represents the trade-off between exploration (of points with high predictive uncertainty) and exploitation (of points with high predictive mean). Thus, by design the acquisition function can be maximized with standard global optimization toolboxes.

A.3 GP kernels and treatment of GP hyperparameters

Although the raw learning curve in DRL is noisy, the transformed version using our proposed curve compression makes the resulting curve smooth. Therefore, we use the two squared exponential kernels for input hyperparameter and training iteration, respectively. That is \( k_i(x, x') = \exp\left(-\frac{|x-x'|^2}{2\sigma^2}\right) \) and \( k_t(t, t') = \exp\left(-\frac{|t-t'|^2}{2\sigma_t^2}\right) \). The observation \( x \) and \( t \) are normalized to \([0, 1]^d \) and the outcome \( y \) is standardized \( y \sim \mathcal{N}(0, 1) \) for robustness. As a result, our product kernel becomes

\[
    k([x, t], [x', t']) = k(x, x') \times k(t, t')
\]

\[
    = \exp\left(-\frac{|x-x'|^2}{2\sigma_x^2} - \frac{|t-t'|^2}{2\sigma_t^2}\right).
\]

The length-scales \( \sigma_x \) and \( \sigma_t \) are learnable parameters indicating the variability of the function with regards to the hyperparameter input \( x \) and number of training iterations \( t \). Estimating appropriate values for them is critical as this represents the GPs prior regarding the sensitivity of performance w.r.t. changes in the number of training iterations and hyperparameters. For extremely large \( \sigma \) we expect the objective function to change very little for different numbers of training iterations. For small \( \sigma \) by contrast we expect drastic changes even for small differences.

We fit the GP hyperparameters by maximizing their posterior probability (MAP), \( p(\sigma, \tau | X, t, y) \).
Figure 8: Illustration of BOIL on a 2-dimensional optimization task of DDQN on CartPole. The augmented observations fill the joint hyperparameter-iteration space quickly to inform our surrogate. Our decision balances utility $\alpha$ against cost $\tau$ for iteration-efficiency. Especially in situations of multiple locations sharing the same utility value, our algorithm prefers to select the cheapest option.
Figure 9: Illustration of the Continuous Multi-task BO (CMTBO) – this is the case of BOIL without using augmented observations (same setting as Fig. 8). This version leads to less efficient optimization for two main reasons. First, the additional iteration dimension requires more evaluation than optimizing the hyperparameters on their own. Second, the algorithm can reselect parameters at lower fidelity (less training iterations) despite having evaluated a higher fidelity already.
\( p(\sigma, x, t, y) \), which, thanks to the Gaussian likelihood, is available in closed form as (Rasmussen 2006)

\[
\ln p(y, X, t, \sigma, \sigma) = -\frac{1}{2} \ln |K + \sigma^2 I_N| \\
-\frac{1}{2} y^T (K + \sigma^2 I_N)^{-1} y + \ln p_{hyp}(\sigma, \sigma) + \text{const}
\]

where \( I_N \) is the identity matrix in dimension \( N \) (the number of points in the training set), and \( p_{hyp}(\sigma, \sigma) \) is the prior over hyperparameters, described in the following.

We optimize Eq. (10) with a gradient-based optimizer, providing the analytical gradient to the algorithm. We start the optimization from the previous hyperparameter values \( \theta_{\text{prev}} \). If the optimization fails due to numerical issues, we keep the previous value of the hyperparameters. We re-fit the hyperparameters every 3 \( \times \) \( d \) function evaluations where \( d \) is the dimension.

**Remark.** Our focus in this paper is to demonstrate the effectiveness on optimizing the learning curve by compressing the curve into a value and augmenting the data for modeling efficiency. Therefore, we have not yet demonstrated the proposed model on various acquisition functions and kernel choices. However, other choices of kernels and acquisition functions are straightforward to be used in our model.

### B Algorithm Illustration

Fig. 8 and Fig. 9 illustrate the behavior of our proposed algorithm BOIL on the example of optimizing the discount factor \( \gamma \) of Dueling DQN (Wang et al. 2016) on the CartPole problem. The two settings differ in the inclusion augmented observations into BOIL in Fig. 8 and CMTBO (or BOIL without augmented observations) in Fig. 9.

In both cases, we plot the GP predictive mean in Eq. (1), GP predictive variance in Eq. (2), the acquisition function in Eq. (3), the predicted function and the final decision function in Eq. (8).

As shown in the respective figures the final decision function balances between utility and cost of any pair \( (\gamma, t) \) to achieve iteration efficiency. Especially in situations where multiple locations share the same utility value, our decision will prefer to select the cheapest option. Using the augmented observations in Fig. 8, our joint space is filled quicker with points and the uncertainty (GP variance) across it reduces faster than in Fig. 9 – the case of vanilla CMTBO without augmenting observations. A second advantage of having augmented observations is that the algorithm is discouraged to select the same hyperparameter setting at lower fidelity than a previous evaluation. We do not add the full curve as this will make the conditioning problem of the GP covariance matrix.

| Table 1: Dueling DQN algorithm on CartPole problem. |
|-----------------------------------------------|
| Variables | Min | Max | Best Parameter \( x^* \) |
| \( \gamma \) discount factor | 0.8 | 1 | 0.95586 |
| learning rate model | \( 1 \times 10^{-6} \) | 0.01 | 0.00589 |
| #Episodes | 300 | 800 | - |

| Table 2: A2C algorithm on Reacher problem. |
|-----------------------------------------------|
| Variables | Min | Max | Best Parameter \( x^* \) |
| \( \gamma \) discount factor | 0.8 | 1 | 0.8 |
| learning rate actor | \( 1 \times 10^{-6} \) | 0.01 | 0.00071 |
| learning rate critic | \( 1 \times 10^{-6} \) | 0.01 | 0.00042 |
| #Episodes | 200 | 500 | - |

### B.1 Experiment settings

We summarize the hyper-parameter search ranges for A2C on Reacher in Table 2, A2C on InvertedPendulum in Table 3, CNN on SHVN in Table 4, and DDQN on CartPole in Table 1. Additionally, we present the best found parameter \( x^* \) for these problems. Further details of the DRL agents are listed in Table 1.

### B.2 Robustness over Different Preference Functions

We next study the learning effects with respect to different choices of the preference functions. We pick three preference functions including the Sigmoid, Log and Average to compute the utility score for each learning curve. Then, we report the best found reward curve under such choices. The experiments are tested using A2C on Reacher-v2. The results presented in Fig. 10 demonstrate the robustness of our model with the preference functions.

### B.3 Examples of Deep Reinforcement Learning Training Curves

Finally, we present examples of training curves produced by the deep reinforcement learning algorithm A2C in Fig. 11. These fluctuate widely and it may not be trivial to define good stopping criteria as done for other applications in previous work (Swersky et al. 2014).

| Table 3: A2C algorithm on InvertedPendulum problem. |
|-----------------------------------------------|
| Variables | Min | Max | Best Parameter \( x^* \) |
| \( \gamma \) discount factor | 0.8 | 1 | 0.95586 |
| learning rate \( q \) model | \( 1 \times 10^{-6} \) | 0.01 | 0.00589 |
| learning rate \( v \) model | \( 1 \times 10^{-6} \) | 0.01 | 0.00037 |
| #Episodes | 700 | 1500 | - |
Figure 10: To highlight the robustness, we examine the results using different preference functions such as Sigmoid curve, Log curve, and Average curve on Reacher experiments. The results include the best found reward curve with different preference choices that show the robustness of our model.
Figure 11: Examples of reward curves using A2C on Reacher-v2 (rows 1 – 3) and on InvertedPendulum-v2 (rows 4 – 6). Y-axis is the reward averaged over 100 consecutive episodes. X-axis is the episode. The noisy performance illustrated is typical of DRL settings and complicates the design of early stopping criteria. Due to the property of DRL, it is not trivial to decide when to stop the training curve. In addition, it will be misleading if we only take average over the last 100 iterations.
Table 4: Convolutional Neural Network on SVHN dataset.

| Variables          | Min | Max | Best Found $x^*$ |
|--------------------|-----|-----|------------------|
| filter size        | 1   | 8   | 5                |
| pool size          | 1   | 5   | 5                |
| batch size         | 16  | 1000| 8                |
| learning rate      | $1e^{-6}$ | 0.01 | 0.000484     |
| momentum           | 0.8 | 0.999| 0.82852          |
| decay              | 0.9 | 0.999| 0.9746           |
| number of epoch    | 30  | 150 | -                |

Table 5: Further specification for DRL agents

| Hyperparameter                  | Value                                      |
|---------------------------------|--------------------------------------------|
| **A2C**                         |                                            |
| Critic-network architecture     | [32,32]                                    |
| Actor-network architecture      | [32,32]                                    |
| Entropy coefficient             | 0.01                                       |
| **Duelling DQN**                |                                            |
| Q-network architecture          | [50,50]                                    |
| $\epsilon$-greedy (start, final, number of steps) | (1.0, 0.05, 10000) |
| Buffer size                     | 10000                                      |
| Batch size                      | 64                                         |
| PER-$\alpha$ (Schaul et al. 2016) | 1.0                                        |
| PER-$\beta$ (start, final, number of steps) | (1.0, 0.6, 1000)   |