Amortized Auto-Tuning: Cost-Efficient Transfer Optimization for Hyperparameter Recommendation

Yuxin Xiao¹, Eric P. Xing¹,3, Willie Neiswanger²,3
¹Carnegie Mellon University, ²Stanford University, ³Petuum, ⁴MBZUAI
yuxinxia@andrew.cmu.edu, epxing@cs.cmu.edu, neiswanger@cs.stanford.edu

Abstract

With the surge in the number of hyperparameters and training times of modern machine learning models, hyperparameter tuning is becoming increasingly expensive. Although methods have been proposed to speed up tuning via knowledge transfer, they typically require the final performance of hyperparameters and do not focus on low-fidelity information. Nevertheless, this common practice is suboptimal and can incur an unnecessary use of resources. It is more cost-efficient to instead leverage the low-fidelity tuning observations to measure inter-task similarity and transfer knowledge from existing to new tasks accordingly. However, performing multi-fidelity tuning comes with its own challenges in the transfer setting: the noise in the additional observations and the need for performance forecasting. Therefore, we conduct a thorough analysis of the multi-task multi-fidelity Bayesian optimization framework, which leads to the best instantiation—AmorTized Auto-Tuning (AT²).

We further present an offline-computed 27-task Hyperparameter Recommendation (HyperRec) database to serve the community. Extensive experiments on HyperRec and other real-world databases illustrate the effectiveness of our AT² method.[1]

1 Introduction

Modern machine learning models typically come with a large number of hyperparameters and are often sensitive to their values. Consequently, researchers have paid increasing attention to automatic hyperparameter tuning [18, 22, 72], which aims to identify a set of optimal hyperparameters for a learning task without human experts. With the aid of optimization histories of past tuning sessions, some methods propose to accelerate new tuning processes via knowledge transfer. Despite their impressive results, these methods come with limitations on their cost-efficiency and flexibility, in the sense that they either make modality-specific one-time predictions [1, 6, 42, 69, 70] or rely on extra information from new tasks [11, 24, 53, 56, 52]. More importantly, they generally operate on the final performance of hyperparameters and ignore low-fidelity information [13, 53, 57, 59, 64]. As we demonstrate via a motivating example in Section 2, this practice incurs an unnecessary cost. It is more resource-efficient to instead utilize cheap-to-obtain low-fidelity tuning observations when carrying out inter-task hyperparameter transfer learning.

However, performing multi-fidelity tuning in the transfer setting is non-trivial. It requires carefully distilling relevant knowledge from the additional multi-fidelity information in existing tasks. It also demands accurate forecasting to extrapolate max-fidelity performance based on corresponding low-fidelity observations. To this end, we resort to the well-established approach of Bayesian optimization (BO) and conduct a thorough analysis of a multi-task multi-fidelity BO framework. In particular, we address the aforementioned challenges by considering a family of kernels and, based on an empirical evaluation, develop an AmorTized Auto-Tuning (AT²) method—the name is derived from the fact that past tuning costs will be written off in future tuning sessions.

We summarize our contributions as follows: (1) To better leverage cheap-to-obtain low-fidelity observations for measuring inter-task dependency efficiently, we conduct a thorough analysis of the

¹AT² and HyperRec are available at https://github.com/xiaoyuxin1002/amortized-auto-tuning
multi-task multi-fidelity BO framework where we empirically evaluate 64 different instantiations.

(2) To motivate our analysis and as a service to the community, we present an offline-computed Hyperparameter Recommendation (HyperRec) database. It consists of 27 unique computer vision tuning tasks and 150 distinct configurations over a 16-dimensional hyperparameter space. (3) Based on the analysis, we propose the AT2 method, which uses a novel task kernel and acquisition function. It outperforms competitive baselines on HyperRec and other real-world tuning databases.

2 Background & Motivation

2.1 Preliminaries of Hyperparameter Transfer Optimization

Consider a black-box function \( f : \mathcal{X} \rightarrow \mathbb{R} \) where the input space \( \mathcal{X} \) is defined as the Cartesian product of the task space \( \mathcal{T} \), the configuration space \( \mathcal{C} \), and the fidelity space \( \mathcal{E} \), i.e., \( \mathcal{X} = \mathcal{T} \times \mathcal{C} \times \mathcal{E} \).

At each iteration, we make a (typically expensive) function evaluation and obtain a noisy observation.

\[ y = f(x) + \epsilon \]

where \( \epsilon \) is drawn from some noise distribution for an input \( x \in \mathcal{X} \). Moreover, the fidelity space can only be queried in incremental order. That is, if we want to query a given \( x \in \mathcal{X} \), where \( \mathcal{X} = \{t,c,e\} \), we must first query all \( e' < e \). Consequently, it incurs a larger computational cost to acquire an observation for a higher fidelity value.

Suppose for a set of past tasks \( \{t_i\}_{i=1}^{T} \), we have collected some subset of associated observations \( \{y_{i,t,c,e}\}_{i=1}^{N} \) via querying the search space. Given a new task \( t^* \), we would like to propose an optimization strategy that aims to identify \( x^* = (t^*, c^*, e^*) \) using as little computation as possible with the help of knowledge transfer from offline observations. Here, \( c^* \) and \( e^* \) are where \( f \) achieves its maximum on \( t^* \), i.e., \( (c^*, e^*) = \arg\max_{c \in \mathcal{C}, e \in \mathcal{E}} f((t^*, c, e)) \).

In this paper, we focus on this setup for the task of hyperparameter transfer optimization, where we treat \( t \) as a single tuning instance, \( c \in \mathcal{C} \) as a hyperparameter configuration, \( e \in \mathcal{E} \) as an epoch value, and \( f(x) \) as the associated validation accuracy. In particular, we are interested in two metrics for the effectiveness of an optimization strategy on a new task \( t^* \): given budget \( Q \), we want to minimize the simple regret \( R_Q = f(x^*) - \max_{q=1,...,Q} f(x_q) \) of queried points \( x_q \), and maximize the final performance \( F_Q = \max_{e \in \mathcal{E}} f((t^*, c^*_Q, e)) \) of the predicted optimal configuration \( c^*_Q \).

2.2 Limitations of Existing Work

Besides the performance metrics introduced above, we would like to further assess the cost-efficiency (E) and flexibility (F) of hyperparameter tuning methods based on the following criteria.

**E1:** (Transferable) The method should leverage the observations of existing tasks and perform knowledge transfer to speed up the tuning process of any new tasks.

**E2:** (Low-fidelity) The method should utilize low-fidelity information and not proceed with max-fidelity performance only.

**E3:** (Cost-aware) The method should respond to different computational costs involved in querying for observations of different tasks or fidelities.

**E4:** (Sequential) The method should actively adapt to any observations received while tuning new tasks and carry out feedback-driven sequential tuning.

**F1:** (Modality-agnostic) The method should be data modality-agnostic and broadly applicable to various data types.

**F2:** (Self-contained) The method should be able to operate on any new tasks without relying on auxiliary information such as extracted metadata or pre-computed representations.

**F3:** (Cold-start friendly) The method should be able to work well under cold start situations and not require any observations on new tasks in order to execute.

To this end, we summarize our evaluation results on existing hyperparameter recommendation literature in Table 1 and give more details in Appendix A. In general, widely-adopted Bayesian optimization (BO) methods [43] define a surrogate model (e.g., Gaussian process [28, 54], neural networks [55], random forests [21]) on the target black-box function and deploy an acquisition function (e.g., GP-UCB [2][58] and GP-EI [25]) to determine future query points. However, vanilla BO methods focus on single-task tuning and require preliminary observations for proper initialization.

One line of extension is multi-fidelity BO methods [20][26][32], which apply cheap approximations to the target function. Some bandit-based [9][38][39] and learning curve modeling [8][60] approaches also examine the multi-fidelity information for early stopping. Hence, they do a better job at leveraging low-fidelity information for single-task tuning, which leads to more effective resource allocation.
Table 1: Evaluation of hyperparameter tuning methods based on cost-efficiency (E) and flexibility (F). We detail the criteria in Section 2.2 and present the full table with additional methods [54, 21, 20, 26, 60, 8, 9, 39, 57, 52, 11, 64, 37, 24, 35, 30, 12, 48, 47, 3, 13, 69, 1, 6, 63] in Appendix A.

In another direction, multi-task BO methods aim to transfer knowledge between multiple optimization problems via methods such as multi-output GPs [11, 52, 59], Bayesian deep learning [57, 64], and Bayesian linear regression [46]. However, they mostly operate on the final (max-fidelity) performance and treat all queries as having equal cost. Even when equipped with the optimization histories of previous tasks, these methods often spend some budget on obtaining initial max-fidelity observations on new tasks so as to measure inter-task similarity before carrying out knowledge transfer. As we will show in the motivating example below, this procedure is unnecessary and, often, unexpectedly costly.

Towards a similar goal, some approaches view hyperparameter transfer learning from a warm-start [12, 30, 47, 48] or recommendation [3, 13, 69, 70] perspective and typically rely on pre-computed task-dependent metadata or representations. A few prediction-only methods [1, 6, 42, 63] have been proposed for specific domains but satisfy neither the sequential tuning nor modality-agnostic criteria.

On account of the analysis above, we draw merits from both multi-task and multi-fidelity BO methods and present an AT2 (Ours) method, which fulfills each of the cost-efficiency and flexibility criteria. In particular, AT2 performs sequential, modality-free tuning of validation accuracy and transfers knowledge from existing to new tasks effectively, even under cold start scenarios, based on cheap-to-obtain low-fidelity observations (instead of auxiliary or full-fidelity information).

Nevertheless, it is a non-trivial task to consider the multi-fidelity information in the transfer setting. For instance, the additional structure given by the multi-fidelity observations from previous tasks demands careful attention. Additionally, in this setting we must forecast the max-fidelity performance of hyperparameters based on their corresponding low-fidelity observations.

2.3 Motivating Example

To illustrate the challenges involved in multi-task multi-fidelity tuning, we implement a motivating example where AT2 is compared against two multi-task baselines under the cold start situation: ABLR [46], which ignores multi-fidelity information, and ABLR-HB [61], which processes multi-fidelity information via the Hyperband [38] regime. Here, we utilize a real-world hyperparameter tuning database, HyperRec (which will be introduced in detail in Section 3.1), and report the results averaged over five train-test task pairs based on the two metrics \( R_Q, F_Q \) discussed in Section 2.1. For \( F_Q \), we use the final performance ranking of the configuration with the highest predicted mean instead of the raw score for a clearer presentation. All three methods are trained with their respective default settings and given an iteration budget four times the max fidelity (i.e., \( Q = 4 \times E_{\text{max}} = 300 \)).

As shown in Figure 1, since ABLR uses max-fidelity observations from the test task, its final performance ranking suffers initially and improves only after making several max-fidelity queries. Meanwhile, when ABLR is still waiting for its first max-fidelity feedback, AT2 and ABLR-HB are able to update their predictions immediately after receiving low-fidelity feedback and quickly recognize promising hyperparameter configurations. This phenomenon renders the cost of max-fidelity initialization in ABLR unnecessary and illustrates the advantage of low-fidelity tuning.

On the other hand, although Hyperband is ideal for the parallel tuning setting when substantial computational resources are accessible, it begins by selecting a large batch of configurations and thus uses excessive computation in the low-fidelity region given the same iteration budget (in terms of total computation, disregarding parallelism). As a result, in our sequential setting, ABLR-HB only...
achieves a lower simple regret than ABLR at around the 80th iteration. Moreover, ABLR-HB’s predicted final performance ranking declines after the 50th iteration. Since ABLR-HB treats the fidelity as a contextual variable, when more multi-fidelity observations become available on the test task, the extrapolation performance begins to suffer, as it becomes difficult to identify an informative subset of training observations and forecast full-fidelity performance. Eventually, ABLR outperforms ABLR-HB in both metrics after initializing on enough full-fidelity observations.

Unlike ABLR-HB, which leaves the task of multi-fidelity tuning to Hyperband, our proposed AT2 method sequentially selects queries for increased cost-efficiency. It quantifies inter-task dependencies based on low-fidelity information and converges to a high-ranking configuration thanks to careful forecasting of validation accuracies. In addition, AT2 also balances exploration and exploitation well and achieves a lower simple regret than ABLR from the beginning. To this end, we focus on developing a multi-task multi-fidelity BO framework and discuss AT2 in detail, in the next section.

3 Methods

3.1 Hyperparameter Recommendation (HyperRec) Database

We first illustrate the problem setting in Section 2.1 with an offline-computed Hyperparameter Recommendation database—HyperRec. HyperRec consists of 27 unique image classification tuning tasks and 150 distinct configurations composed of 16 nested hyperparameters. Each task is evaluated by each configuration for 75 epochs and repeated with two different seeds. We record the validation loss and top one, five, and ten accuracies in HyperRec. More details can be found in Appendix B.

To the best of our knowledge, this is the first hyperparameter recommendation database specifically targeting computer vision tasks. By releasing HyperRec, we seek to serve both the hyperparameter tuning and computer vision communities with a database for testing and comparing the performance of existing and future hyperparameter tuning or image classification algorithms.

3.2 Multi-Task Multi-Fidelity Bayesian Optimization Framework

In what follows, we will describe the overall multi-task multi-fidelity BO framework and then give an extensive study of different implementations. The BO paradigm is characterized by the use of a probabilistic surrogate model of the expensive black-box target \( f(x) \). In this paper, we stick to the popular choice of Gaussian process (GP) for the surrogate model due to its good uncertainty quantification and leave the investigation of other options (e.g., random forest [21]) to future works. To enhance the model scalability, we adopt the stochastic variational GP regression framework [19].

A GP over the input space \( \mathcal{X} \) is a random process from \( \mathcal{X} \) to \( \mathbb{R} \), represented by a mean function \( \mu: \mathcal{X} \to \mathbb{R} \) and a kernel (i.e., covariance function) \( \kappa: \mathcal{X}^2 \to \mathbb{R} \). If \( f \sim \mathcal{G}P(\mu, \kappa) \), then we have \( f(x) \sim \mathcal{N}(\mu(x), \kappa(x, x)) \) for all \( x \in \mathcal{X} \). Consider \( N \) offline observations \( D_N = \{ (x_i, y_i) \}_{i=1}^N \) from \( T \) tasks where \( y_i = f(x_i) + \epsilon_i \in \mathbb{R} \) and \( \epsilon_i \sim \mathcal{N}(0, \eta^2) \). We stack \( D_N \) to form \( \mathbf{X} \in \mathcal{X}^N \) and \( \mathbf{Y} \in \mathbb{R}^N \). When using variational inference, we also learn \( \bar{M} \) inducing inputs \( \mathbf{Z} \in \mathcal{X}^M \) where \( M \ll N \) and the corresponding inducing variables \( \mathbf{u} = f(\mathbf{Z}) \). Here, we let the prior distribution \( \rho(\mathbf{u}) = \mathcal{N}(0, \mathbf{I}) \) and
the variational distribution \( q(u) = \mathcal{N}(m, \Sigma) \). We optimize the GP hyperparameters \( \theta \) and variational parameters \( \varphi \) by maximizing the variational evidence lower bound (ELBO),

\[
\theta^*, \varphi^* = \arg\max_{\theta, \varphi} \text{ELBO} = \arg\max_{\theta, \varphi} \sum_{i=1}^{N} \mathbb{E}_{q_{\theta, \varphi}(f(x(i)))} \left[ \log p(y_i|f(x(i))) \right] - \text{KL} \left[ q_{\varphi}(u) \parallel p(u) \right],
\]

where \( q_{\theta, \varphi}(f(x(i))) \) is the marginal of \( p_\varphi(f(x(i)|u)q_\varphi(u) \). The predictive distribution for query \( x \) is

\[
p_\theta(f(x)|D_N) \approx \int p_\theta(f(x)|u)q_\varphi(u) \, du = \mathcal{N} \left( A m, \kappa(x, x) + A (S - K) A^T \right),
\]

where \( A = kK^{-1}, k \in \mathbb{R}^{1 \times M} \) with \( k_i = \kappa(x, z_i) \), and \( K \in \mathbb{R}^{M \times M} \) with \( K_{i,j} = \kappa(z_i, z_j) \).

After incorporating the information from previous tasks, we can construct an acquisition function \( \phi : \mathcal{X} \rightarrow \mathbb{R} \) for the new tuning task \( t^* \). The next point to query \( x_q = (t^*, c_q, e_q) \) at iteration \( q \) is determined by maximizing the acquisition function, i.e., \( (c_q, e_q) = \arg \max_{c \in \mathcal{C}, e \in \mathcal{E}} \phi((t^*, c, e)) \) (described in detail in Section 3.4). Then we update the model parameters according to Equation 1 after collecting an observation \( y_q \) by querying for \( f(x_q) = f((t^*, c_q, e_q)) \). This iterative process continues until we spend the query budget \( Q \).

Next, we provide a thorough analysis of this general multi-task multi-fidelity BO framework, where we focus on a comparison of options for the key component—the kernel \( \kappa \) in Section 3.3 and conclude with the best instantiation—Amortized Auto-Tuning (AT2) algorithm in Section 3.4.

### 3.3 Kernel Analysis

Since the input space \( \mathcal{X} \) is the product of three spaces, we can use a kernel with the structure

\[
\kappa(x, x') = \kappa((t, c, e), (t', c', e')) = \kappa_T(t, t') \otimes \kappa_C(c, c') \otimes \kappa_E(e, e'),
\]

where \( \otimes \) denotes the Kronecker product. \( \kappa_T : T^2 \rightarrow \mathbb{R}_+ \), \( \kappa_C : C^2 \rightarrow \mathbb{R}_+ \), and \( \kappa_E : E^2 \rightarrow \mathbb{R}_+ \) are the task, configuration, and fidelity kernels, respectively. Below we will discuss kernels that are suitable for each of the three spaces and then carry out an empirical evaluation to find the best combination.

#### 3.3.1 Task Kernel

Based on the example in Section 2.3, we are motivated to take advantage of low-fidelity function queries to define inter-task similarity. One key observation we derived from HyperRec is that if two tasks have similar low-fidelity behaviors, they often share high-scoring configurations. For instance, ACTION40 \([7] \) and CALTECH256 \([16] \) are two tasks in HyperRec. As shown in Figure 2(a), they exhibit similar low-fidelity behavior, and their top five best-performing configurations largely overlap.

Moreover, we can see that this observation is ubiquitous among all task pairs. We select two groups of pairs according to the L2 distance of their optimization landscapes (i.e., between their zero-meaned validation accuracies). As shown in Figure 2(b), task pairs similar in L2 distance share larger portions of high-performing configurations. We, therefore, propose the OptiLand task kernel, which infers the similarity between a new tuning task and past tasks by comparing their low-fidelity performance, in order to perform efficient optimization via knowledge transfer.

Consider a task pair \((t_1, t_2)\) and their respective queries \( X_1 = \{(t_1, c_{1,i}, e_{1,i})\}_{i=1}^{N_1} \) and \( X_2 = \{(t_2, c_{2,i}, e_{2,i})\}_{i=1}^{N_2} \). Among these queries, we focus on their overlapping subset when measuring inter-task dependency, which provides robustness against noisy multi-fidelity observations of existing tasks, as reflected in the motivating example in Section 2.3. We define a matching function to return the set of configuration-fidelity tuples for which we have queried for observations on both tasks:

\[
M((t_1, t_2)) = \{(c, e) \mid (t_1, c, e) \in X_1, (t_2, c, e) \in X_2\}.
\]

The corresponding observation vectors are \( Y_{1|M((t_1, t_2))} \) and \( Y_{2|M((t_1, t_2))} \), respectively. Entries in \( Y_{1|M((t_1, t_2))} \) and \( Y_{2|M((t_1, t_2))} \) are min-max normalized to \([0, 1]\), shifted to have zero mean, and ordered by a common permutation of \( M((t_1, t_2)) \).

Hence, the distance function between the optimization landscapes of \( t_1 \) and \( t_2 \) becomes

\[
D(t_1, t_2) = \frac{\|Y_{1|M((t_1, t_2))} - Y_{2|M((t_1, t_2))}\|_2}{|M((t_1, t_2))|^2}.
\]

Since the observation vectors are normalized, we have \( D(t_1, t_2) \in [0, 1] \). When the number of matched observations \( |M((t_1, t_2))| = 1 \) (e.g., during initialization), we simply use a distance of \( \frac{1}{2} \). Note that both observation vectors are transformed to have zero mean, since we are interested in whether the optimization landscapes of two tasks have similar shapes. In this way, two tasks will have zero distance if one’s landscape is equal to another’s shifted or scaled.
We then define the \texttt{OptiLand} task kernel to assess the dependency between \( t_1 \) and \( t_2 \) as follows:

\[
\kappa_T(t_1, t_2) = \exp \left( -\frac{D(t_1, t_2)}{(\xi \cdot \gamma(t_1, t_2))^2} \right) \quad \text{where} \quad \gamma(t_1, t_2) = \frac{U}{1 + (U - 1) \cdot R(t_1, t_2)}.
\]

Here, \( \xi \in \mathbb{R}_+ \) is the length scale and \( R(t_1, t_2) = \frac{|M(t_1, t_2)|}{|\xi|} \) is the ratio of matched observations. \( \gamma : T^2 \rightarrow \mathbb{R}_+ \) is a scaling function indicating the amount of information we have about the task pair. Intuitively, no matter how many observations we have on \( t_1 \) and \( t_2 \) separately, if we have very few matched observations, we are less confident about how well \( D(t_1, t_2) \) captures the true difference between their optimization landscapes. In this case, we would like to bias the tuning process of the new task towards existing tasks and increase the length scale to allow more knowledge transfer.

Therefore, we use a learnable parameter \( U \) to bound \( \gamma \in [1, U] \). That is, when \( \gamma = 1 \), then the ratio of matched observations is 1, and we leave the length scale alone and let the task kernel control the amount of information transfer. Alternatively, when \( \gamma = 0 \), we scale up the length scale by \( U \) to increase the amount of information transfer. This design is especially useful for the cold start situation. During the early search phase of the new task, configurations queried for the new and old tasks hardly overlap. Hence, we increase the length scale via \( \gamma \) to allow more meaningful knowledge transfer for warm-starting the new task. This artificial upscaling is mitigated as more queries are made on the new task. Again, our claim is well supported by the good initial performance of AT2 under the cold start scenario in the motivating example (Section 2.3).

Besides the proposed \texttt{OptiLand} task kernel, we will compare three other possibilities for \( \kappa_T \). MTBO task kernel \cite{halkia2020model} is defined by a lookup table and optimized by learning the entries in the Cholesky decomposition of the covariance matrix. Some methods \cite{chakraborty2020bayesian} also suggest learning an embedding for each task and apply a linear or second-order polynomial kernel on top of it. We name these two alternatives as \texttt{DeepLinear} and \texttt{DeepPoly} task kernels, respectively.

### 3.3.2 Configuration Kernel

The configuration kernel needs to deal with different hyperparameter types (i.e., numerical or categorical) and partially overlapping hyperparameter configurations. Therefore, Tree configuration kernel \cite{louizos2017learning} advocates treating the configuration space as tree-structured and composites individual hyperparameter kernels in a sum-product way. For our experiments, we use an RBF or index kernel as the individual kernel for numerical or categorical hyperparameters, respectively. Alternatively, Flat configuration kernel discards the tree structure and multiplies all the individual kernels together. Some prior work \cite{shahriari2015taking, chakraborty2020bayesian} recommends encoding the configuration space via deep learning. Hence, we construct a two-layer fully-connected neural network with \texttt{tanh} activation function and learn an embedding input for each categorical hyperparameter. Then \texttt{DeepLinear} or \texttt{DeepPoly} configuration kernels leverage a linear or second-order polynomial kernel based on network outputs, respectively.
We also provide a qualitative analysis of the kernel performance in Figure 3 (full results in Appendix C). We also consider two simple choices for which consists of 30,000 observations. We further sample 1,000 observations from them to form Therefore, we will leverage this composition for our configuration kernel, and AccCurve fidelity kernel gives the highest ELBO score among the 64 candidates. Full results in Appendix C.

### 3.3.3 Fidelity Kernel

The fidelity kernel aims to capture how the validation accuracy changes over epochs. As inspired by [60], we define AccCurve fidelity kernel as a weighted integration over infinite basis functions: \( \kappa_e(e, e') = \int_0^\infty (1 - \exp[-\lambda e]) (1 - \exp[-\lambda e']) d\psi(\lambda). \) When the mixing measure \( \psi \) takes the form of a gamma distribution with parameters \( \alpha, \beta > 0 \), the equation can be simplified into \( \kappa_e(e, e') = 1 + \left( \frac{\beta}{e + e' + \beta} \right)^\alpha - \left( \frac{\beta}{e + \beta} \right)^\alpha - \left( \frac{\beta}{e' + \beta} \right)^\alpha. \) Since the basis function approximates the shape of learning curves, this kernel extrapolates the high-fidelity performance well based on low-fidelity observations. Another popular kernel for modeling multi-fidelity information is Fabola's fidelity kernel [52], where the authors assume a monotonic behavior of function evaluations with fidelity \( e \).

We also consider two simple choices for \( \kappa_e \)—RBF and Matern fidelity kernels.

### 3.3.4 Empirical Evaluation

In the previous sections, we discussed four options for each of the three component kernels, which gives rise to 64 combinations. Here, we identify the best-performing instantiation based on an empirical evaluation. More specifically, we randomly sample four tasks from the HyperRec database, which consists of 30,000 observations. We further sample 1,000 observations from them to form the test set and use the rest as the train set. All of the kernel combinations are trained with the same setting based on the multi-task multi-fidelity BO framework introduced in Section 3.2. Since we are concerned with how well different kernel combinations can explain the data, we report the ELBO on the test set as the quantitative metric in Table 2 (full results in Appendix C).

In general, although the other three task kernels show competitive results, the OptiLand task kernel has the best performance with different configuration and fidelity kernels. We attribute the success to its careful measurement of inter-task similarities based on matched queries. For the configuration kernel, the neural network-based kernels (i.e., DeepLinear and DeepPoly) perform better than the other two options. Finally, AccCurve fidelity kernel better models the shape of learning curves than the other three alternatives. Among the 64 candidates, the combination of OptiLand task kernel, DeepPoly configuration kernel, and AccCurve fidelity kernel achieves the highest ELBO value. Therefore, we will leverage this composition for our AT2 method in the next section.

We also provide a qualitative analysis of the kernel performance in Figure 3 (full results in Appendix C). In particular, we divide the 1,000 observations in the test set into 500 pairs and compare their true distance, defined by the absolute difference (which is bounded by \([0, 1]\)) with the predicted distance, defined as \((1 - \frac{\kappa(x, x')}{\sqrt{\kappa(x, x) \kappa(x', x')}})/2 \in [0, 1]\) (given by the covariance kernel). As shown in Figure 3(b) and (c), an ineffective kernel combination either give random or equal predicted distance regardless of the true distance. In contrast, the predicted distance by the best-performing kernel combination is more aligned with the true distance, which helps justify its quantitative result.

### 3.4 Amortized Auto-Tuning (AT2) Method

Besides the kernel analysis, we propose Max-Trial-GP-UCB, a specially designed acquisition function. Similar to GP-UCB [58], it defines an upper confidence bound \( \phi(x) = \mu(x) + \eta \cdot \sigma(x) \) on \( f(x) \) for a given \( x \). Here, \( \mu(x) \) and \( \sigma(x) \) are the predictive mean and standard deviation, respectively, of the posterior distribution in Equation 2. \( \eta \) is a hyperparameter controlling the trade-off between exploitation and exploration. Since our ultimate goal is to identify the configuration with the highest final performance on the tuning task \( t^{*} \), we choose the next configuration to query as \( c_q = \arg \max_{c \in C} \max_{e \in E} \phi(t^{*}, c, e) \). Suppose that for \( t^{*} \) and \( c \), the maximum queried fidelity so far is \( \epsilon_{\text{max}}[c] \), then we formulate the succeeding query as \( x = (t^{*}, c, \epsilon_{\text{max}}[c] + 1) \). Unlike other multi-fidelity UCB-based acquisition functions [27], Max-Trial-GP-UCB may consider \( \phi \) at a distinct

| Rank | Figure | Task Kernel | Configuration Kernel | Fidelity Kernel | ELBO |
|------|--------|-------------|---------------------|----------------|------|
| 1    | Figure 3 (a) | OptiLand | DeepPoly | AccCurve | 1.4951 |
| 49   | Figure 3 (b) | DeepPoly | DeepPoly | Matern | 0.3053 |
| 64   | Figure 3 (c) | MTBO | Tree | Fabolas | 0.1342 |

Table 2: Quantitative performance of different kernel compositions. The combination of our proposed OptiLand task kernel, DeepPoly configuration kernel, and AccCurve fidelity kernel gives the highest ELBO score among the 64 candidates. Full results in Appendix C.
fidelity for each configuration. Meanwhile, it queries the fidelity space incrementally and factors in different computational costs due to the constraint in our problem setup in Section 2.1.

All together, we present the AmorTized Auto-Tuning (AT2) method as an instantiation of the multi-task multi-fidelity BO framework, consisting of OptiLand task kernel, DeepPoly configuration kernel, AccCurve fidelity kernel, and Max-Trial-GP-UCB acquisition function. AT2 measures inter-task similarity based on low-fidelity observations and enjoys the power of the best-performing kernel ensemble to transfer knowledge to new online tuning tasks in a flexible and cost-effective manner.

4 Experiments

Datasets. Besides our offline-computed database HyperRec, we consider another similar database LCBox [74] in our experiments. We sample 100 configurations from each database to construct the configuration space C. Since training epochs are treated as fidelity values in our setting, we have |E| = 75 in HyperRec and |E| = 52 in LCBox. We further normalize the numerical hyperparameters based on their respective sampling distributions and take y to be the top five validation accuracy in HyperRec and the validation balanced accuracy in LCBox. To assess the generalizability of model performance, we randomly sample five train-test task pairs from each database where one pair consists of four training tasks and one testing task.

Baselines. We compare our AT2 method against a wide spectrum of hyperparameter transfer learning baselines: ABLR [46] applies Bayesian linear regression for each task with a shared representation space; ABLR-HB [61] further utilizes Hyperband [38] for multi-fidelity tuning; Box-BOB [47] constrains the search space of BO based on the best configurations of train tasks; Box–BOHB supplies BOHB [9] with a constrained search space to allow for inter-task knowledge transfer; BOHAMIANN [57] combines neural networks with stochastic gradient Hamiltonian Monte Carlo for better scalability; PMF [13] leverages probabilistic matrix factorization for hyperparameter recommendation; RGPE [11] ensembles single-task GPs as a ranking-weighted mixture. Moreover, Box–BO uses the same configuration and fidelity kernels as AT2 for the BO process. Box–BOB and Box–BOHB define the candidate pool based on the top three best-performing training configurations.

Implementation details. We implement the proposed AT2 method using the GPyTorch package [14]. More specifically, AT2 is initialized with 1,000 inducing points and optimized for 200 epochs with the momentum optimizer (learning rate = 0.02, momentum factor = 0.8) and a linearly decaying scheduler. All the other baselines are trained with their respective default settings and incorporate fidelity value as a contextual variable. We apply our novel Max-Trial-GP-UCB acquisition function to all the methods for selecting the next point to query, and after experimenting with \{0.25, 0.5, 1\}, we set \(\eta = 0.25\) to balance exploration and exploitation.

Quantitative evaluation. To assess the performance of baselines quantitatively, we allow a query budget \(Q\) of 100 iterations and report the results averaged over five train-test task pairs for each database based on the two metrics \((R_Q, F_Q)\) discussed in Section 2.1. Similar to Section 2.3, we use the final performance ranking for \(F_Q\). As shown in Figure 4, although some methods give competitive simple regrets, their predicted final performance rankings deviate. In particular, methods requiring preliminary observations for proper initialization (e.g., BOHAMIANN and PMF) generally do not work well under cold start situations. The final performance rankings delivered by ABLR and ABLR–HB worsen after more observations become available, especially in HyperRec. This suggests that multi-fidelity information requires careful treatment as it is challenging to forecast max-fidelity
Figure 4: Performance of methods on HyperRec and LCBench. The results based on two metrics (simple regret and final performance ranking) are averaged across five train-test task pairs for each database. Lower is better. The predicted final performance rankings are smoothed with a hamming window of 10 iterations. Our proposed AT2 method consistently achieves lower values in both metrics. We omit error bars here for readability and show a version with one standard error in Appendix D.

Qualitative analysis. To better understand how effective AT2 is in transferring knowledge and forecasting high-fidelity performance, we visualize how the predictive mean and standard deviation of the GP surrogate change over iterations. We randomly sample one train-test task pair and 10 configurations from HyperRec and compare the predicted and observed accuracies in Figure 5 (full version in Appendix D). At the start when there are no observations on the new task, AT2 exploits knowledge gained from previous tasks and produces a reasonable approximation of the true landscape albeit with high uncertainties. As more queries are made on the new task over iterations, AT2 can better extrapolate the high-fidelity performance (e.g., the zigzag shape from configuration 4 to 8) based on low-fidelity observations with a reduced standard deviation.

5 Conclusion

In this paper, to achieve cost-efficient hyperparameter transfer optimization, we focus on leveraging cheap-to-obtain low-fidelity tuning observations for measuring inter-task dependencies. Based on a thorough analysis of the multi-task multi-fidelity BO framework, we propose the AmoRtized Auto-Tuning (AT2) method. We further compute a Hyperparameter Recommendation (HyperRec) database offline to serve the community. The compelling empirical performance of our AT2 method on HyperRec and other real-world databases demonstrates the method’s effectiveness. Since our analysis is currently restricted to the GP surrogate, in the future we would like to investigate how other surrogate models (e.g., random forest [21]) perform in our multi-task multi-fidelity BO framework.
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Appendix

A Cost-Efficiency and Flexibility of Existing Work

We assess the cost-efficiency ($E$) and flexibility ($F$) of hyperparameter tuning methods, based on the seven criteria detailed in Section 2.2. In the table below, we extend Table 1 (from Section 2.2) to include a full set of hyperparameter tuning methods.

| Category                | Method          | Cost-Efficiency | Flexibility |
|-------------------------|-----------------|-----------------|-------------|
|                         |                 | $E_1$ $E_2$ $E_3$ $E_4$ | $F_1$ $F_2$ $F_3$ |
| Vanilla BO              |                 |                 |             |
|                         | DNGO [55]       | ✓               | ✓           | ✓           |
|                         | GPBO [54]       | ✓               | ✓           | ✓           |
|                         | ROAR [21]       | ✓               | ✓           | ✓           |
| Multi-fidelity BO       | Fabolas [32]    | ✓               | ✓           | ✓           |
|                         | TSE [20]        | ✓               | ✓           | ✓           |
|                         | MF-GP-UCB [26]  | ✓               | ✓           | ✓           |
| Learning curve modeling | Freeze-Thaw [60]| ✓               | ✓           | ✓           |
|                         | LC Pred [8]     | ✓               | ✓           | ✓           |
| Bandit-based approach   | Hyperband [38]  | ✓               | ✓           | ✓           | ✓           |
|                         | BOHB [9]        | ✓               | ✓           | ✓           | ✓           |
|                         | MFES-HB [39]    | ✓               | ✓           | ✓           | ✓           |
|                         | ABLR-HB [61]    | ✓               | ✓           | ✓           | ✓           |
| Multi-task BO           | MTBO [59]       | ✓               | ✓           | ✓           | ✓           | ✓           |
|                         | BOHAMIANN [57]  | ✓               | ✓           | ✓           | ✓           | ✓           |
|                         | ABLR [46]       | ✓               | ✓           | ✓           | ✓           | ✓           |
|                         | GCP [52]        | ✓               | ✓           | ✓           | ✓           | ✓           |
|                         | RGPE [11]       | ✓               | ✓           | ✓           | ✓           | ✓           |
|                         | FSBO [64]       | ✓               | ✓           | ✓           | ✓           | ✓           |
|                         | Policy Search [37]|              |             |             |             |             |
|                         | DMFBS [24]      | ✓               | ✓           |             |             |             |
|                         | distGP [35]     | ✓               |             |             |             |             |
| Warm-starting method    | Siamese-BHO [30]| ✓               | ✓           | ✓           | ✓           |
|                         | MI-SMBO [12]    | ✓               | ✓           | ✓           | ✓           |
|                         | wsKG [48]       | ✓               | ✓           | ✓           | ✓           |
|                         | Box BO [47]     | ✓               | ✓           | ✓           | ✓           |
| Recommendation method   | SCoT [3]        | ✓               | ✓           | ✓           |
|                         | PMF [13]        | ✓               | ✓           | ✓           |
|                         | Data Grouping [69]|              |             |             |             |             |
|                         | OBBOE [70]      | ✓               | ✓           |             |             |             |
| Domain-specific method  | task2vec [1]    | ✓               | ✓           | ✓           | ✓           |
|                         | DSTL [6]        | ✓               | ✓           | ✓           |
|                         | HyperSTAR [42]  | ✓               | ✓           | ✓           |
|                         | TNP [63]        | ✓               |             |             |             |             |
| Multi-task multi-fidelity BO | AT2 [Ours] | ✓ ✓ ✓ ✓ ✓ ✓ ✓ |

Table 3: Evaluation of hyperparameter tuning methods based on cost-efficiency ($E$) and flexibility ($F$). $E_1$: transferable; $E_2$: low-fidelity; $E_3$: cost-aware; $E_4$: sequential; $F_1$: modality-agnostic; $F_2$: self-contained; $F_3$: cold-start friendly. The details of these criteria are explained in Section 2.2.
## B Generation of HyperRec Database

### B.1 HyperRec Details

The Hyperparameter Recommendation database (HyperRec) consists of 27 unique image classification tasks and 150 distinct configurations sampled from a 16-dimensional nested hyperparameter space. The original image classification dataset of each task is split based on a common ratio: 60% for the training set, 20% for the validation set, and 20% for the testing set. We summarize the details of the tasks in Table 4 and explain the nested hyperparameter space in Appendix B.2.

For each task, we evaluate each configuration during 75 training epochs and repeat this with two randomly sampled seeds. During training, we record the batch-wise cross-entropy loss, the batch-wise top one, five, and ten accuracies, and the training time taken to loop through all the batches. During evaluation, we record the epoch-wise cross-entropy loss and the epoch-wise top one, five, and ten accuracies for the validation and testing sets separately, as well as the evaluation time taken to loop through the two sets.

| Task/Dataset | Number of Images | Number of Classes |
|--------------|------------------|-------------------|
| ACTION40 [71]| 9,532            | 40                |
| AWA2 [66]    | 37,322           | 50                |
| BOOKCOVER30 [23]| 57,000        | 30                |
| CALTECH256 [16]| 30,607         | 257               |
| CARS196 [33] | 16,185           | 196               |
| CIFAR10 [34] | 60,000           | 10                |
| CIFAR100 [34]| 60,000           | 100               |
| CUB200 [62]  | 11,788           | 200               |
| FLOWER102 [43]| 8,189           | 102               |
| FOOD101 [4]  | 101,000          | 101               |
| IMAGENET64SUB1 [51]| 128,112      | 1,000             |
| IMAGENET64SUB2 [51]| 128,112      | 1,000             |
| IMAGENET64SUB3 [51]| 128,112      | 1,000             |
| IP102 [65]   | 75,222           | 102               |
| ISR [50]     | 15,620           | 67                |
| OIPETS [45]  | 7,349            | 37                |
| PLACE365SUB1 [73]| 91,987         | 365               |
| PLACE365SUB2 [73]| 91,987         | 365               |
| PLACE365SUB3 [73]| 91,987         | 365               |
| PLANT39 [15] | 61,486           | 39                |
| RESISC45 [5] | 31,500           | 45                |
| SCENE15 [10, 36]| 4,485           | 15                |
| SDD [29, 7]  | 20,580           | 120               |
| SOP [56]     | 120,053          | 12                |
| SUN397SUB1 [68, 67]| 9,925        | 397               |
| SUN397SUB2 [68, 67]| 9,925        | 397               |
| SUN397SUB3 [68, 67]| 9,925        | 397               |

Table 4: Details on the 27 tasks in HyperRec.
B.2 Nested Hyperparameter Space

Here, we explain the 16-dimensional nested hyperparameter space used in HyperRec. In what follows, \( \mathcal{C}\{\cdots\} \) denotes the categorical distribution, \( \mathcal{U}(\cdot, \cdot) \) denotes the uniform distribution, \( \mathcal{U}\{\cdot, \cdot\} \) denotes the discrete uniform distribution, \( \mathcal{LU}(\cdot, \cdot) \) denotes the log-uniform distribution, and CAWR stands for CosineAnnealingWarmRestarts.

In Table 5, we summarize information about the subset of hyperparameters in HyperRec that are independent of any categorical variables.

| Hyperparameter | Tuning Distribution |
|----------------|---------------------|
| Batch size     | \( \mathcal{U}(32, 128) \) |
| Model          | \( \mathcal{C}\{\text{ResNet34, ResNet50}\} \) |
| Optimizer      | \( \mathcal{C}\{\text{Adam, Momentum}\} \) |
| LR Scheduler   | \( \mathcal{C}\{\text{StepLR, ExponentialLR, CyclicLR, CAWR}\} \) |

Table 5: Details on the hyperparameters that are independent of any categorical variables in HyperRec.

HyperRec involves three categorical hyperparameters: Model, Optimizer, and Learning Rate (LR) Scheduler. In particular, we consider two choices for Model (ResNet34 and ResNet50 [17]), two choices for Optimizer (Adam [51] and Momentum [49]), and four choices for LR Scheduler (StepLR, ExponentialLR, CyclicLR [53], CAWR [40]). The dependent hyperparameters of the categorical variables Optimizer and LR Scheduler in HyperRec are described in Table 6 and Table 7, respectively. Note that the categorical variable Model does not have any dependent hyperparameters in HyperRec.

| Optimizer Choice | Hyperparameter | Tuning Distribution |
|------------------|----------------|---------------------|
| Adam             | Learning rate | \( \mathcal{LU}(10^{-4}, 10^{-1}) \) |
|                  | Weight decay  | \( \mathcal{LU}(10^{-5}, 10^{-3}) \) |
|                  | Beta\(_0\)    | \( \mathcal{LU}(0.5, 0.999) \) |
|                  | Beta\(_1\)    | \( \mathcal{LU}(0.8, 0.999) \) |
| Momentum         | Learning rate | \( \mathcal{LU}(10^{-4}, 10^{-1}) \) |
|                  | Weight decay  | \( \mathcal{LU}(10^{-5}, 10^{-3}) \) |
|                  | Momentum factor | \( \mathcal{LU}(10^{-3}, 1) \) |

Table 6: Details on the hyperparameters that are dependent on Optimizer choices in HyperRec.

| LR Scheduler Choice | Hyperparameter          | Tuning Distribution |
|---------------------|-------------------------|---------------------|
| StepLR              | Step size               | \( \mathcal{U}(2, 20) \) |
|                     | Gamma                   | \( \mathcal{LU}(0.1, 0.5) \) |
| ExponentialLR       | Gamma                   | \( \mathcal{LU}(0.85, 0.999) \) |
| CyclicLR            | Gamma                   | \( \mathcal{LU}(0.1, 0.5) \) |
|                     | Max learning rate       | \( \min(1, LR \times \mathcal{U}(1.1, 1.5)) \) |
|                     | Step size up            | \( \mathcal{U}(1, 10) \) |
| CAWR                | \( T_0 \)               | \( \mathcal{U}(2, 20) \) |
|                     | \( T_{\text{mult}} \)   | \( \mathcal{U}(1, 4) \) |
|                     | \( \text{Eta}_{\text{min}} \) | \( LR \times \mathcal{U}(0.5, 0.9) \) |

Table 7: Details on the hyperparameters that are dependent on LR Scheduler choices in HyperRec.
C Analysis Results of Kernel Combinations

Based on the four options proposed for each of the three component kernels (task, configuration, and fidelity kernels) in Section 3.3, we empirically evaluate the resulting 64 combinations via both quantitative and qualitative measures. We discuss the evaluation results in Section 3.3.4 and present shorter versions of the following tables and figures in Table 2 and Figure 3, respectively.

| Rank | Figure   | Task Kernel | Configuration Kernel | Fidelity Kernel | ELBO  |
|------|----------|-------------|---------------------|----------------|-------|
| 1    | Figure 6 (a) | OptiLand    | DeepPoly            | AccCurve       | 1.4951|
| 2    | Figure 6 (b) | MTBO        | DeepLinear          | Matern         | 1.4296|
| 3    | Figure 6 (c) | OptiLand    | DeepLinear          | AccCurve       | 1.4172|
| 4    | Figure 6 (d) | OptiLand    | DeepPoly            | Matern         | 1.4127|
| 5    | Figure 6 (e) | MTBO        | DeepPoly            | AccCurve       | 1.4121|
| 6    | Figure 6 (f) | DeepPoly    | DeepLinear          | AccCurve       | 1.4017|
| 7    | Figure 6 (g) | OptiLand    | DeepLinear          | Matern         | 1.3871|
| 8    | Figure 6 (h) | DeepPoly    | DeepLinear          | RBF            | 1.3763|
| 9    | Figure 6 (i) | DeepPoly    | DeepLinear          | Matern         | 1.3700|

Table 8: Quantitative performance of different kernel compositions (ranking #1 ~ #9).

Figure 6: Qualitative performance of different kernel compositions (ranking #1 ~ #9).
Table 9: Quantitative performance of different kernel compositions (ranking #10 ∼ #18).

| Rank | Figure | Task Kernel | Configuration Kernel | Fidelity Kernel | ELBO   |
|------|--------|-------------|----------------------|----------------|-------|
| 10   | Figure 7 (a) | OptiLand | DeepLinear | RBF | 1.3590 |
| 11   | Figure 7 (b) | DeepLinear | DeepLinear | RBF | 1.3586 |
| 12   | Figure 7 (c) | DeepLinear | DeepLinear | Matern | 1.3464 |
| 13   | Figure 7 (d) | DeepPoly | DeepLinear | RBF | 1.3460 |
| 14   | Figure 7 (e) | DeepPoly | DeepPoly | RBF | 1.3360 |
| 15   | Figure 7 (f) | MTBO | DeepLinear | AccCurve | 1.3350 |
| 16   | Figure 7 (g) | DeepLinear | DeepLinear | AccCurve | 1.3309 |
| 17   | Figure 7 (h) | MTBO | DeepLinear | RBF | 1.3170 |
| 18   | Figure 7 (i) | OptiLand | Tree | AccCurve | 1.3129 |

Figure 7: Qualitative performance of different kernel compositions (ranking #10 ∼ #18).
Table 10: Quantitative performance of different kernel compositions (ranking #19 ∼ #27).

| Rank | Figure | Task Kernel | Configuration Kernel | Fidelity Kernel | ELBO |
|------|--------|-------------|----------------------|----------------|------|
| 19   | Figure 8 (a) | OptiLand | DeepPoly | RBF | 1.2934 |
| 20   | Figure 8 (b) | DeepPoly | DeepPoly | AccCurve | 1.2925 |
| 21   | Figure 8 (c) | DeepLinear | DeepPoly | AccCurve | 1.2861 |
| 22   | Figure 8 (d) | DeepLinear | Tree | AccCurve | 1.2777 |
| 23   | Figure 8 (e) | MTBO | DeepPoly | Matern | 1.2763 |
| 24   | Figure 8 (f) | DeepLinear | DeepPoly | Matern | 1.2716 |
| 25   | Figure 8 (g) | DeepPoly | Tree | AccCurve | 1.2704 |
| 26   | Figure 8 (h) | MTBO | DeepPoly | RBF | 1.2495 |
| 27   | Figure 8 (i) | OptiLand | Flat | AccCurve | 1.2409 |

Figure 8: Qualitative performance of different kernel compositions (ranking #19 ∼ #27).
| Rank | Figure | Task Kernel | Configuration Kernel | Fidelity Kernel | ELBO  |
|------|--------|-------------|---------------------|----------------|-------|
| 28   | Figure 9 (a) | MTBO       | Tree                | AccCurve       | 1.2121 |
| 29   | Figure 9 (b) | OptiLand   | Tree                | Matern         | 1.1843 |
| 30   | Figure 9 (c) | OptiLand   | Tree                | RBF            | 1.1628 |
| 31   | Figure 9 (d) | DeepPoly   | Tree                | Matern         | 1.1532 |
| 32   | Figure 9 (e) | DeepPoly   | Tree                | RBF            | 1.1431 |
| 33   | Figure 9 (f) | MTBO       | Tree                | RBF            | 1.0923 |
| 34   | Figure 9 (g) | MTBO       | Tree                | Matern         | 1.0864 |
| 35   | Figure 9 (h) | DeepLinear | Tree                | Matern         | 1.0861 |
| 36   | Figure 9 (i) | DeepLinear | Tree                | RBF            | 1.0850 |

Table 11: Quantitative performance of different kernel compositions (ranking #28 ~ #36).

Figure 9: Qualitative performance of different kernel compositions (ranking #28 ~ #36).
Table 12: Quantitative performance of different kernel compositions (ranking #37 ∼ #45).

| Rank | Figure   | Task Kernel | Configuration Kernel | Fidelity Kernel | ELBO  |
|------|----------|-------------|----------------------|-----------------|-------|
| 37   | Figure 10 (a) | OptiLand    | Flat                | RBF             | 1.0633 |
| 38   | Figure 10 (b) | OptiLand    | Flat                | Matern          | 1.0557 |
| 39   | Figure 10 (c) | OptiLand    | DeepPoly            | Fabolas         | 1.0424 |
| 40   | Figure 10 (d) | DeepPoly    | Flat                | AccCurve        | 1.0389 |
| 41   | Figure 10 (e) | DeepPoly    | DeepLinear          | Fabolas         | 0.9881 |
| 42   | Figure 10 (f) | DeepLinear  | DeepPoly            | Fabolas         | 0.9880 |
| 43   | Figure 10 (g) | OptiLand    | Tree                | Fabolas         | 0.9224 |
| 44   | Figure 10 (h) | OptiLand    | Flat                | Fabolas         | 0.9170 |
| 45   | Figure 10 (i) | DeepPoly    | Flat                | RBF             | 0.9100 |

Figure 10: Qualitative performance of different kernel compositions (ranking #37 ∼ #45).
| Rank | Figure   | Task Kernel | Configuration Kernel | Fidelity Kernel | ELBO  |
|------|----------|-------------|---------------------|----------------|-------|
| 46   | Figure 11(a) | DeepPoly   | Flat                | Matern         | 0.8844|
| 47   | Figure 11(b) | DeepPoly   | Flat                | AccCurve       | 0.4301|
| 48   | Figure 11(c) | DeepLinear | Flat                | RBF            | 0.3416|
| 49   | Figure 11(d) | DeepPoly   | DeepPoly            | Matern         | 0.3053|
| 50   | Figure 11(e) | MTBO       | Flat                | AccCurve       | 0.2985|
| 51   | Figure 11(f) | DeepLinear | Flat                | Matern         | 0.2822|
| 52   | Figure 11(g) | MTBO       | Flat                | RBF            | 0.1433|
| 53   | Figure 11(h) | MTBO       | Flat                | Matern         | 0.1406|
| 54   | Figure 11(i) | DeepPoly   | DeepPoly            | Fabolas        | 0.1350|

Table 13: Quantitative performance of different kernel compositions (ranking #46 ~ #54).

Figure 11: Qualitative performance of different kernel compositions (ranking #46 ~ #54).
| Rank | Figure   | Task Kernel | Configuration Kernel | Fidelity Kernel | ELBO |
|------|----------|-------------|---------------------|-----------------|------|
| 55   | Figure 12 (a) | OptiLand | DeepLinear | Fabolas | 0.1350 |
| 56   | Figure 12 (b) | DeepLinear | Flat | Fabolas | 0.1349 |
| 57   | Figure 12 (c) | DeepLinear | Tree | Fabolas | 0.1349 |
| 58   | Figure 12 (d) | DeepLinear | DeepLinear | Fabolas | 0.1349 |
| 59   | Figure 12 (e) | DeepPoly | Flat | Fabolas | 0.1349 |

Table 14: Quantitative performance of different kernel compositions (ranking #55 ~ #59).

Figure 12: Qualitative performance of different kernel compositions (ranking #55 ~ #59).
| Rank | Figure | Task Kernel | Configuration Kernel | Fidelity Kernel | ELBO  |
|------|--------|-------------|----------------------|----------------|-------|
| 60   | Figure 13 (a) | DeepPoly   | Tree                 | Fabolas        | 0.1349|
| 61   | Figure 13 (b) | MTBO       | DeepLinear           | Fabolas        | 0.1342|
| 62   | Figure 13 (c) | MTBO       | Flat                 | Fabolas        | 0.1342|
| 63   | Figure 13 (d) | MTBO       | DeepPoly             | Fabolas        | 0.1342|
| 64   | Figure 13 (e) | MTBO       | Tree                 | Fabolas        | 0.1342|

Table 15: Quantitative performance of different kernel compositions (ranking #60 ~ #64).

Figure 13: Qualitative performance of different kernel compositions (ranking #60 ~ #64).
D Experiment Details

We compare the proposed AT2 method against seven hyperparameter transfer learning baselines, based on our offline-computed database HyperRec and another real-world database LCBench [74]. Figure 14 shows AT2’s ability to transfer knowledge and forecast high-fidelity performance. Figure 15 shows the quantitative performance of AT2 and other baselines with one standard error. The detailed experiment setup is explained in Section 4.

We perform our experiments on an AWS P2 instance with one K80 GPU. It takes around one hour for AT2 to finish training and to run 100 queries on one train-test task pair. The GPyTorch package [14] uses the MIT license, and the LCBench database [74] uses the Apache License Version 2.0. The data used in our experiments contain the validation accuracy of machine learning models, and therefore do not include any personally identifiable information or require the consent of human subjects.

Figure 14: Predictions by AT2 versus observed validation accuracies for one sampled train-test task pair and 10 sampled configurations in HyperRec. The shaded regions indicate one and two predictive standard deviations. At iteration 1, AT2 approximates the optimization landscape of the new tuning task by transferring knowledge from past tasks. As more queries are made on the new task over iterations, AT2 better resembles the observed validation accuracies at both low and high fidelities (i.e., Epoch 0 and 50, respectively).
Figure 15: Performance of methods on HyperRec and LCBench. The results based on two metrics (simple regret and final performance ranking) are averaged across five train-test task pairs for each database. Lower is better. The predicted final performance rankings are smoothed with a hamming window of 10 iterations. The shaded regions represent one standard error of each method. Our proposed AT2 method consistently achieves lower simple regrets and final performance rankings.