Explainability of MLP Based Species Distribution Models: A Case Study

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Abstract: Species Distribution models (SDMs) are widely used to study species occurrence in conservation science and ecology evolution. However the huge amount of data and its complexity makes it difficult for professionals to forecast the evolutionary trends of distributions across the concerned landscapes. As a solution, machine learning (ML) algorithms were used to construct and evaluate SDMs in order to predict the studied species occurrences and their habitat suitability. Nevertheless, it is critical to ensure that ML based SDMs reflect reality by studying their trustworthiness. This paper aims to investigate two techniques: SHapley Additive exPlanations (SHAP) and the Partial Dependence Plot (PDP) techniques to interpret a Multilayer perceptron (MLP) trained on the Loxodonta Africana dataset. Results demonstrate the prediction process and how interpretability techniques could be used to explain misclassified instances and thus increase trust between ML results and domain experts.

1 INTRODUCTION

Environment scientists assert that the magnitude, pace and severity of the current environmental crisis are unprecedented (B.Daley and R.Kent, 2005). Several regions are losing their biodiversity to make way for human dwelling and industry. Therefore, in order to safeguard the environment, it's crucial to implement well planned policies that take into consideration the environmental characteristics and biological outcomes of each region.

As part of the conservation science, having a well-thought-out strategy for managing the environment requires a thorough understanding of its components, namely its climatic conditions and species distribution. However, it's hard to pinpoint the exact location of each individual of each species at any moment. Therefore, species distribution models (SDMs) are used to find whether a species is likely to be present or absent in a geographic location based on its environmental conditions. Their objective is to understand a particular ecosystem, its number of species, the composition of its population, and to predict the spatial and temporal pattern of species occurrence.

The new technologies and the data they gener- ate hold great potential for large-scale environmental monitoring, however traditional statistical approaches limits its usage which inefficiently distill data into relevant information (D.Tuia et al., 2022). Conversely, data science community works to apply information technologies to gather, organize, and analyze biological data (American Museum of Natural History,). Basically, they try to use machine learning (ML) to discover new insights and patterns from all the available expeditions and remote sensing data. ML techniques are useful to perform predictive analytics since it gives a variety of tools to support complex data structures, and thus provides a powerful approach for assessing SDMs challenges. However, according to a review made by Beery et al. despite the considerable use of ML techniques in ecology, SDMs has received relatively little attention from the computer science community (S.Beery et al., 2021).

In fact, ML contributed to this field in a cou-ple of areas, namely climate models that repre- sent our understanding of Earth and climate physics (Rolnick et al., 2019), forest management based on satellite imagery and 3D Deep Learning tech-niques(Liu et

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al., 2021), mapping wetlands distribu- tion in highly modified coastal catchments (Wen and Hughes, 2020),urban vegetation(Abdollahi and Prad- han, 2021)and many more.

There are two categories of ML algorithms: legible white-box algorithms that provide readable rules (SEON, 2022), , and black-boxes which are opaque yet more powerful since they can identify nonlinear relationships in data. To remedy this limitation, interpretability attempts to explain model predictions to understand the reasoning behind the prediction process (AI, 2020), avoid bias and gain trust whether globally or locally. Global interpretability, exam- ines a model's general behavior, whereas local interpretability concentrates on a particular scenario that was supplied as input to the model.

Interpretability techniques have been used to improve the explainability of ML based species distribution models. For instance, Ryo et al. investi- gated explainable AI (xAI) techniques in the context of SDMs based on the African elephant dataset (Ryo et al., 2021). They used random forest (RF) as a black box algorithm to predict the presence/absence values of the studied species. In terms of interpretability, they used: (1) feature permutation importance (FI) and the (2) Partial Dependence Plot (PDP) as global interpretability techniques, FI classifies the predictor variables according to their importance, while PDP demonstrate the marginal effect a feature may have on the ML model predicted outcome (Molnar, 2019), along with (3) Local Interpretable Model-Agnostic Explanation (LIME) (Ribeiro et al., 2016) as a local interpretability technique. According to this study, the most relevant feature based on FI was the precipi- tation of the wettest quarter.

This article aims to evaluate and interpret a basic Multilayer Perceptron (MLP) model trained to forecast the African elephant distribution (GBIF, 2021) using: (1) the SHapley Additive exPlanations (SHAP) (Lundberg and Lee, 2017), a local interpretability method that explains individual predictions based on the game theoretically optimal Shapley values; and (2) the Partial Dependence Plot (PDP): a global interpretability technique that visualizes the marginal effect of an individual feature to the predictive value of the studied model (Molnar, 2019). This paper answers and discusses the following research questions:

- RQ1: What is the overall performance of the con-structed MLP models?
- RQ2: What is the local interpretability of the bestperforming model?
- RQ3: How global interpretability enhances localexplanations?

The main contributions of this study are the following:

- Assessing and comparing the performance of 12 MLP based classifiers that were generated by combining 3 different Hyperparameters using GridSearch.
- Interpreting 3 randomly chosen instances locally using SHAP and comparing them with their true labels.
- Explanation of misclassified instances using PDP.

The remainder of this paper is organized as follows: Section2 introduces explainable AI and the difference between Global and Local Interpretability. Section 3 describes the used dataset and performance metrics to select the best performing model. Section4 presents the experimental design followed during this study. A discussion about the obtained results and findings is presented in Section 5. Section 6 covers the threats to validity and the conclusion.

2 BACKGROUND

This section presents the feed-forward neural network used in this research, along with the used interpretability techniques namely SHAP and PDP.

2.1 Artificial Neural Networks: MLP

ANNs are a collection of simple computational units interlinked by a system of connections (Cheng and Titterington, 1994) that were inspired from the brain's neuron architecture. They are frequently used in data modelling, as they are perceived as better substitute to standard nonlinear regression or cluster analysis prob- lems (Gurney, 1997).

In general, ANNs are organized in layers and this is where the MLP comes in, it is a typical example of the feed-forward ANN where information travels in one direction from input to output (Hakkoum et al., 2021). A MLP is constituted of 3 types of layers: the input layer, which receives the data to be processed, one or more hidden layers, which together constitute the network's true engine, and the output layer.

As to optimize the MLP Hyperparameters tuning phase, GridSearch a technique that specifies a search space as a grid of Hyperparameters and evaluates every position in the grid (Brownlee, 2020)was used.

Table 1: Bioclimatic variables.

Variable	Description	Abbreviations	Range
Elev	Elevation	Elev	[-61 ; 3508]
Bio1	Annual Mean Temperature	AMT	[7,810688 ; 29,427000]
Bio2	Mean Diurnal Range	MDR	[6,640182 ; 18,048876]
Bio3	Isothermality (BIO2/BIO7) (×100)	Isothermality	[26,918064 ; 92,384308]
Bio4	Temperature Seasonality	TempSeasonality	[15,199914;1039,296265]
Bio5	Max Temperature of Warmest Month	MaxTempWM	[17,118000;41,708752]
Bio6	Min Temperature of Coldest Month	MinTempCM	[-9,583250 ; 22,415842]
Bio8	Mean Temperature of Wettest Quarter	MeanTempWQ	[6,682958 ; 31,448957]
Bio12	Annual Precipitation	AnnualPrecip	[3,000000 ; 3369,000000]
Bio13	Precipitation of Wettest Month	PrecipwettestM	[1,000000 ; 535,000000]
Bio14	Precipitation of Driest Month	PrecipDriestM	[0,000000 ; 105,000000]
Bio15	Precipitation Seasonality	PrecipSeasonality	[12,457452 ; 153,643448]
Bio18	Precipitation of Warmest Quarter	PrecipWQ	[0,000000 ; 728,000000]
Bio19	Precipitation of Coldest Quarter	PrecipCQ	[0,000000 ; 948,000000]

2.2 Interpretability

Interpretability is determined by whether the model has a transparent process that allows the users to understand how inputs are mathematically mapped to outputs (Doran et al., 2017). It represents the degree to which a human can consistently predict the model's result, and evaluate the forecasting process by giving the relative importance of each variable.

Interpretability methods can be categorized according to various criteria, depending on how they are used: Intrinsic/ post-hoc; model-specific/ model-agnostic; global/ local (Molnar, 2019). Global interpretability describes how the entire model behaves, meanwhile local interpretability focuses on the prediction of a particular instance; it is similar to a zoom in on a single instance and then examining the reasons behind the model's prediction for this input.

This paper uses SHAP to examine the local interpretability of the best performing MLP model. It explains the model's individual predictions using Shapley values, a cooperative game theory concept that calculates the contribution of each feature to the difference between the predicted value and the aver- age of all predictions. Shapley values compute the marginal contribution of each feature to the end outcome by perturbing the input features and observ- ing how these changes correspond to the final model prediction. The Shapley value is then calculated by taking the average of all marginal contributions (Gopinath and Kurokawa, 2021). SHAP is a model-agnostic method, meaning that SHAP's process remain the same regardless of the used ML algorithm.

In addition to SHAP, PDP was used to study the marginal effect a feature may have on the target variable. It shows whether the relationship between the target and a feature is linear, monotonic or more complex(Molnar, 2019).

3 DATA DESCRIPTION AND PERFORMANCE CRITERIA

The following section describes the used datasets, and introduces the performance measures.

3.1 Data Description

To run a SDM, two types of data are needed: occurrence data, which presents the coordinates of the locations where the studied species occurs, and environ- mental data, that describes the bioclimatic conditions of those locations (EcoCommons, 2022).

For occurrence data GBIF LoxodontaAfricana tabular data were used. It contains 10494 rows and 257 columns, its relevant features are decimal Longitude, decimal Latitude and the occurrenceStatus. The decimal longitude and latitude define the species geographical locations, while the occurrenceStatus presents the occupancy / absence values at those locations.

The original record contains 10466 row of presence data and 28 row of absence data. To resolve this imbalanced data problem a sample of 8019 background points were randomly generated using dismo package in R to sum up with 16511 occurrences of which 8979 are presence data and 8019 are pseudo-absences.

Despite the existence of different methods to generate background points, the randomly selected pseudo-absences yielded the most reliable.

distribution models (Barbet-Massin et al., 2012).

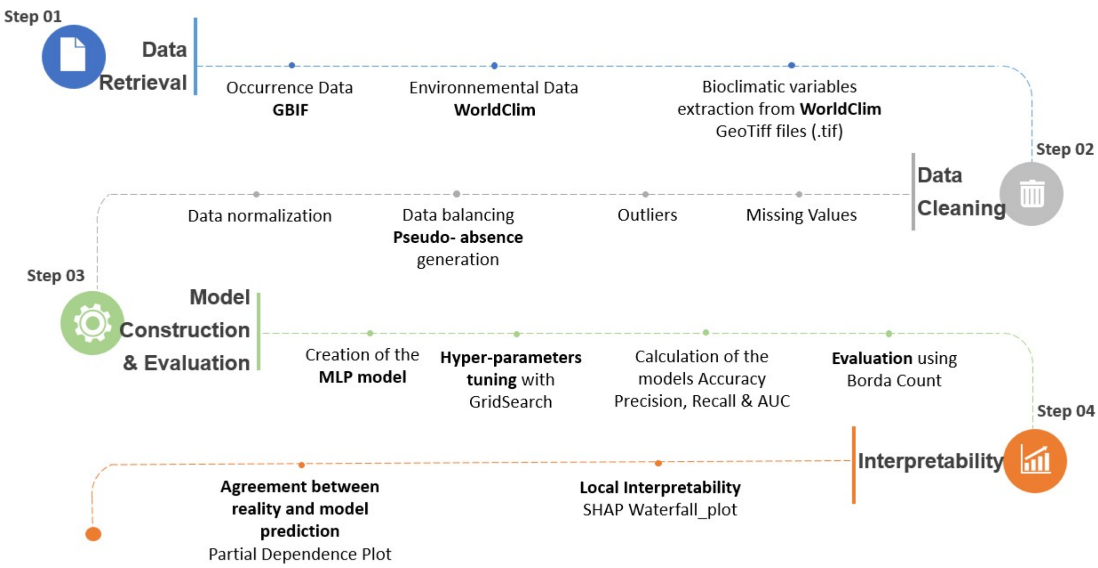

Figure 1: Experimental Design.

It is critical to consider the credibility of the generate background points, a location with no occurrences of the species does not imply the absence of the species in this loca- tion, it could be an area with no data or a location out of land. To avoid such problems the dismo package provides different methods dedicated to SDMs challenges, such as sampling the random points from a study area to form the pseudo-absences afterwards or using a mask to exclude the areas not on land (Spatial Data Science, 2021).

For the environmental data, the WorldClim stan-dard bioclimatic variables were extracted from 19 GeoTiff (.tif) file using 'biovars' function in the dismo R package. Table1 presents the used bioclimatic vari-ables and how they were encoded in this work.

3.2 Performance Criteria

The MLP based models performance is reported and compared in terms of 4 different metrics: Accuracy, Precision, Recall, and AUC. After calculating these metrics, the Borda Count, a ranked voting technique that ranks the models in order of preference, was used to select the best MLP classifier using the accuracy, precision, recall, and AUC metrics as voters (Lipp-man,).

4 EXPERIMENTAL DESIGN

This section describes in details the steps followed in this case study. It starts with model configuration and selection, then the local interpretation using SHAP's Waterfall plots, and finally the PDP plots generation. The steps are showed in detail in Figure1.

4.1 Data Retrieval and Cleaning

As mentioned in section 3, this study used two types of data: Loxodonta Africana occurrence data from GBIF and environmental data from WorldClim,which were concatenated using R based on their com-mon geographic points. Missing values, outliers, data balancing, and normalization were all resolved during the Data Cleaning phase.

4.2 Models Construction

The MLP classifiers were built using one hidden layer. Three different hyper-parameters were used to control the model's learning process: the batch size, which represents the number of samples processed before the model is updated, the solver for weight op-timization where SGD refers to Stochastic Gradient Descent, known as the most basic form of gradient descent while 'Adam' is an extension to SGD that provides faster results (Brownlee, 2017) , however different studies argue that although Adam converges faster, SGD generalizes better than Adam and thus results in improved final performance (Park, 2021). Finally, we have the hidden layer size that represents thenumber of hidden nodes on the first hidden layer, its selected range was chosen as to provide good performance but without requiring a huge amount of time in the training phase since the aim of this empirical evaluation was interpretability and not performance.

GridSearch was employed to optimize the Hyperparameter tuning phase with 10 cross validation training. Table 2 presents the used configuration. Note that the hidden layer sizes were selected based on previous experimentations where the highest performancescores were found close to the mentioned range in table 2. The batch size and the solver values were chosen as a standard configuration commonly found in literature.

Table 2: Hyperparameters configuration.

Hyperparameters	Selected Range
Hidden Layer Size	[(20,),(25,),(30,)]
Batch size	(32,64)
Solver	['sgd', 'adam']

4.3 Interpretability

This step tries to interpret the MLP classifier results locally using SHAP's waterfall plot. It explains a set of 3 different instances that were randomly selected in a way to have one true positive where the model agrees with reality and predicts a high habitat suitability, one true negative where the model accurately predicts a low habitat suitability and one false negative, where the classifier predicts low habitat suitability, while it's not the case in reality.

After the interpretability of the MLP classifier PDP was used to determine if there is an agreement between the classifier predictions, the instances true label and local interpretability results, PDP plots were generated for the 2 first ranked features.

5 RESULTS AND DISCUSSION

This section presents and discusses the results of this empirical study, namely the models performance, and interpretability results.

5.1 Models Evaluation

The Hyperparameters combination gave 12 MLP classifiers. Table 3 describes the overall performance of the 3 first and the last ranked MLP models according to the Borda Count method using accuracy, precision, recall, and AUC as voters. The classifiers are presented according to their assigned ranks. According to Table 3, the top-ranked model has 25 neurons in its hidden layer, 64 as a batch size, which determines the number of training examples utilized in one iteration (Murphy, 2019), and 'sgd' as a solver, which specifies the algorithm weight optimization over the nodes (Fuchs, 2021). To note that this is the classifier used in the interpretability phase.

5.2 Local Interpretability

To test the trustworthiness of individual predictions, a group of 3 instances was randomly chosen, Figure2 shows their relative SHAP's waterfall plot explanations. The waterfall plot's purpose is to show the SHAP values of each feature as well as its im- pact on the final prediction. The model's prediction is represented in the y-axis by f(x), each bar illustrates how the feature helps to push the model's output away from the base value E(x) that indicates the average of the model output over training data.

The features with a right arrow influence the prediction more in favor of an appropriate habitat for African elephants, whilst the features with a left arrow influence the prediction more in favor of the species' inadequacy for such environments.

Equation (4) demonstrates how f(x) is calculated.

$$F(x) = E(x) + \sum SHAPvalues \tag{1}$$

The base value in this study is 0.537, it represents the average of all observations. The model prediction for instance 2 is 1 meaning that the studied species can survive in this location, in this case f(x) is obtained using Equation (4): 0.536 + 0.01 - 0.02 + 0.02 - 0.03 + 0.03 + 0.03 + 0.03 + 0.04 - 0.05 + 0.05 + 0.06 + 0.06 + 0.11 + 0.12 = 0.996 1, it sums the base value E(x) with all SHAP values, the same process is true for the other instances.

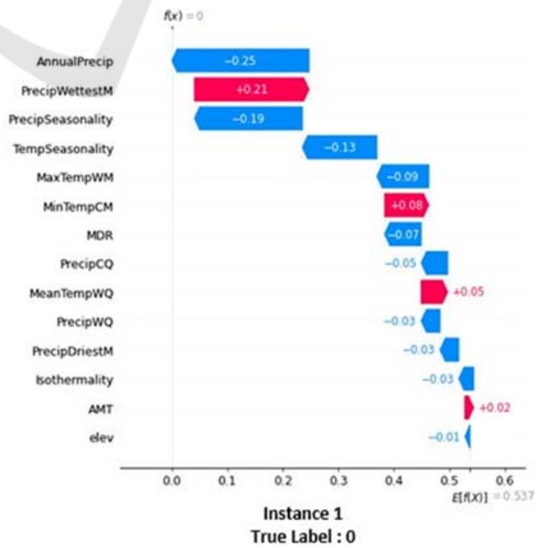

Figure 2: Instance 2 SHAP's waterfall plot.

Table 3: Borda Count Results.

MLP	Accuracy	Precision	Recall	AUC	Rank
[(25,),sgd,64]	0.857059	0.8576	0.856452	0.924786	1
[(30,),adam ,64]	0.854046	0.854450	0.853481	0.923254	2
[(30,),sgd,64]	0.851284	0.851420	0.850775	0.920037	3
[(25,),adam,32]	0.815967	0.816859	0.814878	0.889776	12

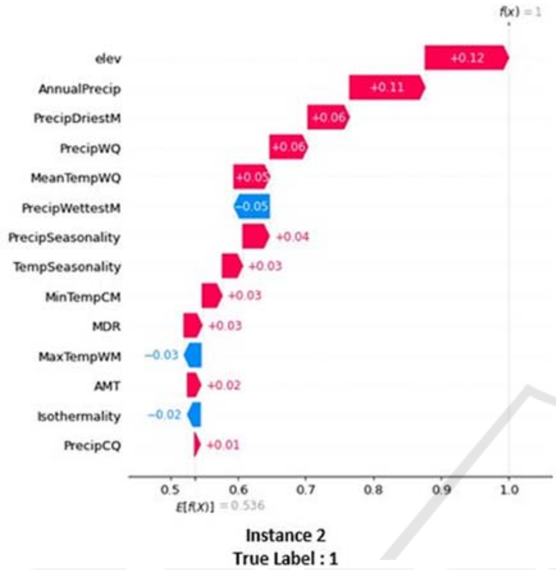

Figure 3: Instance2 SHAP's waterfall plot.

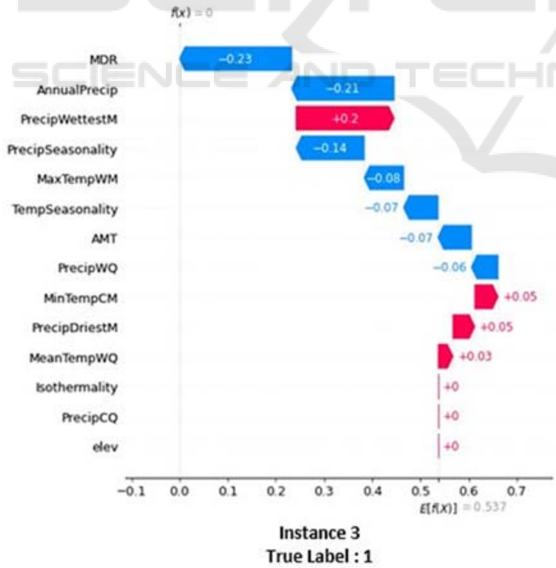

Figure 4: Instance 3 SHAP's waterfall plot.

In the first instance (Figure 2), the classifier pre-dicts a low habitat suitability for the location in question which was mainly proven by SHAP since f(x) =0and the 'AnnualPrecip' variable was ranked the firstamong all other variables with a SHAP value

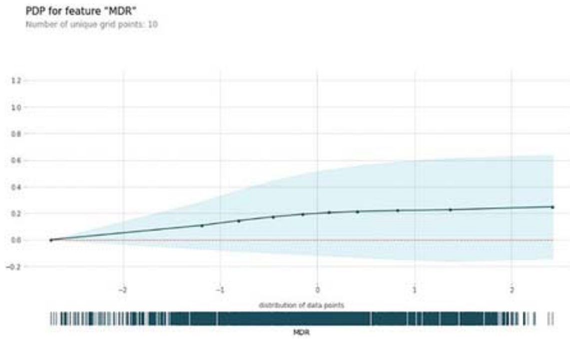

Figure 5: 'MDR' Partial Dependence Plot.

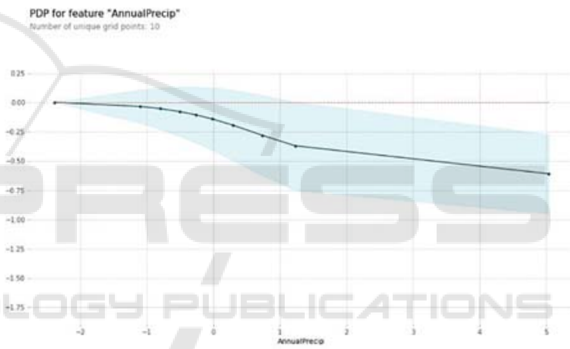

Figure 6: 'Annual Precip' Partial Dependence Plot.

of -0.25.For instance 2 (Figure 3), the MLP classifier pre-dicts a high habitat suitability f(x)=1.It was noticed that according to SHAP the 1st ranked feature was'elev' which increased the base value with 12% in comparison with its initial value. Instance 3 (Figure4) presents a false negative since the classifier predictsa low habitat suitability f(x)=0 while the true label ofthe instance is 1 which means that the models' prediction affirms the absence of the species in this location while it is not the case in reality.

In order to gain a deeper understanding of this in-stance and discover the reasons behind this inaccurate prediction with the point's true label, PDP plots were generated for the first and second ranked features.

Normally 'MDR' ranges from -3.017 to 2.439, in this case it is equal to -0.95. According to the PDP plot in Figure 5, the max reached value at this posi-tion is less than 0.4, which means that the classifier predicts a low habitat suitability and that agrees well with SHAP explanations since f(x) was equal to 0.

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The ‘AnnualPrecip’ range is between -2.388 and 5.115, its value in the studied position is approximately 0.82. According to the PDP plot in Figure 6, the mean reached value in this point is less than -0.25, which agrees with SHAP results where f(x) is equal to 0, and explains more why the model predicted a false 0 since both values 0.4 and -0.25 in the PDP plots (Figure 5 and Figure 6) are far from being around 1.

6 THREATS TO VALIDITY AND CONCLUSION

This work includes limitations that should be taken into account when evaluating its findings. During the data retrieval phase, only one occurrence dataset was used, incorporating additional data types to the used tabular dataset may generate better results.

Optimizing the built MLP classifier and creating more black box models, as well as comparing SHAP with other global and local interpretability techniques would undoubtedly provide better explanations to the misclassified instances.

To conclude, several MLP models were used to study the distribution of the Loxodonta Africana, the top performing model was used to predict the species' occurrence and absence values. Based on SHAP's results, the ‘AnnualPrecip’ contributed significantly to the proposed model's output since the studied species lives in the African Savanna known with its tropical wet and dry climate where rain falls in a single season and the rest of the year is dry.

SHAP allowed the conduction of models analysis in depth and leads the selection of appropriate features making it a suitable explanation technique for biodiversity experts to consider when drawing critical decisions.

Future work would attempt to include more black box models, and compare their performance as well as their interpretability with the obtained results using different techniques such as SHAP's summary plot, FI, and LIME.

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