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Research Article

Increasing the Modelling & Simulations Community Capabilities Through the Use of Datascience: A Review

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ABSTRACT

Data science possesses the capacity to derive significant insights from extensive and complex databases. Nevertheless, the process of interpreting data science is an enormous challenge due to its consistent involvement with vast quantities of unorganised and diverse data. In this research, we have examined a crucial subject in the field of data science: the utilisation of interpretability tools. Our focus is on analysing data science models and methodologies, assessing their efficacy, and clarifying the decision-making process of machine learning algorithms. In summary, we recognise the necessity for additional investigation into interpretability tools to create resilient and transparent tools that will improve the interpretability and reliability of data science models and methodologies.

Keywords:

INTRODUCTION

Everybody loves music recommendations like Spotify or Apple Music, for instance. Thus, everyone is glad when Netflix offers shows up the alley and Instagram shares posts containing the material, which we are interested in, and Google displays ads for products we are thinking about buying. To provide a better and enhanced user experience, all these systems incorporate Machine Learning (ML models, data science, and interpretability. In its operation, the recommendation engine employs ML algorithms, which analyze our listening history and favourite genre, among others. The ML models analyse these and other details very comprehensively and from there make the recommendation. For instance, play the following song that aligns with our music taste: It also gives helpful suggestions, particularly where strategic and/or tactical plans need to be made. They help to augment the customer experience, and they try to predict what the consumer wants. Here, data science plays a principal role in handling and aggregating user data in large quantities. Data scientists use ML algorithms, statistical tools and data visualisation methods in order to analyse the gathered data and enhance the precision of the recommendations. It is worth pointing out that contemporary interpretability tools guarantee the transparency of the recommendation system.

They are useful in helping data scientists make sense of the recommendations made for a certain song or artist. In the process of recommending a song to the user, the system makes the choice depending on the user's profile. SHapley Additive ExPlanations (SHAP) provides a locally interpretable explanation to the user and identifies certain features that reflect the user's choice of this song. This makes the user develop confidence in the system. This ML model needs to sort and categorise the knowledge as structuring information about the genres, artists and users' preferences. If the user complains that the song recommended to him/her is not appropriate, the system gives counterfactual explanations that indicate what changes in the user's profile might lead to a different, and presumably more satisfying, recommendation. To do this, our idea was to try to train a surrogate model that mimics the actions of the complex recommendation model. This less complex model yields the sensitivity analysis of the recommendation to support top-level interpretation that shows the contribution of every feature. Therefore, this integration offers recommendations of the music which we are likely to be interested in. It is a direction that will help to determine which data is important, study significant amounts of information to find useful facts, help enterprises, contribute to the discovery of something new, and contribute to the formation of developments in the sphere of digital technologies. We are getting data analysis from raw data by processing data at various levels at high granularity using data science, and unravelling complex patterns and trends with the help of machine learning (ML). Data science is going to have a large impact on ML because the effectiveness of any machine learning model highly depends on the quality and the amount of data used in the experiment. This paper defines ML as a tool that can be used to analyse big data and obtain vital information from it [1]. They claim to make the right approximations and forecasts for any distinct area of concern. ML models are also very effective in automating jobs that were before very tasking. This means that machine learning can be used in a wide array of areas to minimise the need for human input. Big data analysis is applied in decision support in the ML models [2]. Machine learning algorithms are a very important part of data science as they enable the creation of models to predict future outcomes and see relations in data.

Consequently, if one wishes to effectively communicate about the results of machine learning algorithms to interested stakeholders, one has to opt for graphs and visualisation. The use of data visualisation also helps in finding trends and gaining more insights about the machine learning model. The given field of data science can apply visualisation as one of the most significant tools quite often. The other interpretability is the feature importance. With regards to the music recommendation system, feature importance enables one to determine which of the features or attributes most influence songs and users' behaviour for recommendation. Feature importance can be of great help to the ML model in learning which of the features affect or contribute most to the recommendations. This feature enables the improvement of the system with user feedback and the changing of the preferences, thus relating to a more favourable experience for the listener, where increasing unpredictability of the recommended songs keeps the listener interested. Of late, interpretable tools within data science allow users to better explain what information original complex algorithms have brought, which allows for better decision-making in the process of creating and improving ML models [3, 4]. To explain it in a rather straightforward manner, interpretability tools are best understood as those techniques and methodologies specifically geared towards explaining the decisions and predictions of ML models. Its goals are to increase the comprehensibility of the particulars of models and algorithms that, instead of straightforward human understanding, are often relied upon in human decision making. It allows users to build up trust and explore the model for bias and useful information they can use. Other advantages of interpretability tools are also worth noting; people use these tools to debug errors and inaccuracies, to analyse misclassified or erroneous predictions. With this information, a lot of ideas can be generated concerning the enhancement of the model and the performance in general. ML uses data science as its backbone, and the two work hand in hand to develop strong and accurate models for various uses. Data science, in conjunction with ML, utilises statistical and predictive systems with models that let the system learn from the data and make decisions [5].

LITERATURE REVIEW

These interpretability tools play a crucial role in solving the problem of 'interpretability' in some of the machine learning models, where it might be somewhat challenging to know how the model arrives at a particular decision. Through these tools, practitioners can understand how models work and perform to make decisions on the usage of such models and mechanisms for enhancing them. Because of several factors, such as the creation of confidence in the model and its results, rectifying errors in the model, correcting biases, and total compliance with the laid-down laws. ML models can be interpreted, and thus, the models assist in locating problems or errors. The internal mechanisms of the models can reveal some subtle issues and problems, such as working with biased data, low data quality and logical errors in the model. Whenever there is a need for correcting and fine-tuning of the models, Interpretability plays a very important role in getting to know what has gone wrong and how to rectify it. There are many industries with rules that prescribe the need for explanation and reasoning for the actions of the ML models. This influence occurs due to the following compliance requirements, while interpretability aids in meeting them through explanation regarding the facts and attributes of the model as displayed below: This is especially the case in such fundamental areas as finance, healthcare, and law as well. It is therefore essential to understand how an interpreter builds their decision to uncover bias and assess fairness. Thus, the input features and their weights allow the data scientist to detect that if the models are biased and if some groups are discriminated against. Interpretability enables the fairness of the models and also ensures that the negative effects arising from the use of the models are not inflicted on the disadvantaged groups. Feature importance, that is, determining which features or variables contributed most to the model's decision, is made possible by interpreting ML models. This knowledge gives a better feel of the hidden interactions, trends, and influential variables that are explanatory to the model findings. It permits business domain specialists to come back towards the models, make adjustments and corrections, enhance their understanding of the problem domain, as well as use the result of the model to make decisions. Interpretability helps data scientists to work together with other people involved in a project as well as with other stakeholders. When the data scientist describes the operation of the ML algorithms and furnishes the results of these in a comprehensible manner, the targets of the model are relayed to a nontechnical audience. This fosters teamwork, enhanced decision making, as well as ensures that various sectors are in harmony. Of the available Python packages and techniques, the two that this paper centres its investigation on are the SHAP and Interpret ML interfaces of Generalised Additive Models (GAM). To this end, we implement a survey and a contextual inquiry to examine how data scientists apply interpretability tools in practice and to profile workaday issues in creating and assessing ML models.

METHODOLOGY

Initially, six data scientists working at a big tech company were asked to complete a semi-structured interview. The authors developed and used this particular interview protocol with this end in mind: to bring out problems that are often witnessed in model development and evaluation using ML. They then formulated the interview with the use of the 'open coding' technique and the 'Affinity diagram'. Based on the concerns about real data science projects, they came up with six themes that are the main issues encountered by any data scientist. The six themes described in this paper are presented in Table 1. As the foregoing results have indicated, there are only six interviewees; thus, it is far from possible to claim that the list includes all possible candidates. Nonetheless, the study considered previous work in failure analysis of machine learning and made a consistency check. To address all these problems, we structured our study as a contextual inquiry with an emphasis on problematics. We employed eleven data scientists, each of whom was provided with a Jupyter notebook with a dataset, a pre-trained ML model, an interpretability tool, and a list of questions to address. The main objective was to find out whether the participants could assess where the issues pointed out in the pilot interviews were using the interpretability tool. What is new and relevant to understanding the dynamics of data science practice from a sociotechnical perspective is the observation that contextual analysis uncovers more than a gap or a disconnect; there is a form of dissonance between data scientists' associations with interpretability tools and their supposed purpose. The major part of the participants relied too much on the interpretability tools. Sometimes they fell into the trap of over-relying on some of the artefacts, such as the dataset or the inherent machine learning algorithm. While the idea behind interpretability tools is to help the data scientist understand how an ML model works, some participants used it in the primary sense of trying to explain some observations they had made. In its simplest form, the survey's results can be summarised by the fact that data scientists misuse and over-rely on interpretability tools. In addition, the importance scores and other values are not available in the interpretability tools nor also the visualisation outputs.

Following the contextual inquiry, they created a survey to scale up and quantify their key findings. They conducted the study to shed light on the mental models of data scientists who utilise interpretability tools. Each participant in the contextual inquiry only used one interpretability tool, chosen at random. Manipulation was used to test the participants' perception level, their use of interpretability tools, and their reliance on them for justification. A series of questions was asked of them about their demographics and backgrounds. These questions encompass (1) their current role and its duration; (2) the degree of ML integration in their routine tasks; (3) the duration of their ML work; (4) their familiarity with GAMs and SHAPs, along with interpretability; (5) the duration of their use of interpretability tools and GAMs and SHAP; and (6) their familiarity with the dataset. The results convey the vital differences between GAM-manipulated and SHAP-manipulated, as well as between GAM-normal and SHAP-normal.

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Participants using the GAM algorithm, in particular, had higher accuracy and higher stated confidence in understanding their visualisation.

Additionally, they had less cognitive load than people using SHAP. This explains why GAM interpretations are simpler and easier to comprehend than SHAP interpretations. Although there are no significant differences in the outcomes between manipulated and normal visualisations, the results show that the participants did not fully understand the visualisations produced by the interpretability tools. In addition, they had high standards for these visualisations that went beyond what the tools could do. However, there is still a debate on what interpretability should entail. Furthermore, the primary goal of social science research has been to develop and explain things in a way that allows people to comprehend and use them. As the primary evaluation standards for explanations, the social science literature suggests simplicity, generality, and coherence. The evaluation of explanations includes additional metrics such as knowledge and characteristics responsible for "knowing," as well as the autonomy of individual explanations. This field of work guides the design of explanation systems. For humans, these systems function best. ML researchers specifically designed this technique to address the lack of

user-centric evaluation. This study addressed the complaint by conducting user studies on two pre-existing interpretability tools. Interpretability tools such as GAM and SHAP are highly effective methodologies for comprehending the decision-making processes of ML models.

Table 1: Six themes summarising the common concerns of data scientists

Theme	**Description**
Missing values	Multiple methods for dealing with missing values (e.g., coding as a unique value or imputing with the mean) can cause biases or leakage in the ML models.
Changes in data	Data could change over time (e.g., new categories for an existing feature).
Duplicate data	Unclear or undefined naming conventions could lead to accidental duplication of data
Redundant features	Including the same feature in a variety of ways could distribute importance across all of them, making each appear to be less important.
Ad-hoc categorization	When converting a continuous feature to a categorical feature, one could choose category bins arbitrarily.
Debugging difficulties	Identifying potential model improvements based on only a small number of data points is strenuous.

ROLE OF GAMS

The described ML models are relatively simple, and it is, therefore, natural to interpret them. Statistics is actually at the root of these models. They decompose a learned predictor into additive components that depend on an individual input variable. Either of the modules can be straight or composite. GAMs employ whatever is as complex a forest as, yet can be as accurate. The strength of Interpret ML's implementation of GAM is that every component of it is inherently incorporated as a quantitative visualisation tool for plotting. Stating the technical properties, GAM can be described as an additive model. Here, the authors employ analytically smooth varying functions to measure the effects of the predictive variables. These may be linear or non-linear, and this is concerning the underlying patterns in data observed [6]. In the past, people developed GAMs to encompass aspects of both additive models and generalised linear models. The concept which forms the basis of the GAM framework is an enticing and uncomplicated mental organisation. The framework is: (1) Each predictor and the dependent variable has a smooth, linear or any other type of relationship; the user can calculate these smooth correlations at the same time combine them to predict g(E(Y)). [7–8] Thirdly, the user implements GAMs to data sets that show non-linearity between the dependent and independent variables. They include a random function also known as the distribution function, an additive function and the link function. GAM can also estimate models for standard distribution types of Poisson, normal, gamma and binomial types. Select the spline term with the aid of the degree of freedom, initial smoothing parameter, and the like. Model package: mgcv, gam.

Like all models of aid delivery, GAMs present a lot of benefits as discussed below. The main things that make GAM strong and easy to use are the numerous flexible predictor functions that help GAM to look for some patterns in the given data, the simplicity of the interpreting of GAM and L1 and L2 loss functions, that serve as the method of regularizing the predictor functions, to prevent the model to become over-fitted. When it comes to models with non-linear effects, GAM can propose solutions that are simultaneously interpretable, as well as regularised. Another advantage of GAMs over other potential approaches is the capacity to strike a balance between the interpretable and biased linear model and a fully flexible but non-transparent 'black box' learning algorithm. Moreover, GAM has one more and, in fact, essential advantage, with the help of which we can control the smoothness of the predictor. It thus enables us to exclude unstable, senseless predictor functions within GAM. This is being done by rolling back the smoothness levels. It rationalises merely the fact that, even if the specific dataset with which one works unveils what appears to be 'noisy' relationships, it is indeed possible to start from the assumption that there is an inherent nature of smoothness to the predictive relationships by their nature. They both guarantee that you shall get the right model interpretation and that the results obtained are credible.

Often, the more conventional methods of linear models fail to spot common nonlinear structures that GAMs spot. The relations depicted in Figure 3 vary between sharp oscillations of the response variable, which is typical for the so-called 'hockey stick', as well as several peaks resembling mountain ranges. The following patterns are described in the paper and are presented in Figure 1 in the form of a diagram

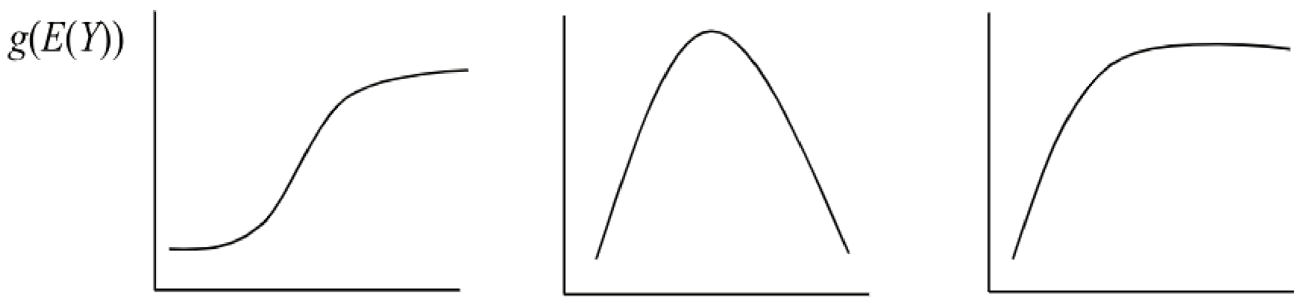

Figure 1: Various patterns of GAM

Although GAM has several advantages, it is not without limitations. Various authors have noted the following drawbacks of GAM: GAMs sometimes suffer from a flaw known as over-fitting. There is also the problem of predictive accuracy, especially when the smoothed variables go above or below the range that was used in the machine learning model training. Another possible concern is that it may not be able to provide sufficient flexibility to capture detailed features of the regression surface to a desirable level [9].

Further, the use of a Smoothing Spline in the construction of a GAM is a tad more complicated than the use of a Natural Spline. The first of these is the fact that one cannot apply least squares in smoothing splines for models. However, this is not a problem when using the so-called 'backfitting algorithm' approach. GAM is extremely useful and comes in handy when the data is not a simple linear model. It has also enabled flexible adaptation to seasonal

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behaviour and the need for parametric forms to be pre-specified [10]. We must agree that GAM is a straightforward, transparent, and adaptable modelling approach able to compete with other widely used techniques. Data scientists should definitely make room in their toolbox for GAM.

ROLE OF SHAP

SHAPs are the techniques that help us provide a post-hoc explanation for predictions made by complex ML models. These models can serve as local interpretable model-agnostic explanations (LIME). These ratings are based on Shapley values, a concept from cooperative game theory. The SHAP Python package can also produce global explanations by aggregating the importance scores for many predictions. SHAP provides information on how each feature affects the target, which helps us understand any ML model. SHAP has many other features, too. By focusing on features that significantly influence the prediction, SHAP can offer a feature for any basic machine learning model used in the selection process [11]. Simply put, SHAP is a cooperative game-theory-based approach. SHAP improves the transparency and interpretability of ML models. By taking into account all subject subsets in the training dataset and computing a weighted sum of the individual contributions, Shapley values achieve fairness [12]. Utilising SHAP is a very easy and simple approach. As explained in Figure 2, we must first construct a model and then use the SHAP library to enhance our ability to address them. Thus, it is possible to point out several discrete types of plots. The user can utilise the following graphs to assess the influence of the attributes: Figure 5, Figure 6, Figure 7, Figure 8, Figure 9, and Figure 10.

Figure 2: SHAP architecture

BAR PLOT

When discussing coding in depth, the usual sequence of steps is as follows: A treatment of developing a predictive model, training the estimator. The idea is that the visualisation helps data scientists to improve the comprehension of the processes that define the possibility of the use of machine learning algorithms and their relation to specific records. SHAP also extends the possibility for youths to PIN, detect and resolve new emerging challenges that eventually

Here, they are grouped to take into consideration the ability to contribute to the forecast. There are no restrictions placed on the absolute values of SHAP; both positive and negative contributing amounts are used. It is possible to host bar plots in either the vertical or horizontal position. A bar plot is a type of graph in which each class has its own bar. The height or the length of each bar represents the frequency or the quantity of data points associated with or connected to that particular category. Bar charts are commonly used in different contexts, such as: One of the abstraction and summarisation methods includes: (1) comparing frequencies or counts, (2) presenting proportions, (3) using temporal changes, (4) comparing multiple variables, and (5) displaying nominal data. The bar plot is used consciously as a visualisation because it unambiguously gives facts.

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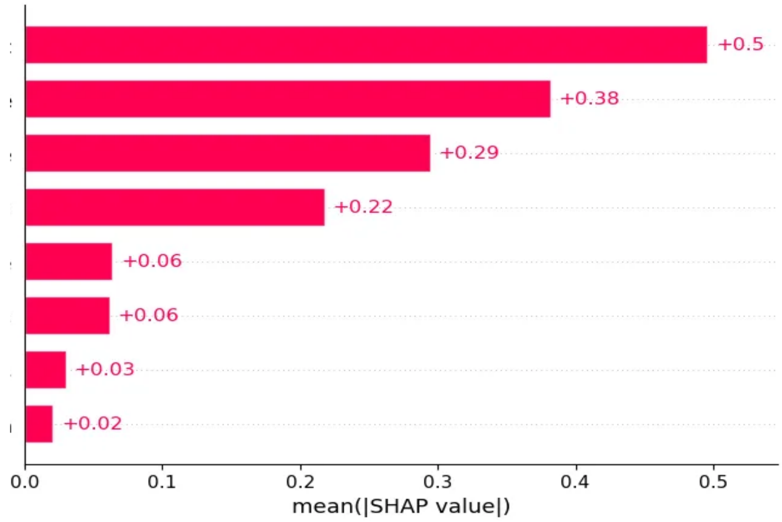

Figure 3: Bar plot to support the SHAP Algorithm

BEESWARM

The primary objective of the beeswarm plot is to provide a concise and comprehensive overview of the key attributes of the dataset and their impact on the output of the model. This summary figure organises the features according to their influence on prediction. However, in this particular scenario, it is also possible to examine the potential impact on the outcome if the feature possessed either greater or lower values. Each individual point on the graph represents a distinct observation.

The horizontal axis represents the SHAP values. We employ colour to indicate the initial value of a characteristic. The colour of the point indicates the value of an observation in comparison to other observations. By default, we organise the features based on the mean absolute value of the SHAP values associated with each characteristic. This ranking assigns greater significance to the overall average impact while downplaying the infrequent yet influential consequences. Alternatively, one can use the method of sorting based on the greatest absolute value to identify features that have significant consequences for specific values.

By default, Beeswarm employs the colours red and blue. Using the colour parameter, however, it is possible to provide a colour map. The beeswarm storyline is the most valuable plot. We attribute this to its ability to visually represent all of the SHAP values. In this instance, the forecast has a negative influence on greater latitudes and longitudes, but lower values have a positive influence.

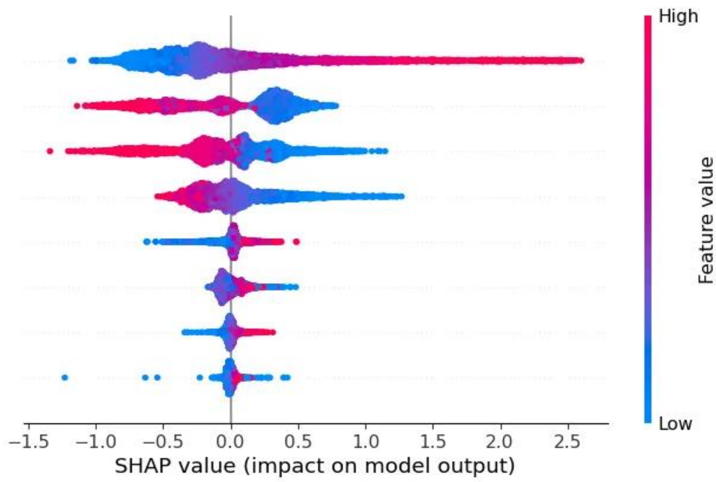

Figure 4: Beeswarm plot for data analysis

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VIOLIN

The violin is an extra way of interpreting the contents of the beeswarm displayed in the shot. This is done to give a more accurate depiction of the density of the body in terms of its shape. A violin plot can be an equally helpful graphical device for representing quantitatively measured data. Moreover, it can be made very plausible. Whereas red regions are dominated by high feature values, blue areas are dominated by low feature values, as is suggested by the hue representing the average feature value at every site.

This graphic is very useful when working with the data that has a multimodal distribution – a distribution that consists of several humps. The particular application of violin plots is to compare the distribution of a specific variable over categories. The violin plot also contains a helpful sign of the nature of the information that it represents.

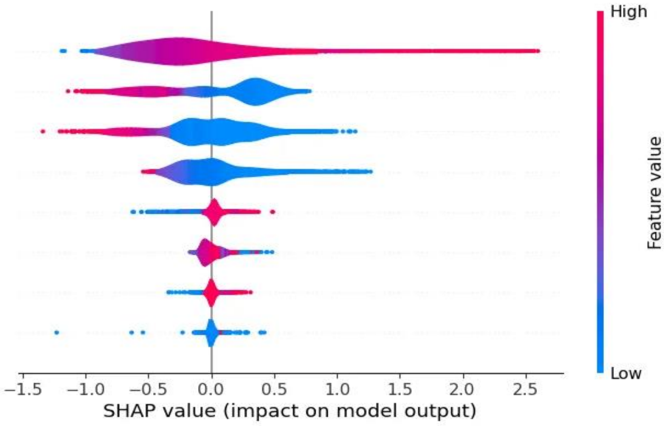

Figure 5: Violin plot

These are the following possibilities within the considered data which the User has available for the local and instance-wise analysis:

LOCAL BAR PLOT

It so graphically visualises the most important features that affect the forecast of an individual observation and the size of its SHAP value.

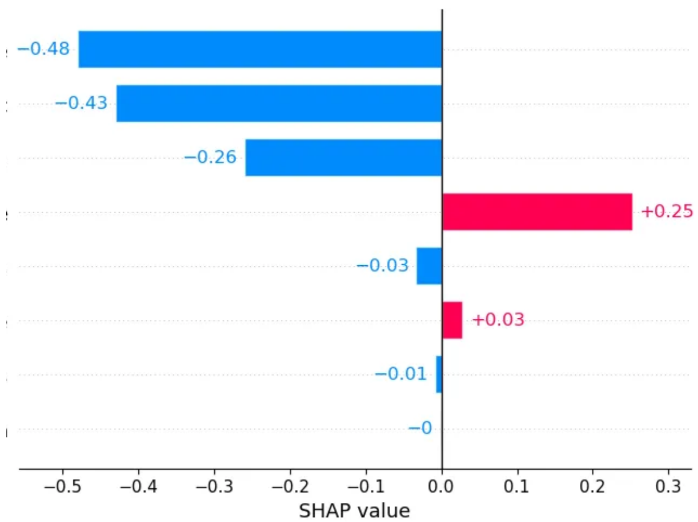

Figure 6: Local bar plot for visualisation

WATERFALL PLOT

The waterfall plot depicts the same values in a form which is different from the above three kinds of plots. The user

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deliberately plots waterfall plots to explain why and what predictions are made in a figure. Thus, it is obligatory to type any row of an explanation, i.e., the criterion of obligatoriness of an input is the existence of at least one row of an explanation.

As shown in the waterfall plot in the lower part of the figure below, each row is the net contribution of each characteristic, whether it is positive or negative. It is sometimes possible to sum up all SHAP values by computing f(x) – E[f(x)].

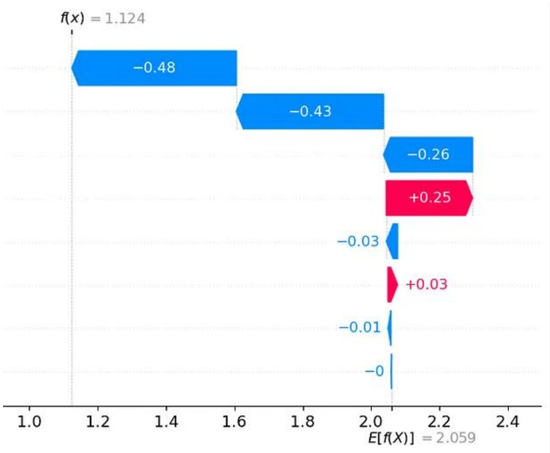

Figure 7: Waterfall plot

Force Plot

A force plot is an alternative approach for assessing the impact of individual features on the prediction of a specific observation. The graph displays positive SHAP values on the left side and negative numbers on the right side. The graph depicts them in direct contrast to each other as they engage in competition.

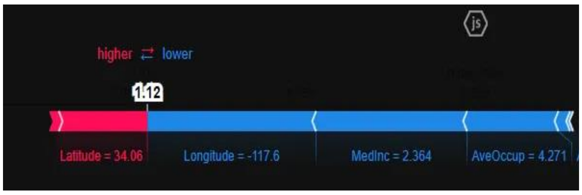

Figure 8: Force plot

SHAP demonstrates the importance or contribution of each feature to the model's prediction. It may demonstrate the local feature contribution for each instance of the problem as well as the global contribution by utilising the feature importance. Since SHAP allows us to understand the features, we can also use it for feature selection. SHAP also has a fast implementation for tree-based models [13]. While SHAP offers numerous benefits, it also has certain limitations. While SHAP can demonstrate the significance of every feature for the ML model's prediction, it does not assess its accuracy [14]. The user cannot use the SHAP values to make causal inferences. This includes determining an event's or target's actual causes. SHAP values will contribute to a prediction that is not the same as the true target [15]. If the model develops or trains incorrectly, it can lead to inherent issues with the SHAP inferences, as SHAP aids in inferring the importance of the feature for the given model. High multicollinearity would cause one variable to have high SHAP values and the other to have zero or very low SHAP values. This might conflict with the notion that features are important. In this case, the problem is with the model's training rather than with how SHAP assigns the values [16]. If the machine first assigns weight to one variable, the contribution of the other correlated variable would be negligible. If the second variable () makes more sense in terms of business logic, this might seem counterintuitive. Shapley values, as a solution to game theory issues, have mathematically satisfying theoretical properties. However, this does not automatically solve the problem of feature importance [17-19]. The SHAP framework is capable of identifying the class of additive feature importance methods.

Parameter	Advantage	Disadvantage	Limitation
GAM	Flexible functions for uncovering hidden patterns	Overfitting	Difficult to fit with a smoothing spline
SHAP	Demonstrates the importance of each feature	The accuracy of the prediction is not assessed	SHAP values are not useful in the case of causal inference

Table 1: Comparison of GAM, SHAP Algorithms [19]

Analysing machine learning models with a wide range of data might be difficult. The SHAP framework facilitates understanding the relative importance of various input variables and their influence on the model's decision-making process on a global scale [20]. The GAM facilitates the examination of intricate associations between dependent and independent variables. The GAM is an expanded version of the linear model that enables the representation of non-linear connections and interactions among variables.

This research study underscores the crucial importance of interpretability tools in the field of data science. The aforementioned tools and methodologies serve as the fundamental basis for constructing transparent and reliable data science models. Diverse domains can apply these models to enhance decision-making processes, foster innovation, and generate societal and economic benefits.

CONCLUSION

Analysing machine learning models with a wide range of data might be difficult. The SHAP framework facilitates understanding the relative importance of various input variables and their influence on the model's decision-making process on a global scale. The GAM facilitates the examination of intricate associations between dependent and independent variables. The GAM is an expanded version of the linear model that enables the representation of non-linear connections and interactions among variables.

This research study underscores the crucial importance of interpretability tools in the field of data science. The aforementioned tools and methodologies serve as the fundamental basis for constructing transparent and reliable data science models. Diverse domains can apply these models to enhance decision-making processes, foster innovation, and generate societal and economic benefits.

FUTURE

Unsurprisingly, the HITL (Human-In-The-Loop) interpretability in the case of the chosen machine learning model implies the input of feedback and domain knowledge from people into the procedure of interpretability. Such an approach recognises the fact that while Artificial Intelligence (AI) models can work alongside interpretability tools, it is equally essential that the intuition of individuals be incorporated when addressing complex models or specialists' challenges. The following are specific scenarios that show how the interpretability of human-in-the-loop systems can make a difference: In the healthcare context, you always aim to involve medical specialists in assessing the relevancy and the clinical applicability of the insights that the models generate to diagnose diseases. Scholars aim at crafting models where a person is in the loop when interpreting the results, which is why researchers follow a guideline of interpretability to make sure that the tool developed will be both reliable and accurate and often conforming to human realistic expectations and standards of the domain of study. The proposed framework of interpretability ensures that the decision-making from the machine learning models is reasonable and has substantial application in the real world. Top of Form

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