iXGB: Improving the Interpretability of XGBoost Using Decision Rules and Counterfactuals

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Abstract: Tree-ensemble models, such as Extreme Gradient Boosting (XGBoost), are renowned Machine Learning models which have higher prediction accuracy compared to traditional tree-based models. This higher accuracy, however, comes at the cost of reduced interpretability. Also, the decision path or prediction rule of XGBoost is not explicit like the tree-based models. This paper proposes the iXGB–interpretable XGBoost, an approach to improve the interpretability of XGBoost. iXGB approximates a set of rules from the internal structure of XGBoost and the characteristics of the data. In addition, iXGB generates a set of counterfactuals from the neighbourhood of the test instances to support the understanding of the end-users on their operational relevance. The performance of iXGB in generating rule sets is evaluated with experiments on real and benchmark datasets, which demonstrated reasonable interpretability. The evaluation result also supports the idea that the interpretability of XGBoost can be improved without using surrogate methods.

1 INTRODUCTION

Tree-ensemble is a class of Machine Learning (ML) models which have gained recent popularity for their efficacy in handling a diverse array of tabular data in real-world applications (Sagi and Rokach, 2021). These tree-ensemble models, *e.g.*, Random Forests (Breiman, 2001), Gradient Boosted Trees (Friedman, 2001), Extreme Gradient Boosting (XGBoost) (Chen and Guestrin, 2016), *etc.* operate by combining the predictive power of multiple decision trees. One of their key strengths is their ability to manage complex relationships within data, making them particularly suitable for datasets characterised by heterogeneity while very little preprocessing is required on the data before model training. The collective strength of individual trees, each contributing a unique perspective, results in a powerful ensemble capable of tackling various predictive tasks.

A major weakness of the tree-ensemble models (*e.g.*, XGBoost) is that they lose interpretability while improving the prediction accuracy. This was showcased by Gunning and Aha (2019) with a notional diagram in their secondary study on the research field of Explainable Artificial Intelligence (XAI). Precisely, these ensemble models divide the input space into small regions and predict from that region. The number of small regions is generally large, theoretically, these regions represent a large number of rules for prediction. This excessive number of rules makes the decision process less interpretable for end-users. Hara and Hayashi (2016) proposed a post-processing method that improves the interpretability of the tree-ensemble models and demonstrated their approach by interpreting predictions from XGBoost. The authors also showed that smaller decision regions refer to more transparent and understandable models. In another work, Blanchart (2021) described a method for computing the decision regions of tree-ensemble models for classification tasks. The authors also utilised counterfactual reasoning alongside the decision regions to interpret the models' decisions. Sagi and Rokach (2021) proposed an approach of approximating an ensemble of trees into an interpretable decision tree for classification problems. Nalenz and Augustin (2022) developed Compressed Rule Ensemble (CRE) to interpret the output of

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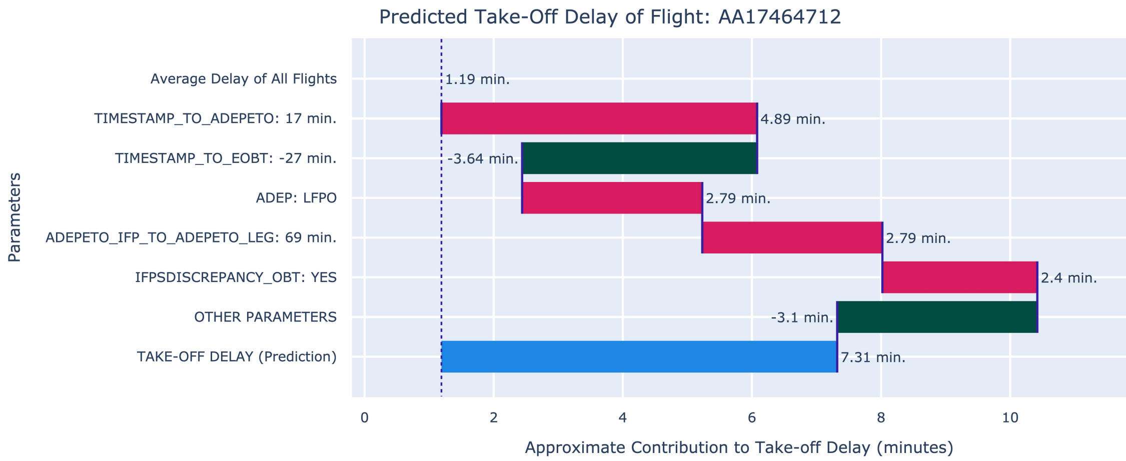


Figure 1: Example of explanation generated for a single instance of flight TOT delay prediction using LIME. The red and green horizontal bars correspond to the contributions for increasing and decreasing the delay respectively, and the blue bar corresponds to the predicted delay.

tree-ensemble classifiers. These studies are the only notable ones found in the literature which contributed to improving the interpretability of the tree-ensemble models for classification tasks with indications towards their use in regression tasks.

From the literature, it is evident that less effort is given towards making the ensemble models (*e.g.*, XGBoost) interpretable for regression tasks. Moreover, different state-of-the-art methods produce explanations that differ in the contents of the output. Under these circumstances, this study aims to improve the interpretability of XGBoost by utilising its mechanisms by design. The main contribution of this study is twofold –

- Explaining the predictions of XGBoost regression models using decision rules extracted from the trained model.
- Generation of counterfactuals from the actual neighbourhood of the test instance.

1.1 Motivation

The work presented in this paper is further motivated by a real-world regression application for the aviation industry. Particularly, the regression task is to predict the flight take-off time (TOT) delay from historical data to support the responsibilities of the Air Traffic Controllers (ATCO). It is worth mentioning that the aviation industry experiences a loss of approximately 100 Euros on average per minute for Air Traffic Flow Management (ATFM) (Cook and Tanner, 2015). The Federal Aviation Administration (FAA)[1] reported in 2019 that the estimated cost due to delay, considering passengers, airlines, lost demand, and indirect costs, was thirty-three billion dollars (Lukacs, 2020). The significant expenses provide the rationale for increased attention towards predicting TOT and reducing delays of flights (Dalmau et al., 2021).

To solve the problem of predicting flight TOT delay, an interpretable system was developed to incorporate the existing operational interface of the ATCOs. In the process, the prediction model was developed with XGBoost and its prediction was made interpretable with the help of several popular XAI tools, such as LIME – Local Interpretable Model-agnostic Explanation. Qualitative evaluation in the form of a user survey was conducted for the developed system with the following scenario –

The current time is 0810 hrs. AFR141 is at the gate and expected to take off from runway 09 at 0910 hrs. It is predicted that this flight will be delayed for unknown minutes. After this, the aircraft has 2 more flights in the day. Concurrently, SAS652 is in the last flight leg of the day and is expected to land on runway 09 at 0916 hrs. Moreover, there is a scheduled runway inspection at 0920 hrs.

The target users of the survey were the ATCOs, both professionals and students. Participants were prompted with several scenarios similar to the scenario stated above and corresponding predictions of the delay with explanation as illustrated in Figure 1, which varied based on the explainability tool used to generate the explanation. At the end of each scenario, the participants were asked to respond to questions to evaluate the effectiveness of the XAI methods in explaining the prediction results.

The outcome of the user survey was deduced as– the contribution to the final delay of the selected

[1]https://www.faa.gov/

features from the XAI methods would not impact the operational relevance of the information received, though the explanations are understandable. This rationalisation was also reflected in the qualitative interviews including the preference for user-centric feature selection in the explanations and their corresponding values on which the practitioners can act to mitigate the issues of delays. Extensive details on the presented use case can be found in a prior work by the authors (Jmoona et al., 2023).

Based on the outcome of the previous study, the aim was to generate a rule set and counterfactuals in support of the prediction from XGBoost so that the understanding of the operational relevance of the selected features is improved. Particularly, XGBoost is an ensemble of decision trees that are interpretable by nature as the prediction rules from a single decision tree are easily obtained (Gunning and Aha, 2019). This intrinsic characteristic of XGBoost created the hypothesis of this work to extract decision rules from the trained XGBoost model and generate counterfactuals that suggest changes in the feature values influencing the prediction.

2 iXGB – INTERPRETABLE XGBoost

The mechanism of the proposed iXGB is illustrated in Figure 2, which utilises the trained XGBoost regression model as the starting point. The principal components of iXGB are the XGBoost regressor, the rule extractor and the counterfactual generator. Among these, the last two are described in the following subsections including the formal definitions from the context of a regression problem where the first component is addressed.

2.1 Definitions

The regression model Ω is defined to predict a continuous target variable $y_i \in \mathcal{Y}$, based on a set of m independent features or attributes $a_1,\ldots,a_m$ represented by the vector $x_i = [x_{i1},\ldots,x_{im}]$ and $x_i \in \mathcal{X}$. The dataset consists of n observations, each comprising a feature vector x_i and its corresponding target value y_i, where $i = 1,\ldots,n$. The objective of the regression model is to learn a mapping function $f(x_i) = \hat{y}_i$ on $(\mathcal{X}_{train}, \mathcal{Y}_{train})$ that can accurately estimate the target variable $y_i \in \mathcal{Y}_{test}$ given the input feature vector $x_i \in \mathcal{X}_{test}$. Here, the $(\mathcal{X}_{train}, \mathcal{Y}_{train})$ and $(\mathcal{X}_{test}, \mathcal{Y}_{test})$ are the training and test sets respectively split from the given dataset at a prescribed ratio.

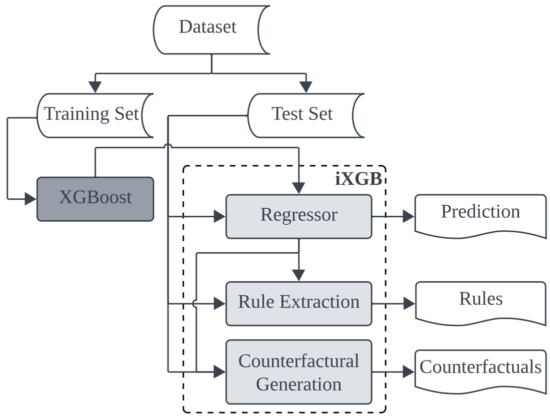


Figure 2: Overview of the mechanism of the proposed iXGB. The grey-coloured boxes with lighter shades depict the principal components of iXGB.

In this study, Ω refers to an XGBoost (Chen and Guestrin, 2016) regression model for which the corresponding f computes the sum of residuals δ from p decision trees d_k, where $k = 1,\ldots,p$ and by definition, $\delta_{d_1} > \delta_{d_2} > \cdots > \delta_{d_p}$. Therefore, f is formalised as –

$$f(x_i) = \sum_{k=1}^{p} \delta_{d_k} \tag{1}$$

iXGB explains $f(x_i)$ as a pair of objects: $\langle r, \Phi \rangle$, where $r = c \rightarrow \hat{y}_i$ describing $f(x_i) = \hat{y}_i$. Here, c contains the conditions on the features $a_1,\ldots,a_m$. And, Φ is the set of counterfactuals. A counterfactual is defined as an instance x'_i as close as possible to a given x_i with different values for at least one or more features a, but for which $f(x_i)$ outputs a different prediction $\hat{y}_i{}'$, *i.e.*, $y_i \neq \hat{y}_i{}'$.

2.2 Extraction of Rules

The decision rules r supporting the prediction $\hat{y}_i$ by the trained XGBoost regressor f is extracted from the last trees (δ_{d_p}) while regressor f predicts y for the q closest neighbours of the instance x_i. The intuition behind using the last tree is that it generates the lowest residual by definition of XGBoost. In other words, the prediction is more accurate than the other trees in f. The closest neighbours of x_i are determined using Euclidean distance metric. The value of q can be determined by changing the value and observing the quality of generated rules. Finally, all rules from the decision paths of closest neighbours and x_i are merged for each feature and the r is obtained. The decision paths of the closest instances are also included to obtain a generalised rule for the decision region. Algorithm 1 presents the steps of extracting rules with iXGB.

Algorithm 1: Rule Extraction.

Input: f: regressor, x_i: test instance, X_{test}: test set, q: number of neighbours
Output: r: decision rule

$CN = \{cn_1, \ldots, cn_q\} \leftarrow q$ closest neighbours of x_i from X_{test} within the its cluster
$DP = \{dp_{x_i}, dp_{cn_1}, \ldots, dp_{cn_q}\} \leftarrow$ decision paths from δ_{d_p} of f for $\{x_i\} \cup CN$
$r \leftarrow$ merge the conditions from DP for each feature a_j, where $j = 1, \ldots, m$
return r

2.3 Generation of Counterfactuals

The pseudo-code for generating counterfactuals is stated in Algorithm 2. In the process of generating the counterfactuals, all the instances of the test set are clustered arbitrarily to form decision boundaries around the instances based on their characteristics. In this study, K-Means clustering is used and the number of clusters is determined with the Elbow method (Yuan and Yang, 2019). Then, the closest neighbours of the test instance x_i in other clusters than its own are selected. The differences in the feature values and the change in predicted values are calculated for x_i versus the closest neighbours. Lastly, the pairs of differences in feature values and the changes in prediction are generated as the set of counterfactuals Φ.

Algorithm 2: Counterfactual Generation.

Input: f: regressor, x_i: test instance, X_{test}: test set, q: number of neighbours
Output: Φ: set of counterfactuals

$C \leftarrow$ form arbitrary number of clusters with the instances of X_{test}
$CN' = \{cn'_1, \ldots, cn'_q\} \leftarrow q$ closest neighbours of x_i in X_{test} which are in different cluster than x_i, *i.e.,* $C(x_i) \neq C(cn'_j)$, where $j = 1, \ldots, q$
$\{\Delta A_1, \ldots, \Delta A_q\} \leftarrow$ differences in the feature values of x_i and CN'
$\{\Delta y'_1, \ldots, \Delta y'_q\} \leftarrow$ differences in the predictions with f for x_i and CN'
$\Phi \leftarrow \{(\Delta A_1, \Delta y'_1), \ldots, (\Delta A_q, \Delta y'_q)\}$
return Φ

3 MATERIALS AND METHODS

The implementation of iXGB was done using Python scripts. Scikit–Learn (Pedregosa et al., 2011) interface was used to build the models of XGBoost regressor and K-Means clustering. The visualisations were generated using Matplotlib (Hunter, 2007) and Seaborn (Waskom, 2021). The datasets and metrics used to evaluate the performance of iXGB are discussed in the following subsections.

3.1 Datasets

Three different datasets were used in the conducted experiments for this study. Among them, the first one is the real-world dataset associated with the motivating study described in Section 1.1, and the other two are benchmark datasets. The summary of the datasets is presented in Table 1 followed by brief descriptions of the datasets below.

Table 1: Summary of the datasets used for evaluating the performance of iXGB.

Dataset	Features	Instances
Flight Delay	5	1000
Auto MPG	7	392
Boston Housing	13	516

The real dataset was collected and processed by EUROCONTROL[2] from the Enhanced Tactical Flow Management System (ETFMS) flight data messages containing all flights in Europe throughout the year 2019, from May to October. For this study, the dataset was acquired from Aviation Data for Research Repository[3]. The dataset consists of fundamental details of the flights, flight status, preceding flight legs, ATFM regulations, weather conditions, calendar information, *etc.* The definitions of the features from the dataset are described in the works of Koolen and Coliban (2020) and Dalmau et al. (2021). Here, the target variable is the flight take-off time delay in minutes. The acquired dataset contained 42 features, whereas only 5 features were considered for this study. The exclusion of the features was done based on the observation of predicting flight take-off delay from two different sets of data as illustrated in Figure 3. In the figure, the prediction performance of XGBoost improves until the top 5 most important features are used from the data. Here, the feature importance values are obtained from the global weights generated by XGBoost.

The benchmark datasets used in the experiments are datasets commonly used to evaluate models built for regression tasks. The first benchmark dataset is the Auto MPG dataset (Quinlan, 1993)

[2]https://www.eurocontrol.int/
[3]https://www.eurocontrol.int/dashboard/rnd-data-archive

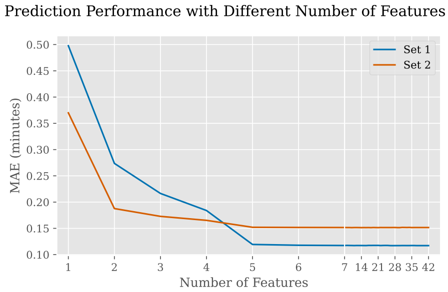


Figure 3: Prediction Performance of XGBoost in terms of MAE for flight delay prediction with different numbers of features ranked by XGBoost feature importance from two different subsets of the data.

containing information about various car models, including attributes such as cylinders, displacement, horsepower, weight, acceleration, model year, and origin in numerical features. The target variable is the miles per gallon, representing the fuel efficiency of the cars. The other benchmark dataset was the Boston Housing dataset (Harrison and Rubinfeld, 1978). It contains both numerical and categorical features, such as per capita crime rate, the average number of rooms per dwelling, distance to employment centres, and others. Here, the target variable is the median value of owner-occupied homes, which is generally utilised as a proxy for housing prices.

3.2 Metrics

The prediction performances of the models are evaluated using Mean Absolute Error (MAE) and standard deviation of the Absolute Error (σ_{AE}). MAE is the average difference between the actual observation y_i and the prediction $\hat{y}_i$ from the model. σ_{AE} signifies the dispersion of the absolute error around the MAE. The measures were calculated using Equations 2 and 3 respectively.

$$MAE = \frac{1}{n}\sum_{i=1}^{n}|y_i - \hat{y}_i| \tag{2}$$

$$\sigma_{AE} = \sqrt{\frac{1}{n}\sum_{i=1}^{n}(|y_i - \hat{y}_i| - MAE)^2} \tag{3}$$

To assess the quality of the extracted decision rules, the metric *coverage* or *support* (Molnar, 2022) was utilised. Coverage is the percentage of instances from the dataset which follow the given set of rules. It is calculated using the Equation 4 –

$$coverage = \frac{|\text{instances to which the rule applies}|}{|\text{instances in the dataset}|} \tag{4}$$

4 EVALUATION AND RESULTS

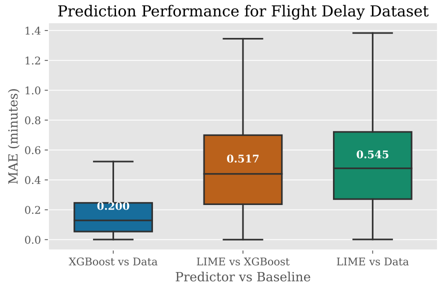
The proposed approach was evaluated through a series of experiments within the context of regression problems. The experimental procedures and the result of the evaluation experiments are presented in this section.

To evaluate the extracted rules and the predictions from iXGB, LIME (Ribeiro et al., 2016) is considered as the baseline, which is widely used in recent literature to generate rule-based explanations (Islam et al., 2022). LIME is developed based on the assumption that the behaviour of an instance can be explained by fitting an interpretable model (*e.g.*, linear regression) with a simplified representation of the instance and its closest neighbours. While predicting a single prediction of a black box model, LIME generates an interpretable representation of the input instance. In this step, it standardises the input by modifying the values of the measurement unit. The standardisation causes LIME to lose the original proportion of values for regression. In the next step, LIME perturbs the values of the simplified input and predicts using the black box model, thus generating the data on which the interpretable model trains. Next, LIME draws samples from the generated data based on their similarity to select the closest neighbours. Lastly, a linear regression model is trained with the sampled neighbours. With the prediction from the linear regression model and the value ranges from the neighbourhood, LIME presents the local explanation with rules.

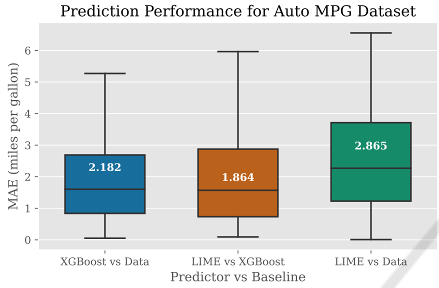
4.1 Prediction Performance

The first evaluation experiment was conducted to assess the prediction performance of the proposed approach. For each dataset described in Section 3.1, the *MAE* and σ_{AE} were calculated using Equations 2 and 3. For iXGB, the predictions remain unchanged as the predictions are directly taken from the XGBoost models which were compared with the target values from the datasets. For LIME, the predictions are compared with the predictions from XGBoost and the target values from the datasets. The results of all the calculations of *MAE* and σ_{AE} are illustrated in Figure 4. For Boston Housing and Flight Delay datasets, it is observed that the error in prediction by iXGB is better than the LIME predictions. However, for all the datasets, the predictions from LIME are more erroneous than iXGB when compared to the original target values from the datasets. These observations advocate that iXGB retains the prediction performance of the

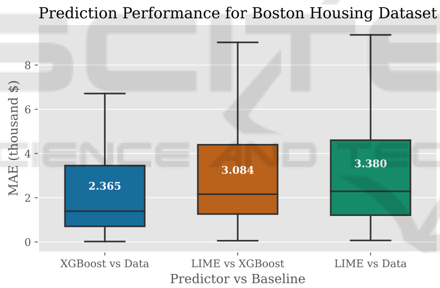
XGBoost regressor than the surrogate LIME.



(a) Flight Delay Dataset.



(b) Auto MPG Dataset.



(c) Boston Housing Dataset.

Figure 4: Comparison of prediction performance of iXGB and LIME in terms of MAE with three different datasets. Blue-coloured coloured box-plots are for iXGB prediction compared with the target values. Red- and green-coloured box-plots are for LIME predictions compared with XGBoost prediction and the target values respectively. The mean values are presented on the corresponding box–plots.

By design, LIME perturbs the input values to generate samples to train an interpretable model (*e.g.*, linear regression) and use that model for generating the local explanations. However, the literature prohibits modification of measurement units for regression tasks since this operation destroys the original proportion of the input values (Letzgus et al., 2022). On the other hand, while explanations are generated with iXGB, the prediction performance of XGBoost is not compromised. Under these circumstances, iXGB can be utilised by replacing the surrogate models for rule-based explanation (*e.g.,* LIME) when performing regression tasks with XGBoost.

4.2 Coverage of Decision Rule

To evaluate the quality of rules generated from iXGB, they were compared with the rules extracted from LIME. For simplicity, only the rules extracted for a single instance of prediction from the Auto MPG dataset by iXGB and LIME are presented. Using Algorithm 1, the following rule (r) is extracted from iXGB considering 5 closest instances from the test set:

```
IF (cylinders < 4.00) AND
   (displacement <= 74.50) AND
   (horsepower >= 96.50) AND
   (2305.00 <= weight < 2337.50) AND
   (13.10 <= acceleration < 13.75) AND
   (model_year <= 72.00) AND
   (origin >= 3.00)
THEN   (mpg = 19.00)
```

And, the decision rule extracted from LIME is:

```
IF (cylinders <= 4.00) AND
   (displacement <= 98.00) AND
   (88.00 < horsepower <= 120.00) AND
   (2157.00 < weight <= 2672.00) AND
   (acceleration <= 14.15) AND
   (model_year <= 73.00) AND
   (origin > 2.00)
THEN   (mpg = 23.66)
```

Table 2: Coverage scores (average ± standard deviation) of the rules extracted from iXGB and LIME. For local explanation, lower values are better which are emphasised with blue fonts.

Dataset	Coverage	
	iXGB	LIME
Auto MPG	2.71 ± 1.55	7.24 ± 13.89
Boston Housing	2.53 ± 1.56	1.36 ± 0.87
Flight Delay	3.06 ± 1.41	20.50 ± 22.29

In both the decision rules, all the features from the dataset are present. Particularly, for the feature `weight` the value range is smaller in the rule extracted from iXGB than the rule extracted from LIME. Again, the conditions are different for the feature `origin` but both the rules indicate values greater or equal to 3.00. While rules were generated considering all the datasets, it was observed that the value ranges from the rules extracted from iXGB are smaller than the rules from LIME for the same instances.

Table 3: Sample set of counterfactuals generated using iXGB from the Auto MPG dataset.

Change in Feature Values							Change in Target
cylinders	***displacement***	***hp***	***weight***	***acceleration***	***model_year***	***origin***	
+1	+43	-2	+42	+2	-2	0	-50%
0	-27	23	-29	-4	-3	+2	-10%
0	-27	+23	-29	-4	-3	+2	-10%
0	+5	+20	+22	-2	-11	0	+20%
0	+15	+30	-8	-6	-11	+2	+45%
0	-22	+11	-13	+2	-11	+2	+75%
0	-27	+23	-36	-4	-1	+2	+90%

Table 4: Sample set of counterfactuals generated using iXGB from the Boston Housing dataset.

Change in Feature Values													Change in Target
crim	***zn***	***indus***	***chas***	***nox***	***rm***	***age***	***dis***	***rad***	***tax***	***prratio***	***blck***	***lstat***	
+1	0	0	0	0	+1	+2	0	0	0	0	-287	+3	-600%
+4	0	0	0	0	0	0	0	0	0	0	-152	+9	-275%
+7	0	0	0	0	0	+5	0	0	0	0	-83	+6	-200%
-1	0	0	0	0	0	+4	0	0	0	0	-33	+5	+40%
+1	0	0	0	0	0	+22	0	0	0	0	-69	+8	+50%

Furthermore, the *coverage* of the rules from iXGB and LIME were calculated using Equation 4. The results for all the datasets are presented in Table 2. The *coverage* values of rules for classification models are expected to be higher for better generalisation (Guidotti et al., 2019). In the case of local interpretability, the rule needs to define a single instance of prediction that is the opposite of generalisation (Ribeiro et al., 2018). This claim is also supported in the works of (Sagi and Rokach, 2021). The authors argued that the tree-ensemble models create several trees to improve the performance of the model resulting in lots of decision rules for prediction. This mechanism makes it harder to be understood by the end users. Thus, the smaller coverage values are considered better in this evaluation.

4.3 Counterfactuals

For all the datasets, the sets of counterfactuals (Φ) were generated by selecting a random instance from the test set to assess the impact on the target when the feature values are changed. The process described in Algorithm 2 was followed to generate the counterfactuals. Here, the counterfactuals are the instances around the boundary of the closest clusters of the selected instance. The number of clusters was chosen with the Elbow method (Yuan and Yang, 2019), which was 7 for the Auto MPG dataset and 5 for both Boston Housing and Flight Delay datasets. Unlike, counterfactuals from a classification task, the boundaries of the clusters formed with the test instances can be referred to as decision boundaries as they are clustered based on the characteristics of the data.

The sample set of counterfactuals from the Auto MPG dataset is presented in Table 3. For the table, it is found that the target value changes when all the feature values are changed except the feature *cylinders* in the first counterfactual. Likewise, for the Boston Housing dataset (Table 4), 8 out of 13 features needed not be changed to find the counterfactuals. Again, changing the values of only 3 features can decrease the target value by 275%. Lastly, the counterfactuals from the Flight Delay dataset are presented in Table 5 which can be interpreted in a similar way to the last two tables. For all the tables with counterfactuals, the feature names are shown as it is present in the dataset since the names are not directly subjected to the mechanism of the proposed iXGB.

The set of counterfactuals for any regression task can support the end users when they need to modify some feature values to achieve any target. Such question can be – *what would it take to increase the target value by some percentage?*. However, the change can be measured both in percentage and absolute values. After all, the counterfactuals would facilitate the decision-making process of end users by

Table 5: Sample set of counterfactuals generated using iXGB from the Flight Delay dataset.

Change in Feature Values					Change in Target
ts_leg_to_ts	***flight_duration_leg***	***ts_to_ta_leg***	***ta_leg***	***ts_ifp_to_ts***	
-118	-56	+9	+4	+3	-10%
+2	+2	+2	+2	+2	-5%
-14	+7	+11	-36	-89	-5%
-21	+35	+25	-5	-34	+5%
+29	+46	-25	-8	-49	+5%

maintaining operational relevance.

5 CONCLUSION AND FUTURE WORKS

XGBoost is widely adopted in regression tasks because of its higher accuracy than other tree-based ML models with the cost of interpretability. Generally, the interpretability is induced to XGBoost through using various XAI methods. These XAI methods (*e.g.*, LIME) rely on perturbed samples to provide explanations for XGBoost predictions. In this paper, iXGB is proposed by utilising the internal structure of XGBoost to generate rule-based explanations and counterfactuals from the same data on which the model trains for prediction tasks. The proposed approach is functionally evaluated on three different datasets in terms of local accuracy and quality of the rules, which shows the ability of iXGB to improve the interpretability of XGBoost reasonably. Future research directions include theoretically grounded evaluation of the proposed approach on more diverse datasets and different real-world problems. Moreover, further investigations are also required to adopt the proposed iXGB for binary and multi-class classification tasks.

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