Abstract

Feature selection is a process <u>that</u> aimings forto reducinge the number of variables when building a prediction model or performing a machine learning procedure. In this paper, we suggestpropose an automated machine learning mechanism for the task of feature selection, which and that relies on the comparison between two methods: Random Forest and XGBoost classifier. We present both backward and forward approaches for the feature selection process, and test our suggested the proposed algorithm on <u>4 four</u> different datasets. In all cases, the results show that the number of features for building the model can be significantly reduced, while retaining high model accuracy is maintained high. Our The proposed automated feature selection method presents an effective and efficient strategy for users to adopt in order to choose accurate algorithms and features that significantly influence the predicted variable.

Feature selection, AutoML, Random forest, XGBoost

1 Introduction

Feature selection is one of the most important tasks and a core concept in machine learning, specifically especially in predictive models. Using irrelevant features when training a model may affect the performance of the model, reduce accuracy, and cause overfitting. By choosing wisely the best and most significant features from the data when building the model, one can avoids overfitting, improves prediction accuracy, and reduces the training time. Feature selection has been widely studied widely in the literature (see, e.g. [?], [?], [?], [?], [?], [?] and many references therein). Feature selection _ and is applied toused in many fields, such as statistical pattern recognition [?], [?], [?], face recognition [?], data mining and machine learning [?], [?], [?], [?], text categorization [?], customer relationship management [?], bioinformatics [?], genomics [?], and cross-project defect prediction [?], and more. Furthermore, inRef. [?], the authors provides a comprehensive survey onf online feature selection with streaming features (i.e., when features are generated dynamically).

Feature selection methods are mainly divided into filter methods, wrapper methods, and embedded methods. Filter methods use variable ranking techniques, and some ranking criteria to decide whether a variable should be removed from the model or not. In wrapper methods, a subset of features is evaluated <u>by</u> using a machine learning algorithm that employs a search strategy to look through the space of possible feature subsets. Each subset is evaluated based on the quality of the performance of a given algorithm. Embedded methods perform feature selection during the <u>execution of the</u> modeling algorithm's execution. For a review of these methods, see Ref. [?].

In tThis paper, we presents an automated feature selection mechanism. After receiving the data, the mechanism first executes two feature selection methods: <u>Random Forest</u> [?] and XGBoost [?]. <u>ThenNext</u>, according to each method, it determines the importance of each feature and, as a result, which features should be used in the model.

Automated machine Elearning (AutoML) is an artificial-intelligence-based method whose purpose tothat automates the process of machine learning by building efficient and high-model -quality machine learning algorithms. A recent comprehensive survey on AutoML can be found in <u>Ref.</u> [?] and references therein.

As mentioned, wWe focus herein this paper on the Random Forest classifier and the XGBoost algorithm. InReference [?], the authors statereports that a feature selection based on the Random Forest classifier has been found to provides multivariate feature importance scores, which are relatively cheap to obtain and which have been successfully applied to high-dimensional data. Random Forest performs an implicit feature selection by using a small subset of "useful variables" for the classification only. This provides, eventually, an indicator of feature relevance. XGBoost is a scalable machine learning system that is commonly applied in tree boosting [?]. InReference [?], the authors states that the XGBoost algorithm provides a trained predictive model that automatically provides estimates the trained feature importance estimates. The XGBoost algorithm improves the performance of the model by alleviating the effects of redundant features and noise. Moreover, the algorithm prevents overfitting through feature subsampling or column subsampling.

Naturally, one of the most interesting issues when performing variable selection is accuracy, see <u>Ref.</u> [?]. That is<u>In other words</u>, we are interested in whether the accuracy achieved fromby using all features in the machine learning model is significantly greater than exceeds the accuracy of the model with when using only the selected (most important) variables; Or, <u>Put</u> another way, we are interested in whether it is sufficientes to use a small (but how small) number of features, and nevertheless achieve almost the same without reducing the accuracy.

Our<u>The</u> proposed automated mechanism <u>iteratively</u> performs the <u>R</u>andom <u>F</u>orest and XGBoost algorithms <u>iteratively</u>. In each iteration, we keep the most important features according to their rank in the <u>R</u>andom <u>F</u>orest and XGBoost classifier, and only use <u>only</u> them when solving some given classification problem. We then calculate the accuracy of this model and compare it with the accuracy of the full model (i.e., a Random Forest or an XGBoost classifier with all features). In the following iteration, we add another feature to the model (according to the ranks of the features), and calculate its accuracy. This procedure stops when there is only a negligible difference between the accuracy of the full model (with all features) and differs only negligibly from that of the partial model (with only the selected features).

The rest of the paper is organized as follows: In Section 2 we describes ourthe proposed algorithm, while inand Section 3 we presents the implementation steps. RThe results and comparisons between the Random Forest classifier and the XGBoost algorithm are given in Section 4. Section 5 concludes the paper.

2 The Method

In this paper, we define an<u>the</u> AutoML method which<u>that</u> performs the procedure of automated feature selection and reduction. The underlying process is as follows:

- 1. Run a selected algorithm on a full dataset *D*, i.e., with all features (in this paper, we apply both the Random Forest classifier and the XGBoost algorithm).
- 2. Let AC(D) be the accuracy of step 1.
- 3. Use a well-defined features importance method f(D) (in this paper work we use the Random Forest classifier as well as and the XGBoost algorithm).
- 4. Sort the f(D) features list by importance. Let $X_1(D)$ denote the first feature in the <u>list of ordered features</u> list (i.e., the most "important" feature), and let $X_n(D)$ denote the last feature in the <u>list of ordered features</u> list (i.e., the most "unimportant" feature).
- 5. **Option A:** <u>BUse the backward approach, i.e.</u>; <u>that is</u>, remove variables until <u>the accuracy between a full model and a partial model exceeds</u> some pre-determined error <u>denoted by</u> *E*. <u>The main steps in tThis</u> approach <u>areuses the following main steps</u>:
 - (a) Let n = be the number of features in the dataset D.
 - (b) Omit $X_n(D)$ from dataset D and create $D_{new} = D[-X_n(D)]$.

- (c) Run the selected algorithm from step 1 on D_{new} .
- (d) Let $AC(D_{ne}w) = \underline{be}$ the accuracy of step 5.A.c.
- (e) While $[AC(D) AC(D_{new}) \le E \text{ and } n > 0]$ do

i. n = n - 1

ii. $D_{new} = D_{new}[-X_n(D)]$

- iii. Run the selected algorithm on D_{new}
- iv. $AC(D_{new})$ = the accuracy of step (e)iii.

Option B: Use the forward approach, i.e.; that is, start with a model consisting of only the predicted (dependent) variable, and add (independent) features to the model, as long as the difference between the accuracy of the full model and the partial model is greater than some error EE. Once the difference is less than E, we stop and use the model with only the selected features. This approach has the following main steps in this approach are:

- (a) Let n = be the number of features in the dataset D and let b = 1.
- (b) Create a new empty dataset D_{new} (which that contains only the (single) dependent variable.
- (c) Add $X_1(D)$ to D_{new} .
- (d) Run the selected algorithm from step 1 on D_{new} .
- (e) Let $AC(D_{new}) = \underline{be}$ the accuracy of step 5.B.d.
- (f) While $[AC(D) AC(D_n ew) > E$ and b < n] do i. b = b + 1
 - ii. $D_{new} = D_{new}[+X_b(D)]$
 - iii. Run the selected algorithm from step 1 on D_{new}
 - iv. $AC(D_{new})$ = the accuracy of step (f)iii.

Note that the parameter E determines a threshold level for error accuracy-It, which should be modified according to various factors and considerations, such as

- the research domain (for example, in the health care domain, the prediction must be very high);
- quality of the data (sample size, missing values, outliers, etc.);
- <u>use-case analysis;</u>

- <u>other statistical measures and factors (dependencies, multi-collinearity, bias, etc.)</u>;
- model flexibility.

We present both the backward and the forward approaches, since because, depending on the research domain, one approach might be more suitable than the other, depending on the research domain. For example, if we assume that <u>an</u> accuracy of 80% is sufficientes, we can apply the forward approach (i.e., add features gradually to the model until this level of accuracy is achieved). On the other handConversely, if we are interested inwant to reducinge the number of features but maintain some minimum deviation from the accuracy of the full model, we will prefer the backward approach.

3 Implementation

To illustrate our suggested the proposed mechanism, we perform the following implementation procedures:

- 1. We test <u>ourthe proposed</u> mechanism on <u>4four</u> different datasets, which are presented and detailed in the sequel. [AU: Do you mean "which will be detailed in a forthcoming presentation"?]In each dataset, we solve some classification problem.
- We use the Random Forest and XGBoost algorithms in two manners:

 (i) we use it for feature selection, and (ii) we use it as the prediction model for the classification problem, and calculate itsthe accuracy. For that purpose To this end, we utilizeuse the libraries sklearn.ensemble.RandomForestClassifier (see Ref. [?] and the xgboost import XGBClassifier).
- 3. We use pandas [?] for handling with our datasets and derive <u>the</u> statistical results and measures.
- 4. We test our suggested the proposed procedure on the following datasets:
 - (a) Dataset 1 is Wine Quality [?]. This dataset consists of 4898 records, 11 features, and a categorical target variable with 11 different classes).
 - (b) Dataset 2 is the Cleveland Heart Disease Dataset [?]. We used the processed cleveland data dataset, which contains 303 records with <u>a</u> total of 14 features, including the classification target (with 5 classes).

- (c) Dataset 3 is breast-cancer-Wisconsin [?]. This dataset consists of 699 records, 10 features, and a categorical target variable (with 2 classes).
- (d) Dataset 4 is the Internet Firewall (see, e.g., <u>Ref.</u> [?]). This dataset consists of 65 532 records and 12 twelve features including the classification categorical target variable (with 4 four different classes).
- 5. We implemented both backward and forward approaches (as described in Section 2) on each of the selected datasets detailed above. For each dataset, we provide the following results:
 - (a) <u>feature importance sorted list derived from the Random Forest</u> classifier and from the XGBoost algorithm;
 - (b) <u>one</u> comparative accuracy graph per model of <u>the</u> backward approach;
 - (c) <u>Aone</u> comparative accuracy graph per model of <u>the</u> forward approach.

At the end of the process, ourthis procedure returns the best model with the optimal number of features selected for each dataset. **TFigure** <u>1 describes</u> the flow of the AutoML implementation steps is described in Figure 1. We start our implementation by splitting the data into a training set and a test set. ThenNext, we run the Random Forest algorithm and generate the feature-importance list. If the generated list is not empty, we drop one feature and rerun the algorithm forto generate <u>a</u> the new list. We then calculate the accuracy and save it in the algorithm's feature-accuracy list. We compile the Random Forest feature accuracy list if the importance is not greater than zero. Furthermore, we perform successively iterations fore the procedure <u>by</u> using the XGBoost algorithm, and compare the accuracy obtained by using the features from the two lists. The final output is the accuracy needed alongsideand the optimal number of features.

Figure 1: Flow chart of the implementation steps.

4 Results

In tThis section we presents the results of our suggested the proposed mechanism for each of the $\frac{4}{10}$ datasets described in Section 2.

4.1 Dataset 1: Wine-quality dataset

Table 1 presents the sorted feature importance list based on the outcomes of both the Random Forest algorithm and the XGBoost algorithm. The results for dataset 1 show that the accuracy of a full Random Forest model (consisting of all features) is 0.6020, while the accuracythat of the full XG-Boost model is 0.6562. Figure 2 presents the accuracy of the fitted Random Forest and XGBoost models under the backward approach. That is In other words, we start with a full model with all 11eleven features and then remove features; according to their importance given in Table 1. In this case, it is evident that reducing the number of features to only 5five (out of 11eleven) does not dramatically influencechange the accuracy of the model. However, it is shown in Figure 2 shows that the accuracy obtained from the XG-Boost method is bettermore accurate than the accuracy of rRandom Forest method.

Figure 3 depicts the accuracy for the forward approach. We start with a model consisting only <u>of</u> the most important feature, which, for both <u>Random Forest and XGBoost</u>, results in <u>a</u> low accuracy of about 0.51. We then add features according to their importance until reaching the desired accuracy. Again, <u>a</u> good accuracy is <u>reachedobtained</u> with only <u>5five</u> features. Both Figures 2 and 3 show that, for dataset 1, the XGBoost model provides betteris more accuracyte than the Random Forest classifier.

| Feature name | Importance Random Forest | Feature name | Importance XGBoost |
|----------------------|--------------------------|----------------------|--------------------|
| Alcohol | 0.242851 | Alcohol | 0.201177 |
| Sulphates | 0.140236 | Total sulfur dioxide | 0.105005 |
| Total sulfur dioxide | 0.115642 | sulphates | 0.101907 |
| Volatile acidity | 0.111605 | Volatile acidity | 0.09821 |
| Density | 0.092982 | Free sulfur dioxide | 0.07577 |
| Chlorides | 0.057417 | Fixed acidity | 0.075138 |
| Citric acid | 0.053522 | pН | 0.074227 |
| Fixed acidity | 0.052005 | Residual sugar | 0.072228 |
| pН | 0.045732 | Citric acid | 0.065855 |
| Residual sugar | 0.044457 | Density | 0.065293 |
| Free sulfur dioxide | 0.043558 | Chlorides | 0.06519 |

Table 1: Feature importance for dataset 1 according to Random Forest and XGBoost.

4.2 Dataset 2: Cleveland heart disease dataset

Table 2 presents the results of the feature importance process executed on dataset 2, as obtained by Random Forest and XGBoost. Note that the ac-

Figure 2: Model accuracy offor the backward approach for applied to dataset $1_{.}$

Figure 3: Model accuracy offor the forward approach for applied to dataset 1.

curacy of the full model according to <u>Random Forest (XGBoost)</u> is 0.5604, and (0.4945-via XGBoost). It is shown in Figure 4 shows that, according to the Random Forest classifier, eliminating variables from the model increases the accuracy. This often occurs since having many variables in the model may cause overfitting and increase the variance. It appears that <u>aA</u> model with <u>2two</u> features <u>reachesattains</u> the best accuracy when using <u>Random</u> Forest, and whereas 4 four features are required when using XGBoost. This is also shown in Figure 5, where the accuracy is given for the forward approach (i.e., when adding features). A model with a single independent feature gives poor accuracy with Random Forest, but, surprisingly, when using a single feature, it does not give the worse accuracy than when using XGBoost. Adding only a single extra feature to the model with Random Forest significantly improves the accuracy, while in the accuracy for the XGBoost model the accuracy rises in a more moderate manner. Overall, it is evident from Figures 4 and 5 that Random Forest results within better accuracy for dataset 2.

Table 2: Feature importance for dataset 2 according to when using Random Forest and XGBoost.

| Feature name | Importance Random Forest | Feature name | Importance XGBoost |
|--------------|--------------------------|--------------|--------------------|
| feature 2 | 0.177796 | feature 11 | 0.153479 |
| feature 11 | 0.146085 | feature 2 | 0.143723 |
| feature 1 | 0.139925 | feature 1 | 0.12426 |
| feature 6 | 0.101466 | feature 5 | 0.083033 |
| feature 4 | 0.098772 | feature 3 | 0.076648 |
| feature 5 | 0.082157 | feature 4 | 0.064499 |
| feature 13 | 0.079420 | feature 12 | 0.063392 |
| feature 3 | 0.045154 | feature 16 | 0.059724 |
| feature 9 | 0.042083 | feature 8 | 0.058084 |
| feature 12 | 0.037607 | feature 13 | 0.052149 |
| feature 10 | 0.035161 | feature 9 | 0.048032 |
| feature 7 | 0.013243 | feature 10 | 0.044038 |
| feature 8 | 0.001131 | feature 7 | 0.028939 |

4.3 Dataset 3: Breast-cancer-Wisconsin dataset

FTable 3 presents the order of feature importance for the breast-cancer dataset, we present the order of feature importance in Table 3. The accuracies of the full Random Forest model and the full XGBoost model is are both about 0.9714 (both are very close). According to For the backward approach, it is depicted in Figure 6 shows that a model with 3three features (out of 10ten), reaches a very good accuracy for the Random Forest classifier (almost as good as for the full model), whilewhereas 6six features provide good accuracy infor the XGBoost model. This phenomenon is also presented appears in the lower part of Figure 7, in which shows the accuracy for the forward approach is shown.

Figure 4: Model accuracy <u>of when applying</u> the backward approach <u>for to</u> dataset 2.

Figure 5: Model accuracy of the when applying the forward approach forto dataset 2.

4.4 Dataset 4: Internet firewall dataset

In this lastfinal example, we consider the firewall data set. Feature importance is given in Table 4. The accuracy of a full Random Forest (XGBoost) model with all 11eleven features is 0.9984 and for XGBoost is (0.9986). However, ourthe results in Figures 8 and 9 show that even a model with only two features reaches almost the same accuracy, either by using either Random

| Feature name | Importance Random Forest | Feature name | Importance XGBoost |
|--------------|--------------------------|--------------|--------------------|
| feature 7 | 0.256161 | feature 7 | 0.565556 |
| feature 8 | 0.233745 | feature 8 | 0.231707 |
| feature 4 | 0.155182 | feature 3 | 0.056456 |
| feature 3 | 0.128431 | feature 4 | 0.050602 |
| feature 5 | 0.092941 | feature 2 | 0.044598 |
| feature 2 | 0.080215 | feature 9 | 0.024274 |
| feature 9 | 0.034542 | feature 6 | 0.010903 |
| feature 6 | 0.015189 | feature 5 | 0.010789 |
| feature 10 | 0.002378 | feature 10 | 0.005116 |
| feature 1 | 0.001223 | feature 1 | 0 |

Table 3: Feature importance for dataset 3 according to <u>Random Forest</u> and XGBoost.

Figure 6: Model accuracy of when applying the backward approach forto dataset 3.

Forest or XGBoost.

5 Concluding remarks

In tThis paper we presenteds an automated feature importance method based on the Random Forest and XGBoost algorithms. For a given dataset, the proposed mechanism suggests which features should be used in the model and which should be omitted from it while maintaining high accuracy. Reducing the number of features may reduce the complexity of the model, and, as shown in our examples, does not influence drastically onaffect perfor-

Figure 7: Model accuracy of the when applying the forward approach forto dataset 3.

Figure 8: Model accuracy of the when applying the backward approach forto dataset 4.

mance (i.e., model accuracy). Specifically, we test <u>ourthe proposed</u> method on <u>four</u> different datasets by solving <u>somea</u> classification problem. For each dataset, we first <u>performedapply</u> the <u>Random Forest</u> and the XGBoost algorithms to derive <u>the</u> feature importance. <u>ThenNext</u>, according to the importance of features, we <u>employeduse</u> the backward approach (i.e., starting with a full model and removing variables according to <u>some</u> accuracy criteria) and

| Feature name | Importance Random Forest | Feature name | Importance XGBoost |
|----------------------|--------------------------|----------------------|--------------------|
| Destination Port | 0.225071 | Elapsed Time | 0.793872 |
| Elapsed Time | 0.192756 | Destination Port | 0.083326 |
| NAT Source Port | 0.144005 | Bytes | 0.077337 |
| NAT Destination Port | 0.120887 | Packets | 0.03966 |
| Packets | 0.074335 | NAT Source Port | 0.00164 |
| Bytes | 0.065065 | Bytes Received | 0.001225 |
| pkts received | 0.050558 | Bytes Sent | 0.001096 |
| Bytes Sent | 0.046179 | NAT Destination Port | 0.001009 |
| Source Port | 0.040731 | Source Port | 0.000374 |
| Bytes Received | 0.038632 | pkts received | 0.000265 |
| pkts sent | 0.001781 | pkts sent | 0.000197 |

Table 4: Feature importance for dataset 4 according to <u>R</u>andom <u>F</u>orest and XGBoost.

Figure 9: Model accuracy of the when applying the forward approach forto dataset 4.

the forward approach (i.e., starting with an empty model and adding variables according to some pre-determined criteria). The measured accuracy is referred to as a classification model, which we conducted implement using Random Forest. For all datasets, we conclude, in all datasets, that the number of features used for building the model may be reduced by half (and even by more than that), while keeping the model accuracy very close to the accuracy of a full model (with all features). The results also show that, for some datasets, the Random Forest classifier outperforms XGBoost (datasets 2 and 3), whilewhereas, for dataset 1, the XGBoost gives better accuracy.

For dataset 4, both methods yield quite the same accuracy, except for the case when only a single feature is used, in this which case Random Forest is better. This automated feature selection method presents an effective process offor selecting the optimal number of features for predictive machine learning models, thus enhancing the accuracy of the fit. Implementing a machine learning model with the appropriate features increases the model's performance and reduces the computational costs. Overall, the method is efficient and states which features strongly influence the response variable.