EVALUATING RECOMMENDER SYSTEMS FOR AI-DRIVEN DATA SCIENCE

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ABSTRACT

We present a free and open-source platform to allow researchers to easily apply supervised machine learning to their data. A key component of this system is a recommendation engine that is bootstrapped with machine learning results generated on a repository of open-source datasets. The recommendation system chooses which analyses to run for the user, and allows the user to view analyses, download reproducible code or fitted models, and visualize results via a web browser. The recommender system learns online as results are generated. In this paper we benchmark several recommendation strategies, including collaborative filtering and metalearning approaches, for their ability to learn to select and run optimal algorithm configurations for various datasets as results are generated. We find that a matrix factorization-based recommendation system learns to choose increasingly accurate models from few initial results.

Keywords Artificial Intelligence · Automated Machine Learning

1 Introduction

Experimental data is being collected faster than it can be understood across scientific disciplines [1]. The hope of many in the data science community is that widely accessible, open-source artificial intelligence (AI) tools will allow scientific insights from these data to keep abreast of their collection [2]. AI is expected to make significant improvements to scientific discovery, human health and other fields in the coming years. In this light, the key promise of AI is the automation of learning from large sets of collected data. However, at the same time that data collection is outpacing researchers, methodological improvements from the machine learning (ML) and AI communities are outpacing their dissemination to other fields. As a result, AI and ML remain steep learning curves for non-experts, especially for researchers pressed to gain expertise in their own disciplines.

It is clear from this situation that specialized researchers would benefit greatly from increasingly automated, accessible and open-source tools for AI. With this in mind, we present an open-source, free AI platform, PennAI, that is designed for the non-expert to quickly conduct a ML analysis on their data. PennAI uses a web browser-based user interface (UI) to display a user’s datasets, experiments, and results. Central to PennAI’s ease of use is a bootstrapped recommendation system that automatically configures and runs supervised learning algorithms catered to the user’s datasets and previous results. In addition to streamlining the ML process for new users, PennAI provides a research platform for AI researchers who can quickly plug in their own automatic machine learning (AutoML) methods and use PennAI as a test-bed for methods development. The project is documented and maintained on Github [2].

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2 http://github.com/EpistasisLab/pennai
In this paper, we focus on the AI strategy used to automatically run analyses for the user. The underlying methods are based on recommender systems, which are well known inference methods underlying many commercial content platforms, including Netflix [3], Amazon [4], Youtube [5], and others. Our goal is to assess the ability of state-of-the-art recommender systems to learn the best ML algorithm and parameter settings for a given dataset over a set number of iterations in the context of previous results. We compare collaborative filtering (CF) approaches as well as metalearning approaches on a set of 135 open-source classification problems. We find that collaborative filtering algorithms based on matrix factorization perform well in choosing the best analysis, and are able to learn an optimal algorithm setting from few results. We demonstrate that over time, the learning system is able to generate increasingly accurate recommendations.

2 Background

In this section, we briefly reviewAutoML methodologies, which are a key component to making data science approachable to new users. We then describe recommender systems, the various methods that have worked in other application areas, and our motivation for applying them to this relatively new area of AutoML.

2.1 Automated Machine Learning

AutoML is a burgeoning area of research in the ML community that seeks to automatically configure and run learning algorithms without human intervention. A number of different learning paradigms have been applied to this task, and tools are available to the research community as well as commercially. A competition around this goal has been running since 2015 focused various budget-limited tasks for supervised learning [6].

A popular approach arising from the early competitions is sequential model-based optimization via Bayesian learning [7], represented by the auto-Weka and auto-sklearn packages [8, 9]. These tools parameterize the combined problem of algorithm selection and hyperparameter tuning and use Bayesian optimization to select and optimize algorithm configurations. It is worth noting this parameterization of the problem can be handled with other learning approaches, for example in Hyperopt [10].

Auto-sklearn incorporates metalearning into the optimization process [11] to narrow the search space of the optimization process. The idea behind metalearning in this context is that the “metafeatures” from the datasets, such as predictor distributions, variable types, cardinality etc. provide valuable information about algorithm performance that can be leveraged to choose an appropriate algorithm configuration. Auto-sklearn uses this approach to narrow the search space of their learning algorithm. PoSH auto-sklearn [13] an update to auto-sklearn, bootstrapped auto-sklearn with an extensive analysis to minimize the configuration space. ML pipelines were optimized on a large number of datasets beforehand, and the pipelines were narrowed to those that performed best over all datasets. This tool effectively replaced metalearning with bootstrapping; our experiments provide some evidence supporting a similar strategy.

Another popular method for AutoML is tree-based pipeline optimization tool TPOT [14]. TPOT uses an evolutionary computation approach known as genetic programming to optimize syntax tree representations of ML pipelines. Complexity is controlled via multi-objective search. Benchmark comparisons of TPOT and auto-sklearn show trade-offs in performance for each [15].

There are many commercial tools providing variants of AutoML as well. Many of these platforms do not focus on choosing from several ML algorithms, but instead provide automated ways of tuning specific ones. Google has created AutoML tools as well using neural architecture search [16], a method for configuring the architecture of neural networks. This reflects their historical focus on learning from sequential and structured data like images. H2O uses genetic algorithms to tune the feature engineering pipeline of a user-chosen model. Intel has focused on proprietary gradient boosted ensembles of decision trees [6].

A main paradigm of many AutoML is that they wrap several ML analyses, thereby obscuring the analysis from the user. Although this does indeed automate the ML process, it also removes the user from the experience. In contrast to these strategies, PennAI uses a recommender system as its basis of algorithm recommendation with the goal of providing a more intuitive and actionable user experience.

There has been limited research utilizing recommender systems as AutoML approaches. One recent exception is Yang et al. [17], who found that non-negative matrix factorization could be competitive with auto-sklearn for classification. A recent workshop also solicited discussion of algorithm selection and recommender systems, although most research of this nature is interested in tuning the recommendation algorithms themselves [18].
Ultimately, the best algorithm for a dataset is highly subjective: a user must balance their wants and needs, including the accuracy of the model, its interpretability, the training budget and so forth. PennAI’s coupling of the recommendation system approach with the UI allows for more user interaction, essentially by maintaining their ability to “look under the hood”. The user is able to fully interface with any and all experiments initialized by the AI in order to, for example, interrupt them, generate new recommendations, download reproducible code or extract fitted models and their results. Although the experiments in this paper use accuracy as the focus for generating recommendations, the general strategy opens the door for future versions that explicitly incorporate user feedback on the models that are generated in order to tailor the analysis to the user’s preferences.

By developing PennAI as a free and open-source tool, we also hope to contribute an extensible research platform for the ML and AutoML communities. The code is developed on Github and documents a base recommender class that can be written to the specification of any learning algorithm. We therefore hope that it will serve as a framework for bring real world users into contact with cutting edge methodologies.

2.2 Recommender Systems

Recommender systems are typically used to recommend items, e.g. movies, books, or other products, to users, i.e. customers, based on a collection of user ratings of items. The most popular approach to recommender systems is collaborative filtering (CF). CF approaches rely on user ratings of items to learn the explicit relationship between similar users and items. In general, CF approaches attempt to group similar users and/or group similar items, and then to recommend similar items to similar users. CF approaches assume, for the most part, that these similarity groupings are implicit in the ratings that users give to items, and therefore can be learned. However, they may be extended to incorporate additional attributes of users or items [19].

Recommenders face challenges when deployed to new users, or in our case, datasets. The new user cold start problem [20] refers to the difficulty in predicting ratings for a user with no data by which to group them. With datasets, one approach to this problem is through metalearning. Each dataset has quantifiable traits that can be leveraged to perform similarity comparisons without relying on algorithm performance history. In our experiments we benchmark a recommender that uses metafeatures to derive similarity scores for recommendations, as has been proposed in previous AutoML work [9, 12].

Recommender systems are typically used for different applications than AutoML, and therefore the motivations behind different methods and evaluation strategies are also different. For example, unlike typical product-based recommendation systems, the AI automatically runs the chosen algorithm configurations, and therefore receives more immediate feedback on its performance. Since the feedback is explicitly the performance of the ML choice on the given dataset, the ratings/scores are reproducible, less noisy, and less sparse than user-driven systems. This robustness allows us to measure the performance of each recommendation strategy reliably in varying training contexts. As another example, many researchers have found in product recommendation that the presence or absence of a rating may hold more weight than the rating itself, since users choose to rate or to not rate certain products for non-random reasons [21]. This observation has led to the rise of implicit rating-based systems, such as SVD++, that put more weight on presence/absence of ratings. In the context of AutoML, it is less likely that the presence of results for a given algorithm configuration imply that it will outperform others. Furthermore, the goal of advertising-based, commercial recommendation systems may not be to find the best rating for a user and product, but to promote engagement of the user, vis-a-vis their time spent browsing the website. To this end, recommender systems such as Spotlight [23] are based on the notion of sequence modeling: what is the likelihood of a user interacting with each new content given the sequence of items they have viewed? Sequence-based recommendations may improve the user experience with a data science tool, but we contend that they do not align well with the goals of an approachable data science assistant.

3 Methods

In this section we first describe the user experience of PennAI, and then describe recommenders that we benchmark in our experiments for automating the algorithm selection problem. Fig. I gives an overview of the data science pipeline. Users upload datasets through the interface or optionally by pointing to a path during startup. At that point, users can choose between building a custom experiment (manually configuring an algorithm of their choice) or simply clicking the AI button. Once the AI is requested, the recommendation engine chooses a set of analyses to run. The AI can be configured with different termination criteria, including a fixed number of runs, a time limit, or running until the user turns it off. As soon as the runs have finished, the user may navigate to the results page, where several visualizations of model performance are available (Fig. I C).
PennAI is available as a docker image that may be run locally or on distributed hardware. Due to its container-based architecture, it is straightforward to run analysis in parallel, both for datasets and algorithms, by configuring the docker environment. For more information on the system architecture, refer to the Appendix.

3.1 Recommendation System

In order to use recommender systems as a data science assistant, we treat datasets as users, and algorithms as items. The goal of the AI is therefore as follows: given a dataset, recommend an algorithm configuration to run. Once the algorithm configuration has been run, the result is now available as a rating of that algorithm configuration on that dataset, as if the user had rated the item. This is a nice situation for recommender systems, since normally users only occasionally rate the items they are recommended. We denote this knowledge base of experimental results as \( D = \{ r_{ad}, r_{be}, \ldots \} \), where \( r_{ad} \) is the test score, i.e. rating, of algorithm configuration \( a \) on dataset \( d \). In our experiments the test score is the average 10-fold CV score of the algorithm on the dataset.

With a few notable exceptions discussed below, the recommenders follow this basic procedure:

1. Whenever new experiment results are added to \( D \), update an internal model mapping datasets \( d \) to algorithm configurations, \( a \).
2. Given a new recommendation request, generate \( \hat{r}_{ad} \), the estimated score of algorithm configuration \( a \) on dataset \( d \). Do this for every \( ad \) pair that has not already been recommended.
3. Return recommended algorithm configurations in accordance with the termination criterion, in order of best rating to worst.

Note that the knowledge base \( D \) can be populated not only by the AI, but by the user through manual experiments (Fig. 1A) and by the initial knowledge base for PennAI. In production mode, the knowledge base is seeded with approximately 1 million ML results generated on 165 open-source datasets, detailed here \[24\]. The user may also specify their own domain-specific cache of results. Below, we describe several recommender strategies that are benchmarked in the experimental section of this paper. Most of these recommenders are adapted from the Surprise recommender library \[25\].

3.1.1 Neighborhood Approaches

We test four different neighborhood approaches to recommending algorithm configurations that vary in their definitions of the neighborhood. Three of these implementations are based the \( k \)-nearest neighbors (KNN) algorithm, and the other uses co-clustering. For each of the neighborhood methods, similarity is calculated using the mean squared deviation metric.

In the first and second approach, clusters are derived from the results data directly and used to estimate the ranking of each ML method by computing the centroid of rankings within the neighborhood. Let \( N^k(a) \) be the \( k \)-nearest neighbors of algorithm configuration \( a \) that have been run on dataset \( d \). For KNN-ML, we then estimate the ranking from this neighborhood as:

\[
\hat{r}_{ad} = \frac{\sum_{b \in N^k(a)} \text{sim}(a, b) \cdot r_{bd}}{\sum_{b \in N^k(a)} \text{sim}(a, b)} \quad (1)
\]

For KNN-data, we instead define the neighborhood over datasets, with \( N^k(d) \) consisting of the \( k \) nearest neighbors to dataset \( d \) that have results from algorithm \( a \). Then we estimate the rating as:

\[
\hat{r}_{ad} = \frac{\sum_{e \in N^k(d)} \text{sim}(d, e) \cdot r_{ae}}{\sum_{e \in N^k(d)} \text{sim}(d, e)} \quad (2)
\]

Instead of choosing to define the clusters according to datasets or algorithms, we may define co-clusters to capture algorithms and datasets that cluster together. This is the motivation behind co-clustering \[26\], the third neighborhood-based approach in this study. Under the CoClustering approach, the rating of an algorithm configuration is estimated as:

\[
\hat{r}_{ad} = \bar{C}_{ad} + (\mu_a - \bar{C}_a) + (\mu_d - \bar{C}_d) \quad (3)
\]

where \( \bar{C} \) is the average rating in cluster \( C \). As Eqn. \[3\] shows, clusters are defined with respect to \( a \) and \( d \) together and separately. Co-clustering uses a \( k \)-means strategy to define these clusters. In case the dataset is unknown, the average algorithm rating, \( \mu_a \), is returned instead; likewise if the algorithm configuration is unknown, the average dataset rating \( \mu_d \) is used. In case neither is known, the global average rating \( \mu \) is returned.
Figure 1: Overview of the UI. A) Users upload datasets and choose a custom experiment (right), or allow the AI to run experiments of its choosing by clicking the AI button. B) Experiments are tabulated with configuration and performance information. The user may download scripts to reproduce the experiment in python, or export the fitted model. C) The results page displays experiment information and statistics of the fitted model, including various performance measures (confusion matrix, receiver operating characteristic (ROC) curve, etc.) as well as feature importance scores for the independent variables.
Finally, we test a metalearning method dubbed **KNN-meta**. In this case, the neighborhood is defined according to metafeature similarity, in the same way as other approaches [11][12][9]. We use a set of 45 metafeatures calculated from the dataset, including properties such as average correlation with the dependent variable; statistics describing the mean, max, min, skew and kurtosis of the distributions of each independent variable; counts of types of variables; and so on.

Rather than attempting to estimate ratings of every algorithm, KNN-meta maintains an archive of the best algorithm configuration for each dataset experiment. Given a new dataset, KNN-meta calculates the $k$ nearest neighboring datasets and recommends the highest scoring algorithm configurations from each dataset. KNN-meta has the advantage in cold starts since it does not have to have seen a dataset before to reason about its similarity to other results; it only needs to know how its metafeatures compare to previous experiments. KNN-meta has the limitation, however, that it can only recommend algorithm configurations that have been tried on neighboring datasets. In the case that all of these algorithm configurations have already been recommended, KNN-meta will recommends uniform-randomly from algorithms and their configurations.

### 3.1.2 Singular Value Decomposition

The singular value decomposition (SVD) recommender is a CF method popularized by the top entries to the Netflix challenge [3]. Like other top entrants [27][28], SVD is based on a matrix factorization technique that attempts to minimize the error of the rankings via stochastic gradient descent (SGD). Each rating is estimated as

$$\hat{r} = \mu + b_d + b_a + q_a^T p_d$$

(4)

where $\mu$ is the average score of all datasets across all learners; $b_a$ is the estimated bias for algorithm $a$, initially zero; $b_d$ is the estimated bias for dataset $d$, initially zero; $q_a$ is a vector of factors associated with algorithm $a$ and $p_d$ is the vector of factors associated with dataset $d$, both initialized from normal distributions centered at zero. Ratings are learned to minimize the regularized loss function

$$L = \sum_{r_{ad} \in D} (r_{ad} - \hat{r}_{ad})^2 + \lambda (b_d^2 + b_a^2 + ||q_a||^2 + ||p_d||^2)$$

(5)

One of the attractive aspects of SVD is its ability to learn latent factors of datasets and algorithms ($q_d$ and $q_d$) that interact to describe the observed experimental results without explicitly defining these factors, as is done in metalearning. A historical challenge of SVD is its application to large, sparse matrices, such as the matrix defined by datasets and algorithms (in our experiments this matrix is about 1 million elements). SVD recommenders address the computational hurdle by using SGD to estimate the parameters of Eqn. 4 using available experiments (i.e. dataset ratings of algorithms) only [29]. SGD is applied by the following update rules:

$$b_d \leftarrow b_d + \gamma (c_{ad} - \lambda b_d)$$

(6)

$$b_a \leftarrow b_a + \gamma (c_{ad} - \lambda b_a)$$

$$p_d \leftarrow p_d + \gamma (c_{ad} q_a - \lambda p_d)$$

$$q_a \leftarrow q_a + \gamma (c_{ad} p_d - \lambda q_a)$$

where $c_{ad} = r_{ad} - \hat{r}_{ad}$. To facilitate online learning, the parameters in Eqn. 6 are maintained between updates to the experimental results, and the number of iterations (epochs) of training is set proportional to the number of new results.

### 3.1.3 Slope One

Slope one [30] is a simple recommendation strategy that models algorithm performance on a dataset as the average deviation of the performance of algorithms on other datasets with which the current dataset shares at least one analysis in common. To rate an algorithm configurations $a$ on dataset $d$, we first collect a set $R_a(d)$ of algorithms that have been trained on $d$ and share at least one common dataset experiment with $a$. Then the rating is estimated as

$$\hat{r}_{ad} = \mu_d + \frac{1}{|R_a(d)|} \sum_{b \in R_a(d)} dev(a, b)$$

(7)

### 3.1.4 Benchmark Recommenders

As a control, we test two baseline algorithms: a random recommender and an average best recommender. The **Random** recommender chooses uniform-randomly among ML methods, and then uniform-randomly among hyperparameters for that method to make recommendations. The **Average** recommender keeps a running average of the best algorithm configuration as measured by the average validation balanced accuracy across experiments. Given a dataset request, the Average recommender recommends algorithm configurations in order of their running averages, from best to worst.
4 Experiments

The goal of our experiments is to assess different recommendation strategies in their ability to recommend better algorithm configurations for various datasets as they learn over time from previous experiments. The diagram in Fig. 2 describes the experimental design used to evaluate recommendation strategies under PennAI.

Datasets  We assess each recommender on 135 open-source classification datasets, varying in size and origin. We use datasets from the Penn Machine Learning Benchmark (PMLB) [31]. PMLB is a curated and standardized set of hundreds of open source supervised machine learning problems from around the web (sharing many in common with OpenML [32]). In previous work, we conducted an extensive benchmarking experiment to characterize the performance of different ML frameworks on these problems [31, 24]. The benchmark assessed 13 ML algorithms over a range of hyperparameters detailed in Table 1 on these problems. This resulted in a cache of over 1 million ML results across a broad range of classification problems which we use here to assess the performance of each recommender with a known ranking of algorithms for each dataset. For the experiment in this paper, we use a subset of these results consisting of 12 ML algorithms (dropping one of three naïve Bayes algorithms) with 7580 possible hyperparameter configurations, shown in Table 1.

Experiment  The experiment consists of 300 repeat trials for each recommender. In each trial, the recommender begins with a knowledge base of $n_{init}$ experiments that consist of single ML runs on single datasets. For each iteration of the experiment, the recommender is asked to return $n_{recurr}$ recommendations for a randomly chosen dataset. Once the recommendation is made, the results for the recommended algorithm configurations are fed back to the recommender as updated knowledge. Thus, the recommender behaves as a reinforcement learning experiment in which the actions taken by the recommender (i.e., the recommendations it makes) determine the information it is able to learn about the relationship between datasets and algorithm configurations.

We conduct experiments varying $n_{init} \in [10, 50, 100]$ and $n_{recurr} \in [10, 50, 100]$. This allows us to assess the sensitivities to 1) starting with more information and 2) exploring more algorithm options during learning.

Assessment  Since we have the complete results of ML analyses on our experiment datasets, we are able to assess recommendations in terms of their closeness to the best configuration, i.e. that configuration with the best performance on a dataset over all results obtained in our exhaustive benchmark. Each algorithm configuration is primarily assessed according to its balanced accuracy ($BA$), a metric that takes into account class imbalance by averaging accuracy over classes [33]. We define the best balanced accuracy on a given dataset as $BA_{d}^{*}$. Then the performance of a recommendation is assessed as the relative distance to the best solution, as:

$$\Delta \text{Balanced Accuracy}_{ad} = \frac{(BA_{d}^{*} - BA_{ad})}{BA_{d}^{*}}$$  \hspace{1cm} (8)
In addition to Eqn. 8, we assess the AI in terms of the number of datasets for which it is able to identify an “optimal” configuration. Here we define “optimal” algorithm configurations to be those that score within some small threshold percentage of the best performance for a dataset. This definition of optimality is of course limited both by the finite search space defined by Table 1 and by the choice of thresholding, which we range from 1%-5%. Nonetheless, this definition gives a practical indicator of the extent to which AI is able to reach the global best performance.

Table 1: Analyzed algorithms with their parameters settings. The methods and parameters are named according to Scikit-learn nomenclature[34].

| Algorithm name | Parameter Values |
|----------------|------------------|
| AdaBoostClassifier | learning_rate [0.01, 0.1, 0.5, 1.0, 10.0, 50.0, 100.0] |
| BernoulliNB | alpha [0.0, 0.1, 0.25, 0.5, 0.75, 1.0, 5.0, 10.0, 25.0, 50.0] |
| DecisionTreeClassifier | max_features [0.0, 0.1, 0.25, 0.5, 0.75, 0.9, 1.0] |
| ExtraTreesClassifier | max_features [0.0, 0.05, 0.1, 0.2, 0.25, 0.3, 0.35, 0.4, 0.45, 0.5] |
| GradientBoostingClassifier | loss ["deviance"] |
| KNeighborsClassifier | n_neighbors [1, 2, ..., 25] |
| LogisticRegression | C [0.0001, 0.001, 0.01, 0.1, 0.5, 1.0, 10.0, 50.0, 100.0] |
| MultinomialNB | alpha [0.0, 0.1, 0.25, 0.5, 0.75, 1.0, 5.0, 10.0, 25.0, 50.0] |
| PassiveAggressiveClassifier | loss ["hinge", "squared_hinge"] |
| RandomForestClassifier | max_features [0.0, 0.05, 0.1, 0.15, 0.2, 0.25, 0.3, 0.35, 0.4, 0.45, 0.5] |
| SGDClassifier | penalty ["l2", "l1"] |
| SVC | C [0.01] |
5 Results

Results for the PMLB experiment are shown in Figures 3-5. Recommenders are first compared in terms of median $\Delta$ Balanced Accuracy in Fig. 3. In Fig. 4 we look at the fraction of datasets for which SVD is able to find an optimal configuration under different experiment treatments. Finally we visualize the behavior of a subset of recommenders in Fig. 5 in order to gain insight into which algorithms are being selected and how this compares to the underlying distribution of algorithm performance in the knowledgebase.

Figure 3: Experiment results for each recommendation strategy. Each plot shows the median $\Delta$ Balanced Accuracy (Eqn. 8) for 300 trials with error bars denoting 95% confidence intervals. From left to right, the number of recommendations made per dataset increases; from top to bottom, the number of experiments in the initial knowledgebase increases.
Let us first focus on the performance results in Fig. 3. We find in general that the various recommender systems are able to learn to recommend algorithm configurations that increasingly minimize the gap between the best performance on each dataset (unknown to the AI) and the current experiments. SVD performs the best, tending to reach good performance more quickly than the other recommendation strategies, across treatments. KNN-data and KNN-ml are the next best methods across treatments; KNN-ML shows a sensitivity to the number of recommendations per iteration, indicating it requires more results to form good clusters. For most experimental treatments, there is a gap between those three methods and the next best recommenders, which vary between SlopeOne, KNN-meta, and CoClustering for different settings.

As we expected due to its cold-start strategy, KNN-meta turns out to work well initially, but over time fails to converge on a set of high quality recommendations. The collaborative filtering recommenders are generally able to learn quickly from few examples compared to the metalearning approach. This difference in performance has been found in other domains, particularly movie recommendations [35].

Given 100 initial experiment results and 10 recommendations per iteration, the SVD recommender converges to within 5% of the optimal performance in approximately 100 iterations, corresponding to approximately 7 training instances per dataset. Note that the performance curves begin to increase on the right-most plots that correspond to 100 recommendations per dataset. In these cases, the recommender begins recommending algorithm configurations with lower rankings due to repeat filtering, described in Section 3.

Figure 4: Cumulative success rates for every dataset in the knowledgebase, starting with all other experiment results. The success rate is the fraction of datasets for which the recommender has trained an algorithm configuration that achieves a test set balanced accuracy within 1-5% of the best performance on that dataset. As the number of recommendations/evaluations increases, the success rate improves, until 100% of datasets have an optimal configuration chosen by the AI.

In Fig. 4, we look deeper into SVD’s performance since it is shown to perform the best in terms of $\Delta$ Balanced Accuracy. As described earlier, we are interested in capturing a notion of “optimality”, which we define as being within a small threshold percentage of the best performance on a dataset, where the best performance is determined using the exhaustive experiments in our previous work [31, 24]. In this case, we wish to know how many evaluations it takes for the AI to recommend an optimal configuration across all the datasets. We perform a leave-one-out style analysis, meaning that the AI is trained on results from all other datasets prior to iteratively making recommendations for a given dataset. This leave-one-out analysis corresponds to the applied case, in which PennAI is deployed with a pre-trained recommender and must run experiments for a newly uploaded dataset. We repeat this analysis for all datasets and to calculate the rate of success, using thresholds of 1-5% to define success/optimality. Each of these thresholds is shown as a separate line in Fig. 4.

Let us first focus on the most stringent success criteria: a 1% threshold for determining success/optimality. Fig. 4 shows that the SVD recommender is able to recommend an optimal algorithm configuration on its first recommendation for
21% of the datasets. It reaches a 50% success rate after 16 evaluations, an 80% success rate after 532 evaluations, and a 98% success rate after 4242 evaluations. These evaluations correspond to searching 0.2%, 7%, and 56% of the algorithm configuration space, respectively. According to a relaxed threshold of 5%, SVD is able to recommend successful configurations for 95% of datasets in 453 iterations.

Figure 5: Heatmaps of three different recommendation strategies on the PMLB benchmark showing how often each ML was recommended. These plots show the experiment treatment with \( n_{\text{recs}} = 50 \) and \( n_{\text{init}} = 10 \). The top left figure is derived from the true data, and represents the average frequency of top-ranking algorithms across all of the datasets (note that the uniformity is due to the shuffling of the datasets for each trial). The right top figure shows SVD’s performance; over several iterations, it learns to approximate the frequency distribution of best ML models, i.e. GradientBoostingClassifier, followed by RandomForestClassifier, ExtraTreesClassifier, and SGDClassifier. The bottom left shows the same plot for KNN-ML, which more heavily weights SGDClassifier in the final iterations. The bottom right plot shows SlopeOne’s behavior which is to recommend GradientBoostingClassifier and SGDClassifier most frequently at different points in time.

The final set of plots in Fig 5 show the frequency with which SVD, KNN-ML, and SlopeOne recommend different algorithms in comparison to the frequency of top-ranking algorithms by type (the top left plot). Here we see that SVD gradually learns to recommend the top five algorithms in approximately the same ranking as they appear in the knowledgebase. This lends some confidence to the relationship that SVD has learned between algorithm configurations and dataset performance.

6 Conclusion

In this paper we propose a data science tool for non-experts that generates increasingly reliable ML recommendations tailored to the needs of the user. The web-based interface provides the user with an intuitive way to launch and monitor analyses, view and understand results, and download reproducible experiments and fitted models for offline use. The learning methodology is based on a recommendation system that can learn from both cached and generated results. We demonstrate through the experiments in this paper that collaborative filtering algorithms can successfully learn to produce intelligent analyses for the user starting with sparse data on algorithm performance. We find in particular that a matrix factorization algorithm, SVD, works well in this application area.

PennAI automates the algorithm selection and tuning problem using a recommendation system that is bootstrapped with a knowledgebase of previous results. The default knowledgebase is derived from a large set of experiments conducted on 165 open source datasets. The user can also configure their own knowledgebase of datasets and results catered to their application area. We hope in the future to provide these for various learning domains, including electronic health records and genetics.

We also hope that PennAI can serve as a testbed for novel AutoML methodologies. In the near term we plan to extend the methodology in the following ways. First, we plan to implement a focused hyperparameter tuning strategy that can fine-tune the models that are recommended by the AI, similar to auto-sklearn \([9]\) or Hyperopt \([10]\). We plan to make this process transparent to the user so that they may easily choose which models to tune and for how long. We also plan to increasingly automate the data preprocessing, which is, at the moment, mostly up to the user. This can include processes from imputation and data standardization to more complex operations like feature selection and engineering.
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Appendix

System Architecture

PennAI is a multi-component architecture that uses a variety of technologies including Docker\textsuperscript{5}, Python, Node.js\textsuperscript{6}, scikit-learn\textsuperscript{7}, FGLab\textsuperscript{8} and MongoDB\textsuperscript{9}. The project contains multiple docker containers that are orchestrated by a

\textsuperscript{5}https://www.docker.com/
\textsuperscript{6}https://nodejs.org
\textsuperscript{7}http://sklearn.org
\textsuperscript{8}https://kaixhin.github.io/FGLab/
\textsuperscript{9}https://www.mongodb.com/
docker-compose file. The central component is the controller engine, a server written in Node.js. This component is responsible for managing communication between the other components using a REST API. A Mongodb database is used for persistent storage. The UI component is a web application written in javascript that uses the React library to create the user interface and the Redux library to manage UI state. The interface supports user interactions including uploading datasets for analysis, requesting AI recommendations for a dataset, manually specifying and running machine learning experiments, and displaying experiment results in an intuitive way. The AI engine is written in Python. As users make requests to perform analysis on datasets, the AI engine will generate new machine learning experiment recommendations and communicate them to the controller engine. The AI engine contains a knowledgebase of previously run experiments, results, and dataset metafeatures that it uses to inform the recommendations it makes. The knowledgebase is bootstrapped with a collection of experiment results generated from the PMBL benchmark datasets. Instructions and code templates are provided to allow easy integration of custom recommendation systems. The machine learning component is responsible for running machine learning experiments on datasets. It has a Node.js server that is used to communicate with the controller engine, and uses python to execute Scikit-learn experiments on datasets and communicate results back to the central server. A PennAI instance can support multiple instances of machine learning engines, enabling multiple experiments to be run in parallel. Fig. 6 shows how each component interacts in PennAI.