HYPERPARAMETER TRANSFER ACROSS DEVELOPER ADJUSTMENTS

Anonymous authors
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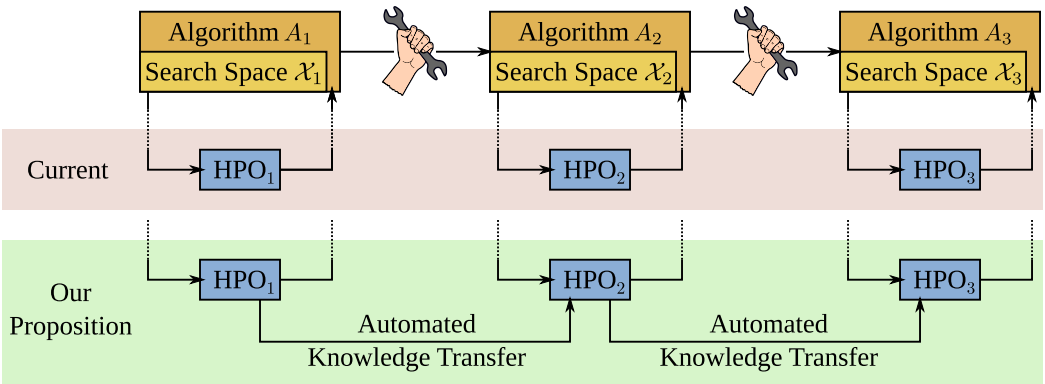
ABSTRACT

After developer adjustments to a machine learning (ML) algorithm, how can the results of an old hyperparameter optimization (HPO) automatically be used to speedup a new HPO? This question poses a challenging problem, as developer adjustments can change which hyperparameter settings perform well, or even the hyperparameter search space itself. While many approaches exist that leverage knowledge obtained on previous *tasks*, so far, knowledge from previous *development steps* remains entirely untapped. In this work, we remedy this situation and propose a new research framework: hyperparameter transfer across adjustments (HT-AA). To lay a solid foundation for this research framework, we provide four simple HT-AA baseline algorithms and eight benchmarks changing various aspects of ML algorithms, their hyperparameter search spaces, and the neural architectures used. The best baseline, on average and depending on the budgets for the old and new HPO, reaches a given performance 1.2–3.6x faster than a prominent HPO algorithm without transfer. As HPO is a crucial step in ML development but requires extensive computational resources, this speedup would lead to faster development cycles, lower costs, and reduced environmental impacts. To make these benefits available to ML developers off-the-shelf and to facilitate future research on HT-AA, we provide python packages for our baselines and benchmarks.



Graphical Abstract: Hyperparameter optimization (HPO) across adjustments to the algorithm or hyperparameter search space. A common practice is to perform HPO from scratch after each adjustment or to somehow manually transfer knowledge. In contrast, we propose a new research framework about automatic knowledge transfers across adjustments for HPO.

1 INTRODUCTION: A NEW HYPERPARAMETER TRANSFER FRAMEWORK

The machine learning (ML) community arrived at the current generation of ML algorithms by performing many iterative adjustments. Likely, the way to artificial general intelligence requires many more adjustments. Each algorithm adjustment could change which settings of the algorithm's hyperparameters perform well, or even the hyperparameter search space itself (Chen et al., 2018; Li et al., 2020). For example, when deep learning developers change the optimizer, the learning rate's optimal value

likely changes, and the new optimizer may also introduce new hyperparameters. Since ML algorithms are known to be very sensitive to their hyperparameters (Chen et al., 2018; Feurer & Hutter, 2019), developers are faced with the question of how to adjust their hyperparameters after changing their code. Assuming that the developers have results of one or several hyperparameter optimizations (HPOs) that were performed before the adjustments, they have two options:

1. Somehow manually transfer knowledge from old HPOs.

This is the option chosen by many researchers and developers, explicitly disclosed, e.g., in the seminal work on AlphaGo (Chen et al., 2018). However, this is not a satisfying option since manual decision making is time-consuming, often individually designed, and has already lead to reproducibility problems (Musgrave et al., 2020).

2. Start the new HPO from scratch.

Leaving previous knowledge unutilized can lead to higher computational demands and worse performance (demonstrated empirically in Section 5). This is especially bad as the energy consumption of ML algorithms is already recognized as an environmental problem. For example, deep learning pipelines can have CO_2 emissions on the order of magnitude of the emissions of multiple cars for a lifetime (Strubell et al., 2019), and their energy demands are growing furiously: Schwartz et al. (2019) cite a "300,000x increase from 2012 to 2018". Therefore, reducing the number of evaluated hyperparameter settings should be a general goal of the community.

The **main contribution** of this work is the introduction of a new research framework: *Hyperparameter transfer across adjustments (HT-AA)*, which empowers developers with a third option:

3. Automatically transfer knowledge from previous HPOs.

This option leads to advantages in two aspects: The automation of decision making and the utilization of previous knowledge. On the one hand, the automation allows to benchmark strategies, replaces expensive manual decision making, and enables reproducible and comparable experiments; on the other hand, utilizing previous knowledge leads to faster development cycles, lower costs, and reduced environmental impacts.

To lay a solid foundation for the new HT-AA framework, our **individual contributions** are as follows:

- We formally introduce a basic version of the HT-AA problem (Section 2).
- We provide four simple baseline algorithms for our basic HT-AA problem (Section 3).
- We provide a comprehensive set of eight novel benchmarks for our basic HT-AA problem (Section 4).
- We show the advantage of transferring across developer adjustments: some of our simple baseline algorithms outperform HPO from scratch up to 1.2–3.6x on average depending on the budgets (Section 5).
- We empirically demonstrate the need for well-vetted algorithms for HT-AA: two baselines modelled after actually-practiced manual strategies perform horribly on our benchmarks (Section 5).
- We relate the HT-AA framework to existing research efforts and discuss the research opportunities it opens up (Section 6).
- To facilitate future research on HT-AA, we provide open-source code for our experiments and benchmarks and provide a python package with an out-of-the-box usable implementation of our HT-AA algorithms.

2 Hyperparameter Transfer Across Adjustments

After presenting a broad introduction to the topic, we now provide a detailed description of hyperparameter transfer across developer adjustments (HT-AA). We first introduce hyperparameter optimization, then discuss the types of developer adjustments, and finally describe the transfer across these adjustments.

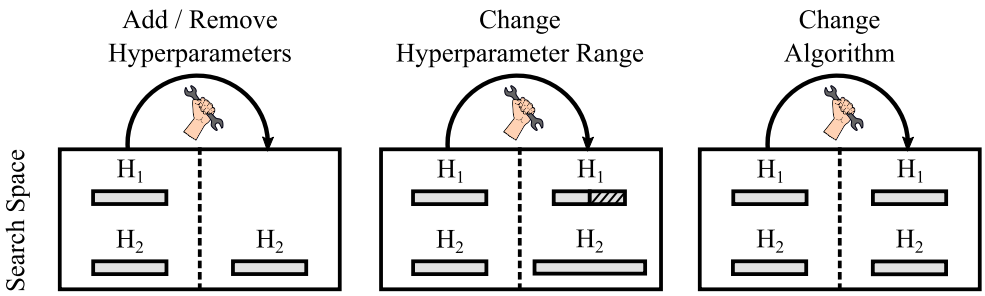


Figure 1: Developer adjustments from the perspective of hyperparameter optimization.

Hyperparameter optimization (HPO) The HPO formulation we utilize in this work is as follows:

$$\underset{\boldsymbol{x}\in\mathcal{X}}{\text{minimize}}\, f_{\mathcal{A}}(\boldsymbol{x}) \quad \text{with } b \text{ evaluations} \qquad , \tag{1}$$

where $f_{\mathcal{A}}(\boldsymbol{x})$ is the objective function for ML algorithm $\mathcal{A}$ with hyperparameter setting $\boldsymbol{x}$, b is the number of available evaluations, and $\mathcal{X}$ is the search space. We allow the search space $\mathcal{X}$ to contain categorical and numerical dimensions alike and consider only sequential evaluations. We refer to a specific HPO problem with the 3-tuple $(\mathcal{X},\, f_{\mathcal{A}},\, b)$. For a discussion on potential extensions of our framework to different HPO formulations, we refer the reader to Section 6.

Developer adjustments We now put developer adjustments on concrete terms and introduce a taxonomy of developer adjustments. We consider two main categories of developer adjustments: ones that do not change the search space $\mathcal{X}$ (homogeneous adjustments) and ones that do (heterogenous adjustments). Homogeneous adjustments could either change the algorithm's implementation or the hardware that the algorithm is run on. Heterogeneous adjustments can be further categorized into adjustments that add or remove a hyperparameter (hyperparameter adjustments) and adjustments that change the search space for a specific hyperparameter (range adjustments). Figure 1 shows an illustration of the adjustment types.

Knowledge transfer across adjustments In general, a continuous stream of developer adjustments could be accompanied by multiple HPOs. We simplify the problem in this fundamental work and only consider the transfer between two HPO problems; we discuss a potential extension in Section 6. The two HPO problems arise from adjustments Ψ to a ML algorithm $\mathcal{A}_{\text{old}}$ and its search space $\mathcal{X}_{\text{old}}$, which lead to $\mathcal{A}_{\text{new}}, \mathcal{X}_{\text{new}} := \Psi(\mathcal{A}_{\text{old}},\, \mathcal{X}_{\text{old}})$. Specifically, the hyperparameter transfer across adjustments problem is to solve the HPO problem $(\mathcal{X}_{\text{new}},\, f_{\mathcal{A}_{\text{new}}},\, b_{\text{new}})$, given the results for $(\mathcal{X}_{\text{old}},\, f_{\mathcal{A}_{\text{old}}},\, b_{\text{old}})$. Compared to HPO from scratch, developers can choose a lower budget b_{new}, given evidence for a transfer algorithm achieving the same performance faster.

3 Baseline Algorithms for HT-AA

In this section we present four baselines for the specific instantiation of the hyperparameter transfer across adjustments (HT-AA) framework discussed in Section 2. We resist the temptation to introduce complex approaches alongside a new research framework and instead focus on a solid foundation. Specifically, we focus on approaches that do not use any knowledge from the new HPO for the transfer and include two baselines that are modelled after actually-practiced manual strategies. We first introduce the basic HPO algorithm that the transfer approaches build upon, then introduce notation for two decompositions of HPO search spaces across adjustments, and finally, we present the four baselines themselves.

3.1 Preliminaries

Background For basic hyperparameter optimization and parts of the transfer algorithms, we employ Bayesian optimization (BO) (Shahriari et al., 2016) with Gaussian processes (Rasmussen & Williams, 2006). Given observations $\mathcal{D} = \{(\boldsymbol{x}_k,\, f_{\mathcal{A}}(\boldsymbol{x}_k)\}_{k=1}^{n}$, BO fits a probabilistic model $p(f_{\mathcal{A}} \mid \mathcal{D})$ for the

objective function $f_{\mathcal{A}}$. Then, to decide which hyperparameter setting to evaluate next, BO maximizes an acquisition function $\alpha(\boldsymbol{x} \mid \mathcal{D})$, which uses this probabilistic model. Here, we use Gaussian process regression to fit a model, and the widely used expected improvement (Jones et al., 1998) as the acquisition function. In our experiments, we use the BO implementation from the SMAC3 package (Lindauer et al., 2017) with default kernels, hyperparameters, and optimization procedures. In the following we will refer to BO with Gaussian processes with GP.

Search space decomposition: Hyperparameter adjustments For hyperparameter adjustments the new search space $\mathcal{X}_{\text{new}}$ and the old search space $\mathcal{X}_{\text{old}}$ only differ in hyperparameters, not in hyperparameter ranges, so we can decompose the search spaces as $\mathcal{X}_{\text{new}} = \mathcal{X}_{\text{only-new}} \times \mathcal{X}_{\text{both}}$ and $\mathcal{X}_{\text{old}} = \mathcal{X}_{\text{both}} \times \mathcal{X}_{\text{only-old}}$, where $\mathcal{X}_{\text{both}}$ is the part of the search space that remains unchanged across adjustments (see Figure 2 for reference). All baselines use this decomposition and project the hyperparameter settings that were evaluated in the old HPO from $\mathcal{X}_{\text{old}}$ to $\mathcal{X}_{\text{both}}$.

Search space decomposition: Range adjustments A range adjustment can remove values from the hyperparameter range or add values. For an adjustment of hyperparameter range $\mathcal{X}_{old}^{H_i}$ to $\mathcal{X}_{\text{new}}^{H_i}$ this can be expressed as $\mathcal{X}_{\text{new}}^{H_i} = \mathcal{X}_{\text{both}}^{H_i} \cup \mathcal{X}_{\text{both,range-only-new}}^{H_i}$ with $\mathcal{X}_{\text{both}}^{H_i} = \mathcal{X}_{old}^{H_i} \setminus \mathcal{X}_{\text{both,range-only-old}}^{H_i}$.

3.2 Only Optimize New Hyperparameters

A common strategy by developers to manually transfer across adjustments is to set previous hyperparameters in $\mathcal{X}_{\text{both}}$ to the best setting of the previous HPO and only optimize hyperparameters in $\mathcal{X}_{\text{only-new}}$ (Agostinelli et al., 2014; Huang et al., 2017; Wu & He, 2018). If the previous best setting is not a valid configuration anymore, i.e., it has values in $\mathcal{X}_{\text{both,range-only-old}}^{H_i}$ for a hyperparameter H_i still in $\mathcal{X}_{\text{both}}$, this strategy uses the best setting that still is a valid configuration. In the following, we refer to this strategy as *only-optimize-new*.

3.3 Drop Unimportant Hyperparameters

A strategy inspired by manual HT-AA efforts is to only optimize important hyperparameters. The utilization of importance statistics was, for example, explicitly disclosed in the seminal work on AlphaGo (Chen et al., 2018). Here, we determine the importance of each individual hyperparameter with functional analysis of variance (fANOVA) (Hutter et al., 2014) and do not tune hyperparameters with below mean importance. Therefore, this strategy only optimizes hyperparameters in $\mathcal{X}_{\text{only-new}}$ and hyperparameters in $\mathcal{X}_{\text{both}}$ with above mean importance. In the following, we refer to this strategy as *drop-unimportant*.

3.4 First Evaluate Best

The *best-first* strategy uses only-optimize-new for the first evaluation, and uses standard GP for the remaining evaluations. This strategy has a large potential speedup and low risk as it falls back to standard GP.

3.5 Transfer GP (TGP)

The transfer GP (TGP) strategy uses a Gaussian process fitted on the results of the previous HPO projected to $\mathcal{X}_{\text{both}}$ with $\mathcal{X}_{\text{both}}$ as the search space. To choose the values for hyperparameters in $\mathcal{X}_{\text{only-new}}$, TGP uses a random sample (Figure 2). Further, as in the basic GP strategy, TGP uses a random sample over $\mathcal{X}_{\text{new}}$ in ½ of cases, and after $\dim(\mathcal{X}_{\text{new}})$ evaluations, TGP uses a Gaussian process fitted on the new observations. TGP is similar to only-optimize-new, but instead of using the best previous values of previously existing hyperparameters at each step, the algorithm samples from a model fitted on the projected results of the previous HPO until a model is fit on the new observations.

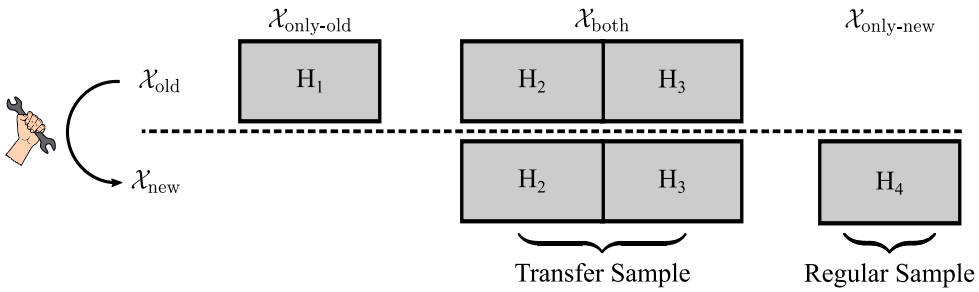


Figure 2: Example search space decomposition for a hyperparameter addition and removal.

4 BENCHMARKS FOR HT-AA

We introduce eight novel benchmarks for the basic hyperparameter transfer across adjustments (HT-AA) problem discussed in Section 2. As is common in hyperparameter optimization research, we employ tabular and surrogate benchmarks to allow cheap and reproducible benchmarking (Perrone et al., 2018; Falkner et al., 2018). Tabular benchmarks achieve this with a lookup table for all possible hyperparameter settings. In contrast, surrogate benchmarks fit a surrogate model for the objective function (Eggensperger et al., 2014). We base our surrogate models and lookup tables on code and data from existing hyperparameter optimization (HPO) benchmarks (detailed in Appendix A) that, together, cover four different machine learning algorithms: a fully connected neural network (FCN), neural architecture search for a convolutional neural network (NAS), a support vector machine (SVM), and XGBoost (XGB). While the NAS and FCN benchmarks are based on lookup tables, the SVM and XGB based benchmarks use surrogate models. For each of these base benchmarks, we simulate two different types of developer adjustments (Table 1), to arrive at a total of eight benchmarks. Additionally, for each algorithm and adjustment, we consider multiple tasks in our benchmarks. Further, we provide a python package with all our benchmarks and refer the reader to Appendix A for additional details on the benchmarks.

Table 1: Developer adjustments and types of adjustments in the benchmarks.

Benchmark	Adjustments	Adjustment Type
FCN-A	Increase #units-per-layer 16×	Homogeneous
	Double #epochs	Homogeneous
	Fix batch size hyperparameter	Heterogeneous
FCN-B	Add per-layer choice of activation function	Heterogeneous
	Change learning rate schedule	Homogeneous
NAS-A	Add 3x3 average pooling as choice of operation to each edge	Heterogeneous
NAS-B	Add node to cell template (adds 3 hyperparameters)	Heterogeneous
XGB-A	Expose four booster hyperparameters	Heterogeneous
XGB-B	Change four unexposed booster hyperparameter values	Homogeneous
SVM-A	Change kernel	Homogeneous
	Remove hyperparameter for old kernel	Heterogeneous
	Add hyperparameter for new kernel	Heterogeneous
SVM-B	Increase range for cost hyperparameter	Heterogeneous

5 EXPERIMENTS AND RESULTS

In this section, we empirically evaluate the four baseline algorithms presented in Section 3 as solutions for the hyperparameter transfer across adjustments problem. We first describe the evaluation protocol used through all studies and then present the results.

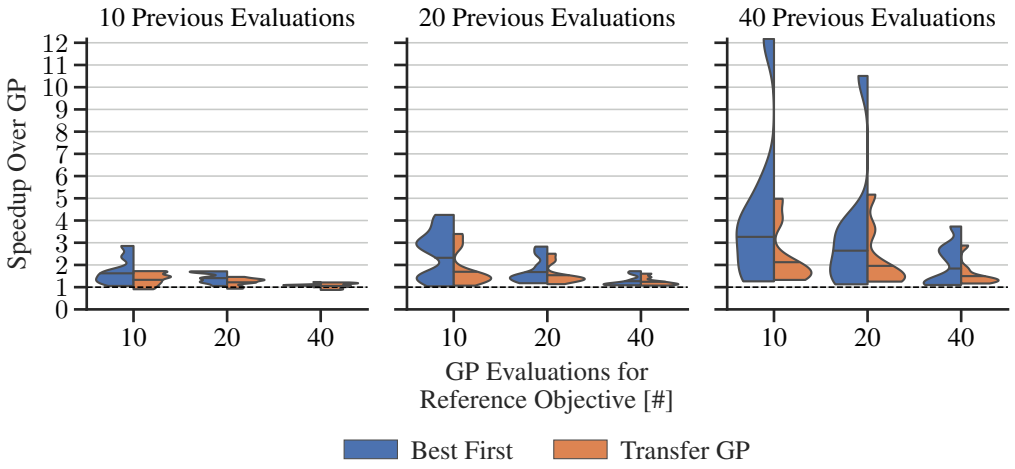


Figure 3: Speedup to reach a given reference objective value compared to GP for best-first and transfer GP across 8 benchmarks. The violins estimate densities of benchmark geometric means. The horizontal line in each violin shows the geometric mean across these benchmark means. #Evaluations for the old HPO increases from left to right. The x-axis shows the budget for the GP reference. Note that the GP runs we used to determine the reference objective are different to the ones that we show the speedups over.

Evaluation protocol We use the benchmarks introduced in Section 4 and focus on the speedup of transfer strategies over Bayesian optimization with Gaussian processes, which we refer to as GP. Specifically, we measured how much faster a transfer algorithm reaches a given objective value compared to GP in terms of the number of evaluations. We repeated all measurements across 25 different random seeds and report results for validation objectives, as not all benchmarks provide test objectives, and to reduce noise in our evaluation. We terminate runs after 400 evaluations and report ratio of means. To aggregate these ratios across tasks and benchmarks, we use the geometric mean. We use the geometric mean, as, intuitively, two speedups of e.g., 0.1x and 10x average to 1x, and not 5.05x. We want to note that the standard mean is an upper bound for the geometric mean, so using the geometric mean in fact makes the speedups slightly less impressive than had we used the standard arithmetic mean. To determine the target objective values, we measured GP's average performance for 10, 20, and 40 evaluations. We chose this range of evaluations as a survey among NeurIPS2019 and ICLR2020 authors indicates that most hyperparameter optimizations (HPOs) do not consider more than 50 evaluations (Bouthillier & Varoquaux, 2020). Further, for transfer approaches, we perform this experiment for different evaluation budgets for the HPO before the adjustments (also for 10, 20, and 40 evaluations).

Results The transfer GP (TGP) and best-first strategy lead to large speedups, while drop-unimportant and only-optimize-new perform poorly. On average and depending on the budgets for the old and new HPO, TGP reaches the given objective values 1.1–2.1x faster than GP, and best-first 1.1–3.3x faster. The combination of TGP and best-first leads to further speedups over best-first if the budget for the old HPO was 20 or 40, and when the old budget and new budget both equal 10. These additional average speedups when combining TGP with best-first are between 0.1 and 0.3. We visualize these results with violin plots (Figure 4 and Figure 3), as they take into account the multi modality of the results, and also provide a table with exact averages (Table 2). There are two main trends visible: (1) The more optimal the target objective, the smaller the speedup, and (2) the higher the budget for the previous HPO, the higher the speedup. For a more fine-grained visualization that shows violin plots over task means for each benchmark, we refer to Appendix B. The approaches inspired by actually-practiced manual strategies, drop-unimportant and only-optimize-new, do not reach the performance of GP in a large percentage of cases, even while given at least 10x the budget compared to GP (Figure 5). These high failure rates makes an evaluation for the speedup unfeasible and indicates that actually-practiced manual strategies perform worse than starting from scratch. For the failure rates for GP, TGP, and best-first (0-0.8%) we refer the reader to Appendix C.

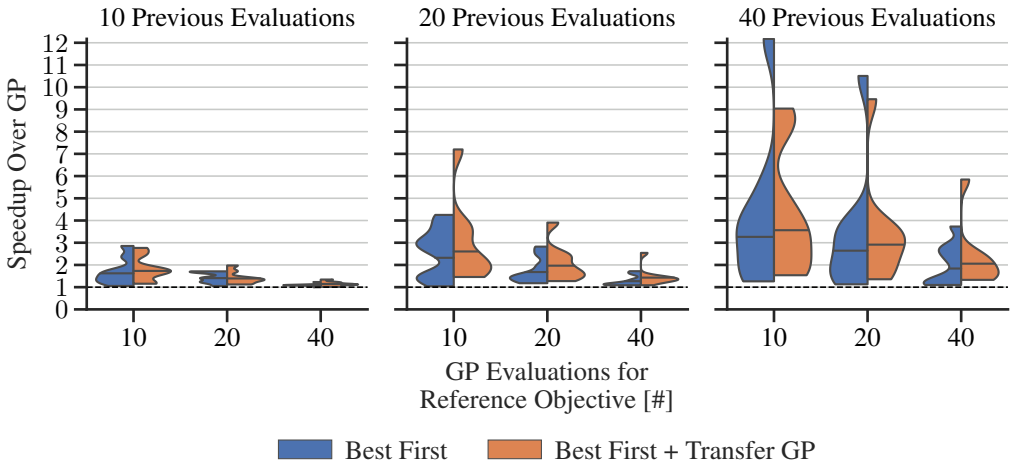


Figure 4: Speedup to reach a given reference objective value compared to GP for best-first and combined best-first with transfer GP across 8 benchmarks. The violins estimate densities of benchmark geometric means. The horizontal line in each violin shows the geometric mean across these benchmark means. #Evaluations for the old HPO increases from left to right. The x-axis shows the budget for the GP reference. Note that the GP runs we used to determine the reference objective are different to the ones that we show the speedups over.

Table 2: Average speedup across benchmarks for different #evaluations for the old and new HPO.

#Evals Old	#Evals New	Best First	Transfer GP	Best First + Transfer GP
10	10	1.6	1.3	**1.7**
	20	**1.4**	1.2	**1.4**
	40	1.1	1.1	**1.2**
20	10	2.3	1.7	**2.6**
	20	1.7	1.5	**2.0**
	40	1.3	1.2	**1.4**
40	10	3.3	2.1	**3.6**
	20	2.6	2.0	**2.9**
	40	1.8	1.5	**2.1**

Additionally, we provide a study on the improvement in objective value for a fixed number of evaluations in Appendix D; in Appendix E we show the results of a control study that compares GP with different ranges of random seeds; and in Appendix F we compare random search and a popular HPO algorithm with GP to validate its reliability.

6 Related Work and Research Opportunities

In this section, we discuss work related to hyperparameter transfer across adjustments (HT-AA) and present several research opportunities in combining existing ideas with HT-AA.

Transfer learning Transfer learning studies how to use observations from one or multiple source tasks to improve learning on one or multiple target tasks (Zhuang et al., 2019). If we view the HPO problems before and after specific developer adjustments as tasks, we can consider HT-AA as a specific transfer learning problem. As developer adjustments may change the search space, HT-AA would then be categorized as a heterogeneous transfer learning problem (Day & Khoshgoftaar, 2017).

Transfer learning across adjustments Recently, Berner et al. (2019) transferred knowledge between deep reinforcement learning agents across developer adjustments. They crafted techniques

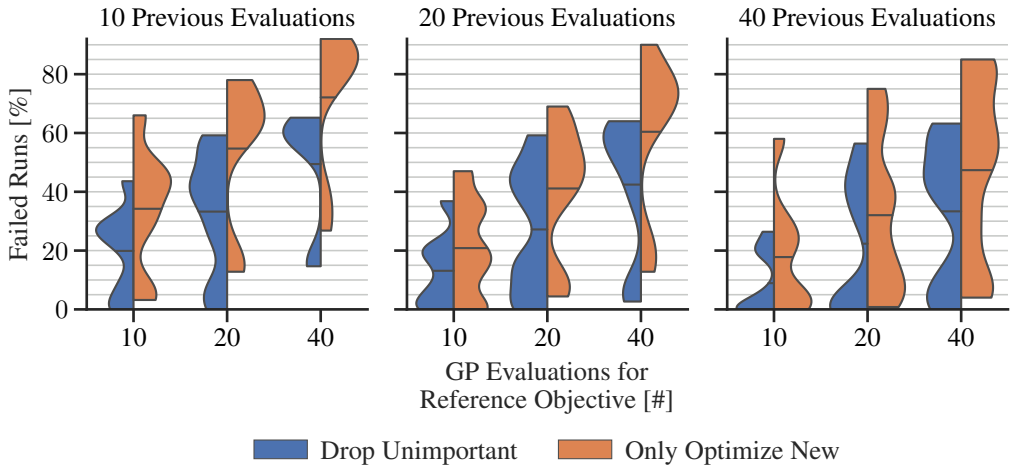


Figure 5: Percent of runs that do not reach the reference objective for drop-unimporant and only-optimize-new. Each data point for the violins represents the mean percentage of failures for a benchmark. The line in each violin shows the mean across these benchmark means. #Evaluations for the old HPO increases from left to right. The x-axis shows the budget for the GP reference.

to preserve, or approximately preserve, the neural network policy for each type of adjustment they encountered. Their transfer strategies are inspired by Net2Net knowledge transfer (Chen et al., 2015), and they use the term surgery to refer to this practice. Their work indicates that transfer learning across adjustments is not limited to knowledge about hyperparameters, but extends to a more general setting, leaving room for many research opportunities.

Continuous knowledge transfer In this paper, we focus on transferring knowledge from the last HPO performed, but future work could investigate a continuous transfer of knowledge across many cycles of adjustments and HPOs. Transferring knowledge from HPO runs on multiple previous versions could lead to further performance gains, as information from each version could be useful for the current HPO. Such *continuous* HT-AA would then be related to the field of continual learning (Thrun & Mitchell, 1995; Lange et al., 2020).

Hyperparameter transfer across tasks (HT-AT) There exists an extensive research field that studies the transfer across *tasks* for HPOs (Vanschoren, 2018). The main difference to hyperparameter transfer across *adjustments* is that the former assumes an unchanging search space, whereas dealing with such changes is one of the main challenges in HT-AA. In HT-AT, the search space and the ML algorithm remain unchanged, but the task that the algorithm is applied to changes. Another difference is that most work on HT-AT considers large amounts of meta-data; up to more than a thousand tasks and function evaluations (Wang et al., 2018; Metz et al., 2020).

Homogeneous hyperparameter transfer across adjustments (homogeneous HT-AA) problems, where none of the adjustments changes the search space, are syntactically equivalent to HT-AT problems. For this homogeneous HT-AA, existing approaches for HT-AT could, in principle, be applied without modification; this includes, for example the transfer acquisition function (Wistuba et al., 2018), multi-task bayesian optimization (Swersky et al., 2013), multi-task adaptive bayesian linear regression (Perrone et al., 2018), ranking-weighted gaussian process ensemble (Feurer et al., 2018), and difference-modelling bayesian optimisation (Shilton et al., 2017).

Further, an adaptation of across-task strategies to the across-adjustments setting could lead to more powerful HT-AA approaches in the future. Finally, the combination of across-task and across-adjustments hyperparameter transfer is an exciting research opportunity that could provide even larger speedups than either transfer strategy on its own.

Advanced hyperparameter optimization HT-AA can be combined with one of the many extensions to the basic hyperparameter optimization (HPO) formulation. One such extension is multi-

fidelity HPO, which allows the use of cheap-to-evaluate approximations to the actual objective (Li et al., 2017; Falkner et al., 2018). Similarly, cost-aware HPO adds a cost to each hyperparameter setting, so a cost model can prioritize the evaluation of cheap hyperparameter settings over expensive ones (Snoek et al., 2012). Yet another extension is to take different kinds of evaluation noise into account (Kersting et al., 2007) or to consider not one, but multiple objectives to optimize for (Khan et al., 2002). All these HPO formulations can be studied in conjunction with HT-AA, to either provide further speedups or deal with more general optimization problems.

Guided machine learning The field of guided machine learning (gML) studies the design of interfaces that enables humans to guide ML processes (Westphal et al., 2019). An HT-AA algorithm could be viewed as a ML algorithm that receives incremental guidance in the form of arbitrary developer adjustments; the interface would then be the programming language(s) the ML algorithm is implemented in.

On a different note, gML could provide HT-AA algorithms with additional information about the adjustments to the ML algorithm. For example, when adding a hyperparameter, there are two distinctions we can make: Either an existing hyperparameter is exposed (e.g., the dropout rate was previously hardcoded as 0.5, and is now tuned) , or a new component is added to the algorithm that introduces a new hyperparameter (e.g., a new learning rate schedule that introduces a decay hyperparameter) . From the HPO problem itself, we cannot know which case it is, and neither which fixed value an exposed hyperparameter had. Guided HT-AA algorithms could ask for user input to fill this knowledge gap. Alternatively, HT-AA algorithms with code analysis could automatically extract this knowledge from the source code.

Programming by optimization Relatedly, the programming by optimization (PbO) framework (Hoos, 2012) proposes the automatic construction of a search space of algorithms, based on code annotations, and the subsequent automated search in this search space. While this framework considers evolving search spaces over incremental developer actions, each task and development step restarts the search from scratch. This is in contrast to our hyperparameter transfer framework that alleviates the need to restart from scratch after each developer adjustment.

7 Conclusion

In this work, we introduced hyperparameter transfer across developer adjustments to improve efficiency during the development of ML algorithms. In light of rising energy demands of ML algorithms and rising global temperatures, more efficient ML development practices are an important issue now and will become more important in the future. As already two of the simple baseline algorithm considered in this work lead to large empirical speedups, our new framework represents a promising step towards efficient ML development.

References

Forest Agostinelli, Matthew Hoffman, Peter Sadowski, and Pierre Baldi. Learning activation functions to improve deep neural networks. *arXiv preprint arXiv:1412.6830*, 2014.

James S Bergstra, Rémi Bardenet, Yoshua Bengio, and Balázs Kégl. Algorithms for hyper-parameter optimization. In *Advances in neural information processing systems*, pp. 2546–2554, 2011.

Christopher Berner, Greg Brockman, Brooke Chan, Vicki Cheung, Przemysław Dębiak, Christy Dennison, David Farhi, Quirin Fischer, Shariq Hashme, Chris Hesse, et al. Dota 2 with large scale deep reinforcement learning. *arXiv preprint arXiv:1912.06680*, 2019.

Xavier Bouthillier and Gaël Varoquaux. Survey of machine-learning experimental methods at NeurIPS2019 and ICLR2020. Research report, Inria Saclay Ile de France, January 2020. URL `https://hal.archives-ouvertes.fr/hal-02447823`.

Tianqi Chen, Ian Goodfellow, and Jonathon Shlens. Net2net: Accelerating learning via knowledge transfer. *arXiv preprint arXiv:1511.05641*, 2015.

Yutian Chen, Aja Huang, Ziyu Wang, Ioannis Antonoglou, Julian Schrittwieser, David Silver, and Nando de Freitas. Bayesian optimization in alphago. *arXiv preprint arXiv:1812.06855*, 2018.

Oscar Day and Taghi M Khoshgoftaar. A survey on heterogeneous transfer learning. *Journal of Big Data*, 4(1):29, 2017.

Xuanyi Dong and Yi Yang. Nas-bench-201: Extending the scope of reproducible neural architecture search. In *International Conference on Learning Representations*, 2019.

K. Eggensperger, F. Hutter, H. Hoos, and K. Leyton-Brown. Surrogate benchmarks for hyperparameter optimization. In *ECAI workshop on Metalearning and Algorithm Selection (MetaSel'14)*, 2014.

Stefan Falkner, Aaron Klein, and Frank Hutter. BOHB: Robust and efficient hyperparameter optimization at scale. In *Proceedings of the 35th International Conference on Machine Learning (ICML 2018)*, pp. 1436–1445, July 2018.

Matthias Feurer and Frank Hutter. Hyperparameter optimization. In Frank Hutter, Lars Kotthoff, and Joaquin Vanschoren (eds.), *Automatic Machine Learning: Methods, Systems, Challenges*, pp. 3–38. Springer, 2019. Available at `http://automl.org/book`.

Matthias Feurer, Benjamin Letham, and Eytan Bakshy. Scalable meta-learning for bayesian optimization. *arXiv preprint arXiv:1802.02219*, 2018.

Holger H Hoos. Programming by optimization. *Communications of the ACM*, 55(2):70–80, 2012.

Gao Huang, Zhuang Liu, Laurens Van Der Maaten, and Kilian Q Weinberger. Densely connected convolutional networks. In *Proceedings of the IEEE conference on computer vision and pattern recognition*, pp. 4700–4708, 2017.

F. Hutter, H. Hoos, and K. Leyton-Brown. An efficient approach for assessing hyperparameter importance. In E. Xing and T. Jebara (eds.), *Proceedings of the 31th International Conference on Machine Learning, (ICML'14)*, pp. 754–762. Omnipress, 2014.

Donald R Jones, Matthias Schonlau, and William J Welch. Efficient global optimization of expensive black-box functions. *Journal of Global optimization*, 13(4):455–492, 1998.

Kristian Kersting, Christian Plagemann, Patrick Pfaff, and Wolfram Burgard. Most likely heteroscedastic gaussian process regression. In *Proceedings of the 24th international conference on Machine learning*, pp. 393–400, 2007.

Nazan Khan, David E Goldberg, and Martin Pelikan. Multi-objective bayesian optimization algorithm. In *Proceedings of the 4th Annual Conference on Genetic and Evolutionary Computation*, pp. 684–684. Citeseer, 2002.

Aaron Klein and Frank Hutter. Tabular benchmarks for joint architecture and hyperparameter optimization. *arXiv preprint arXiv:1905.04970*, 2019.

Daniel Kühn, Philipp Probst, Janek Thomas, and Bernd Bischl. Automatic exploration of machine learning experiments on openml. *arXiv preprint arXiv:1806.10961*, 2018.

Matthias De Lange, Rahaf Aljundi, Marc Masana, Sarah Parisot, Xu Jia, Ales Leonardis, Gregory Slabaugh, and Tinne Tuytelaars. A continual learning survey: Defying forgetting in classification tasks, 2020.

Hao Li, Pratik Chaudhari, Hao Yang, Michael Lam, Avinash Ravichandran, Rahul Bhotika, and Stefano Soatto. Rethinking the hyperparameters for fine-tuning. In *International Conference on Learning Representations*, 2020. URL `https://openreview.net/forum?id=B1g8VkHFPH`.

L. Li, K. Jamieson, G. DeSalvo, A. Rostamizadeh, and A. Talwalkar. Hyperband: Bandit-based configuration evaluation for hyperparameter optimization. In OpenReview.net (ed.), *Proceedings of the International Conference on Learning Representations (ICLR'17)*, 2017.

M. Lindauer, K. Eggensperger, M. Feurer, S. Falkner, A. Biedenkapp, and Hutter F. Smac v3: Algorithm configuration in python. `https://github.com/automl/SMAC3`, 2017.

Luke Metz, Niru Maheswaranathan, Ruoxi Sun, C. Daniel Freeman, Ben Poole, and Jascha Sohl-Dickstein. Using a thousand optimization tasks to learn hyperparameter search strategies, 2020.

Kevin Musgrave, Serge Belongie, and Ser-Nam Lim. A metric learning reality check. *arXiv preprint arXiv:2003.08505*, 2020.

Valerio Perrone, Rodolphe Jenatton, Matthias W Seeger, and Cédric Archambeau. Scalable hyperparameter transfer learning. In *Advances in Neural Information Processing Systems*, pp. 6845–6855, 2018.

C. Rasmussen and C. Williams. *Gaussian Processes for Machine Learning*. The MIT Press, 2006.

Roy Schwartz, Jesse Dodge, Noah A Smith, and Oren Etzioni. Green ai. *arXiv preprint arXiv:1907.10597*, 2019.

B. Shahriari, K. Swersky, Z. Wang, R. Adams, and N. de Freitas. Taking the human out of the loop: A review of Bayesian optimization. *Proceedings of the IEEE*, 104(1):148–175, 2016.

Alistair Shilton, Sunil Gupta, Santu Rana, and Svetha Venkatesh. Regret Bounds for Transfer Learning in Bayesian Optimisation. In Aarti Singh and Jerry Zhu (eds.), ., volume 54 of *Proceedings of Machine Learning Research*, pp. 307–315, Fort Lauderdale, FL, USA, 20–22 Apr 2017. PMLR. URL `http://proceedings.mlr.press/v54/shilton17a.html`.

J. Snoek, H. Larochelle, and R. P. Adams. Practical Bayesian optimization of machine learning algorithms. In P. Bartlett, F. Pereira, C. Burges, L. Bottou, and K. Weinberger (eds.), *Proceedings of the 26th International Conference on Advances in Neural Information Processing Systems (NIPS'12)*, pp. 2960–2968, 2012.

Emma Strubell, Ananya Ganesh, and Andrew McCallum. Energy and policy considerations for deep learning in NLP. In *Proceedings of the 57th Annual Meeting of the Association for Computational Linguistics*, pp. 3645–3650, Florence, Italy, July 2019. Association for Computational Linguistics. doi: 10.18653/v1/P19-1355. URL `https://www.aclweb.org/anthology/P19-1355`.

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

Sebastian Thrun and Tom M. Mitchell. Lifelong robot learning. *Robotics and Autonomous Systems*, 15(1):25 – 46, 1995. ISSN 0921-8890. doi: https://doi.org/10.1016/0921-8890(95)00004-Y. URL `http://www.sciencedirect.com/science/article/pii/092188909500004Y`. The Biology and Technology of Intelligent Autonomous Agents.

Joaquin Vanschoren. Meta-learning: A survey. *arXiv preprint arXiv:1810.03548*, 2018.

Zi Wang, Beomjoon Kim, and Leslie Pack Kaelbling. Regret bounds for meta bayesian optimization with an unknown gaussian process prior. In S. Bengio, H. Wallach, H. Larochelle, K. Grauman, N. Cesa-Bianchi, and R. Garnett (eds.), *Advances in Neural Information Processing Systems 31*, pp. 10477–10488. Curran Associates, Inc., 2018.

Florian Westphal, Niklas Lavesson, and Håkan Grahn. A case for guided machine learning. In Andreas Holzinger, Peter Kieseberg, A Min Tjoa, and Edgar Weippl (eds.), *Machine Learning and Knowledge Extraction*, pp. 353–361, Cham, 2019. Springer International Publishing. ISBN 978-3-030-29726-8.

Martin Wistuba, Nicolas Schilling, and Lars Schmidt-Thieme. Scalable gaussian process-based transfer surrogates for hyperparameter optimization. *Machine Learning*, 107(1):43–78, 2018.

Yuxin Wu and Kaiming He. Group normalization. In *Proceedings of the European conference on computer vision (ECCV)*, pp. 3–19, 2018.

Fuzhen Zhuang, Zhiyuan Qi, Keyu Duan, Dongbo Xi, Yongchun Zhu, Hengshu Zhu, Hui Xiong, and Qing He. A comprehensive survey on transfer learning. *arXiv preprint arXiv:1911.02685*, 2019.

A BENCHMARK SUITE DETAILS

A.1 OVERVIEW

Table 3: Benchmarks overview

Benchmark	#Hyperparameters Old	#Hyperparameters New	#Tasks	Metric
FCN-A	6	5	4	MSE
FCN-B	6	8	4	MSE
NAS-A	6	6	3	Accuracy
NAS-B	3	6	3	Accuracy
XGB-A	5	9	10	AUC
XGB-B	6	6	10	AUC
SVM-A	2	2	10	AUC
SVM-B	2	2	10	AUC

A.2 FCN-A & FCN-B

Base benchmark We use code and data from (Klein & Hutter, 2019). We use the tasks HPO-Bench-Protein, HPO-Bench-Slice, HPO-Bench-Naval, and HPO-Bench-Parkinson.

Budget For FCN-A the budget is set to 100. For FCN-B, additional to the changes in the search space (Table 6), the budget is increased from 50 to 100 epochs.

Table 4: Values for integer coded hyperparameters in FCN benchmarks

Hyperparameter	Values
# Units Layer $\{1, 2\}$	(16, 32, 64, 128, 256, 512)
Dropout Layer $\{1, 2\}$	(0.0, 0.3, 0.6)
Initial Learning Rate	(0.0005, 0.001, 0.005, 0.01, 0.05, 0.1)
Batch Size	(8, 16, 32, 64)

Table 5: Search spaces in FCN-A. Numerical hyperparameters are encoded as integers, see Table 4 for specific values for these hyperparameters.

Steps	Hyperparameter	Range/Value	Prior
1	# Units Layer 1	1	-
1	# Units Layer 2	1	-
1	Batch Size	$\{0, \ldots, 3\}$	Uniform
1, 2	Dropout Layer 1	$\{0, \ldots, 2\}$	Uniform
1, 2	Dropout Layer 2	$\{0, \ldots, 2\}$	Uniform
1, 2	Activation Layer 1	{ReLu, tanh}	Uniform
1, 2	Activation Layer 2	{ReLu, tanh}	Uniform
1, 2	Initial Learning Rate	$\{0, \ldots, 5\}$	Uniform
1, 2	Learning Rate Schedule	Constant	Uniform
2	# Units Layer 1	5	-
2	# Units Layer 2	5	-
2	Batch Size	1	-

Table 6: Search spaces in FCN-B. Numerical hyperparameters are encoded as integers, see Table 4 for specific values for these hyperparameters.

Steps	Hyperparameter	Range/Value	Prior
1	Activation Layer 1	tanh	-
1	Activation Layer 2	tanh	-
1	Learning Rate Schedule	Constant	-
1, 2	# Units Layer 1	$\{0, \ldots, 5\}$	Uniform
1, 2	# Units Layer 2	$\{0, \ldots, 5\}$	Uniform
1, 2	Dropout Layer 1	$\{0, \ldots, 2\}$	Uniform
1, 2	Dropout Layer 2	$\{0, \ldots, 2\}$	Uniform
1, 2	Initial Learning Rate	$\{0, \ldots, 5\}$	Uniform
1, 2	Batch Size	$\{0, \ldots, 3\}$	Uniform
2	Activation Layer 1	{ReLu, tanh}	Uniform
2	Activation Layer 2	{ReLu, tanh}	Uniform
2	Learning Rate Schedule	Cosine	-

A.3 NAS-A & NAS-B

Base benchmark We use code and data from (Dong & Yang, 2019). We use the tasks CIFAR10, CIFAR100, and ImageNet.

Table 7: Search spaces in NAS-A.

Steps	Hyperparameter	Range/Value	Prior
1, 2	$0 \to 2$	{ none, skip-connect, conv1x1, conv3x3, avg-pool3x3 }	Uniform
1, 2	$0 \to 3$	{ none, skip-connect, conv1x1, conv3x3, avg-pool3x3 }	Uniform
1, 2	$2 \to 3$	{ none, skip-connect, conv1x1, conv3x3, avg-pool3x3 }	Uniform
2	$0 \to 1$	{ none, skip-connect, conv1x1, conv3x3, avg-pool3x3 }	Uniform
2	$1 \to 2$	{ none, skip-connect, conv1x1, conv3x3, avg-pool3x3 }	Uniform
2	$1 \to 3$	{ none, skip-connect, conv1x1, conv3x3, avg-pool3x3 }	Uniform

Table 8: Search spaces in NAS-B.

Steps	Hyperparameter	Range/Value	Prior
1	$0 \to 1$	{ none, skip-connect, conv1x1, conv3x3 }	Uniform
1	$0 \to 2$	{ none, skip-connect, conv1x1, conv3x3 }	Uniform
1	$0 \to 3$	{ none, skip-connect, conv1x1, conv3x3 }	Uniform
1	$1 \to 2$	{ none, skip-connect, conv1x1, conv3x3 }	Uniform
1	$1 \to 3$	{ none, skip-connect, conv1x1, conv3x3 }	Uniform
1	$2 \to 3$	{ none, skip-connect, conv1x1, conv3x3 }	Uniform
2	$0 \to 1$	{ none, skip-connect, conv1x1, conv3x3, avg-pool3x3 }	Uniform
2	$0 \to 2$	{ none, skip-connect, conv1x1, conv3x3, avg-pool3x3 }	Uniform
2	$0 \to 3$	{ none, skip-connect, conv1x1, conv3x3, avg-pool3x3 }	Uniform
2	$1 \to 2$	{ none, skip-connect, conv1x1, conv3x3, avg-pool3x3 }	Uniform
2	$1 \to 3$	{ none, skip-connect, conv1x1, conv3x3, avg-pool3x3 }	Uniform
2	$2 \to 3$	{ none, skip-connect, conv1x1, conv3x3, avg-pool3x3 }	Uniform

A.4 SVM-A & SVM-B

Base benchmark We use an open source implementation by the HPOlib authors following Perrone et al. (2018). This implementation uses data from Kühn et al. (2018) and employs a random forest as a

surrogate model (Eggensperger et al., 2014). For our benchmarks, we randomly selected the ten tasks monks-problems-2, tic-tac-toe, kc2, monks-problems-1, qsar-biodeg, nomao, pc3, bank-marketing, ada-agnostic, and hill-valley.

Table 9: Search spaces in SVM-A.

Steps	Hyperparameter	Range/Value	Prior
1	Kernel	Radial	-
1	Degree	$\{2, \ldots, 5\}$	Uniform
1, 2	Cost	$[2^{-10}, 2^{10}]$	Log-uniform
2	Kernel	Polynomial	-
2	γ	$[2^{-5}, 2^{5}]$	Log-uniform

Table 10: Search spaces in SVM-B.

Steps	Hyperparameter	Range/Value	Prior
1	Cost	$[2^{-5}, 2^{5}]$	Log-uniform
1, 2	γ	1	-
1, 2	Degree	5	-
1, 2	Kernel	{Polynomial, Linear, Radial}	Uniform
2	Cost	$[2^{-10}, 2^{10}]$	Log-uniform

A.5 XGB-A & XGB-B

Base benchmark We use an open source implementation by the HPOlib authors following Perrone et al. (2018). This implementation uses data from Kühn et al. (2018) and employs a random forest as a surrogate model (Eggensperger et al., 2014). For our benchmarks, we randomly selected the ten tasks monks-problems-2, tic-tac-toe, kc2, monks-problems-1, qsar-biodeg, nomao, pc3, bank-marketing, ada-agnostic, hill-valley

Table 11: Search spaces in XGB-A

Steps	Hyperparameter	Range/Value	Prior
1	Colsample-by-tree	1	-
1	Colsample-by-level	1	-
1	Minimum child weight	1	-
1	Maximum depth	6	-
1, 2	Booster	Tree	-
1, 2	# Rounds	$\{1, \ldots, 5,000\}$	Uniform
1, 2	Subsample	$[0, 1]$	Uniform
1, 2	Eta	$[2^{-10}, 2^{0}]$	Log-uniform
1, 2	Lambda	$[2^{-10}, 2^{10}]$	Log-uniform
1, 2	Alpha	$[2^{-10}, 2^{10}]$	Log-uniform
2	Colsample-by-tree	$[0, 1]$	Uniform
2	Colsample-by-level	$[0, 1]$	Uniform
2	Minimum child weight	$[2^{0}, 2^{7}]$	Log-uniform
2	Maximum depth	$\{1, \ldots, 15\}$	Uniform

Table 12: Search spaces in XGB-B

Steps	Hyperparameter	Range/Value	Prior
1	Colsample-by-tree	1	-
1	Colsample-by-level	1	-
1	Minimum child weight	1	-
1	Maximum depth	6	-
1, 2	Booster	{ Linear, Tree }	-
1, 2	# Rounds	$\{1, \ldots, 5,000\}$	Uniform
1, 2	Subsample	$[0, 1]$	Uniform
1, 2	Eta	$[2^{-10}, 2^{0}]$	Log-uniform
1, 2	Lambda	$[2^{-10}, 2^{10}]$	Log-uniform
1, 2	Alpha	$[2^{-10}, 2^{10}]$	Log-uniform
2	Colsample-by-tree	1	-
2	Colsample-by-level	0.5	-
2	Minimum child weight	10	-
2	Maximum depth	10	-

B DETAILED SPEEDUPS

B.1 TRANSFER GP AND BEST-FIRST VS. GP

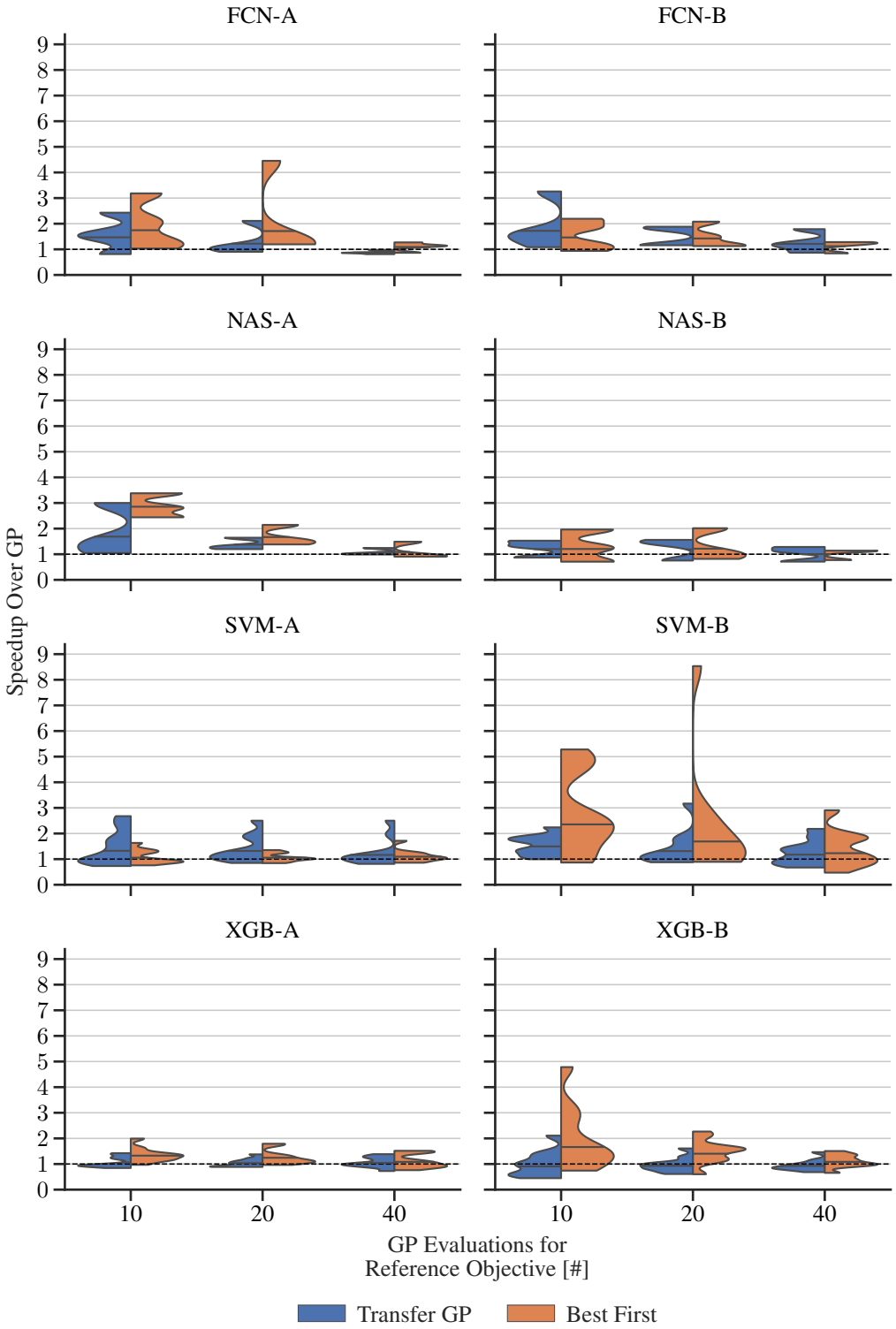


Figure 6: Speedup of transfer GP and best-first over GP across tasks for each of 8 benchmarks. The previous HPO has a budget of 10 evaluations here.

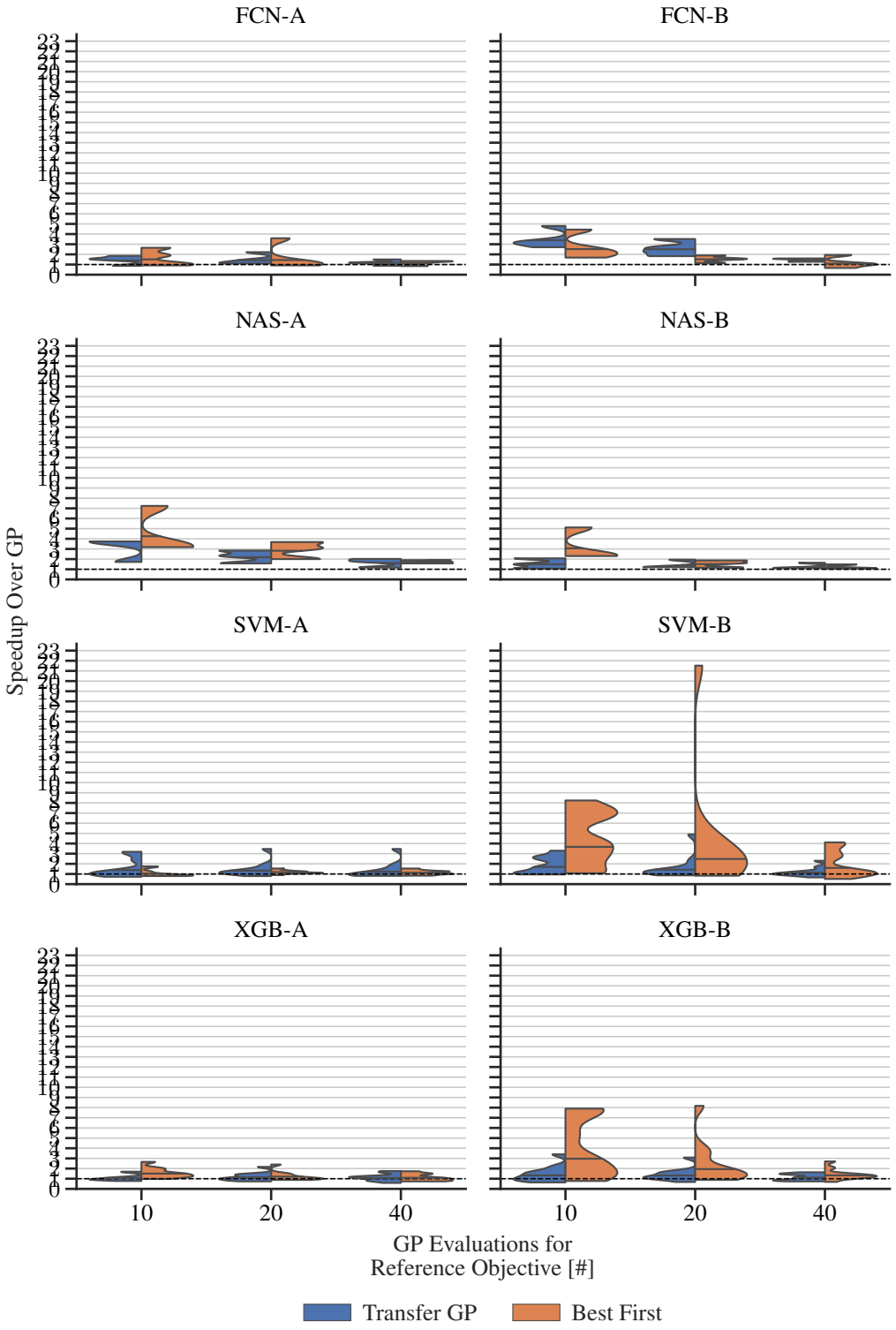


Figure 7: Speedup of transfer GP and best-first over GP across tasks for each of 8 benchmarks. The previous HPO has a budget of 20 evaluations.

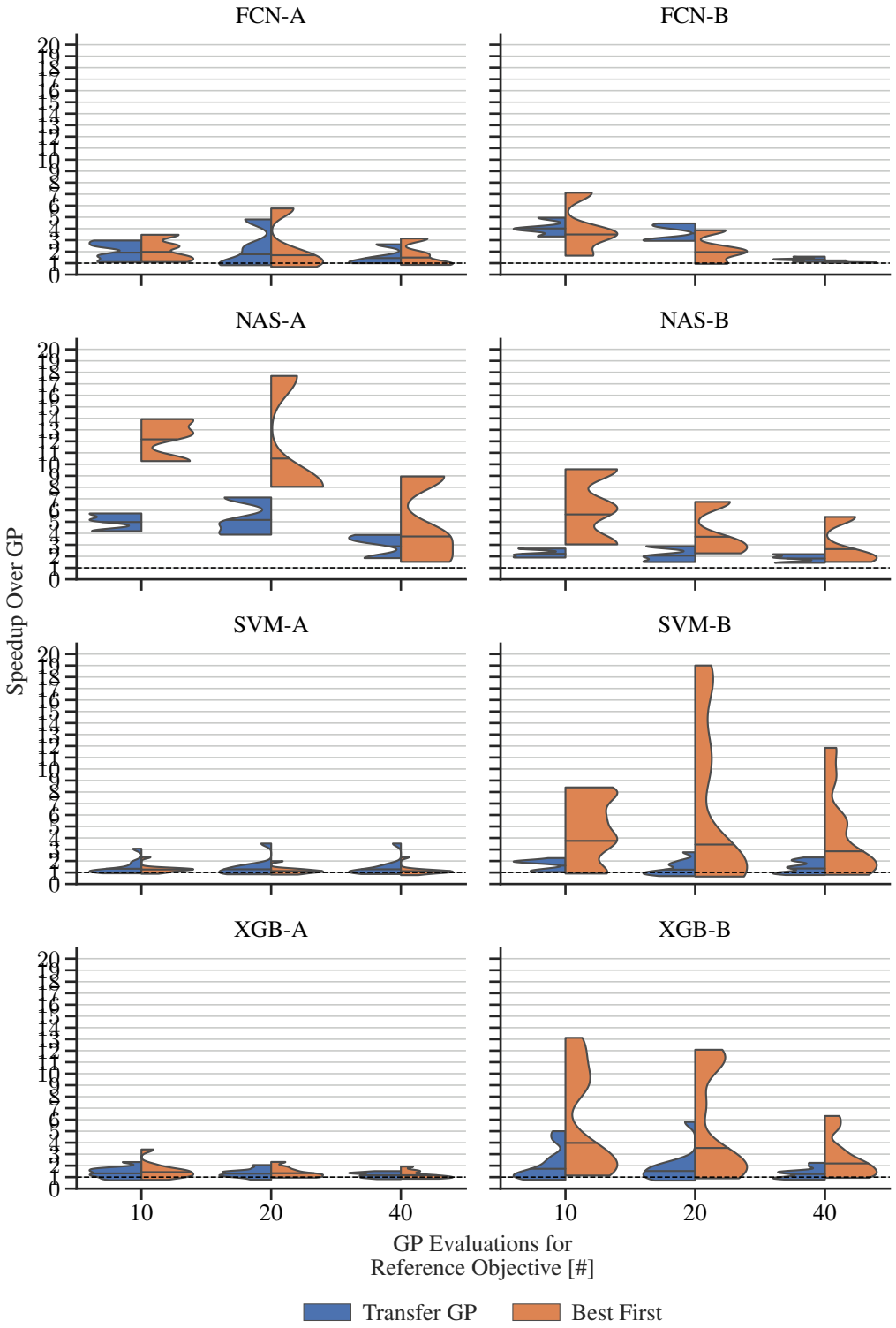


Figure 8: Speedup of transfer GP and best-first over GP across tasks for each of 8 benchmarks. The previous HPO has a budget of 40 evaluations.

B.2 BEST-FIRST AND COMBINED TRANSFER GP WITH BEST-FIRST VS. GP

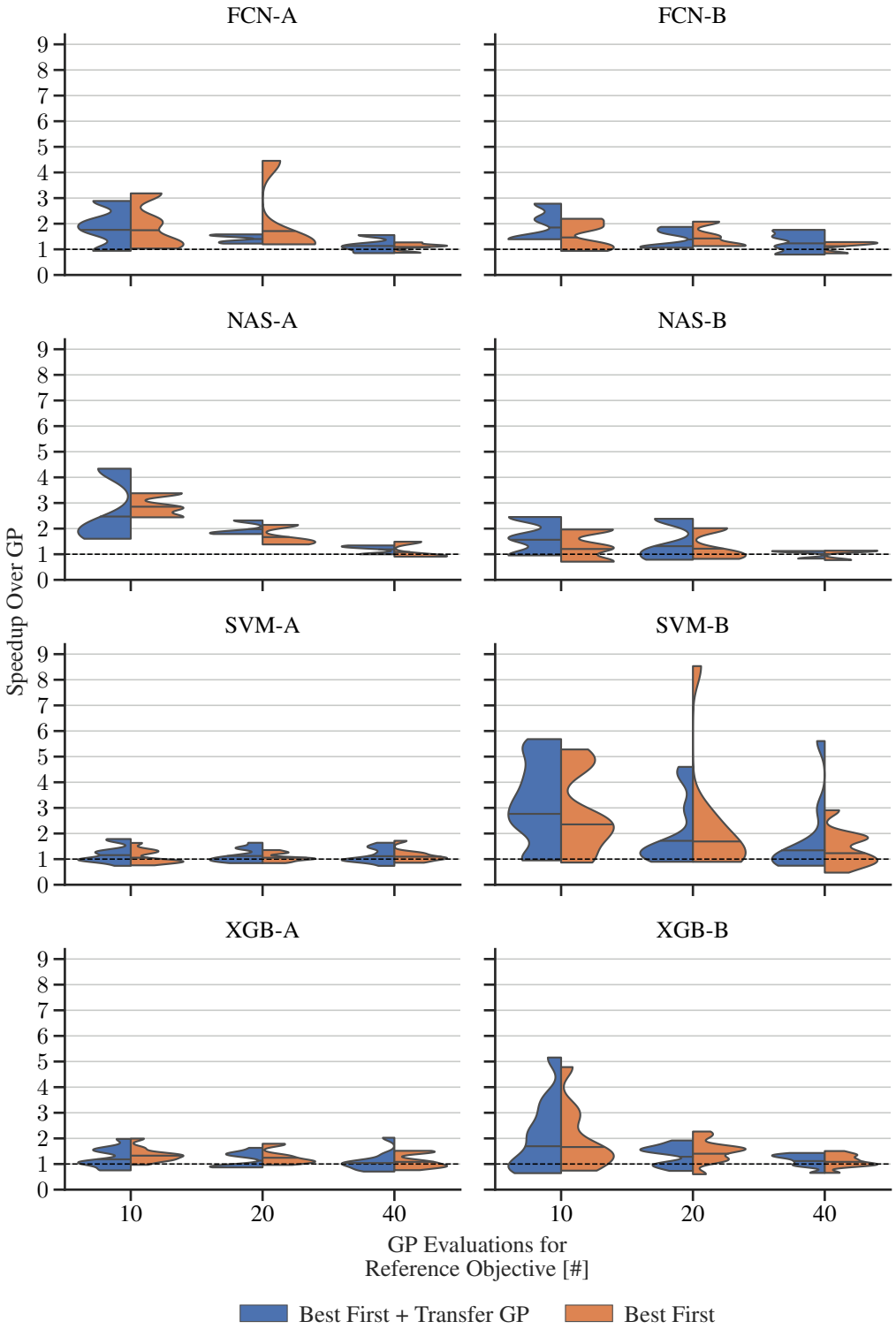


Figure 9: Speedup of transfer GP and best-first over GP across tasks for each of 8 benchmarks. The previous HPO has a budget of 10 evaluations here.

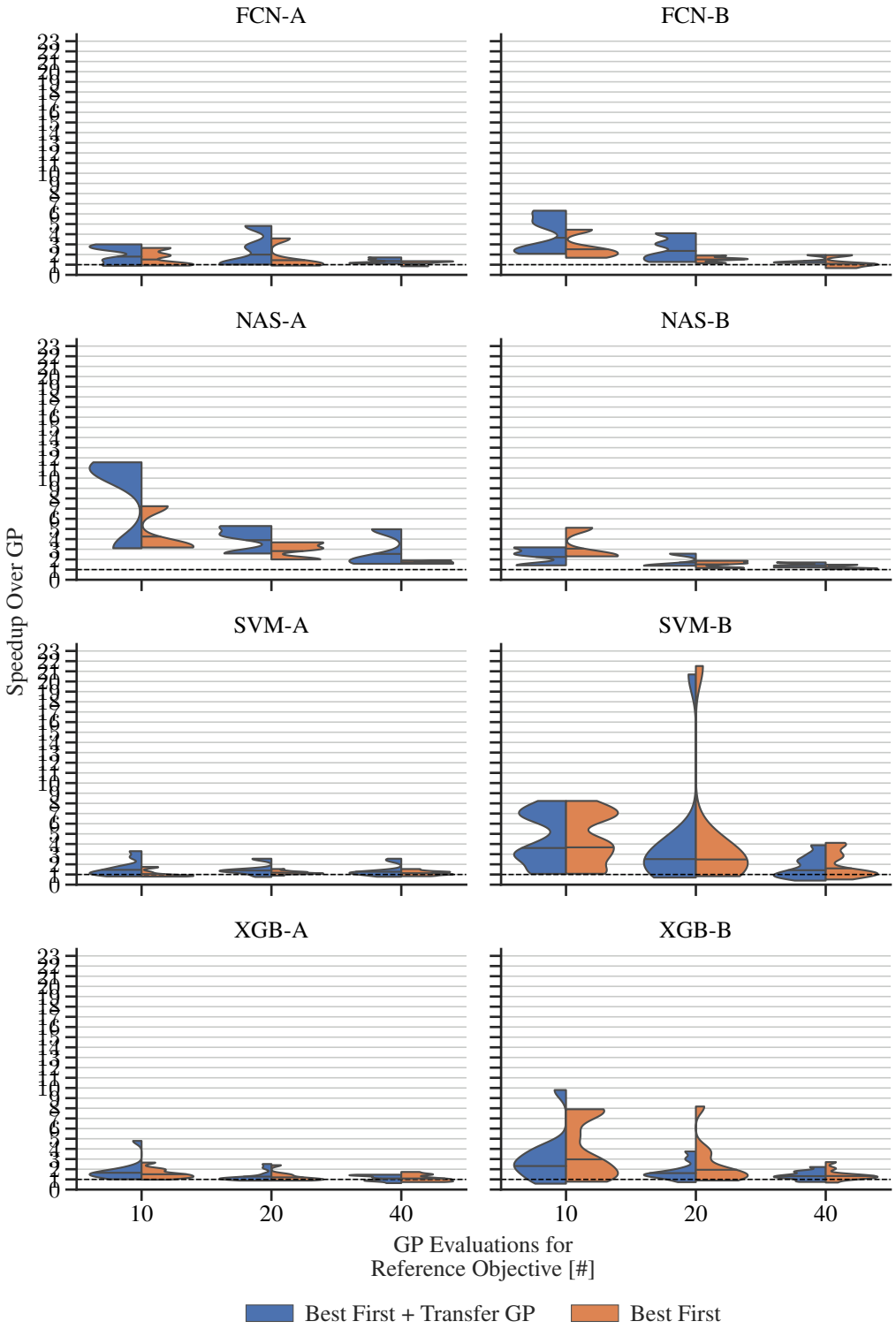


Figure 10: Speedup of transfer GP and best-first over GP across tasks for each of 8 benchmarks. The previous HPO has a budget of 20 evaluations.

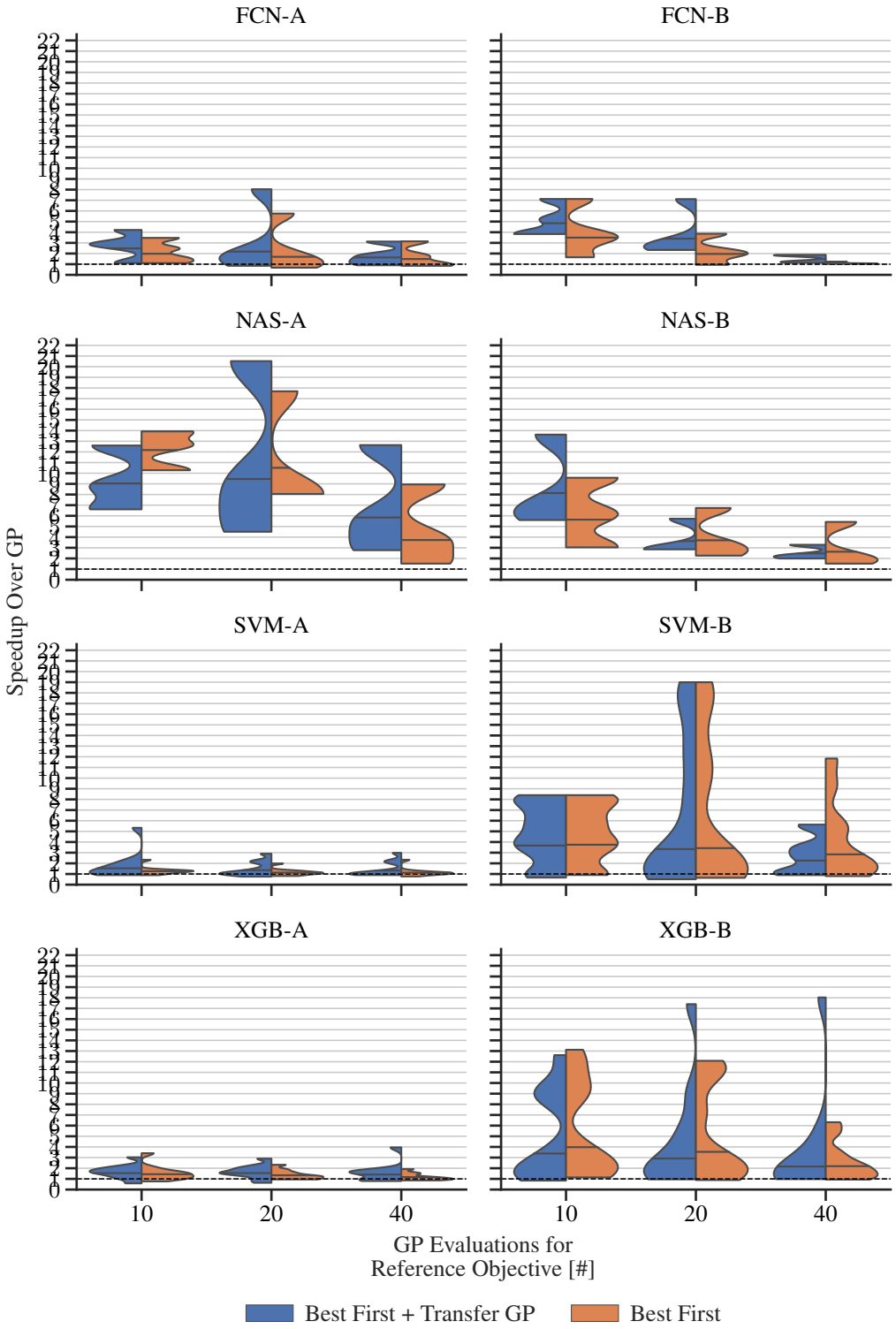


Figure 11: Speedup of transfer GP and best-first over GP across tasks for each of 8 benchmarks. The previous HPO has a budget of 40 evaluations.

C FAILURE RATES

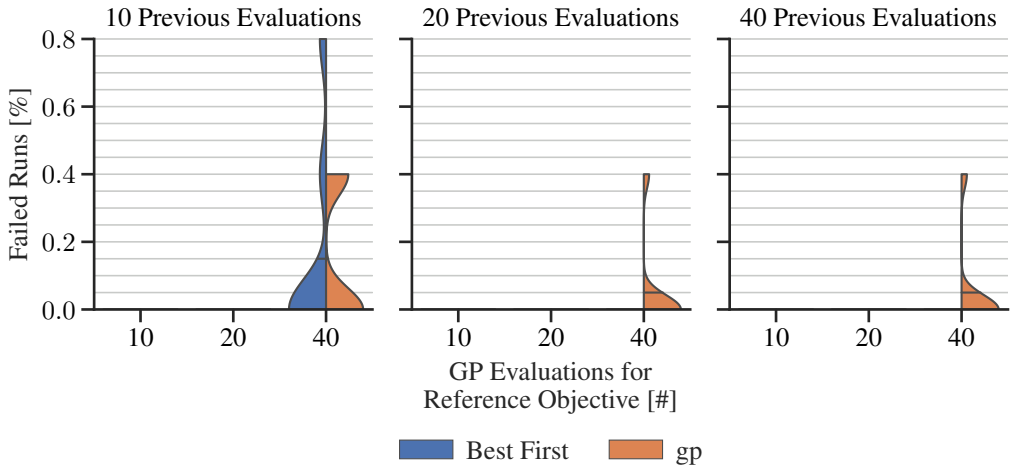


Figure 12: Failure rates for best-first and GP across 8 benchmarks. The violins estimate densities of the task means. The horizontal line in each violin shows the mean across these task means. The plots from left to right utilize increasing budget for the pre-adjustment hyperparameter. The x-axis shows the budget for the GP reference.

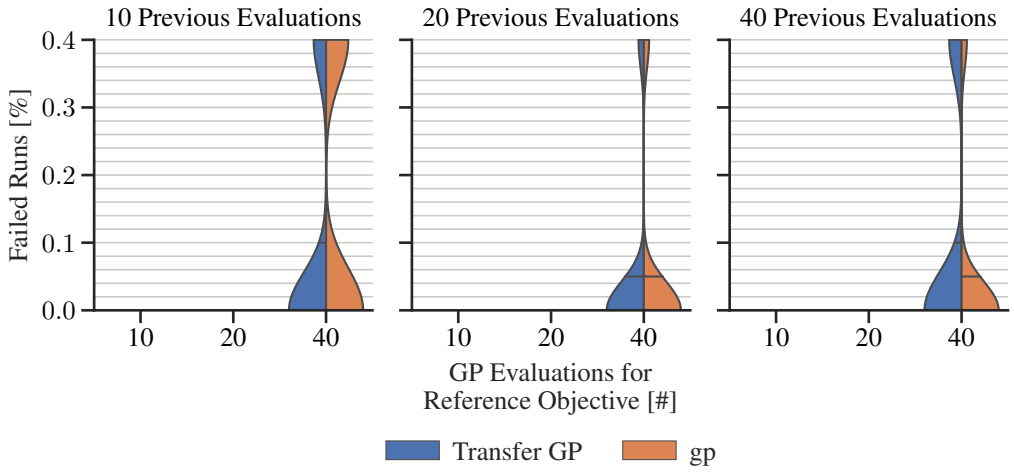


Figure 13: Failure rates for transfer GP and GP across 8 benchmarks. The violins estimate densities of task means. The horizontal line in each violin shows the mean across these task means. #Evaluations for the old HPO increases from left to right. The x-axis shows the budget for the GP reference.

D OBJECTIVE IMPROVEMENTS

For the improvement plots, we show the difference of means normalized with respect to the standard deviation of the control algorithm. This metric is known as glass delta. As some benchmarks had a standard deviation of 0, we added a small constant in those cases. We chose this constant according to the 0.2-quantile of the observed values. For the plots we clip the improvement to $[-100, \infty)$, as for some plots there are extreme outliers.

D.1 TRANSFER GP AND BEST FIRST VS. GP

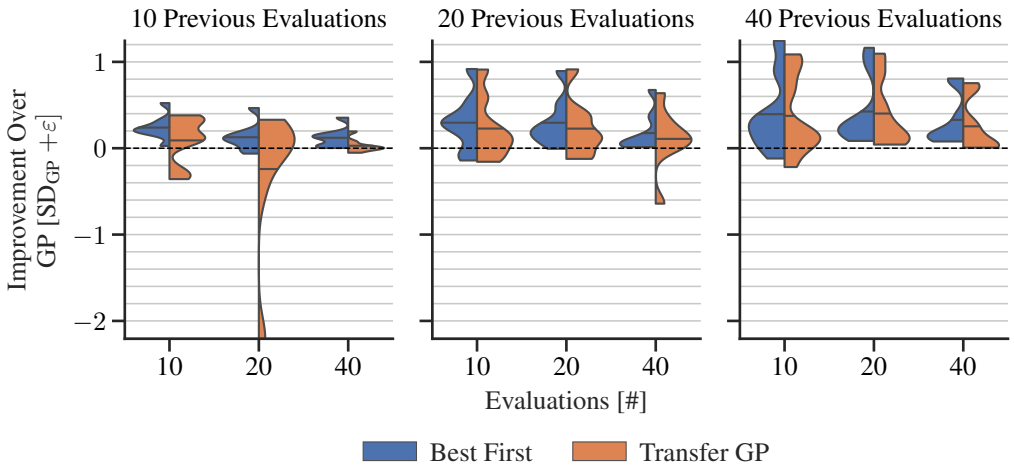


Figure 14: Standardized objective improvements of Transfer GP and best-first over GP across 8 benchmarks. The violins estimate densities of the benchmark means. The horizontal line in each violin shows the mean across these benchmark means. #Evaluations for the old HPO increases from left to right. In each plot, the evaluation budget increases.

D.2 TRANSFER GP COMBINED WITH BEST FIRST AND BEST FIRST VS. GP

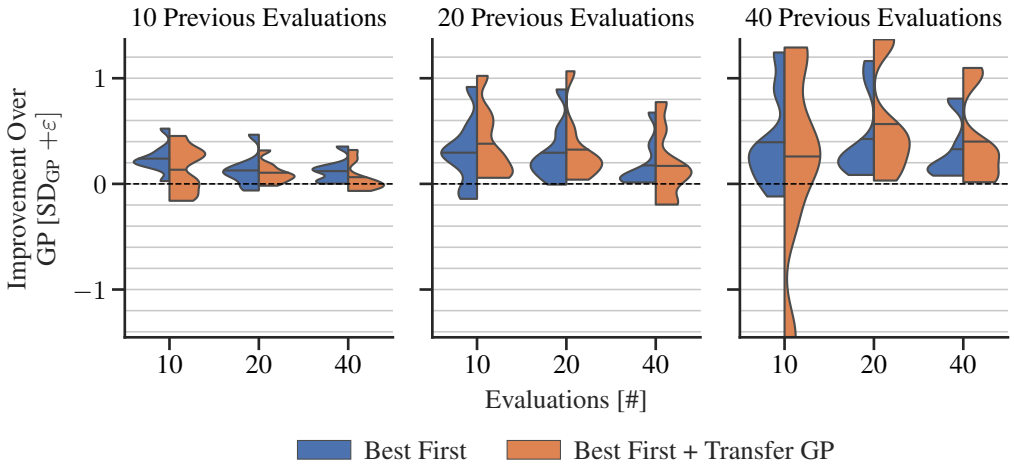


Figure 15: Standardized objective improvements of Transfer GP combined with best-first, and best-first over GP across 8 benchmarks. The violins estimate densities of the benchmark means. The horizontal line in each violin shows the mean across these benchmark means. #Evaluations for the old HPO increases from left to right. In each plot, the evaluation budget increases.

D.3 Only Optimize New and Drop Unimportant vs. GP

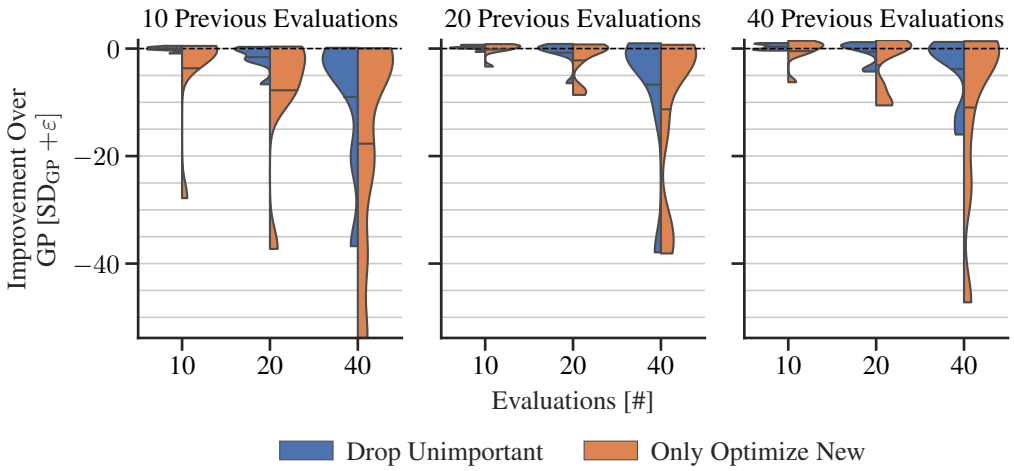


Figure 16: Standardized objective improvements of only-optimize-new and drop-unimportant over GP across 8 benchmarks. The violins estimate densities of the benchmark means. The horizontal line in each violin shows the mean across these benchmark means. #Evaluations for the old HPO increases from left to right. In each plot, the evaluation budget increases.

E Control Study: GP for Different Random Seed Ranges

As a sanity check, and to gauge the influence of random seeds, we compare GP to itself with different random seed ranges (GP_1 and GP_2). We observe little differences in GP_1 and GP_2 compared to the differences between GP and the transfer approaches (Figure 17).

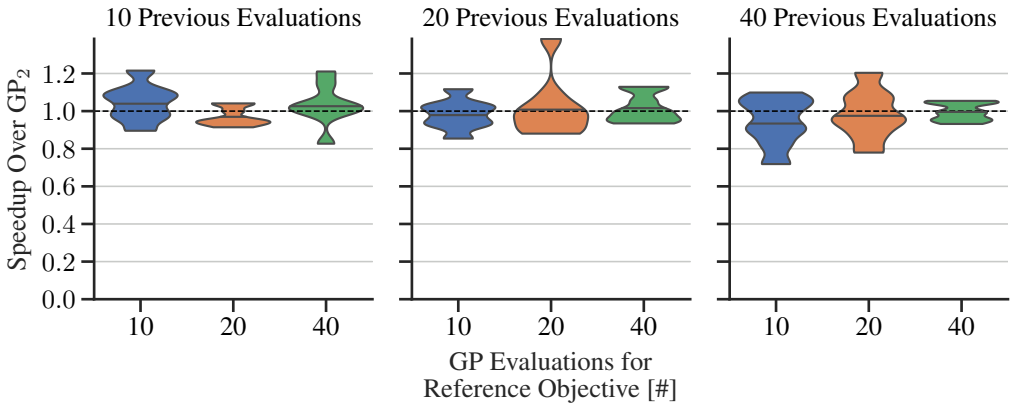


Figure 17: Speedup of GP_1 over GP_2 across 8 benchmarks. The violins estimate densities of the benchmark geometric means. The horizontal line in each violin shows the geometric mean across these benchmark means. #Evaluations for the old HPO increases from left to right. The x-axis shows the budget for the GP reference.

F Control Study: Reliability of GP

As a sanity check for the reliability of GP, we compare GP to random search in Figure 18, and to TPE (Bergstra et al., 2011) in Figure 19. We use the GP implementation and hyperparameter settings from Falkner et al. (2018).

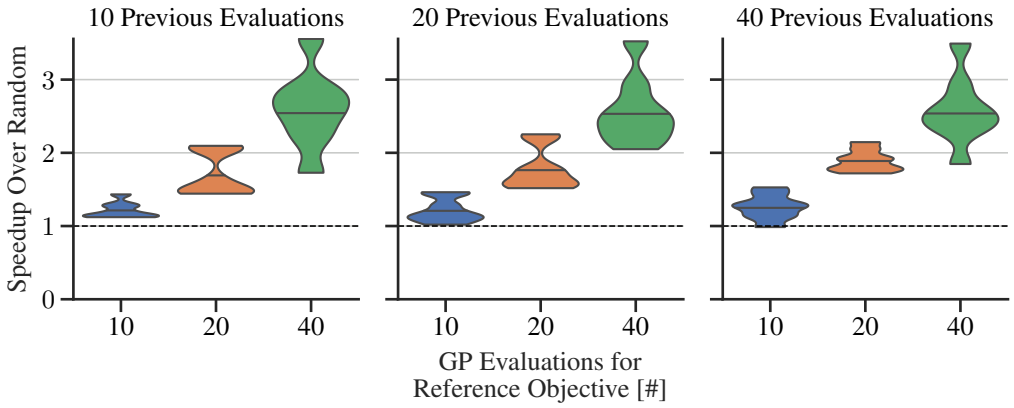


Figure 18: Speedup of GP over random search across 8 benchmarks. The violins estimate densities of the benchmark means. The horizontal line in each violin shows the geometric mean across these benchmark means. #Evaluations for the old HPO increases from left to right. The x-axis shows the budget for the GP reference.

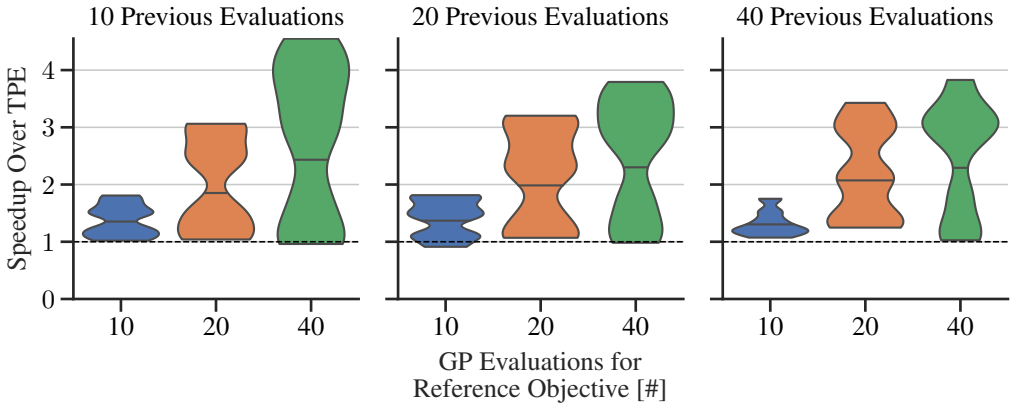


Figure 19: Speedup of GP over TPE across 8 benchmarks. The violins estimate densities of the benchmark means. The horizontal line in each violin shows the geometric mean across these benchmark means. #Evaluations for the old HPO increases from left to right. The x-axis shows the budget for the GP reference.