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EXPLAINING XGBOOST PREDICTIONS WITH SHAP VALUE: A COMPREHENSIVE GUIDE TO INTERPRETING DECISION TREE-BASED MODELS

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Abstract. Understanding the factors that affect Key Performance Indicators (KPIs) and how they affect them is frequently important in sectors where data and data science are crucial. Machine learning is utilized to model and predict pertinent KPIs in order to do this. Interpretability is important, nevertheless, in order to fully comprehend how the model generates its predictions. It enables users to pinpoint which traits have aided the model's ability to learn and comprehend the data. A practical approach for evaluating the contribution of input attributes to model learning has evolved in the form of SHAP (SHapley Additive exPlanations offer an index for evaluating the influence of each feature on the forecasts made by the model. In this paper, it is demonstrated that the contribution of features to model learning may be precisely estimated when utilizing SHAP values with decision tree-based models, which are frequently used to represent tabular data.

Keywords: SHAP value, machine learning, decision tree-based model, feature importance.

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Introduction

Machine learning models have gained a lot of popularity recently since they give us insightful predictions. Yet, the predictions generated by these models can be difficult to comprehend, making it difficult for us to understand why a certain prediction was made. Although the decision trees used by the well-known machine learning algorithm XGBoost for classification and regression tasks are complicated, it might be difficult to grasp their results. SHapley Additive exPlanations (SHAP) value plays a role in this.

A technique called SHAP can be used to explain the predictions that a machine learning model makes. Each component of the model is given a numerical number to indicate how much it contributed to a certain prediction. These numbers can make it easier and more accurate for us to comprehend how the model generates its predictions.

Let's look at an example to see how SHAP values operate. Imagine that we have a dataset of property prices and that our goal is to estimate the cost of a house depending on its size and the number of bedrooms. This dataset can be utilized to train an XGBoost model, which predicts a price of $500,000 for a three-bedroom, 2,000-square-foot home. We now need to know why the model made this forecast.

The contributions of the various features can be separated into the prediction using SHAP values. In this instance, $300,000 and $200,000, respectively, might be the SHAP values for square footage and bedroom count. This suggests that the square footage, rather than the number of bedrooms, is the factor that has the most impact on the price estimate.

Another type of visualization known as a SHAP summary plot can be made using SHAP values (Mitchell et al., 2022). This graph displays the average SHAP value for each feature across all dataset instances. It can be used to determine which elements are most crucial for the model's predictions and how each one affects the forecasts as a whole.

The SHAP dependence plot is an additional helpful tool for analyzing XGBoost forecasts with SHAP values. This plot displays the appropriate SHAP values and illustrates the relationship between a single character and the model's predictions. It can be used to spot any non-linear interactions between the features and the predictions as well as to see how the model's predictions change as a feature's value varies (Covert & Lee, 2021).

SHAP values can be used for feature engineering and model debugging, in addition to explaining to users why a model predicts certain things (Chen et al., 2021). Users can determine which elements are most important to the model's predictions by looking at the SHAP values for those features, as well as which features might be unnecessary or even harmful to the model's performance. The model or dataset can then be improved using this knowledge, potentially leading to an increase in accuracy and readability (Wang et al., 2022).

Overall, SHAP values are an effective tool that can aid in our understanding of the XGBoost models' predict simply and understandably model's decision-making process in a simple and understandable way, and they may also be utilized for feature engineering and model debugging. Understanding the output of these models will become increasingly critical as machine learning plays an increasingly significant part in decision-making. Tools like SHAP values will be crucial for gaining this knowledge (Gebreyesus et al., 2023).

In this study, it is investigated how to interpret XGBoost model predictions using SHAP (SHapley Additive exPlanations) values. When utilizing sophisticated models like XGBoost, SHAP values offer a thorough and understandable manner to comprehend the contribution of each feature to the model's prediction. By analyzing SHAP values, it may be learned how the model generates its predictions and which attributes are responsible for them.

It is shown that the contribution of features to model learning may be correctly quantified by using SHAP values with decision tree-based models, which are often used to represent tabular data (Rozemberczki et al., 2022). This enables users to see the characteristics that have improved the model's capacity to learn from and understand the data, offering deeper insights into the variables that influence KPIs and how they do so.

Overall, this study emphasizes the significance of interpretability in machine learning and shows how to use SHAP values with decision tree-based models to present a realistic method for assessing the contribution of input variables to model learning.

The novelty of the research described in the passage is as follows:

- The study highlights the problem of interpretability in machine learning when it comes to understanding the underlying mechanisms.
- The study focuses on using machine learning to anticipate and model spatial phenomena, which is a growing area of research.

- The study gives comprehensive recent developments in local interpretation techniques that are opening the black box of machine learning models and enabling analysts to explain how a prediction is made for each observation.
- The study specifically tests the precision of the SHAP value method for assessing the contribution of features to decision tree-based model learning.
- The results of the study confirm that the SHAP value method can accurately evaluate the contribution of features to model learning when the model is used. This finding suggests that the SHAP value method can be a useful tool for understanding the mechanisms of machine learning models in spatial data modeling.
- Finally, it is emphasized the importance of assessing the effectiveness of the SHAP value method as a trustworthy analysis technique through comparable verification. This highlights the need for ongoing research to ensure that the methods used in spatial data modeling are reliable and accurate.

The paper is organized as follows: Section 1 presents the related works. Basic concepts of SHAP Value are outlined in Section 2. Section 3 presents the experimental part, including results from both "Experiments on data without the difference in resolution" and "Experiments on data with the difference in resolution". The last Section provides the conclusion and outlines the outlook for future research.

1. Related works

In this section, it is presented the importance of features in the data and what kind of methods can be used for that with the help of related works from the literature.

To find out the importance of features in the data, various methods can be used. Some of the commonly used methods are:

Univariate Feature Selection: This method involves evaluating each feature independently using statistical tests or other criteria, and selecting the most important features based on their individual performance (Jain & Saha, 2022; Fagrou et al., 2022; Fayaz et al., 2022).

Recursive Feature Elimination (RFE): This method involves iteratively removing the least important features from the dataset until the desired number of features is obtained. The importance of features is determined by their contribution to the performance of a machine-learning algorithm (Lee et al., 2022; Kilincer et al., 2023; Kumari et al., 2023).

Principal Component Analysis (PCA): This method involves transforming the data into a new set of uncorrelated variables, called principal components, which capture the most significant information in the data. The importance of features is determined by the amount of variance explained by each principal component (Liu et al., 2023; Dargaud et al., 2023; Serrão et al., 2023).

Feature Importance using Tree-Based Models: This method involves using decision tree-based models such as Random Forest, XGBoost, or Gradient Boosting, to determine the importance of each feature in the model. The importance of features is measured based on their contribution to reducing impurity or error in the model (Liu & Aldrich, 2023; Kim et al., 2023; Awotunde et al., 2023).

SHAP values: This method involves computing the contribution of each feature to a machine learning model's prediction using game theory. SHAP values provide an intuitive way

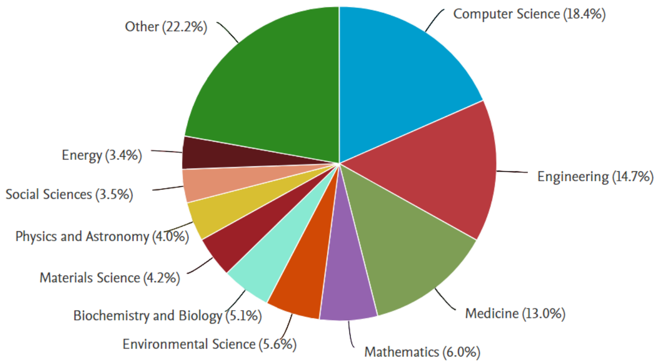

Figure 1. Subject areas of SHAP value

to understand the contribution of each feature to the model's prediction (Mangalathu et al., 2020; Rozemberczki et al., 2022; Merrick & Taly, A 2020).

Overall, the choice of method depends on the nature of the data and the specific problem being addressed. It is often advisable to use multiple methods to obtain a more comprehensive understanding of the importance of features in the data.

Considering the subject areas of 913 publications scanned in Scopus and using SHAP Value, the fields of computer science, engineering, and medicine are in the first three places except for another field. Figure 1 shows the main subject areas of SHAP value in these publications.

XGBoost is used in 243 of these studies. It is demonstrated that the SHAP value may typically accurately assess the contribution of features to model learning using an experiment in which the SHAP value is derived for a model trained by XGBoost using table data produced in an XGBoost model.

The selected papers which are examined for this study are presented in Table 1 in detail.

2. Basic concept of SHAP value

SHAP Value explains the output of any machine learning model by providing an explanation for every feature's contribution to the model's score for a specific instance (Bowen & Ungar, 2020). The SHAP Value approach is based on game theory and connects optimal credit allocation with local explanations using the classic Shapley values and their extensions. The input for SHAP Value is a training model f and the specific instance x, and the output is the contribution of each feature to the model score f(x). The SHAP Value is additive, and the sum of all contributions is exactly f(x).

Cooperative game theory (Chalkiadakis et al., 2011; Alparslan Gök et al., 2010) is used in the concept of SHAP Value to quantify the level of contribution a member has made in a partnership. SHAP Value's foundation is based on the Shapley value, which has been extensively studied in cooperative game theory literature (Futagami et al., 2021). The SHAP Value approach is helpful when the distinct values that each feature can take vary significantly

Table 1. The examined classification of some related works used SHAP value and XGBoost

Paper	Problem addressed	Methodology	Data used	Main contribution	Results	Implications	Limitations
Wang et al. (2022)	Improve process management in wastewater treatment plants	SHAP values for feature importance in tree-based machine learning	Data from wastewater treatment plants	Introduces the use of SHAP values in wastewater treatment plants and demonstrates their usefulness in process analytics	Improved understanding of the processes in wastewater treatment plants and identification of important process variables	Can lead to better process control and optimization in wastewater treatment plants	Limited to only one wastewater treatment plant, and therefore the results may not be generalizable to other plants. Limited to using only tree-based machine learning methods.
Loecher (2022)	Address the bias in feature importance measures in tree ensembles	MDI (Mean Decrease Impurity) and SHAP values for feature importance in tree ensembles	Various datasets used in machine learning research	Proposes a method to debias feature importance measures in tree ensembles and demonstrates its effectiveness	Reduced bias in feature importance measures and improved interpretability of tree ensembles	Can improve the reliability and interpretability of machine learning models that use tree ensembles for feature importance analysis	Limited to tree-based models only. The method may not always perform better than existing debiasing methods.
Li et al. (2022)	Predict beach water quality	Tree-based ensemble model for predicting beach water quality	Beach water quality data	Develops an interpretable tree-based model for predicting beach water quality	Accurate prediction of beach water quality with an interpretable model	Can help manage and improve beach water quality	Limited to only one beach location, and therefore the results may not be generalizable to other locations. Limited to using only tree-based machine learning methods.
Liu and Aldrich (2023)	Explain anomalies in coal data	Shapley and tree-based models for explaining anomalies in coal data	Coal proximity and coal processing data	Provides a method for explaining anomalies in coal data using Shapley and tree-based models	Identification and explanation of anomalies in coal data	Can improve the understanding of coal data and inform decision-making	Limited to only one coal processing plant, and therefore the results may not be generalizable to other plants. Limited to using only tree-based machine learning methods.

End of Table 1

Paper	Problem addressed	Methodology	Data used	Main contribution	Results	Implications	Limitations
Gebreyesus et al. (2023)	Optimize data center operations	SHAP values for feature selection in data center optimizations	Data center optimization data	Uses SHAP values for feature selection in data center optimizations	Improved performance and efficiency of data center operations with SHAP-based feature selection	Can optimize data center operations and improve energy efficiency	Limited to using data from only one data center, and therefore the results may not be generalizable to other data centers. Limited to using only tree-based machine learning methods.
Ullah et al. (2023)	Predict electric vehicle charging behavior	SHAP values for machine learning modeling of EV charging behavior	Electric vehicle charging data	Develops a model for predicting EV charging behavior using SHAP values	Accurate prediction of EV charging behavior using SHAP values	Can inform the design and deployment of EV charging infrastructure	Limited to a specific geographic area, and therefore the results may not be generalizable to other areas. The study is limited to using only XGBoost and SHAP for machine learning.
Jas and Dodagoudar (2023)	Assess soil liquefaction potential	XGBoost-SHAP for assessing soil liquefaction potential	Soil liquefaction data	Uses XGBoost-SHAP for assessing soil liquefaction potential	Accurate assessment of soil liquefaction potential with XGBoost-SHAP	Can inform decisions related to soil liquefaction potential and hazard mitigation	Limited to using only XGBoost and SHAP for machine learning. Limited to using only one type of soil data.
Arboleda-Florez and Castro-Zuluaga (2023)	Interpret demand forecasts	SHAP values for interpreting demand forecasts	Direct sales demand data	Uses SHAP values for interpreting demand forecasts	Improved interpretation and understanding of demand forecasts with SHAP values	Can improve the accuracy and usefulness of demand forecasts	Limited to using only one type of product data. Limited to using only tree-based machine learning methods.

between features, or when a feature's variance in values is lower than that of other features, as demonstrated in our experiments. By providing an explanation for each feature's contribution to the model's output, SHAP Value enables us to interpret the model's behavior and identify important features for better decision-making.

When the number of features is M, the input $x' \in \{0,1\}^M$, which is a simplified input vector x, is locally linearly approximated by the model f.

Using f_x, the contribution of feature i φ_i to model f is calculated as follows:

$$\varphi_i(f,x) = \sum_{z' \subseteq x'} \frac{|z'|!\left(M-|z'|-1\right)!}{M!}\left[f_x(z') - f_x(z' \setminus i)\right]. \tag{1}$$

Then, $z' \in x'$ is the whole subset of x' nonzero elements and $|z'|$ represents the number of nonzero elements in the feature vector z'.

For all input combinations that can be compared with and without feature i, take the average of the differences $f_x(z') - f_x(z' \setminus i)$. Omitting the details of the simplification process and input formulation can be focused on the conditions that the simplified model needs to satisfy. These include local accuracy, which ensures that the model performs well on specific subsets of data, as well as missingness, which ensures that the model can handle missing data appropriately. Additionally, consistency is important to ensure that the model produces consistent and reliable results across different subsets of data. These conditions are critical to ensuring that the simplified model is effective and can be used to generate reliable predictions.

3. Experiment

In order to assess the usefulness of the SHAP value in situations where the distinct values that each feature can take vary significantly, it is conducted two experiments and present the process and results below. Specifically, it is interested in cases where certain features had a lower variance in values compared to others or where the resolution of a feature was low, as is the case with XGBoost based on metric gain (Li, 2022). In such scenarios, default Feature Importance settings may not be sufficient as they only provide an average improvement evaluation criterion for a trained model (Chen & Guestrin, 2016).

To test the efficacy of the SHAP value in such cases, we replicated the difference in resolution between features and calculated the SHAP value. Our experiments demonstrate that the SHAP value can be a valuable tool in identifying important features even in scenarios where there is significant variance in the number of distinct values that each feature can take. These findings suggest that the SHAP value can be a useful technique for analyzing and interpreting machine learning models in various real-world applications.

3.1. Experiments on data without the difference in resolution

Let us consider the case where there is no difference in resolution between features.

For training purposes, an artificial dataset of 10,000 rows is generated in this study. The dataset consists of five features, denoted as $x_i (i = 1, 2, 3, 4, 5)$ which are modeled by a normal distribution $N(0,30^2)$ with a mean of 0 and a standard deviation of 30. An error term b is also incorporated, which follows a normal distribution $N(0,10^2)$ with a mean of 0 and a standard deviation of 10. The training data is then generated using the following formula:

$$y = 15x_1 + 10x_2 + 5x_3 + x_4 + 0.3x_5 + b\,. \tag{2}$$

To ensure consistency, it is necessary to generate each feature as a random number sequence with the same distribution, resulting in a roughly equal number of unique values for each feature. Table 2 shows the hyperparameter settings used by the XGBoost package to train the artificially generated dataset as a regression problem using the package mind.

Table 2. The hyperparameter settings

learning_rate	0.01
colsample_bytree	0.3
max_depth	5
alpha	10

Figure 2 displays the output of the SHAP value package (Mitchell et al., 2022), which computes and presents values that are relevant to the analysis at hand. These values provide important insights into the influence of specific features on the model's prediction and can be used to identify potential areas of improvement or to validate the model's performance.

The x_i coefficient in Eq. (2) is thought to accurately reflect the genuine feature importance in this situation since the five characteristics, $x_i (i = 1,2,3,4,5)$, are generated with an equal mean and variance. The SHAP value calculated in Figure 2 is x_1 : 334.1, x_2 : 206.6, x_3 : 93.3, x_4 : 18.6, x_5 : 9.6. However, since the ratio is about the same as each term's coefficient in Eq. (2), it appears that the feature value importance can be roughly and fairly precisely calculated.

For comparison, the default Feature Importance of the XGBoost package is also calculated and presented in Figure 3.

The feature value of x_5 in the XGBoost default is greater than x_3, and x_4, and virtually equal to x_2, which runs counter to how Eq is generated (2).

When taking this into account and comparing Figures 2 and 3, it appears that SHAP can more properly determine the feature relevance.

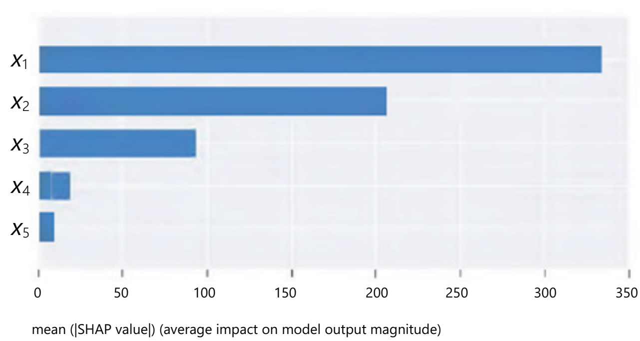

Figure 2. SHAP value of Experiment 3.1

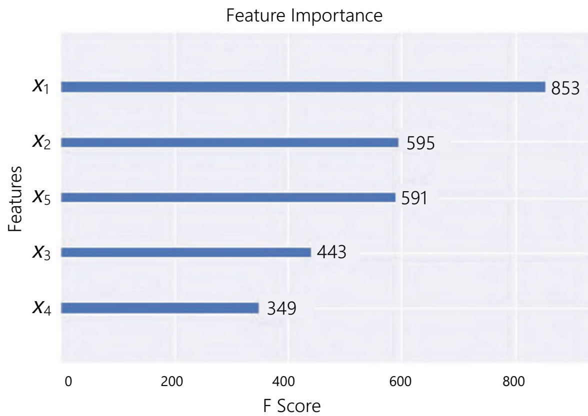

Figure 3. XGBoost feature importance of Experiement 3.1

3.2. Experiments on data with the difference in resolution

Let us consider the case where there is a difference in resolution between features. For simplicity, we generated the feature $x_i (i = 1, 2, 3, 4, 5)$ in the same way as in Section 4.1, and then rounded the feature x_2 to the tenths to lower the resolution. In addition, the training data y is generated by the following formula:

$$y = 10x_1 + 10x_2 + 5x_3 + x_4 + 0.3x_5 + b . \tag{3}$$

The XGBoost model was trained on a dataset, with a focus on two features, x_1, and x_2, which share the same coefficient but have different resolutions. The resulting SHAP value and default feature importance of XGBoost are visualized in Figures 4 and 5, respectively. These figures provide valuable insights into how the model weights the importance of each feature and how it affects the outcome. By analyzing these visualizations, one can gain a better understanding of how the model makes predictions and identify any potential biases or shortcomings.

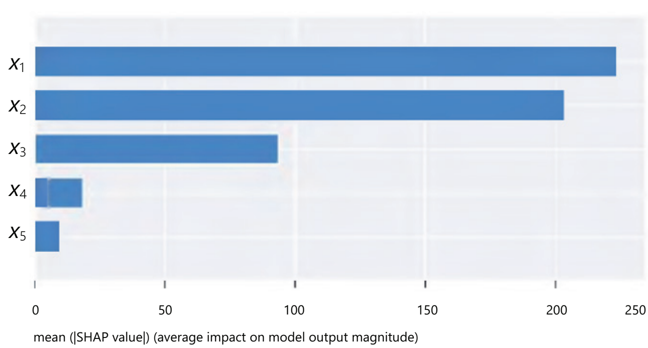

Figure 4. SHAP Value of Experiement 3.2

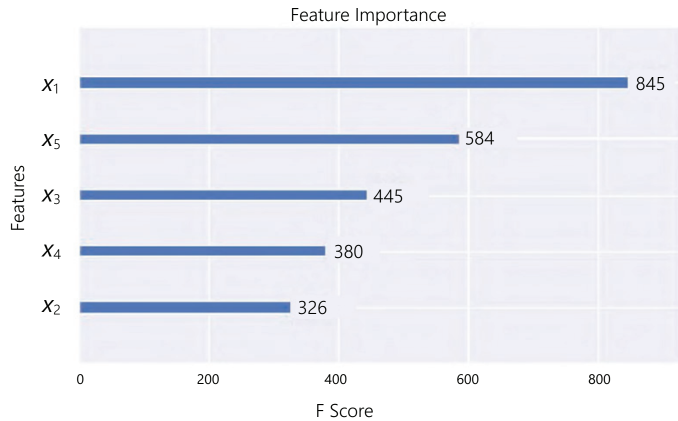

Figure 5. XGBoost feature importance of Experiement 3.2

Conclusions

This study investigates the effectiveness of the SHAP value method for feature importance analysis in spatial data modeling. The findings demonstrate that SHAP value is a reliable and accurate technique for assessing the contribution of features to decision tree-based model learning in spatial data analysis. This enables spatial analysts to identify spatial correlations and visualize them on maps in applications using geocoded spatial data.

It is emphasized that a more accurate data set is essential to assess the SHAP function effectively. Furthermore, a comparable verification is carried out to determine the effectiveness of SHAP value as a trustworthy analysis technique, and reliable results are obtained.

The study makes a significant contribution to addressing the significant problem of interpretability in spatial data modeling and highlights the potential of local interpretation techniques such as SHAP value for overcoming this challenge. In summary, valuable insights into the practical application of SHAP value for spatial data modeling are obtained, and new avenues for further research in this area are opened up.

In conclusion, while creating machine learning prediction models for KPIs, interpretability is crucial. By offering information on the contribution of each feature to the model's learning, SHAP values provide a mechanism to accomplish this. In fields where data is essential, SHAP values are a useful tool for analyzing machine learning models since they can precisely assess the impact of each attribute.

Outlook

Future works could address a number of topics pertaining to how to understand XGBoost forecasts using SHAP values.

First off, even though the focus of this article is decision tree-based models, SHAP values can also be applied to other machine learning model types, like neural networks and random forests. The application of SHAP values to these models and how their interpretations differ from those of decision tree-based models could be the subject of future study.

Second, the usage of SHAP values for interpretability is the main focus of this guide. Nevertheless, feature engineering and feature selection can also be done with SHAP values. Future research could look into how SHAP values can be utilized to discover which characteristics are most crucial and eliminate unimportant or harmful features in order to enhance the performance of machine learning models.

Thirdly, even though SHAP values are an effective tool for understanding machine learning models, calculating them can be computationally expensive. Future research might look into ways to speed up the calculation of SHAP values so that users can access them more quickly.

Last but not least, even though this article offers a thorough overview of reading XGBoost predictions with SHAP values, other techniques or tools might be utilized in addition to SHAP values to increase interpretability. Future studies could examine these techniques and how they can be applied to shed more light on how machine learning models function.

Overall, the topic of using SHAP values to interpret machine learning models is one that is rapidly emerging, and there are a lot of promising areas that need to be further investigated.

It can be enhanced the interpretability, performance, and accessibility of machine learning models in a variety of applications by further developing and broadening our understanding of SHAP values.

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