Task Selection for AutoML System Evaluation

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Abstract Our goal is to assess if AutoML system changes - i.e., to the search space or hyperparameter optimization - will improve the final model’s performance on production tasks. However, we cannot test the changes on production tasks. Instead, we only have access to limited descriptors about tasks that our AutoML system previously executed, like the number of data points or features. We also have a set of development tasks to test changes, ex., sampled from OpenML with no usage constraints. However, the development and production task distributions are different leading us to pursue changes that only improve development and not production. This paper proposes a method to leverage descriptor information about AutoML production tasks to select a filtered subset of the most relevant development tasks. Empirical studies show that our filtering strategy improves the ability to assess AutoML system changes on holdout tasks with different distributions than development.

1 Introduction

Successful deployment of machine learning models requires many design choices, often requiring expertise. Automatic Machine Learning (AutoML) systems mechanize this process. A typical AutoML system consists of many components, including feature engineering, model selection & optimization [1–3], and hyperparameter optimization [4–7].

Providers usually deploy an AutoML system as a service, which they want to improve by rolling out changes and assessing system performance. Due to providers limited visibility into production tasks (abbreviated prod.) supplied by actual clients, it is impossible to run system experiments on these tasks. Instead, providers have a set of opensourced development tasks (abbreviated dev.) [8–16] which can be used to assess system changes.

However, the distribution of the dev. tasks may be wildly different from the received prod. tasks – see (App.)endix Fig. 1 and 2. Fig. 1 displays the distribution of selected model types for a set of prod. and dev. tasks, showing a significant difference, which could – for example – lead us to pursue DNN improvements when a random forest is used most often in prod. Therefore, testing the impact of a change on real users is a non-trivial task unaddressed by existing papers on benchmarking [1–3, 17–19]. Our contributions in this paper include:

1. Proposing a framework to select a filtered subset of dev. tasks so the performance delta – on a change to our AutoML system – is similar between filtered and prod. tasks.
2. Proposing task selection methods and comparing their trade-offs in large-scale experiments.
3. Showing specific examples of methods which improve our ability to accurately assess AutoML system changes when we have task distribution shift, as in production setups.
2 Background and Key Concepts

Notations used in the paper are summarized in Appendix Table 1.

The Production AutoML System: The key components of our AutoML system include the search space, hyperparameter optimizer, and how we assess performance. The AutoML system is a service used on varied machine learning tasks for commercial applications, supporting multi-modal datasets with image, natural language text, and tabular data. Specific details are in App. Sec. C.1, summarized here: We use a conditional search space, with a root parameter for the algorithm choice (Fig. 1) and sub-parameters conditioned on the root choice. A wide range of hyperparameters are tuned, including optimizer, model choice, regularization, and feature engineering. Vizier [20] is our hyperparameter optimizer, supporting user-specified parameters controlling the HPO.

Changes to the AutoML System: AutoML service providers constantly make changes to the AutoML system in order to improve performance. By change, we mean moving from an AutoML system with a baseline setup to a modified setup. Generally, we can view each setup as an arbitrary AutoML system; thus, the change can encode almost any reasonable system modification. System changes can be partitioned into those affecting the AutoML system/search space, and those for the hyperparameter optimizer. We look at both in our experiments in Sec. 4.1.

Tasks: AutoML service providers receive a stream of tasks from their end-users. Here, a task is a dataset and a problem statement specifying what is to be solved and the relevant metric. For example, stating that we have a binary classification problem for some specified label, and the goal is maximizing AUC. Our systems run on two sets of tasks: Development tasks (dev.) are gathered from various open-source repositories (such as OpenML [8]), have no restrictions and thus can be easily used to evaluate our service. The second set is Production tasks (prod.), which are those received by our service from a client and can only be run for the exact client-specified purpose. This setup has parallels with meta-learning (ex., task splits), but with additional issues and information/constraints available for providers.

Unique Production Issues for AutoML Service Providers: AutoML service providers have limited visibility into the uses of the ML system in product applications. This could, for example, be to comply with privacy regulations and the terms of service. Similarly, providers may not want to risk evaluating experiments on model changes in live production environments. These constraints force providers to assess system performance on dev. tasks.

System descriptors: AutoML service providers often have access to common descriptors about the executed tasks. These include task descriptors, containing info about only the task, such as the number of data points or number/modality of features. Alternatively, system descriptors contain info about both the task and our AutoML system. For example, the performance (ex., accuracy) of a model on a task with some hyperparameter values.
Figure 3: Left: How a filter is used to select relevant filtered, development tasks (given production task descriptors), which are evaluated on a system change for yes/no deployment decisions. Right: The filter is tuned for effective deployment decisions, but we cannot evaluate changes on production – see Sec. 2 – so we select holdout tasks with no constraints to use as a proxy.

3 Problem Setup

We propose a method allowing us to better assess AutoML system changes in prod. tasks by using their task descriptor to select relevant dev. tasks. More formally, we assume that when making a roll-out decision on a change, the service provider has descriptors for: (a) dev. tasks on the baseline setup. (b) prod. tasks on the baseline setup. (c) dev. tasks on the modified setup.

Assessing AutoML system changes then boils down to the following steps – see Fig. 3, left. (1) Filtering a subset of dev. tasks that more closely match prod. tasks. (2) Assessing the change on the filtered subset of dev. tasks. (3) Roll out the change to production if the modified setup improves over the baseline setup on the filtered subset of dev. tasks. In this paper, we propose a framework to design filters to perform step 1 of the above.

Since we are limited in using prod. tasks for the purpose of this paper, we divide the dev. tasks into two sets as a proxy. From here on, train tasks represent the role of dev. tasks and holdout tasks are a proxy for prod. tasks. Fig. 3 illustrates this setup. In App. Sec. D we describe a method to assess if a change to our AutoML system improves performance across a distribution of tasks by first measuring improvement on each task, then aggregating improvement measures across tasks.

3.1 Filtering Tasks

The first step to assessing AutoML system changes is filtering dev. tasks that closely match the holdout tasks (a proxy for prod. tasks). Our filtering problem uses descriptor info from holdout tasks to select a filtered subset of the dev. tasks. This section presents different filtration strategies and then shows a method to evaluate the strategies.

3.1.1 Similarity Filters. First, we design filters for a single holdout task, which we later aggregate into filters for multiple tasks. Intuitively, similarity filter methods take a way to measure the similarity between training tasks and a holdout task – denoted a similarity metric – then returns the top \( n \) tasks. Alg. 1 shows a skeleton for the proposed similarity filter parameterized by the number of returned tasks (filter length) and the similarity metric. The returned item is a filter function taking train tasks and a holdout task, then returning a filtered subset of the train tasks.

**Algorithm 1** simFilter(length, simMetric)

1: def filter(trainTasks, holdoutTasks):
2:    sims = simMetric(trainTasks, holdoutTasks)
3:    mostSimTasks = argsort(sims)[:length]
4:    return trainTasks[mostSimTasks]
5: return filter  # Note - this returns a function
3.1.2 Similarity Metrics. Our similarities metrics use the different types of info available to AutoML service providers in our setup, including: (a) task descriptors, (b) system descriptors. We also describe a similarity forming a heuristic performance bound. Sec. 4.4 lists other metrics that could be considered, but we did not use.

Task descriptor similarity: For descriptors like the number of data points or features, we can reasonably rank train tasks in their euclidean distance from the holdout task, which we simply use as the similarity metric (Alg. 2).

Performance descriptor similarity: For descriptors like the performance on different hyperparameter values, we can not simply compute a euclidean distance to the holdout task as with task descriptors. Instead we propose to use the following intuition: similar tasks have nearby qualities for hyperparameter values. Instead of evaluating train tasks on hyperparameter configurations used for the holdout tasks on the baseline setup, we estimate train tasks performance with a surrogate model. Then the correlation between the predicted quality and the actual quality from the holdout tasks is used as the similarity. Specific details are in App. Sec. D.3.

Oracle Similarity: We would like a (relatively tight) upper bound on the possible performance of a similarity filter, to see how performant our filters are. Intuitively, we approximate this by constructing a filter using extra info about holdout tasks, which cannot be accessed via stored descriptors. Specifically, we re-run the holdout tasks with changes and simply compute correlations in task quality. See App. Sec. D.3 for more details. This strategy is only a heuristic a upper bound and cannot be used on actual prod. tasks, but proves useful in our experiments nonetheless.

3.1.3 Constructing Filters for Multiple Holdout Tasks: Our prior sections looked at filters with one holdout task. However, we want filters for multiple holdout tasks because we have multiple tasks in prod. A simple approach for transforming a single holdout task filter is taking the union of the filtered tasks over every holdout task. However, this does not control the number of filtered tasks and can include rarely selected train tasks. We apply a filter for each holdout task and have them vote on the selected tasks. Once the votes are collected, we return the top \( n \) tasks for a user-specified \( n \). App. Alg. 9 shows our voting method, and App. Sec. D.3.1 discusses design choices.

3.1.4 How to evaluate a filter with a loss. Now that we have a set of filters defined, we want to evaluate them. An ideal filter has the same result for changes on the filtered and holdout tasks. Hence, comparing the evaluation results with changes should inform us of filter strength. We show an example system change evaluating method in App. Alg. 4 (EvalSystemChange).

We propose a filter evaluation technique (EvalFilter) in Alg. 3 via a loss comparing system change results. EvalFilter inputs a change to evaluate, a set of training & holdout tasks, and a filter, then returns the scalar difference between the change’s loss on filtered and holdout tasks.

We measure the difference between the change’s loss on the filtered and holdout tasks with a log-loss because this is a common choice for comparing (log)probs – ex., as in logistic regression – and our change’s loss is a (log)probability. The log-loss is \( t \log(y) + (1 - t) \log(1 - y) \), where \( y, t \) are the probs. of improvement on the filtered and holdout tasks, respectively. Fig. 4 shows this loss with our oracle similarity and simple baselines, illustrating the range of values we should expect.

Algorithm 2 distanceSimMetric(trainTasks, holdoutTask)

1: featureDistances = empty list
2: for trainTask in trainTasks do
3: \( d = \text{distance}(\text{trainTask.descriptor}, \text{holdoutTask.descriptor}) \)
4: add \( d \) to featureDistances
5: trainTaskSimilarities = \( 1 / \text{featureDistances} \)
6: return trainTaskSimilarities

Algorithm 3 EvalFilter(filter, trainTasks, holdoutTasks, change=(baselineSetup, modifiedSetup))

1: filteredTasks = filter(trainTasks, holdoutTasks.descriptors)
2: \( y = \text{EvalSystemChange(filteredTasks, change)} \) \( \triangleright \) The filtered task improvement probability
3: \( t = \text{EvalSystemChange(holdoutTasks, change)} \) \( \triangleright \) The holdout task improvement probability
4: return \( \logLoss = t \log(y) + (1 - t) \log(1 - y) \) \( \triangleright \) Can clip \( y, t \) to prevent \( \infty \)
4 Experiments

First, we investigate the setup for our problem in Sec. 4.1. Next, we explore our filtering problem in Sec. 4.2, showing that our filters improve over standard approaches. App. Sec. E contains additional details for our experiments, including computational requirements.

4.1 Experimental Setup

To preface the filtering results in Sec. 4.2, we first provide our setup, including: (a) changes made to our AutoML system. (b) the train and holdout task partitions. In our experiments we focus on binary classification with AUC as the quality, and say a system has performed better – on a single run, for a single task – if the quality measured is higher.

**Changes made to the AutoML system for experiments:** We take a default setup and contrast with modified setups as in App. Alg. 4. Our default uses a full, conditional search space for a fixed wall-clock time budget. We use a diverse range of modifications – see App. Sec. E.2.1 – including setups to assess changes to: (1) search space, restricting to only a DNN. (2) hyperparameter optimizer by turning on transfer learning from [20]. (3) Vizier optimizer budget allowing 5× more wall-clock time for hyperparameter queries. (4) the entire AutoML system by changing the underlying library used to implement the different learning algorithms. App. Fig. 8 displays the quality distribution for setups on various tasks, showing changes affect model quality in varied ways. Some tasks have positively correlated qualities, while some are anti-correlated, showing a simple similarity metric used in App. Alg. 8.

**Training and holdout task selection for experiments:** Since we cannot use the prod. tasks for this paper, we divide the dev. tasks into two sets, train tasks and holdout tasks. We do this in two major ways for the results presented here: (a) The dev. tasks are assigned into either train or holdout at random, so the distribution of train and holdout tasks is similar. (b) The dev. tasks are partitioned into all OpenML tasks for train and all other tasks for holdout to simulate distribution shift. See App. Table 2 for more details on specific tasks.

4.2 Filtering Problem Results

First, we compare different filters in Sec. 4.2.3. Then, we use filters when holdout tasks are from a different distribution in Sec. 4.2.4, demonstrating our proposed filters improve our ability to assess AutoML system change performance effects on holdout tasks with realistic distribution shifts. We also include investigations of design choices including evaluating AutoML system changes (Sec. 4.2.1), filter strength (Sec. 4.2.2), and which changes filtration is useful for (Fig. 5).

**4.2.1 Investigating design choices for evaluating changes to AutoML Systems.** Alg. 4 evaluates our system changes and has arguments of the evaluation tasks and system change (from a baseline setup to a modified setup). App. Fig. 10 contrasts the improvement probability for different AutoML system changes and task sizes, showing how the improvement probability depends on the change.
Density

Improvement probability for holdout and randomly filtered tasks

Figure 5: We look at the distribution of evaluate change results on a baseline random filter – i.e., the improvement probability given the change. Left: The resulting distribution when restricting the system search space to DNN only, and we sample our train and holdout tasks the same distribution. We contrast this with other setups highlighted in red. Middle: The holdout tasks are sampled from a different distribution than train as specified in Section 4.1. Right: We vary the system change to increase the compute budget by 5x.

we make to our system. Some changes – like increasing the compute budget – almost always improve performance, showing an example where the selected task does not affect the result.

We also display different numbers of tasks, showing how Alg. 4 behaves as we vary the filter and holdout sizes, verifying we can compare improvements on the differently sized filter and holdout as in later experiments (ex., Fig. 6 or 7). App. Fig. 11 contrasts runs with a probability estimate using one or multiple task evaluations, showing that more evaluations allow us to assess the improvement probability better.

4.2.2 Investigating how we evaluate filters. We now wield our ability to evaluate a change’s loss in our AutoML system for evaluating filters. Alg. 3 computes a loss for a filter given a set of train tasks, holdout tasks, and a system change with the difference between losses on the filtered and holdout tasks (for the change). This loss depends on the number of filtered and holdout tasks, how the train and holdout tasks differ, and the system change. As such, we vary these in our experiments.

Fig. 5, left, evaluates the random task filter with the same train and holdout task distributions, showing the same results distributions with moderate variance. Here, filtering will only provide benefit if we have a limited number of tasks output by the filter.

Fig. 5, middle, evaluates the random task filter while varying the train and holdout task distributions, showing that random selection performs poorly under mismatch. Here, we can benefit from a better filtering approach than the baseline strategy of random.

Fig. 5, right, evaluates the random filter while varying the AutoML system change showing all filters perform equally well – with near 0 loss as in App. Fig. 13 – if a change always improves performance. Here, filtering will provide little to no benefit for any number of filtered tasks, because all tasks perform similarly.

App. Fig. 12 repeats these plots while varying the number of filtered and holdout tasks, showing we can compare the improvement probability distribution for differing task sizes.

4.2.3 Comparing filtering strategies on 1 holdout task. Fig. 6 shows that various filtration strategies offer improvements in filter loss over a random filter baseline, even as we vary the filter lengths, similarities, and system changes. When we select all tasks, then all filters perform equally. Here, performance descriptor similarity is the best feasible filter for non-maximal tasks sizes, which we hypothesis is due to using extra info about the system, and not just the task.

Also, App. Fig. 14, 15 and 16 show the best filtration will depend on the chosen system change by repeating this for more filtering strategies and system changes. Further, App. Fig. 16 verifies that most filter loss differences pass a significance test.

4.2.4 Comparing filtering strategies on multiple holdout tasks: We construct multi-holdout-task filters using single-holdout-task filters (App. Alg. 9). We are particularly interested in holdout tasks with a distribution shift as a proxy for production. Fig. 7 shows the absolute filter performance for various
Loss diff. from random baseline

Number of tasks selected by filter

Change = Default → DNN Only

Approximate Oracle Similarity Filter

Figure 6: We display the 5-sample mean loss differences between filter strategies and a random baseline.

Left: We show filter strategies in each color – see App. Fig. 14 for other system changes.

Right: We show the largest possible loss difference for system changes in each color with our heuristic upper bound – see App. Fig. 15 for other filters.

filters (each line), numbers of holdout tasks (left → right), and task distributions (top → bottom). Performance for all filters was similar at about 8 selected tasks, so we display at most 12. We use 30 total tasks allocating the remaining 18 to holdout.

In Fig. 7, top – where we sample the train and holdout tasks from the same distribution – we do not see a benefit from filtering. The maximal filter size – where all strategies are equal, and we use all tasks – performs best because using more tasks is better when distributions match.

Most importantly, in the bottom of Fig. 7 – where we sample the train and holdout tasks from different distributions – filtering improves our ability to assess AutoML system change’s affects on performance with larger holdout sizes. Notably, the best filters only uses 3 tasks, with the # data points then performance descriptor similarity.

4.3 Takeaways

We see clear performance boosts from the filtering strategies when we have a limited number of holdout tasks, or the holdout task distribution is different from training. As such, we have the following takeaways for practitioners:

1. If there are many prod. tasks, and the distribution differs from dev., filtering helps – Fig. 7, bottom. Task (with # datapoints) and performance descriptor similarity performed best.

2. Using filtering, we saw similar performance using only \( \approx 20\% \) of the tasks, providing a use-case for cheaper benchmarking with only \( \approx 20\% \) the cost even with no prod. distribution shift – Fig. 7.

3. The best filter will depend on the system changes we use – Sec. 4.2.3.

4.4 Future Directions

Our primary goal is showing our filtering paradigm allows us to create simple filters that can select valuable tasks for assessing AutoML system changes – not to construct complex filters. The next step is designing better filters because our simple baselines performed best. More complicated filters – like KNNs – could rank tasks using all available descriptor information. Alternatively, looking at more sophisticated metrics like problem complexity measures could be fruitful.

We also found that simple task similarity metrics performed best, but these encode minimal information about the task. Investigating why these simple metrics performed robustly is interesting for future work. Also, we explored a range of changes to the system, hoping our results apply to other AutoML systems, but this should be experimentally verified. Finally, our filtering methods readily scale to magnitudes larger development task sets, so looking at how we should vary filtering in this regime may be necessary.
Figure 7: We show different filters’ absolute performance as we vary the number of holdout tasks, where we sample the holdout tasks from varying distributions described in Sec. 4.1. Top: The random baseline always performs better with more tasks. All methods perform equally well with many holdout tasks, as expected due to matching distributions. Bottom: Our filters improve performance over the random baseline for any number of holdout tasks.

5 Limitations & Broader Impact

Limitations: We used the improvement probability to assess system performance when evaluating system changes, but this might not accurately reflect a provider’s risk tolerances. Users should select an appropriate scalar measure of system performance. Another limitation is that using improvement probability may not give helpful answers for changes that consistently improve performance, like increasing compute budget. There are other performance metric choices, like changes in the mean quality. Also, we explored a limited number of ways to measure task distribution mismatch – there are various other strategies.

Broader Impact Statement: While there are important impacts from using AutoML in general, we focus on a specific impact of our filtering formulation: Our method allows us to assess changes to our system using fewer development tasks, which could help reduce the environmental impact of benchmarking our system. For example, our best-performing filter used only 20% of the available training tasks. However, this could create unintended biases by using fewer datasets. Also, our method could help service users who are specifically concerned with privacy. We should further investigate which groups most benefit from this.

6 Related work

Our related work covers: AutoML broadly, AutoML systems we hope to apply our method on, then methods to evaluate those AutoML systems. Additional related work is in App. Sec.B.

AutoML: [21] contains an overview of key AutoML components – including hyperparameter optimization [22], meta-learning [23], and neural architecture search [24].

AutoML Systems: We can apply our filters to arbitrary AutoML systems used for production. This includes various publicly available AutoML systems like Auto-WEKA [25], Auto-MEKA [26], Hyperopt-Sklearn [27], Auto-sklearn [28], Auto-Net [29], TPOT [30], adaptive TPOT [31], the automatic statistician [32], AlphaD3m [33], H20 [34], SmartML [35], ML-Plan [36], Mosaic [37], RECIPE [38], Alpine Meadow [39], ATM [40], Rafiki [41] We focus on systems for multiple models, but some systems focus on DNNs including MetaQNN [42], Auto-Keras [43], and the various papers on Neural Architecture Search [44–48].

Evaluating AutoML Systems: There are various proposed benchmarks including HPO-B [2], HPOBench [3], AutoML Benchmark [49], and other varied studies [1, 17–19, 50]. [51] outline fundamental AutoML evaluation practices. Competitions are another method to provide common
goals for AutoML systems, including the AutoML Challenges [52], the AutoDL challenge [53] and NeurIPS BBO Challenge [54].

Filtering for AutoML: There are fewer works on filtering strategies in AutoML. The closest work we are aware of in this vein is Oboe [55] using collaborative filtering on the matrix of qualities for many tasks for time-constrained HO.

7 Conclusion
We were motivated by assessing if AutoML system changes – i.e., the search space or HPO – will improve the final output model’s performance on a separate set of prod. tasks. But, we cannot run the system changes prod. tasks, so we assess them on dev. tasks. However, the set of dev. and prod. tasks differ, leading us to pursue changes improving dev. and not prod. We proposed the filtering problem, leveraging available descriptor info about holdout tasks to select useful dev. tasks. Then we proposed various filtration strategies, which we used in large-scale empirical studies. We showed that the filters improved our ability to assess if system changes improve performance on holdout tasks from different distributions than training, such as in prod. We hope this helps build the set of benchmarking strategies for more sophisticated and realistic setups, allowing people to better deploy AutoML systems. We also believe this provides a fruitful avenue of research in stronger filtration strategies, leveraging the broad body of work on task relationship learning.

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Appendix

A Glossary

| Table 1: Glossary |
|-------------------|
| **Search Space** | The set of all possible hyper-parameters. |
| **Task** | The specification of the dataset and the learning problem. |
| (Prod.)uction tasks | Tasks observed in the production environment, presented by customers. |
| (Dev.)elopment tasks | Tasks used for development, constituting open-source datasets. |
| **Filter** | An algorithm for choosing a subset. |
| **Train tasks** | A subset of the dev. tasks used for designing a filter. |
| **Holdout tasks** | A subset of the dev. tasks used as a representative of production tasks for evaluating a filter. |
| **Filtered tasks** | Subset of train tasks chosen by a filter. |
| **Quality** | A scalar quantity depicting the performance of a model on a task. |
| **Baseline Setup** | Some default AutoML setup. |
| **Modified Setup** | A non-default AutoML setup. |
| **Change** | A combination of a baseline and modified setup. |
| **UB** | Upper bound |
| **DNN** | Deep Neural Network |

B Additional Related work

Hyperparameter optimization in AutoML: There are various scalable methods for HO using more information than quality evaluations [64–70], which can have their own pitfalls [71, 72]. However, we focus on black-box HO like Bayesian optimization [6, 73–76]. [77] focus on Bayesian optimization for AutoML. We use Vizier [20], which supports various black-box optimizers including Bayesian Optimization.

C Additional Background

C.1 The Production AutoML System

C.1.1 The Search Space. Our AutoML system explores jointly algorithm selection and hyper-parameters [78], modeled as a conditional search space, with a root parameter for the algorithm choice and conditional sub-parameters conditioned on the choice of the root node. Our included learning algorithms are Feed-forward Neural Networks (DNNs), Random Forests, Gradient Boosted Decision Trees, Linear models, Sparse Linear Model with feature crosses (Cross) similar to RuleFit [79], and ensembles of Linear and DNNs using AdaNet [80].

C.1.2 The Hyperparameter Optimizer. We use Vizier [20, 81] to optimize our hyperparameters, which supports various user-specified parameters controlling the HPO. Vizier supports various underlying HPO algorithms – ex., random search, and Bayesian optimization. We can specify parameters controlling the underlying HPO algorithms – including exploration rate, whether to use transfer learning and how to apply early stopping.

C.1.3 Assessing System Performance. We focus on binary classification problems for simplicity here, but our work generalizes for an arbitrary scalar quality measure. Specifically, we measure the AUC on the validation subset for the best model selected from the search space by our hyperparameter optimizer. The system has performed better if we measure a higher quality on a single run for a single task.
D The Filtering Problem

Evaluating Changes to the AutoML System: To assess if some change to our AutoML system improves performance across a distribution of tasks, we first measure improvement on each task and then aggregate the improvement measures across tasks. Note that quality measures between tasks are not directly comparable. For example, even if two tasks use the same quality metric, such as AUC, the scale might be different. In other words, an AUC of 0.92 might be suitable for one task, while non-suitable for another task where 0.99 AUC is possible. To be able to compare quality across tasks, we measure improvement on a task with the probs. of the quality improving (Alg. 4).

To aggregate the improvement measure (i.e., probs. of improvement) across tasks, we could simply take the mean of the probabilities. Instead, we use the mean of logits – a simple transformation mapping the probs. to \((-\infty, \infty)\) – then going back to probs. with the inverse-logit (Alg. 4).

Algorithm 4 EvalSystemChange(tasks, change=(baselineSetup, modifiedSetup))

1: for task in tasks do ▶ compute every taskLoss for each task
2: get baselineQualities from baselineSetup ▶ An array of qualities – ex., from a database
3: get modifiedQualities for each run with modifiedSetup
4: probImproved = fraction of pairings with modifiedQuality > baselineQuality
5: taskLoss = logit(probImproved) ▶ Loss is log-odds of improvement probability with change
6: return expit(meanTaskLoss) ▶ Aggregate with mean, and take inverse logit for a probability

D.1 How Filters work

Algorithm 5 abstractFilter(trainTasks, holdoutTaskDescriptors)

1: Construct a list L containing elements of trainTasks, given holdoutTaskDescriptors
2: return L

D.2 How to Compare Filters

Algorithm 6 contrastFilters(newFilter, baselineFilter, baselineSetup, modifiedSetup, taskPartitions)

1: Initialize loss storage arrays newFilterLosses, baselineFilterLosses
2: for each trainTasks, holdoutTasks in taskPartitions do
3: newFilterLoss = EvalFilter(newFilter, trainTasks, holdoutTasks, baselineSetup, modifiedSetup)
4: baselineFilterLoss = EvalFilter(newFilter, trainTasks, holdoutTasks, baselineSetup, modifiedSetup)
5: Store newFilterLoss and baselineFilterLoss
6: Compute summary of loss distributions – ex., the difference in the mean losses, or a significance test to see if newFilter’s loss is lower, significantly.
7: return filter loss distribution summary

D.3 Similarity Metrics

Performance descriptor similarities: Alg. 7 uses a surrogate model to estimate the performance of the hyperparameter configurations on a train task by taking the hyperparameter values as input features. The intuition is that similar tasks perform similarity on the same hyperparameter values. Instead of actually evaluating the train tasks on all hyperparameter configuration used for the holdout tasks on the baseline setup we estimate training performance using a surrogate model.
The surrogate model is trained for each train task on past runs on all baseline setups. Then the trained surrogate model are used to predict what performance metric will be for the hyperparameter values that were applied to holdout task tasks on the baseline setup. These predictions give an idea of how the train tasks would have performed on the set of hyperparameter values used for the holdout tasks. The correlation between the predicted quality/objective metric and the actual metrics from the holdout tasks are computed and used as a similarity measure between the train tasks and the holdout task. We outline this method in Alg. 7.

**Algorithm 7** performanceDescriptorSimilarity(trainTasks, holdoutTask)

1: trainTaskSimilarities = empty list
2: Train surrogate models for each task in trainTasks.
3: holdoutTaskHparamConfigs, holdoutTaskQuality = fetch past runs for holdoutTask for baseline setup
4: for trainTask in trainTasks do
5: surrogateModel = Fetch surrogate model for trainTask
6: estimatedQuality = surrogateModel(holdoutTaskHparamConfigs)
7: similarity = Compute a correlation coefficient for holdoutTaskQuality and estimatedQuality
8: store similarity for task in trainTaskSimilarities
9: return trainTaskSimilarities

**Approximate oracle similarity:** When developing our filters, it would be desirable to have a (relatively tight) upper-bound on the possible performance given our limited access to info about the holdout tasks. For example, once we approach this performance then we know it is not worth attempting to design better filters. This also allows us to better gauge the magnitude of improvement over a random task selection baseline.

We propose a heuristic to approximate an upper-bound on the filter performance using limited descriptors about holdout data, with a filter which uses the unrestricted descriptors about holdout data. This setup allows re-running the holdout data with AutoML system changes. If we can access this info about holdout tasks, then we wouldn’t need to filter. We would simply evaluate our changes on holdout tasks as is standard practice. Nonetheless, this is useful to bound possible filter performance.

Specifically, in App. Alg. 8 we compute the similarity by simply computing the correlation in qualities between a train task and test task – sampled over different setups to our AutoML system. The choice of setups to sample over, and the correlation coefficient to compute are user-specified. This is heuristic with no strong guarantees, but proves useful in our experiments. Experiments for App. Alg. 8 are in Sec. E.2.2.

**Algorithm 8** oracleSimilarity(trainTasks, holdoutTask)

1: trainTaskSimilarities = empty list
2: for trainTask in trainTasks do
3: trainQualities, holdoutQualities = empty lists
4: for setup in systemSetups do
5: store trainQuality = Run the train task with the setup
6: store holdoutQuality = Run the holdout task with the setup
7: similarity = compute a correlation coefficient for trainQualities and holdoutQualities
8: store similarity for task in trainTaskSimilarities
9: return trainTaskSimilarities

**D.3.1 Constructing Filters for Multiple Holdout Tasks.** For Alg. 9, the number of filtered tasks for the inner, single-task filter and the outer multi-task filter can be different, but we keep them the same for simplicity in our experiments. Also, each filtered task receives a single vote of equal weight.
We can use more complicated strategies like weighted votes – e.g., based on similarity scores – but these were unnecessary for our experiments.

**Algorithm 9** VotingFilter(trainTasks, testTasks, filterLength, innerFilter)

1: initialize voteCounts = dictionary of how many votes each train task received
2: for testTask in testTasks do
3:   filteredTasks = innerFilter(trainTasks, testTask)
4:   for filteredTask in filteredTasks do
5:     voteCounts[filteredTask] += 1
6: return the top filterLength tasks with the most votes in voteCounts

**D.3.2 How to compare filters.** Once we can evaluate a filter’s loss, we use this to compare different filters. App. Alg. 6 shows a skeleton for our method of comparing filters, with relevant experiments in Sec. 4.2.3. We look at two simple strategies: First, we compute the cross-entropy loss for each filter – i.e., the filter log-loss averaged over different train and test task partitions – and report the difference in cross-entropies as the magnitude of improvement between filtering strategies (Fig. 6). Second, we use a significance test on the difference in cross-entropy for the filters (Fig. 16).

**E Experiments**

**E.1 Compute Requirements**

The total compute requirement is equivalent to running 60k CPUs for 1 day, consuming 10 PiB of memory on average.

| Datasets                  | OpenML [8] (Phishing Websites, Adult [9], Bank Marketing [10], Churn, Electricity, Kr-vs-kp, Numerai28.6, Sick, Spambase, Nomao [11], Jm1, Internet Advertisements, Phoneme, Madelon [12], Bioresponse, Wilt [13]), Civil Comments [14], Imdb, Census, Yelp sentiment [15], Criteo [16] |
|---------------------------|--------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| Search Space              | Random Forest, Linear, Deep Neural Networks, Gradient Boosted Decision Trees, AdaNet, Linear Feature Cross                                                                                                                                                  |
| Data Splits               | 80-10-10 split, uniformly at random.                                                                                                                                                                                                                        |

**E.2 Experimental Setup**

**E.2.1 Changes made to the AutoML system for experiments.**

![Figure 8](image-url) We show the distribution of qualities for our setups on various pairs of OpenML tasks. Each setups qualities are shown in a different color. For each task and setup, we have multiple observations over re-runs, so we plot every pairing of the tasks qualities for each setup.
E.2.2 Approximate Oracle Similarity Results. Fig. 9 display the matrix of similarities from Alg. 8, computed using the system setups from Sec. E.2.1, showing non-trivial task relationships.

![Approximate Oracle Similarity Matrix]

Figure 9: We show the matrix of approximate oracle similarities where each row and column correspond to a single task.

E.3 Filtering Problem Results

E.3.1 Investigating design choices for evaluating changes to AutoML Systems.

![Evaluation Probability Comparison]

Figure 10: We contrast runs of EvalSystemChange (Alg. 4) showing the improvement probability for different AutoML system changes as we vary the number of tasks.

![Probability Estimation Comparison]

Figure 11: We contrast runs of Alg. 4 with a probability estimate using a single task evaluation, with a probability estimate using multiple task evaluations.
Figure 12: We look at the distribution of evaluate change results – i.e., the improvement probability given the change – on both the randomly filtered tasks and the holdout tasks, as we vary the number of filtered and holdout tasks. For all results we use 5 quality samples. Takeaway: We should account for how we select the number of filtered tasks and holdout tasks when assessing filters.

E.3.2 Investigating how we evaluate filters.

Figure 13: We show the distribution of filter loss values from different samplings of train tasks and holdout tasks, for the changes in Fig. 5.

E.3.3 Comparing different filtering strategies.

Figure 14: The mean of the differences between a filter strategy with a random baseline – multiple filter strategies are displayed in each color.
Figure 15: The mean of the differences between a filter strategy with a random baseline – multiple system changes are displayed in each color. Takeaway: The approximate oracle similarity filter always improves performance over the random baseline. The performance descriptor similarity improves performance over the random baseline when assessing changing to the search space, but not for changes to the implementation.

Figure 16: The mean of the differences in quality, relative to a random baseline, and filtered to only show values with a significance level greater than .05 between a filter strategy with a random baseline – for different changes in setups. Takeaway: The significance filtered results are similar to their respective unfiltered results in Fig. 14 and 15.