Toward Efficient Automated Feature Engineering

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Abstract—Automated Feature Engineering (AFE) refers to automatically generate and select optimal feature sets for downstream tasks, which has achieved great success in real-world applications. Current AFE methods mainly focus on improving the effectiveness of the produced features, but ignoring the lowefficiency issue for large-scale deployment. Therefore, in this work, we propose a generic framework to improve the efficiency of AFE. Specifically, we construct the AFE pipeline based on reinforcement learning setting, where each feature is assigned an agent to perform feature transformation and selection, and the evaluation score of the produced features in downstream tasks serve as the reward to update the policy. We improve the efficiency of AFE in two perspectives. On the one hand, we develop a Feature Pre-Evaluation (FPE) Model to reduce the sample size and feature size that are two main factors on undermining the efficiency of feature evaluation. On the other hand, we devise a two-stage policy training strategy by running FPE on the pre-evaluation task as the initialization of the policy to avoid training policy from scratch. We conduct comprehensive experiments on 36 datasets in terms of both classification and regression tasks. The results show 2.9% higher performance in average and 2x higher computational efficiency comparing to state-of-the-art AFE methods.

Index Terms—approximate hashing, automated feature engineering, MinHash, off-policy, reinforcement learning

I. INTRODUCTION

Feature engineering refers to the process of feature generation and selection to convert raw data into effective features for machine learning tasks. Due to the lack of domain knowledge, traditional manual feature engineering is labor-intensive and time-consuming [1]. To overcome the limitation, <u>A</u>utomated <u>F</u>eature <u>E</u>ngineering (AFE) is proposed to automatically generate and select optimal feature sets [2], [3]. On the one hand, AFE can significantly reduce human efforts and benefit the deployment in large-scale big data systems; on the other hand, AFE can also discover new knowledge from the data that is hardly achieved by traditional manual data engineering.

Current studies in AFE focus on leveraging the Reinforcement Learning paradigm to explore possible feature candidates and exploit generated features to downstream machine learning tasks for selecting optimal feature sets. For example, Nargesian *et al.* proposed Learning Feature Engineering (LFE) with focusing on extracts useful transformations from past feature engineering experiences [4]; Khurana *et al.* developed a new transformation graph with Directed Acyclic Graph (DAG) to



(1) Sample Percentage vs. Perfor-(2) Sample Percentage vs. Computamance. tion Time.

Fig. 1: Sample size vs. performance and computation Time.

represent relationships between different transformed versions of the data, and Q-learning was used to learn a performanceguided strategy for effective feature transformation from historical instances [5]. In order to resolve the feature space explosion problem on high-order transformations, Chen *et al.* proposed Neural Feature Search (NFS) that utilized Recurrent Neural Network (RNN)-based controller to transform each raw feature through a series of transformation functions, and policy gradient was used to train this controller [6].

While promising feature sets produced, these state-of-theart AFE methods suffer from low-efficiency issue, especially in terms of time consumption for complex machine learning tasks. Taking NFS as an example. We investigate the time consumption of NFS on four datasets with different sizes, and present the empirical results in Table I. The results show that for each dataset, only about 0.1% of the time is spent on feature generation, but about 90% of the time is consumed on evaluating new features. The observation indicates that the efficiency of AFE is largely impeded by the feature evaluation step. Moreover, with the sample size increasing, the feature evaluation would take much more time, which even exacerbates the low-efficiency issue. Unfortunately, few efforts are put on improving the efficiency of AFE methods.

Therefore, in this work, we aim to study how to accelerate AFE. As the feature evaluation step takes the most of time, we propose to improve the efficiency of AFE by optimizing the feature evaluation process. Specifically, we optimize the feature evaluation process from two perspectives: (1) reducing the sample size for evaluation; (2) reducing the size of candidate features for evaluation. Next, we introduce the two perspectives as follows:

Dataset	Instances\Features	New Features	Generation Time	Eval. New Features Time	Total Time
PimaIndian	768\8	1195	354ms	205s	225s
credit-a	690\6	890	192ms	139s	155s
diabetes	768\8	1174	334ms	203s	223s
german credit	1001\24	3730	1291ms	654s	732s

TABLE I: One epoch of NFS time consuming on four datasets.

(1) Reducing the sample size for evaluation. In traditional pipeline of AFE, the feature evaluation is conducted over the whole dataset. However, not all samples are necessary for determining the quality of the generated features. We empirically investigate the contribution of the sample size on the feature performance. Specifically, we randomly sample different percentage of four datasets, and calculate the performance of the selected features and the corresponding running time. We conduct the operation for ten times, and present the average results in Figure 1. The results show that ignoring when the sample size achieves a certain scale, the performance of the selected features remains relatively stable. With more samples getting involved in, it barely enhances the quality of the selected features, but raises unacceptable surge in time consumption. The observation suggests that reducing the sample size is a promising direction for accelerating the feature evaluation process without sacrificing the feature quality.

(2) reducing the size of candidate features for evaluation. In addition to sample size, the size of candidate features is another important factor to affect the running time of evaluation. Intuitively, more features lead to larger candidate space for evaluation in feature selection, resulting in larger running time. Moreover, traditional AFE methods directly evaluate the features on the downstream tasks. However, the downstream tasks are usually complex and time-consuming, which even significantly retards the feature evaluation process. Therefore, reducing the size of candidate features prior to the formal evaluation (downstream tasks) is a potential solution.

Nevertheless, it is challenging to achieve the goal. The reasons are as follows: First, since AFE aims to provide a generic feature-refinement pipeline for different datasets with various sizes, the reducing process demands to work for arbitrary sample sizes. Second, different datasets have features with diverse semantic meanings, thus, how to determine a feature as a candidate for evaluation across datasets in a unified manner is non-trivial. Third, it is even more challenging to combine reducing the size of samples and candidate features without violating each requirement. Therefore, to tackle the above challenges, we propose to develop a simple and fast yet reasonable auxiliary evaluation task to pre-evaluate the validness of features to filter the candidate features prior to the formal evaluation. The proposed auxiliary evaluation task, namely Feature-Validness Task, is a binary classification task that justifies whether one feature is selected as a candidate for the formal evaluation. The Feature-Validness Task takes features as input, where one feature is denoted by respective values in samples. We pre-train a binary classification model, namely Feature Pre-Evaluation (FPE) Model, for the Feature-Validness Task using a group of public datasets as prior knowledge, and apply the well-trained model for pre-evaluation of the candidate features. In this case, all the features are required to be represented as a fixed size of samples. To achieve the goal, we further propose a Hashing-based method to project arbitrary sample sizes into a fixed number, which naturally fulfill the requirement for reducing sample sizes.

Along this line, we propose an efficient AFE framework with accelerating AFE via reducing the size of samples and candidate features simultaneously. Specifically, we formulate AFE as an off-policy reinforcement learning problem following the convention of AFE. Different from existing AFE methods, generated features from agents would be first preevaluated by the pre-trained FPE model to reduce the feature size with compressing samples to improve the efficiency. Then, to further reduce the costs on exploring promising feature transformation actions, we develop a two-stage training strategy: (1) quick initialization with FPE model, and (2) formal training. In stage 1, we only use FPE model as the evaluation to quickly discover promising feature transformation actions. During stage 1, the policy is initialized by borrowing knowledge from the pre-trained FPE model, and one replay buffer is constructed to record potentially good actions. After several epochs of training in stage 1, we formally convert the evaluation to the downstream tasks in stage 2. Trough this way, the proposed framework can improve the training efficiency by avoiding learning the policy from scratch. Our contributions can be listed as follows:

- To the best of our knowledge, we are the first to study how to improve the efficiency of AFE.
- Through empirical studies, we identify the core reason of the low-efficiency issue of AFE as the inefficient feature evaluation process.
- We propose an efficient AFE framework by reducing the size of samples and candidate features simultaneously through a faster auxiliary feature evaluation task with sample hashing.
- We develop a two-stage training strategy to improve the efficiency of policy learning.
- We conduct comprehensive experiments on 36 datasets in terms of both classification and regression tasks. The results show 2.9% higher performance in average and 2x higher computational efficiency comparing to stateof-the-art methods.

II. PROBLEM FORMULATION

In this section, we introduce the formulation of AFE. For tabular datasets, the general pipeline of AFE can be abstracted into two steps: feature generation and selection. As shown in Figure 2(1), the original features are first transformed into generated features through a series of combinatorial transformation functions. Then the selection method selects effective features from the generated features based on the evaluation results in downstream tasks. Then, the evaluation results will be further used as the feedback to improve the selection method and transformation functions to continue



(1) General Process of Automated Feature Engineering (2) Automated Feature Engineering with RL Fig. 2: From traditional AFE to RL-based AFE.

generating and selecting features until the selected features satisfy the evaluation requirement for the downstream tasks. Formally, given a dataset $\mathcal{D}\langle \mathbf{F}, \mathbf{y} \rangle$ with N original features $\mathbf{F} = \{f^{[1]}, f^{[2]}, ..., f^{[N]}\}$ with label \mathbf{y} , we use $A_{\mathcal{T}}(\mathbf{F}, \mathbf{y})$ to represent the evaluation score of the downstream task \mathcal{T} on dataset \mathcal{D} . The original feature set \mathbf{F} is transformed into $\check{\mathbf{F}}$ through a set of transformation functions (*e.g.*, addition, multiplication, logarithm, etc). The AFE is to find the optimal transformed feature set \mathbf{F}^* where $A_{\mathcal{T}}(\mathbf{F}^*, \mathbf{y})$ is maximized, such that $\mathbf{F}^* = \operatorname{argmax} A_{\mathcal{T}}(\check{\mathbf{F}}, \mathbf{y})$.

In this work, we formulate AFE in a reinforcement learning setting, as shown in Figure 2(2). We outline the definitions for the key elements as follows:

- Environment. In our design, the environment is the feature subspace of generated feature space. Whenever a feature agent issues an action to generate a new feature, the state of the feature subspace (environment) changes.
- Agents. Suppose there are N original features in the dataset, we define N agents to generate features. Specifically, each agent will generate new features based on the given original feature. In other words, considering one original feature and the respective newly generated features as a subgroup of the state space, there are N feature subgroups. Each agent will be responsible for one feature subgroup.
- **State Space.** We define the state *s* as the selected features. The dimension (size) of the state space is the size of the selected feature. The selected features include the original features and the newly generated features. Once a newly generated feature is discriminated as a good feature, the feature will be included into the state. Therefore, with more newly generated features added into the state, the state space will keep expanding until the feature engineering process finishes.
- Action. We define the action *a* as the feature transformation. Each agent will take actions (feature transformation) over the respective feature subgroup. The feature transformation is in the format of OPERATOR(feature_1, feature_2), where OPERATOR is a feature transformation operator that takes two features as input and outputs a new feature, and feature_1 and



feature₂ are two features from one feature subgroup. We consider two types of feature transformation operators: (i) unary operator (including logarithm, min-maxnormalization, square root, and reciprocal), in this case, feature₁ and feature₂ are the same feature; (ii) binary operator (including addition, subtraction, multiplication, division, and modulo operation), in this case, feature₁ and feature₂ are two different features.

- **Transition.** We illustrate the transition process in Figure 3. For simplicity, we take the transition from s_t to s_{t+1} as an example. The agent first sample two features from the respective feature subgroup in s_t with replacement. Then, the agent takes actions according to the policy to generate new features. The newly generated features will be discriminated as qualified or unqualified. Once confirmed as qualified, the newly generated feature will be selected and added to the respective feature subgroup to construct new state s_{t+1} .
- Evaluation Task. The evaluation task aims to examine the effectiveness of the generated and selected features. There are two types of evaluation tasks: (1) pre-evaluation task, that is to reduce the feature size through quick binary classification; and (2) downstream task, that is the formal evaluation task to evaluate and select the generated features. Following the convention of AFE [6], we utilize Random Forest as the model for downstream tasks. Details will be introduced in Section III-B.
- **Reward.** We define the performance gain on the evaluation task as the reward *r*.

Based on the above definition, we take one agent as example



Fig. 4: An illustration of feature generation using RNN-based agent. An RNN implements an agent of the raw feature. s_t is state, a_t is action, h_t is action probability distribution, f_t is generated features, r_t is the reward of new features. The initial state is the original feature. The evaluation task returns the reward r_t to the h_t through backpropagation on the loss function Equ. 1 and updates h_t .

to show how the proposed RL-based AFE generates features. For each feature, we exploit a RNN as the agent to take actions. Specifically, we maintain the hidden state of RNN as the probability distribution to sample an action (feature transformation function) to perform. For the first round generation, we set the action probability distribution as uniform distribution, and the original feature set as the input. For the tth round generation, we take the probability distribution h_{t-1} updated from the (t-1)-th round generation, and current state (feature set) s_t of RL as the input to RNN. RNN would output the updated probability distribution h_t . We sample an action a_t based on the updated probability distribution h_t . Then, we generate new features f_t by applying the action a_t on the feature set s_t . The updated state (feature set) s_{t+1} is the combination of the input feature set s_t and the generated feature set f_t . Moreover, the generated features f_t will be evaluated on the evaluation tasks and obtain the reward r_t . The action probability distribution h_t will be further updated based on the reward r_t by Equ. 1. Finally, the updated distribution h_t will be taken as the hidden state of RNN to perform the next round feature generation.

The loss function of our RNN is as Equ. 1. Agent loss function is constructed by three parts. r is the reward, h is the action probability distribution, and θ is the weight of RNN.

$$\mathcal{L}(\theta, h, r) = \log(\operatorname{argmax}(h)) * r + \log(h) * h + ||\theta||^2 \quad (1)$$

The notations used in this paper are summarized in Table II.

III. E-AFE

In this section, we introduce our proposed framework in detail. We start with overall framework of our proposed *E*-*AFE*. Then, we present FPE model for reducing sample and feature size. Moreover, we introduce the two-stage training strategy for enhancing the learning efficiency. Finally, we provide a theoretical analysis of the algorithm complexity.

A. Framework Overview

Figure 5 shows an overview of the proposed framework. The core elements of E-AFE includes two parts: (1) FPE model, which is to reduce the sample size and candidate feature size

TABLE II: Notations for E-AFE

Notations	Meaning
$\mathcal{D}\langle \mathbf{F},\mathbf{y} angle$	Dataset \mathcal{D} with feature F and label y
\mathcal{T}^{+}	Downstream task (classification or regression)
$A_{\mathcal{T}}(\mathbf{F},\mathbf{y})$	Score of a downstream task \mathcal{T} on (\mathbf{F}, \mathbf{y})
Ě	A set of generated feature
\mathcal{D}^i	The <i>i</i> -th taining set
\mathcal{D}_{i}^{i}	The i -th residual dataset (drawed j -th feature)
$\mathcal{V}^{'}$	Validation set
A_0^i	The score of <i>i</i> -th original training set
A_i^i	The score of residual dataset \mathcal{D}_{i}^{i}
d	MinHash signature output dimension
Н	Approximate hashing features
L	Labels of negative/positive feature (0 or 1)
thre	Threshold of score gain for feature labels (0 or 1)
Rec, Prec	Recall, Precision
$\mathcal{C}_{\mathcal{D}}$	The FPE model
N	The number of features on a target dataset
T	Sample of an episode
s_t	State at time t for one agent
a_t	Action at time t of one agent
r_t	Reward at time t of one agent
γ	Discount factor in range [0,1]
h_t	Action probability distribution at time t of one agent

for improving the evaluation efficiency; (2) two-stage policytraining strategy, which is to boost the learning efficiency by avoiding training from scratch. Specifically, for each original feature, the agent will first generate features following the pipeline as shown in Figure 4. Then, the generated features are fed into the FPE model to reduce sample size with the hashing module, and reduce the candidate feature size with a binary classifier pre-trained by the pre-evaluation task. During the policy training procedure, we will initialize the policy with taking the pre-evaluation task as the evaluation task to train for several epochs. Meanwhile, we construct a replay buffer to record promising actions. Then, we continue to train the policy with real downstream tasks. The proposed framework continue to be trained until the optimal features are achieved.

B. Feature Pre-Evaluation (FPE) Model

As discussed in Section I, sample size and feature size are two vital factors to compromise the efficiency of AFE. Therefore, we develop FPE model to help reduce the sample and feature size to accelerate AFE. Specifically, FPE model consists of two modules: (1) sample compressor, which is to reduce sample size with hashing operations; and (2) feature pre-selector, which is to reduce candidate feature size for evaluation tasks with pre-trained binary classifier.

Sample Compressor. Figure 1 indicates that not all samples are necessary for feature evaluation. Therefore, a method for reducing the sample size is highly desired. Moreover, different datasets have various sizes. To be generalized across datasets, the compression method also expects to compress arbitrary input sizes into the fix one. Therefore, in this work, we adopt hashing techniques as the sample compressor to reduce sample size. Specifically, we take MinHash as the hashing function family. The basic idea of MinHash is to assign the target dimension hashing values, and select d instances with the minimum hashing values as the compressed results [7].

In our sample compressor case, given a dataset (tabular data) $\mathcal{D} \in \mathbb{R}^{M \times N}$ with N features (column) and M samples (row).



Fig. 5: Framework Overview.

We take samples (row) as the target dimension, and input into MinHash. Suppose the expected sample size is d, we expect the compressed dataset with selected d samples should also preserve the sample similarities in the original M-sample dataset. Then the compression process can be represented as

$$\tilde{\mathcal{D}} = \text{MinHash}(\mathcal{D}, d),$$

s.t. $|\text{sim}(\mathcal{D}^1, \mathcal{D}^2) - \text{sim}(\tilde{\mathcal{D}}^1, \tilde{\mathcal{D}}^2)| < \epsilon$ (2)

where $\mathcal{D} \in \mathbb{R}^{M \times N}$ and $\tilde{\mathcal{D}} \in \mathbb{R}^{d \times N}$ denote the original dataset and compressed dataset, respectively, and ϵ denotes a very small constant. D^1 and D^2 are the two datasets whose similarity is to be calculated.

Feature Pre-Selector. Since evaluating features directly on downstream tasks is time-consuming, we develop a fast yet effective pre-evaluation task to pre-select candidate features. Specifically, we pre-train a binary classifier on public datasets to distinguish the effective features from the generated feature set. Formally, given n public datasets, and each dataset is $\mathcal{D}^i = [k^i, m^i], i \in [1, n]$, which include m^i original features and k^i instances. The downstream task \mathcal{T} calculates the original performance score as A_0 . Then, we leave out the j-th feature from *i*-th original dataset to construct the residual dataset \mathcal{D}^i_j . We compare the performance score between A_0 and A^i_j to determine whether the *j*-th feature is effective. Then, the labeling process of feature effectiveness can be represented as

$$\begin{aligned}
\mathbf{A}_{0}^{i} &= \mathcal{T}(\mathcal{D}^{i}), \ i \in [1, n] \\
\mathcal{D}_{j}^{i} &\leftarrow \mathcal{D}^{i} - \mathbf{F}_{j}^{i} \\
\mathbf{A}_{j}^{i} &= \mathcal{T}(\mathcal{D}_{j}^{i}), \ j \in [1, m^{i}], i \in [1, n] \\
\mathbf{L}_{j}^{i} &= \operatorname{sgn}(\mathbf{A}_{0}^{i} - \mathbf{A}_{j}^{i} + thre)
\end{aligned}$$
(3)

where thre is the threshold of score gain; sgn(z) = 1 if z > 0 and sgn(z) = 0 (or equivalently -1) otherwise; **L** is the label vector. Consequently, the effective feature is labeled as 1, otherwise 0. thre is set a small value, such as 0.01. This value is to set the boundary of the binary classification, which is larger than 0, so that better features can be found. If set to 0, many features that are not significantly improved for downstream tasks may be retained. The size of this threshold



is also set according to the recall effect. For example, as shown in Figure 6.

Once the label vector is obtained, we pre-train a binary classifier $\mathcal{C}_{\mathcal{D}}$ paramterized by ϕ through taking the samplecompressed features as input. We select effective features (labeled as 1) as the candidate as the input to evaluation tasks in RL-based AFE. Although the pre-evaluation task is still based on real downstream tasks, once well-trained, the binary classifier can infer the effectiveness of given features quickly. Model Optimization. We exploit cross-entropy as the loss function and take maximizing recall as the optimization target. The objective is to find the optimal sample compressor with the optimal compression size d complying with best featureeffectiveness classifier. Therefore, we consider the sample compressor as the hyperparameter by fine-tuning the hashing function options and compression size d to train the featureeffectiveness classifier. Formally, the predicted label vector L can be represented as

$$\mathbf{H} = \mathrm{MinHash}(\mathcal{D}, d)$$

$$\tilde{\mathbf{L}} = \mathrm{sgn}(\mathcal{C}_{\mathcal{D}}(\mathbf{H}))$$
(4)

Then, according to the ground-truth L and prediction L, we calculate the precision Prec and recall Rec as

$$Prec = \operatorname{Precision}(\mathbf{L}, \mathbf{L}) \tag{5}$$

$$Rec = \text{Recall}(\mathbf{L}, \mathbf{L})$$

Then, the objective can be represented as

$$\mathcal{C}_{\mathcal{D}}^{*}, \operatorname{MinHash}^{*}, d^{*} \leftarrow \operatorname*{argmax}_{\mathcal{C}_{\mathcal{D}}, \operatorname{MinHash}, d} \operatorname{Rec},$$

s.t. $\operatorname{Prec} > 0 \text{ and } \operatorname{Rec} < 1,$ (6)

Algorithm 1 Feature Pre-Evaluation (FPE) Model

Input: *n* public dataset \mathcal{D} for training, every dataset has $k^i, i \in [1, n]$ samples and $m^i, i \in [1, n]$ features. \mathcal{V} is the validation set. \mathcal{T} is the downstream task. **d** is the vector of MinHash signature output dimension for an approximate feature. *thre* is the threshold of score gain for feature labels (0 or 1). MinHash is hash function set.

Output: Trained FPE model C_D , MinHash function and Min-Hash output dimension d.

1: while Select $d \in \mathbf{d}$ or MinHash Function do 2: Let A = [], L = [], Rec = []./*Training model with cross-entropy*/ 3: for $i = 1 \rightarrow n$ do 4: Get \mathbf{A}_0^i by Equ. (3) on \mathcal{D}^i . 5: 6: for $j = 1 \rightarrow m^i$ do Draw sub dataset $\mathcal{D}_j^i \leftarrow \mathcal{D}^i - \mathbf{F}_j^i$. 7: Get \mathbf{A}_{j}^{i} by Equ. (3) on \mathcal{D}_{j}^{i} . 8: if $\mathbf{A}_0^i - \mathbf{A}_j^i > thre$ then 9: 10: $\mathbf{L}_{i}^{i} \leftarrow 1$ else 11: $\mathbf{L}_{i}^{i} \leftarrow 0$ 12: end if 13: $\mathbf{H}_{i}^{i} \leftarrow \text{MinHash}(\mathbf{F}_{i}^{i}, d)$ as Equ. (4) 14: 15: end for end for 16: /*Validating model for recall*/ 17: $\tilde{\mathbf{L}} = \operatorname{sgn}(\mathcal{C}_{\mathcal{D}}(\mathbf{H}))$ as Equ. (4) 18: $Rec = \text{Recall}(\mathbf{L}, \mathbf{L})$ as Equ. (5) 19: 20: end while 21: /*Train and fine-tune the FPE model*/ 22: $\mathcal{C}^*_{\mathcal{D}}$, MinHash^{*}, $d^* \leftarrow \operatorname{argmax} (Rec)$ as Equ. (6) $\mathcal{C}_{\mathcal{D}}, \widetilde{MinHash}, d$ 23: **return** $\mathcal{C}^*_{\mathcal{D}}$, MinHash^{*}, d^*

where $C_{\mathcal{D}}^*$, MinHash^{*} and d^* are optimal classifier, and the corresponding hashing function and compressed sample size, respectively. We perform stochastic gradient descent (SGD) to train and fine-tune the FPE model. Algorithm 1 shows the calculation details of FPE model.

C. Two-Stage Training Strategy

We integrate the well-trained FPE model into the RL-based AFE framework to construct E-AFE, as shown in Figure 5. The conventional training process of RL-based AFE methods suffer from exhaustively exploring the action-state space, which wastes a lot of running time to reach the optimum. Therefore, to solve the problem, we propose the two-stage training strategy by borrowing external knowledge from pre-trained FPE model to avoid learning policy from scratch. The two-stage training strategy includes: (1) quick initialization with FPE model, and (2) formal training.

Stage 1: Quick Initialization with FPE Model The benefits of FPE model lie in two aspect. On the one hand, FPE model is trained on various public datasets, which contain rich external knowledge of feature characteristics; On the other hand, the well-trained FPE can directly infer the effectiveness of the

Algorithm 2 Two-Stage Policy Training Strategy

Input: Trained FPE model $C_{\mathcal{D}}$. Features **F** of the target dataset. MinHash function. MinHash output dimension *d*. **Output**: Maximize score of downstream task

- 1: /*Stage 1: Quick Initialization with FPE Model*/
- 2: while Choose agent one by one do
- 3: Agent sample action with equal rate
- 4: Action generates new feature $\tilde{f} \in \tilde{\mathbf{F}}$
- 5: Evaluate \hat{f} by Equ. (7)
- 6: **if** \tilde{f} is positive feature **then**
- 7: Store this feature to replay buffer
- 8: else
- 9: Dropout this feature
- 10: end if
- 11: Get A_t^h by Equ. (8)
- 12: Get return U_t^h by Equ. (9) for every agent
- 13: end while
- 14: Agents initialization complete
- 15: /*Stage 2: Formal Training*/
- 16: while Get feature from replay buffer do
- 17: Sample feature transformation with action prob.
- 18: Generate new features by transformation
- 19: Save score of the downstream task
- 20: Get return U_t^{λ} by Equ. (10).
- 21: end while
- 22: Trained agents
- 23: return Maximize score of downstream task

generated features, which saves substantial time comparing to the downstream task evaluation. Therefore, at the initialization stage, we omit the downstream task evaluation, but directly take the results from FPE model as the reward to update the policy of *E-AFE*. Formally, we compute the reward of each action as follows: for taking action a_t , the improvement r_t is the score A_t of state s_t minus A_{t-1} of state s_{t-1} , which means the gain of performing a_t intuitively. Then, we utilize the $\lambda - return \ U_t^{\lambda}$ that combines all k - step returns U_t as the final reward signal for action a_t . We define A^O and A^h as the performance score of the original dataset and compressed dataset by FPE model, respectively. ΔA_{max} and ΔA_{min} are the maximize and minimize score gain of input space. Then, the accumulated reward can be computed as

$$p = \mathcal{C}_{\mathcal{D}}(\mathsf{MinHash}(f, d)) \tag{7}$$

$$A_t^h = \begin{cases} A^O + \frac{0.5 - p}{0.5} (\Delta A_{max} - thre), p \in [0, 0.5) \\ A^O + \frac{0.5 - p}{0.5} (thre - \Delta A_{min}), p \in [0.5, 1] \end{cases}$$
(8)

where, *thre* is the threshold of score gain for feature labels (0 or 1). \check{f} is a new feature from the test set. p is the output probability of the binary classifier.

$$r_{t}^{h} = A_{t}^{h} - A_{t-1}^{h}$$
$$U_{t}^{h} = r_{t}^{h} + \gamma r_{t+1}^{h} + \dots + \gamma^{k} r_{t+k}^{h} = \sum_{k=0}^{t} \gamma^{(t-k)} r_{k}^{h}$$
(9)

Stage 2: Formal Training After several epochs of training in stage 1, we then change the evaluation task to the real downstream task. We take the output of FPE model (preselected feature with reduced sample and feature size) as the candidate features to formally train the policy, where the reward is computed as the performance gain on the downstream tasks. To be consistent with the stage 1, we represent the accumulated rewards for stage 2 as:

$$r_{t} = A_{t} - A_{t-1}$$

$$U_{t} = r_{t} + \gamma r_{t+1} + \dots + \gamma^{k} r_{t+k} = \sum_{k=0}^{t} \gamma^{(t-k)} r_{k}$$

$$U_{t}^{\lambda} = (1-\lambda) \sum_{k=1}^{N \times T} \lambda^{k-1} U_{t},$$
(10)

where A_t and A_{t-1} are evaluation scores of two successive feature sets on the downstream tasks, respectively.

Policy Learning. To explore the optimal actions (feature transformations), we train agents to maximize their expected return, represented by $J(\theta^{[1]}, ..., \theta^{[j]}, \theta^{[N]})$, where the *j*-th agent is parameterized by $\theta^{[j]}$. Then, the expected return can be represented as

$$J(\theta^{[1]}, ..., \theta^{[N]}) = \mathbb{E}_{P(a_{1:N \times T}; \ \theta^{[1]}, ..., \theta^{[N]})} \left[\sum_{t=1}^{N \times T} U_t^{\lambda} \right]$$
(11)

To achieve an empirical approximation, we utilize the REIN-FORCE [8] rule and Monte Carlo simulation [9] to update the parameters:

$$\nabla_{\theta^{[1]},...,\theta^{[N]}} J(\theta^{[1]},...,\theta^{[N]}) \approx \frac{1}{m} \sum_{k=1}^{m} \sum_{t=1}^{N \times T} \nabla_{\theta^{[1]},...,\theta^{[N]}} \log \mathbb{P}(a_t | a_{1,t-1}; \ \theta^{[1]},...,\theta^{[N]}) U_{t,[k]}^{\lambda}$$
(12)

where m is the number of batch size that the agent samples per epoch and $U_{t,[k]}^{\lambda}$ is the cross-validation score that the k-thsample achieves. Algorithm 2 shows the calculation details of the two-stage training strategy.

D. Theoretical Analysis

We first analyze the complexity of the proposed FPE model on reducing sample and feature sizes. The training complexity of FPE is related to the size of search space and datasets. Suppose there are h hash functions in search space, the α candidate options of the sample size d. In the training process, given n public datasets $\mathcal{D}^i = [k^i, m^i], i \in [1, n]$, and vvalidation set $\mathcal{V}^{\gamma} = [j^{\gamma}, t^{\gamma}], \gamma \in [1, v]$, the training complexity of FPE model in stage 1 is $O((h \cdot \alpha \cdot d) \cdot (n \cdot k \cdot m) \cdot (v \cdot j \cdot t))$. When we integrate FPE model in RL-based AFE, the FPE model serves as a sample compressor and feature pre-selector via quick inference. With the two-stage training strategy, *E*-*AFE* evaluates the generated feature with the binary classifier first and then with the downstream tasks. Formally, given N agents (original features) with k samples, each agent performs T times of feature transformations to get m generated features. The complexity in the first training stage is $O(d \cdot k \cdot m \cdot N \cdot T)$. After initialization from stage 1, we continue to train the policy with cross-validation downstream tasks. Suppose the downstream task of RF cross-validation complexity is O(c), the policy update *epoch*, the dropout rate is *ratio*, and the complexity of the stage 2 is $O(c \cdot N \cdot T \cdot epoch \cdot ratio)$.

Then, the two-stage policy training complexity of *E-AFE* is $O((h \cdot \alpha \cdot d) \cdot (n \cdot k \cdot m) \cdot (v \cdot j \cdot t)) + O(c \cdot N \cdot T \cdot epoch \cdot ratio).$ Stage 1 runs the inference process of the FPE model, which is far less than the cross-validation time of RF and can be excluded. If you consider deploying to multiple target datasets, the FPE model can be reused, and the training time of the FPE model is much shorter than the deployment time. Therefore $O(c \cdot N \cdot T \cdot epoch \cdot ratio) >> O((h \cdot \alpha \cdot d) \cdot (n \cdot k \cdot m) \cdot$ $(v \cdot j \cdot t)$, the finally complexity is $O(c \cdot N \cdot T \cdot epoch \cdot t)$ ratio). Compared to the state-of-the-art AFE method NFS, its complexity is $O(c \cdot N \cdot T \cdot epoch \cdot ratio)$. Our method drop rate is more than 0.5. Our algorithm guarantees 2x faster than NFS when running the same epoch without early stopping. As the drop rate increases, our algorithm is faster. The drop rate increase positively correlates with the FPE model's ability to recall good new features on the current dataset.

IV. RESULTS AND DISCUSSION

In this section, we conduct extensive experiments to answer the following research questions: Q1: How is the performance of our *E-AFE* in online AFE tasks as compared to state-ofthe-art methods? Q2: How is the performance of *E-AFE* variants with different combinations of key components in the RL framework? Q3: How is the performance of *E-AFE* with a different RL framework? Q4: Is deep learning better than feature engineering for the tabular dataset? Q5: How do the key hyperparameter settings impact *E-AFE* 's performance? Q6: Why MinHash is chosen? Q7: Are the results robust to other downstream tasks? Q8: Is the performance improvement robust? Q9: How the method is performing with increasing numbers of features and larger datasets? In the following subsections, we first present the experimental settings and then answer the above research questions in turn.

A. Experimental Settings

1) Data Description: We collect 239 public datasets for pre-training FPE, and 36 datasets for downstream task evaluations. Specifically, the collected public datasets are from OpenML¹ with 141 classification datasets and 98 regression datasets. And the datasets for downstream tasks include 26 classification datsets and 10 regression datasets. Detials about the datasets can be found in Table III.

¹http://www.openml.org

TABLE III: Comparison results on 36 target datasets. C\R is the downstream type. C is classification. R is regression. $RTDL_N$ (DL_N) is ResNet with RF from RTDL [10]. AutoFS_R (FS_R) [11], [12] is feature selection from randomly generated features. NFS [6] is feature generation and evaluation. The FE|DL method is to put the features selected by feature engineering into the deep learning process. The DL|FE method puts the original features into the deep learning training and then puts the output features into the feature engineering method for feature selection. $E-AFE_D$ is the ablation study of E-AFE, replacing the approximate hashing model with a random dropout method. $E-AFE_R$ is the ablation study of E-AFE, replacing the RL framework with policy gradient method like NFS [6] used. $E-AFE^P$ is E-AFE with PCWS [13]. $E-AFE^I$ is E-AFE with ICWS [14]. $E-AFE^L$ with LICWS [15]. E-AFE use CCWS [16]

Dataset	C∖ R	Samples\ Features	FS_R	DL_{N}	NFS	FE DL	DL FE	E - AFE_R	E-AFE _D	E - AFE^L	E-AFE ^P	E-AFE ^I	E-AFE
Higgs Boson	C	50000\28	0.723	0.756	0.731	0.779	0.836	0.725	0.802	0.821	0.833	0.816	0.836
A. Employee	C	32769\9	0.948	0.484	0.950	0.677	0.532	0.943	0.950	0.950	0.951	0.950	0.951
PimaIndian	C	768\8	0.779	0.743	0.790	0.787	0.797	0.783	0.792	0.793	0.797	0.795	0.798
SpectF	C	267\44	0.871	0.639	0.876	0.760	0.684	0.862	0.900	0.903	0.900	0.892	0.903
SVMGuide3	C	1243\21	0.842	0.728	0.846	0.741	0.793	0.843	0.875	0.872	0.879	0.881	0.881
German Credit	С	1001\24	0.775	0.681	0.780	0.692	0.712	0.773	0.810	0.796	0.816	0.813	0.816
Bikeshare DC	R	10886\11	0.978	0.945	0.990	0.973	0.993	0.983	0.992	0.991	0.993	0.993	0.993
Housing Boston	R	506\13	0.709	0.648	0.710	0.670	0.720	0.693	0.798	0.813	0.819	0.817	0.821
Airfoil	R	1503\5	0.784	0.697	0.796	0.723	0.741	0.781	0.790	0.795	0.810	0.807	0.810
AP. ovary	С	275\10936	0.852	0.659	0.864	0.684	0.671	0.858	0.879	0.880	0.876	0.879	0.884
Lymphography	C	148\18	0.895	0.000	0.922	0.000	0.000	0.921	0.960	0.958	0.960	0.961	0.964
Ionosphere	C	351\34	0.934	0.883	0.957	0.906	0.913	0.944	0.973	0.977	0.964	0.970	0.977
Openml 618	R	1000\50	0.619	0.072	0.640	0.678	0.143	0.635	0.728	0.729	0.731	0.737	0.737
Openml 589	R	1000\25	0.737	0.578	0.754	0.765	0.647	0.748	0.757	0.754	0.762	0.762	0.764
Openml 616	R	500\50	0.609	0.000	0.673	0.510	0.000	0.653	0.675	0.676	0.689	0.680	0.689
Openml 607	R	1000\50	0.634	0.025	0.688	0.603	0.027	0.678	0.728	0.729	0.727	0.733	0.734
Openml 620	R	1000\25	0.705	0.047	0.732	0.741	0.078	0.727	0.736	0.734	0.747	0.741	0.748
Openml 637	R	500\50	0.608	0.016	0.634	0.539	0.039	0.633	0.624	0.635	0.642	0.636	0.646
Openml 586	R	1000\25	0.749	0.521	0.780	0.612	0.542	0.780	0.790	0.793	0.781	0.784	0.793
Credit Default	C	30000\25	0.782	0.678	0.815	0.738	0.693	0.812	0.819	0.821	0.821	0.816	0.822
Messidor features	С	1150\19	0.743	0.731	0.757	0.765	0.793	0.756	0.781	0.783	0.790	0.784	0.793
Wine Q. Red	C	999\12	0.671	0.387	0.692	0.514	0.421	0.691	0.716	0.717	0.720	0.723	0.723
Wine Q. White	C	4900\12	0.652	0.371	0.687	0.403	0.469	0.671	0.708	0.708	0.705	0.708	0.708
SpamBase	С	4601\57	0.934	0.939	0.938	0.949	0.949	0.935	0.949	0.949	0.949	0.944	0.949
AP. lung	C	203\10936	0.962	0.944	0.966	0.955	0.985	0.964	0.983	0.985	0.979	0.985	0.985
credit-a	C	690\6	0.782	0.798	0.793	0.802	0.815	0.789	0.810	0.814	0.893	0.815	0.815
diabetes	C	768\8	0.778	0.695	0.784	0.714	0.748	0.782	0.798	0.798	0.781	0.784	0.798
fertility	C	100\9	0.896	0.474	0.900	0.513	0.486	0.900	0.916	0.911	0.919	0.913	0.920
gisette	C	2100\5000	0.951	0.950	0.952	0.960	0.978	0.950	0.971	0.973	0.969	0.978	0.978
hepatitis	C	155\6	0.877	0.162	0.884	0.253	0.195	0.873	0.910	0.894	0.910	0.887	0.910
labor	С	57\8	0.876	0.862	0.930	0.899	0.964	0.930	0.964	0.957	0.960	0.960	0.964
lymph	C	138\10936	0.961	1.000	0.964	1.000	1.000	0.964	0.992	1.000	0.990	0.994	1.000
madelon	C	780\500	0.742	0.564	0.751	0.681	0.638	0.740	0.860	0.860	0.864	0.864	0.867
megawatt1	C	253\37	0.899	0.620	0.913	0.743	0.693	0.904	0.943	0.941	0.937	0.942	0.945
secom	C	470\590	0.922	0.030	0.929	0.092	0.092	0.927	0.930	0.929	0.932	0.932	0.932
sonar	C	208\60	0.740	0.699	0.770	0.769	0.840	0.768	0.840	0.842	0.833	0.837	0.842

2) Evaluation Protocols and Metrics: The following metrics are used for evaluating our proposed method. TP, TN, FP, FN are true positive, true negative, false positive and false negative for all classes. **Precision** is given by $\frac{TP}{TP+FP}$. **Recall** is given by $\frac{TP}{TP+FN}$. **F1-score** is the harmonic mean of precision and recall, given by $\frac{2 \times Precision \times Recall}{Precision+Recall}$. **1-relative absolute error** (1-rae) is given by $1 - rae = 1 - \sum_{j=1}^{j} \frac{|\tilde{y}-y|}{|\tilde{y}-y|}$, where y is the actual target, \bar{y} is the mean of y, and \tilde{y} is prediction results by model. We use F1-score for the classification problem, and use 1-rae for the regression problem.

3) Baseline Methods: We compare the performance of our method (namely *E-AFE*) against the following baseline algorithms.

(1)NFS. Neural Feature Search (NFS) [6] is the most accurate method at present. It uses RF as the downstream task. For a fair comparison, we use RF in other comparison methods.

(2) $RTDL_N$. RTDL [10] concludes that ResNet-like archi-

tecture is effective for tabular deep learning. Our ResNet [17] method is derived from RTDL. First, we divide each target dataset into train, validation, and test sets for RTDL. After training and validating the ResNet in the framework of RTDL, we change the downstream task of ResNet, softmax, into RF, then test the modified ResNet model.

(3) $AutoFS_R$. The RL framework of AutoFS [11], [12] can't consider feature generation. So we generated features randomly and selected features by AutoFS.

4) Reproducibility and Parameter Settings: We implemented our RL framework based on TensorFlow and chose Adam [18] as our optimizer to learn the model parameters. The learning rate is 0.01. The batch size is 32. We use four unary operations, such as logarithm, min-max-normalization, square root, and reciprocal, and five binary operations, such as addition, subtraction, multiplication, division, and modulo operation. Our default MinHash signature output dimension is 48, and the MinHash function is CCWS. The maximum order is 5. Threshold *thre* is 0.01. The training epoch of the two-stage policy training strategy is 200, respectively.

B. Performance Comparison (Q1)

We evaluated the performance of all compared algorithms on 26 classification and 10 regression datasets and reported the evaluation results in Table III, IV, and Figure 7. To reduce the feature space, *E-AFE* first conducts feature selection of less than maximum features according to the feature importance via RF on the 36 raw target datasets. Then, In the learning curve, we sample score results when the training epoch is 0, 10, 30, 60, 90, 120, 150, or 200. From the evaluation results, we summarize several key observations as follows:

We can observe that the learning speed of E-AFE is more than 2x that of NFS [6] when the learning curve is saturated. The evaluated features of E-AFE are less than 50% of other methods. In the two-stage training strategy, by dropping some bad generated features, E-AFE can significantly improve the learning speed of AFE. Comparing time with the same score, E-AFE is 10x faster than NFS in some datasets. E-AFE^L, E-AFE^P and E-AFE^I are all variants of E-AFE, just using different MinHash functions.

AutoFS_R [11] has not had enough generated features for feature selection, and the final score is less than *E-AFE*. AutoFS [11], [12] with random feature generation does not fully mine the knowledge of feature generation. The randomly generated feature set does not have enough good features to give AutoFS for feature selection.

The score of $RTDL_N$ [10] is the lowest. The ResNet feature extractor is not suitable for tabular datasets at any time. We believe that the convolution kernel of the CNN network is specially designed for data types such as images, and it is not ideal for tabular data processing.

C. Model Ablation Study of E-AFE (Q2)

In addition to comparing *E-AFE* with state-of-the-art techniques, we aim to understand the proposed framework better and evaluate the critical components of the FPE model. Mainly, we aim to answer the following question: How is the performance of *E-AFE* variants with different combinations of critical components in the RL framework? Hence, in our evaluation, we consider the random drop feature method $E-AFE_D$ for the ablation study:

In Table III, IV, and Figure 7, the score of comparison between E-AFE and E-AFE_D, our FPE model gets a higher score. According to evaluated generated features by downstream task, our method is mostly evaluated less than other methods. The results of E-AFE_D prove that the new features have redundancy for AFE. The above ablation study results also demonstrate that our method does learn more effective knowledge of discarding redundant features than dropping new features randomly.

D. Effect of RL in E-AFE Framework (Q3)

To show the effect of the RL framework in our developed E-AFE, we replaced our designed RL framework with the policy gradient method E-AFE_R for the ablation study:

TABLE IV: Comparison of feature evaluation numbers of one epoch in the target dataset. AutoFS_R (FS_R) [11], [12] is feature selection from randomly generated features. NFS [6] is feature generation and evaluation. E- AFE_D is the ablation study of E-AFE, replacing the approximate hashing model with a random dropout method.

1				
Dataset	FS_R	NFS	$E-AFE_D$	E-AFE
Higgs Boson	4640	4585	2273	2182
A. Employee	1440	1322	667	603
PimaIndian	1280	1230	585	474
SpectF	7040	6964	3372	3116
SVMGuide3	3360	3269	1577	1573
German Credit	3840	3748	1634	1473
Bikeshare DC	1600	1537	743	327
Housing Boston	1920	1826	898	559
Airfoil	800	698	333	161
AP. ovary	8000	7905	3937	4008
Lymphography	2880	2809	1339	1160
Ionosphere	5440	5364	2600	2139
Openml 618	8000	7905	3903	1572
Openml 589	4000	3889	1934	975
Openml 616	8000	7917	3967	2009
Openml 607	8000	7900	3960	1671
Openml 620	4000	3883	1924	929
Openml 637	8000	7894	4040	2038
Openml 586	4000	3891	1996	932
Credit Default	3680	3593	1823	1608
Messidor features	3040	2958	1470	1448
Wine Q. Red	1760	1665	867	806
Wine Q. White	1760	1646	849	596
SpamBase	9120	9016	4347	4015
AP. lung	8000	7905	3954	3966
credit-a	960	898	415	483
diabetes	1280	1208	589	489
fertility	1440	1361	670	552
gisette	8000	7875	3954	3667
hepatitis	960	836	407	363
labor	1280	1202	596	695
lymph	8000	7891	4042	4033
madelon	8000	7923	3549	3549
megawatt1	5760	5695	2845	2319
secom	3200	3087	1559	1647
sonar	9600	9501	4747	4762

Table III shows that our RL framework method E-AFE is better than E-AFE_R. Figure 5 shows that our RL framework explores knowledge from offline public datasets and exploits new knowledge online from a target dataset. Especially our method not only use the final result of the downstream task but also cache the intermediate result of the downstream task in the process of training agents. This RL framework is also the source of improving the score of our method compared with the NFS [6] method, which uses the policy gradient to train the controller and get a result at the final test. However, NFS omitted the cross-validation results in the training process, resulting in time-consuming and poor results.

E. Comparison with DNN method (Q4)

To compare the feature engineering method with the deep learning method, we invite the RTDL [10] method for baseline.

In Table III, we can see that feature engineering-related methods are more robust than ResNet from RTDL. The results of ResNet have 0.0 or near 0.0. We consider that ResNet is less useful in mini datasets, such as Lymphography and hepatitis. In the mini dataset, NFS [6] and *E-AFE* have



Fig. 7: Performance comparison. We show the converging curve of four methods on target datasets. *E-AFE* is our method. AutoFS_R [11], [12] is feature selection from randomly generated features. NFS [6] is feature generation and evaluation. *E-AFE_D* is the ablation study of *E-AFE*, replacing the approximate hashing model with a random dropout method.

significant advantages to ResNet. However, if the dataset is large, ResNet performs similarly to NFS [6] and E-AFE, such as Higgs Boson, SpamBase, AP. lung, and gisette. The robustness loss of DNN results comes from its pre-division of data sets into training, validation, and test sets. Especially for small data sets, this partition is a fatal disadvantage. The

robust result comes from the cross-validation downstream task of the feature engineering-related method, though this crossvalidation is very time-consuming. We also mix deep learning and feature engineering methods in Table III, and DL|FE and FE|DL also support the above analysis results.

F. Hyperparameter Sensitivity Studies (Q5)

E-AFE involves several parameters (e.g., Threshold *thre*, MinHash signature output dimension and Maximum Order). To investigate the robustness of our method, we examine how the different choices of parameters affect the performance of *E-AFE*. Except for the parameter being tested, we set other parameters at the default values.

We use auto-sklearn for training and validation the FPE model. *thre* divides the features into positive and negative ones. The FPE model is trained on the approximate hashing features from the original public training set and validated on the approximate hashing features from the validation set.

Figure 8 shows the evaluation results on data as a function of one selected parameter when fixing others. Overall, we observe that *E-AFE* is not strictly sensitive to these parameters, demonstrating our proposed framework's robustness. In particular, we can observe that score achieves better performance with the decrease of the threshold. The reason is that a smaller threshold has a larger recall for the validation set. The MinHash output length have something with the score. The reason is that the approximate features generated by the hash function can affect training results. This paper uses a variety of hash functions and different compressed feature lengths to generate approximate features. If the MinHash signature output dimension set is too small, it will extract too little information from the original feature and is not conducive to hash model training. Some datasets may get a better score with the maximum order increase, but the evaluated features and training time will increase significantly. Our experiments set the maximum order as 5 due to the effectiveness and computational cost trade-offs.





G. MinHash Explanations and Signature Sensitivity (Q6)

On the one hand, MinHash can map arbitrary size samples into the fixed size (like other Hash functions do), which is necessary for across datasets data engineering; on the other hand, one unique property of MinhHash is to quickly estimate the similarity between two samples with hashing signature, which can capture and preserve the relationships between samples during hashing, leading to limited information loss caused by compression [7]. Table III shows little difference in the effect obtained by different MinHash functions.

H. Replace downstream task (Q7)

We add one more experiment to verify that the features generated by our AFE are also robust to other downstream

TABLE V: Comparison results on 36 datasets. C is classification, R is regression. AutoFS_R [11], [12] is feature selection from randomly generated features. NFS [6] is feature generation and evaluation. SVM is support vector machines, NB is gaussian naive bayes for classification, GP is gaussian processes for regression, MLP is multi-layer perceptron.

	-	AutoFS _B			NFS			E-AFE		
Dataset	C/R	SVM	NB GP	MLP	SVM	NB GP	MLP	SVM	NB GP	MLP
fertility	C	0.880	0.670	0.760	0.870	0.140	0.300	0.880	0.880	0.900
hepatitis	С	0.794	0.819	0.561	0.774	0.316	0.329	0.813	0.826	0.813
labor	C	0.648	0.839	0.482	0.582	0.667	0.333	0.876	0.911	0.808
PimaIndian	C	0.762	0.749	0.569	0.638	0.352	0.469	0.779	0.772	0.626
credit-a	C	0.655	0.657	0.536	0.545	0.555	0.445	0.733	0.748	0.713
diabetes	C	0.762	0.757	0.509	0.642	0.352	0.397	0.770	0.768	0.638
german credit	C	0.713	0.727	0.663	0.688	0.302	0.390	0.734	0.754	0.731
ionosphere	C	0.937	0.869	0.539	0.632	0.442	0.388	0.952	0.906	0.821
sonar	C	0.558	0.590	0.518	0.447	0.441	0.335	0.683	0.667	0.721
spambase	С	0.606	0.826	0.899	0.568	0.388	0.399	0.810	0.847	0.914
SPECTF267	C	0.790	0.670	0.701	0.775	0.513	0.323	0.839	0.794	0.798
AP. lung	C	0.695	0.936	0.626	0.586	0.404	0.339	0.936	0.946	0.867
lymph	C	0.899	0.935	0.682	0.499	0.456	0.363	0.928	0.950	0.884
lymphography	C	0.810	0.713	0.570	0.563	0.465	0.352	0.852	0.838	0.768
madelon	C	0.664	0.504	0.535	0.469	0.468	0.435	0.751	0.621	0.578
megawatt1	C	0.893	0.806	0.565	0.873	0.166	0.222	0.897	0.893	0.893
messidor features	C	0.693	0.611	0.517	0.513	0.467	0.476	0.709	0.643	0.673
AP. ovary	C	0.804	0.789	0.636	0.695	0.284	0.280	0.822	0.829	0.775
secom	C	0.934	0.720	0.906	0.925	0.262	0.712	0.934	0.919	0.931
A. Employee	C	0.942	0.912	0.890	0.942	0.746	0.683	0.942	0.942	0.942
svmguide3	C	0.762	0.817	0.763	0.749	0.240	0.314	0.817	0.825	0.778
Wine Q. Red	C	0.511	0.528	0.475	0.425	0.459	0.334	0.537	0.553	0.527
Wine Q. White	C	0.458	0.436	0.374	0.441	0.159	0.337	0.477	0.479	0.476
credit default	C	0.779	0.380	0.660	0.778	0.222	0.492	0.808	0.780	0.777
gisette	C	0.580	0.555	0.880	0.498	0.486	0.506	0.962	0.900	0.920
higgs boson	C	0.704	0.685	0.695	0.669	0.331	0.432	0.735	0.701	0.720
Bikeshare DC	R	0.977	0.773	0.998	0.976	0.773	0.998	0.977	0.773	0.999
boston housing	R	0.614	0.468	0.509	0.612	0.467	0.476	0.614	0.468	0.525
Airfoil	R	0.680	0.311	0.323	0.670	0.311	0.323	0.680	0.314	0.341
openml 618	R	0.631	0.523	0.218	0.630	0.523	0.438	0.633	0.523	0.671
openml 589	R	0.638	0.548	0.543	0.637	0.548	0.249	0.641	0.548	0.605
openml 616	R	0.552	0.486	0.324	0.549	0.486	0.459	0.558	0.486	0.636
openml 607	R	0.623	0.485	0.369	0.620	0.485	0.497	0.624	0.485	0.606
openml 620	R	0.619	0.521	0.340	0.618	0.518	0.488	0.622	0.521	0.265
openml 637	R	0.519	0.468	0.404	0.517	0.468	0.409	0.523	0.473	0.575
openml 586	R	0.647	0.523	0.756	0.646	0.523	0.726	0.649	0.523	0.759

tasks. Specifically, we cache the features generated by different AFEs and replace Random Forest with other models (*i.e.*, taking widely-used SVM as an exmaple) to evaluate the quality of these features. We also list the results in Table V for your reference. The results indicate that with our proposed framework, the features obtained from random forest can consistently outperform baselines using SVM, which indicates the features selected by our method are robust to other models.

I. Improvement analysis (Q8)

TABLE VI: P-value of *E-AFE* with other baseline methods

P-value	$AutoFS_R$ E-AFE	$RTDL_N \mid E-AFE$	NFS E-AFE
Performance	5.08×10^{-2}	9.87×10^{-7}	1.83×10^{-1}
Time	1.97×10^{-6}	2.75×10^{-11}	3.75×10^{-6}

Specifically, we calculate the p-value of the improvement over each baseline method in terms of both effectiveness (accuracy) and efficiency (running time) to check the significance. The results in Table VI indicate that for efficiency, p-value of improvement over baselines NFS, $AutoFS_R$, and $RTDL_N$ are 3.75×10^{-6} , 1.97×10^{-11} , and 2.75×10^{-11} , respectively, which shows that the improvement on efficiency is statistically significant; for effectiveness, the improvement over $RTDL_N$ is statistically significant with p-value as 9.87×10^{-7} , and the improvement over $AutoFS_R$ is statistically near-significant with p-value as 5.08×10^{-2} . But the effectiveness improvement over NFS is not statistically significant with the p-value as 1.83×10^{-1} . The reason is that the difference of our method over NFS is mainly on developing the two-stage training strategy with reduced sample/feature size to improve the efficiency, while both of the two methods exploits reinforcement learning-based crossvalidation for feature evaluation. Thus, the improvement on efficiency is statistically significant, while the effectiveness improvement is incremental.

J. Scalability analysis (Q9)



(1) Performance (2) Performance (3) Performance (4) Performance vs. Feature Num- vs. Sample Number vs. Feature Num- vs. Sample Number ber ber

Fig. 9: Time or performance improvement vs. feature or sample size.

Figure 9 results show the relationship between running time and performance improvement with data size. The performance improvement of E-AFE on larger datasets are better on smaller dataset, which demonstrate scalability ability of our proposed method.

V. RELATED WORK

A. Automated Feature Engineering

AFE method can be divided into three types: (1)The downstream task has no feedback to the feature generator. ExploreKit [19] performs all transformation functions on the dataset. AutoLearn [2] preprocesses raw features and discards features with low information gain. Learning Feature Engineering (LFE) [4] uses feature-class representation and a set of Multi-Layer Perception (MLP) classifiers to predict whether the transformation result is better than the original feature. (2)The downstream task gives feedback to the feature generator with RL. Transformation Graph [5] builds DAG and uses Q-learning to exploit high-order features. Neural Feature Search (NFS) [6] predicts the most appropriate transformation for each feature by policy gradient for better feature generation. Group-wise Reinforcement Feature Generation (GRFG) [20] proposes a principled framework to address the automation, explicitness, optimal issues in representation space reconstruction. (3)Feature selection with RL ignores feature generation. Multi-Agent Reinforcement Learning Feature Selection (MARLFS), Interactive Reinforced Feature Selection (IRFS), Single-Agent Reinforcement Learning Framework (SADRLFS), Monte Carlo based reinforced feature selection (MCRFS), Group-based Interactive Reinforced Feature Selection (GIRFS) and Combinatorial Multi-Armed Bandit (CMAB) on feature selection [11], [12], [21]-[26] use RL in feature selection. However, those RL frameworks can't consider feature generation.

B. Approximate Feature

To speed up feature engineering, many methods to obtain an approximate dataset from the original dataset are proposed. We summarize four classes of approximate feature methods. (1)Meta-Feature. Previous approaches used hand-crafted metafeatures, including information-theoretic and statistical metafeatures, to represent datasets [19], [27]-[29]. Meta-Feature Extractor (MFE) [30], [31] extracts meta-features from the dataset to improve the reproducibility of machine learning. Automatic generation of meta-features [32] presents a framework to generate meta-features in the context of meta-learning systematically. ExploreKit [19] generates two types of metafeatures: dataset-based and candidate features-based. (2)Lowrank matrix approximation [33], [34] finds a smaller rank matrix similar to the original matrix. (3)Quantile Data Sketch was used in LFE [4] to represent feature values. (4)Hashing method. Feature Hashing [35] introduces specialized hash functions with unbiased inner products that are directly applicable to a large variety of kernel methods. Hash kennel [36], [37] computes the kernel matrix for data streams and sparse feature spaces.

VI. CONCLUSION REMARKS

In this paper, we studied how to improve the efficiency of AFE. Based on the empirical studies, we identified that the time-consuming feature evaluation procedure is the core reason of interfering with AFE's running efficiency. We further validated that smaller sample size and feature size would accelerate feature evaluation. Therefore, we proposed to improve the efficiency of AFE by reducing the sample and feature size. Specifically, we develop FPE model, including a sample compressor with MinHash to reduce sample size, and a feature pre-selector with a pre-trained binary classifier to distinguish the effectiveness of the generated features. Moreover, we devised a two-stage training strategy to first initialize the policy using the binary feature-effectiveness classification as the evaluation task to borrow external knowledge from the pretrained FPE. The enhanced initialization provideed the AFE policy with a good starting point for exploring the optimal actions, which further significantly save the running time. Finally, we conduct extensive experiments on 36 datasets on both the classification and regression tasks. When compared to state-of-the-art AFE methods, the results show 2.9 percent higher average performance and 2x higher computational efficiency. The improvements over both the effectiveness and efficiency proved that FPE model can remove the redundancy in candidate features.

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