Abstract

Building a good predictive model requires an array of activities such as data imputation, feature transformations, estimator selection, hyper-parameter search and ensemble construction. Given the large, complex and heterogenous space of options, off-the-shelf optimization methods are infeasible for realistic response times. In practice, much of the predictive modeling process is conducted by experienced data scientists, who selectively make use of available tools. Over time, they develop an understanding of the behavior of operators, and perform serial decision making under uncertainty, colloquially referred to as educated guesswork. With an unprecedented demand for application of supervised machine learning, there is a call for solutions that automatically search for a good combination of parameters across these tasks to minimize the modeling error. We introduce a novel system called APRL (Autonomous Predictive modeler via Reinforcement Learning), that uses past experience through reinforcement learning to optimize such sequential decision making from within a set of diverse actions under a time constraint on a previously unseen predictive learning problem. APRL actions are taken to optimize the performance of a final ensemble. This is in contrast to other systems, which maximize individual model accuracy first and create ensembles as a disconnected post-processing step. As a result, APRL is able to reduce up to 71% of classification error on average over a wide variety of problems.

1 Introduction

In recent years, applied machine learning has received significant attention. There is an increasing availability of digitally recorded and disseminated information that can be used to build predictive models in various domains across the industry, academia and government. The building of reliable predictive models is a task primarily conducted by data science teams. The primary objective of a data scientist is to try various tools and techniques at her disposal, aggregate the effective operations based on results, fine tune them, and finally test before deploying a generalizable predictive modeling solution. The downside of a data scientist-centric approach is the high cost and high turn around time. There is a significant supply-demand deficit of data scientists [4]. Moreover, not every small organization can afford a highly qualified team of data scientists.

This has lead to an increased demand for automated machine learning (AutoML) techniques that computationally solve some or all of the steps involved in the applied machine learning process. AutoML as an optimization problem is challenging. It involves a vast and diverse space of options, making it computationally prohibitive to run optimization solvers for obtaining solutions in realistic time frame using affordable resources. For instance, feature transformations for a single feature, using a modest number of unary functions, say 30, with a combination depth of 3, itself leads to \( 3^{30} \) configurations to chose from; Sklearn’s Random Forest Classifier provides 17 hyper-parameters with varying range of possible values – some continuous, some discrete; selecting the optimal ensemble base models from a set of many constructed models, is yet another combinatorial problem, and so on. One alternative direction is the use of historical information obtained from model building exercises. Different works recently have been able to learn useful clues from historical information to short-circuit the search on the vast space. For instance, in Bayesian Learning, priors on various options are learned, in reinforcement learning-based techniques, pruning or search strategies are tuned using prior runs, or associating feature distribution characteristics with suitable actions, etc.

Another direction for AutoML is based is the use of approximations and heuristics for specific tasks such as feature engineering, without considering other aspects such as estimator selection. In this context, it should be noted that the choice of learning algorithm often greatly influences the choice of effective feature engineering transformations, and vice versa. While the collective use of such individual optimizers may not aim towards a global optimal solution for the ML choice optimization, they are used effectively by practitioners. Since these techniques are usually based on task specific heuristics or approximations, it is difficult to integrate them in a unified framework. The proposed approach in this paper dwells on the idea of using both – historical information and task-specific heuristics algorithms.

In the process of trying different options such as a particu-
lar feature transformation, using a particular estimator or cer-
tain choice of hyper-parameters, produce several transformed
versions of the data or a slightly different model. Amongst
several such trials on the way, only one or a few models con-
structed are deemed winners and adopted. However, upon
carefully selecting a subset of these subpar models, simple
but effective ensembles can be created that outperform the
impact of the best one alone, owing to their mutual diversity
besides the individual strength. APRL goes a step further and
not only makes ensembles from the subpar models obtained in
the process, but also explicitly creates models that max-
imize the performance of the final ensembles. We use rein-
forcement learning (RL) to devise an exploration strategy that
guides the process to take actions that minimize the ensemble
generalization error (EGE) of a proposed final ensemble.
Minimizing the EGE directly results in finding a combina-
tion of high accuracy and highly diverse models, which is
the recipe for a successful ensemble. To this end, we present
a fast, greedy algorithm to select a subset of models from a
large subset, that minimize EGE. In this paper, we describe
the core ideas behind APRL, which includes modeling the
action space, exploration process, rewards through ensemble
generalization and policy learning through reinforcement
learning.

2 Related Work

In existing work on AutoML, Auto-sklearn [10] and Auto-
WEKA [31; 22] use sequential parameter optimization based
on Bayesian Optimization to determine effective predictive
modeling pipelines by combining data pre-processors, trans-
formers and estimators. Both variants are based on the gen-
eral purpose algorithm configuration framework SMAC [14]
to find optimal machine learning pipelines. In order to ap-
ply SMAC, the problem of determining the appropriate ML
approach is cast into a configuration problem where the se-
lection of the algorithm itself is modeled as a configuration.
Auto-sklearn also supports warm-starting the configuration
search by trying to generalizes configuration settings across
data sets based on historic performance information. Auto-
sklearn is of particular interest in the context of this paper as
it constructs an ensemble of classifiers instead of a sin-
gle classifier. It uses ensemble selection from [5] which is a
greedy algorithm that starting from an empty set of models
incrementally adds a model to the working set in each step if
it results in maximizing the improvement of predictive per-
formance of the ensemble.

Another approach for automated ML is based on genetic
algorithms [28]. While it does not create ensembles, it could
compose them based on derived models as the authors point
out. More interestingly, the approach presented in [1] uses
multi-objective genetic programming to evolve a set of accu-
rate and diverse models via biasing the fitness function ac-
cordingly.

There is a diverse set of approaches towards automated fea-
ture engineering which are summarized below. FICUS [24]
performs a beam search over the space of possible features,
constructing new features by applying constructor functions.
Its is guided by heuristic measures based on information
gain in a decision tree. Data Science Machine by [15] ap-
plies all transformations on all features at once (but no se-
quence of transformations), then performing feature selection
and model hyper-parameter optimization over the augmented
dataset. FEADIS [9] works through a combination of ran-
dom feature generation and feature selection. ExploreKit [16]
expands the feature space explicitly, one feature at a time.
It employs learning to rank the newly constructed features
and evaluating the most promising ones. LFE [27], [26]
directly predicts the most useful transformation per feature
based on learning effectiveness of transforms on sketched
representations of historical data through a perceptron. Cog-
nito [21], [18] presents a rule based hierarchical exploration
of transforms. [30] and [17] summarize some of the work in
feature engineering over the years.

The most relevant feature engineering approach to the
work presented in this paper is [20], which is based on trial
or exploration of different transformation functions and find-
ning sequences with higher returns based on initial feedback.
Their trials are organized in a hierarchical, directed acyclic
graph and the goal is the minimization of model error. Their
exploration policy is trained through reinforcement learning
on historical ML problems. In this paper, we also employ
a hierarchical structure for exploration, with a much diverse
space of actions including ensembles, hyper-parameters, es-
timator selection. Along with that, our reward mechanism
reflects the need to optimize for ensemble goals of both, high
accuracy and diversity instead of model accuracy alone, and
use multiple estimators instead of just single one.

Model ensembles are used extensively in machine learn-
ing to aggregate the output of several weak predictors into
a single strong predictor [8]. Different methods to ensen-
ble ensure diversity through different means. For example,
Random Forests by [2] use systematic randomization to cre-
ate data subsets and perturbation in branch splitting to reduce
variance in a large number of decision trees. The aggregation
is a simple unweighted average.

In the given context, we areas dealing with specific ensen-
bles needs. Due to the associated cost of exploration involving
model building and validation, there is a moderate number of
base models (typically 10-100), all of which are fairly corre-
lated to each other, with small differences. The mutual cor-
relation is because all of them contain an overlapping set of
( original) features, apart from different transformed features,
which often causes mild to moderate deviation in models’ be-
behavior, or none. Hence, a simple averaging of all base models
seems ineffective, and a rather careful selection of base mod-
els is required. We also observe that performance oriented
exploration can often overfit the training data, but presents a
blessing in disguise for ensembles, when handled appropri-
ately [29]. We acknowledge that other known mechanisms to
improve model diversity can be used along with our proposed
methods, such as the use of different hyper-parameter config-
urations, random subset selection, amongst others. In fact,
these mechanisms are complimentary to the core idea sug-
ggested in this paper. To further emphasize the benefits of the
core approach, we present promising results with simple av-
eraging instead of employing more sophisticated approaches
such as stacking [13] or boosting [12], that are obvious addi-
tions to our ongoing work.

There exists a body of work on generating diversity for ensembles. [25], for instance, generate artificial examples to construct diverse predictors whose ensemble provides good gains. [7] and [33] introduce diversity based on feature selection through hill climbing algorithms. A survey of diversity promoting methods is presented by [3]. Reinforcement learning has been used as a metalearning too in the domain of deep neural network tuning recently [11]. However, it should be noted that there are significant differences in the structure of deep learning tuning problem compared to that of regular predictive modeling that involves different learning algorithms, explicit and more diverse feature engineering, etc. We similar approach to AutoML for maximizing ensembles through feature engineering was using reinforcement learning [19] but not performing estimator selection and hyper-parameter optimization.

3 APRL Overview

Figure 1 illustrates APRL’s approach. The cornerstone of APRL is an agent that iteratively decides the action to perform, based on two factors – the performance of various actions until that moment and time remaining until when the problem must be solved. APRL is presented with a classification or regression problem in terms of feature vectors \((X)\) and a target vector \((y)\), and the time constraint \((t_{max})\) in which to build a model. In each iteration, the agent has to decide to perform an action from a choice of many available ones. It can apply one of the following, to either the given data \((X, y)\) or a version of it that has been derived in the course of this exploration: (a) feature transformations; (b) estimator selection and model building; (c) hyper-parameter optimization for a model and transformation. The process of taking such actions is called data science exploration or simply exploration, which is illustrated in Figure 2. Due to the hierarchical nature of the abstract representation, it is called an exploration tree.

![APRL Overview Diagram](image)

Figure 1: APRL approach overview. Given a supervised ML problem \((X, y)\) and a time constraint \(t_{max}\), the system generates an ensemble after iterative exploration through multiple transforms, estimators and hyper-parameters.

Applying a feature transformation to a feature-set means generating new features by applying the corresponding function on all possible input features (or feature combinations for non-unary functions), and appending them to the original feature set. For example, applying a logarithm transform, \(\log(X)\) means creating new features by \(\log(x_i) \forall x_i \in X\), such that feature \(x_i\) contains only positive values. Similarly, \(f_{\text{frequency}}\) transform function, that creates a new feature by counting the number of occurrences of a value is done only for discreet values transforms, and so on. As described in the related work section, in general, feature transformation can be performed in several ways. It may be done iteratively by adding one new feature at a time using one transform, or in contrast, by adding them in bulk by applying multiple transforms on all given features, usually followed by an intense feature selection process. We adopt a middle of the road approach where, in one iteration, we apply one transform to all valid input feature candidates. In this paper, we present results using a set of 9 different transformation functions: \(\text{freq}, \text{pca}, \text{round}, \text{minmaxscaler}, \text{tanh}, \text{groupby+stddev}, \text{cbrt}, \text{sigmoid}, \text{stidscaler}\), and a special feature selection transformation that can remove unnecessary features from the input. The selection is based on historical performance. The approach is independent of the the actual transformations used and additional or fewer transformations may be specified, including domain specific ones.

The second category of actions is the choice of a particular estimator, such as \(\text{Random Forest}, \text{Gradient Boosted Trees}, \text{K-nearest neighbors}\), etc., to be chosen on a transformed (or original) data with its default hyper-parameters, which has not been done so far. The third category of actions is that of a hyper-parameter optimization routine to be run on for data node in the tree. We use a hyper-parameter optimization routine based on black-box optimization using radial basis functions [6]. The action specifies a data node, the estimator, hyper-parameter optimization, and the allocated time for it. Additionally, the result of each hyper-parameter optimization step is treated as a starting value set for the next action belonging to the same estimator type.

At each iteration, the agent enumerates all actions possible from the current state of the tree (without repetition) and ranked as per the expected long term benefit. The action with the highest expected benefit is chosen and applied. From one state of the tree to the next, the list of possible actions changes. Additionally, the perceived benefit of the actions change as well. The task of taking the best action, given the state of the exploration is performed by the agent based upon a policy, II that it learns historically on other learning problems using reinforcement learning. Further details on the agent’s policy learning, definition of states, and such provided in Section 4.

At each node with an estimator, plain or with hyper-parameter optimization, an prediction of the labels is performed through 5-fold cross validation. The predictions thus generated are required to compute the ensemble generalization error (EGE) for a potential ensemble that may contain that node. It is further used to compute \(E_{\text{min},}\), a quantity that reflects the minimum value of EGE for an ensemble from any subset of the nodes of a given tree. This quantity is used as a feedback reward for the agent to learn its policy. Further details are presented in Section 5.
4 Learning Exploration Policy for Agent

We model the exploration process as a Markov Decision Process (MDP), where a state of the system contains all the required information to take the next action at any point. The state at any iteration is described by a combination of the exploration tree state (entire tree up to that point with all details such as gain in model accuracy due to transforms, estimators, EGE, etc.) and the fraction of remaining time \((t_{\max} - t)/t_{\max}\) where \(t = 0\) at the beginning. Let the entire set of states be \(S\). An action for this MDP is the application of a particular transformer, estimator or HPO on a node of the tree at that state. Let the entire set of actions be \(C\). A policy, \(\Pi : S \rightarrow C\), guides which action should be taken for a given state. We first learn \(\Pi\) iteratively through RL on a set of many prediction problems, and apply it to use for an unseen data.

The “remaining time budget fraction” is a part of the state definition because it is used to determine whether to explore more (i.e., experiment with different transformations and estimators, usually at the beginning of a run) or exploit more (i.e., focus more towards steps that will likely give a desired result based on the exploration so far). It decides whether to focus on exploiting gains (depth) or exploring (breadth) or a compromise, in different regions of the graph, at different steps. Overall, the policy selects the action with the highest expected long-term reward contribution; however, upon evaluating a new node’s actual immediate contribution, the expectations are often revised and explore/exploit gears are (implicitly) calibrated through the policy. For example, upon finding an exceptionally high improvement at a node during early stages, the (breadth) exploration can be temporarily localized under that node instead of the same level as it. Overall, value estimation is a function based on multiple attributes of the MDP state such as current remaining budget, tree structure and relative performance at various nodes, etc. Note that this particular explore-exploit tradeoff is implicitly learned as a part of the policy. Note that this runtime explore-exploit tradeoff is different from the explore-exploit tradeoff seen during RL training in context of selecting actions to balance reward and not getting stuck in a local optimum, which is controlled explicitly. We employed an \(\epsilon\)-greedy methodology, where an action is chosen at random with probability \(\epsilon\) (random exploration), and from the current policy with probability \(1 - \epsilon\) (policy exploitation). The trade-off is exercised randomly and is independent of the state of MDP. The value of \(\epsilon\) is constant and is chosen based on experimentation.

At step \(i\), the occurrence of an action results in a estimator node, \(n_i\), and the best ensemble error \(E_{\min}(n_i)\) for a subset of \(\{0, 1, \ldots, n_i\}\) is obtained using Algorithm 1. To each step, we attribute an immediate scalar reward (with a slight abuse of notation):

\[
r_i = \frac{E_{\min}(\text{nodes}(T_{i-1})) - E_{\min}(\text{nodes}(T_i))}{E_{\min}(\{X_0\})}
\]

with \(r_0 = 0\), by definition. Also, \(E_{\min}(\{X_0\})\) is the 5-fold CV performance using any particular estimator. The cumulative reward is then used to update the policy through RL.
lative reward over time from state $s_i$ onwards is defined as $R(s_i) = \sum_{j=0}^{N} \gamma^j r_{i+j}$, where $\gamma \in [0,1)$ is a discount factor, which prioritizes earlier rewards over the later ones. Here, we find the optimal policy $\Pi^*$ which maximizes the cumulative reward. The general result of Q-learning [32] to learn the action-value Q-function, for each state, $s \in S$ and action, $c \in C$, with respect to policy $\Pi$ is:

$$Q(s,c) = r(s,c) + \gamma R^\Pi(\delta(s,c))$$

where $\delta : S \times C \rightarrow S$ is a hypothetical transition function, and $R^\Pi(s)$ is the cumulative reward after state $s$. The optimal policy is found as:

$$\Pi^*(s) = \arg \max_c [Q(s,c)]$$

Due to the extremely large state space, $|S|$, it becomes infeasible to learn the Q-function directly. Instead, we utilize a linear approximation for the Q-function, $Q(s,c) = w.f(s)$, where $w$ is a weight vector and $f(s)$ is a vector of the state characteristics such as: (a) average model performance for a circular node (average of all estimators through it); (b) best performance for a circular node; (c) Average performance of an estimator type; (d) average gain in accuracy for a transform; (e) best gain in accuracy for a transform; (f) Remaining time; (g) Total allocated time (h) Count of numerical features; (i) Count of categorical features; (j) Whether it contain date/time; (k) Remaining time budget fraction times value of (a); (l) Remaining time budget fraction times value of (b), and so on.

Hence, we approximate the Q-function values with linear combinations of characteristics of a state of the MDP. The update rule for $w$ is as follows, where $g'$ is the state of the tree at step $j + 1$, and $\alpha$ is the value for learning rate:

$$w^j \leftarrow w^j + \alpha.(r_j + \gamma \cdot \max_{c \in C} Q(g',c') - Q(g,c)).f^j(s)$$

5 Ensemble Generalization Error

We now describe the criterion to compute the ensemble generalization error (EGE) for a given set of base models and an algorithm to select a subset from a given set of models that maximizes the EGE. While it is used to create a final ensemble, more importantly it is also used to compute a reward for the RL training and runtime stages as described in the previous section.

Krogh et al. [23] provide a useful expression for computing the ensemble generalization error. For a number of base models and the output of model $\alpha$ on input $x$ be $V^\alpha(x)$. Let a weighted average ensemble output on $x$ be:

$$\nabla(x) = \sum_{\alpha} w_\alpha V^\alpha(x)$$

The ambiguity on input $x$ of a single member of the ensemble is defined as $\alpha^\alpha = (V^\alpha(x) - \nabla(x))^2$. The overall ambiguity of the ensemble on input $x$ is:

$$\bar{a}(x) = \sum_{\alpha} w_\alpha \alpha^\alpha = \sum_{\alpha} w_\alpha (V^\alpha(x) - \nabla(x))^2$$

This is the variance of the weighted ensemble around the weighted mean. Let $y(x)$ be the true outcome value for input $x$. The squared errors for the model $\alpha$ and the ensemble respectively are: $e^\alpha(x) = (f(x) - V^\alpha(x))^2$, and $e(x) = (f(x) - \nabla(x))^2$. Now, let the weighted average error of the models be $\bar{e}(x) = \sum_\alpha w_\alpha e^\alpha(x)$. By rearrangement, we obtain, $e(x) = \bar{e}(x) - a(x)$. Averaging the above over several inputs:

$$E = \bar{E} - \bar{A} \tag{2}$$

which states that the generalization error of the ensemble equals the weighted average of the generalization errors of the individual models ($\bar{E} = \sum_\alpha w_\alpha E^\alpha$) minus the weighted average of the ambiguities of the individual models ($\bar{A} = \sum_\alpha w_\alpha A^\alpha$). $E^\alpha$ and $A^\alpha$ are model $\alpha$’s average error and ambiguity, respectively.

The significance of the result by [23] in Equation 2, is that it can help evaluate the relative performance of different model sets through individual model performance and a measure of average ambiguity. However, selecting the best subset of models that minimizes this error is a combinatorially hard problem. Knapsack-type approximation algorithms do not work in this case because we need to minimize the difference of two unrelated quantities. We also explored set coverage style of solutions but found them to be inadequate because this problem is not about coverage (correctly predicted) by sets (as models) as much as it is about an example being covered by enough (possibly a majority) of sets. We adopt this particular measure and choice of ensemble style because of its ease of computation, especially in an incremental manner with respect to adding newer models.

Data: $\hat{Y}$ (Prediction vectors from available models)

$M \leftarrow \phi$

while $|\hat{Y}| > 0$ do

$\hat{y}^* \leftarrow \arg \min_{\hat{y} \in \hat{Y}} E(M \cup \hat{y})$

if $E(M \cup \hat{y}^*) < E(M)$ then

$M \leftarrow M \cup \hat{y}^*$

$N \leftarrow \hat{Y} - \hat{y}^*$

else

break

end

Result: $M$

Algorithm 1: Greedy model subset selection: given a set of predictions from models, the algorithm selects a subset based on $E(M)$. We call this subroutine $E_{\min}(M)$.

We propose an effective greedy algorithm to find the suitable subset of ensemble constituents in an efficient manner. Algorithm 1 iterates over all the predictions of all currently available models, and continues adding the predictions to the set of selected ones, $M$, as long as adding them improves $E(M)$. The advantage of this algorithm is its simplicity and efficiency, and it works well in practice. It is important to note that the simplicity of the formula chosen, enables the computation of $E(M + n)$ efficiently in an incremental manner, using $E(M)$, $n$ and certain bookkeeping by utilizing the
definition of generalization error from Equation 2. We omit
the details here. The algorithm subroutine is referred to as
$E_{min}(M)$. This algorithm can be made more effective by the
two following steps. First, apart from adding a new model to
the bag once it satisfies $E(M \cup \hat{y}^*) \leq E(M)$, we also con-
sider dropping it, in spite of satisfying the condition. Second,
along with the first step) replacing $E(M \cup \hat{y}^*) \leq E(M)$
with $E(M \cup \hat{y}^*) \leq E(M) + \phi$, where $\phi$ is a small, positive
constant. This enables growing the ensemble to a bigger size
at the cost of a tiny increase in EGE in the short term. How-
ever, these make the $E_{min}$ algorithm more expensive. For
the purpose of this paper, we will stick with the simpler Al-
gerism 1. Note that this algorithm is somewhat similar but
different in essential aspects compared to [5], which is based
on a hill-climbing optimization after constructing an ensem-
ble and computing validation score on a hold-out set, and is
arguably slower for an incremental setting.

6 Experiments
Agent’s exploration strategy was learned based on 62 datasets
obtained from various open source repositories, primarily
from OpenML 1 and other propriety data. Different values
of $t_{max}$ (5, 10, 15 … 120 in minutes) were used during train-
ing: 10 transformations including feature selection, 4 estima-
tors for classification and 3 in case of regression. We used
learning rate parameter, $\alpha = 0.05$, discount factor $\gamma = 0.99$,
and tried three values for $\epsilon$ (0.15,0.20,0.25), and finally used
$\epsilon = 0.2$ based on external validation.

We evaluated our work on 56 binary classification data
problems from OpenML. Note that these data are different
from those used to train the agent. We summarize all the
results, while providing details for a subset of 10 amongst
them. The subset was chosen based on the lowest 10 base
Area under ROC curve for a plain random forest classifier
on the data. Our evaluation through out is based on splitting
33% of the data for evaluation using a fixed seed (1)
through Sklearn’s train_test_split. The optimizers (ours or
AutoSklearn) was only provided with the remaining 67% of
the rows and all numbers reported were based on testing on
the unseen 33%, using the metric Area under ROC curve. We
report the relative reduction in AUC error compared to a base
estimator as a measure of comparing across different mod-
els and aggregating results across different datasets. It is de-
scribed as: 
\[
\frac{(1-AUC_{base}) - (1-AUC_{opt})}{1-AUC_{base}}
\]
We additionally report a summary of results of a set of regression problems in terms
of relative reduction of root mean squared error.

6.1 Comparison to base estimators and
Autosklearn
Table 1 presents the AUC scores for Random Forest and XG-
Boost algorithms upon running APRL and AutoSklearn for
30 minutes each, for 10 binary classification datasets. It com-
pares APRL and AutoSklearn based upon reduction in the
initial error (1-AUC) over each base estimator. It can be seen
that APRL consistently achieves lower modeling error rates.
Additionally, results for 56 binary (including the 10) classifi-
cation datasets are summarized.

6.2 Optimization Performance with Varying Time
Figure 3 displays the mean reduction in AUC error for the 56
and 10 set classification data for AutoSklearn and APRL over
varying time constraints for optimization. In all cases, we can
see increasing but diminishing returns with increasing time.
Also, APRL performs better in each case.

6.3 APRL vs FE alone vs FE+Ensemble
For the 10 datasets listed in Table 1, upon allotting 30 minutes
of runtime for each of the following: (a) APRL was able to
reduce AUC error by 61% compared to (b) 36% of feature
engineering alone (using XGBoost) on our implementation of
the system described in [20], and (c) 44% for ensemble using
Algorithm 1 on feature engineering solution from part-b.

6.4 Regression performance
For 9 regression datasets, APRL was able to reduce root mean
squared error by 31% over Random Forest Regressor on an
average, compared to 19% reduction by AutoSklearn over
Random Forest Regressor, by running each for 30 minutes.

7 Conclusion
In this paper, we presented a novel automated machine learn-
ing framework called APRL, that produces effective en-
ssembles using multiple data transformations, estimators and
hyper-parameter optimization steps. At the heart of APRL
is an autonomous agent that performs time-aware contex-
tual decision making of various data science operations. It
was constructed by learning an efficient strategy for data sci-
cence exploration through reinforcement learning on histori-
cal datasets. To the best of our knowledge, it is the first of
its kind where exploration is primarily guided by the need to
optimize ensembles, as well as the first one to use reinforce-
ment learning. We demonstrated the impact of our method
by showing benefits against plain models, feature engineering

1https://www.openml.org/
Tables 1: Comparing the accuracy of Random Forest, XGBoost Classifier with AutoSklearn and APRL ran for 30 minutes each. The fractional improvement is reported over reduction in error (1 - AUC) over the corresponding base model's.

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