Methods for understanding the variable importance of local explanations of black-box models

Abstract

Artificial Intelligence (AI) has seen a revitalization in recent years from the use of increasingly hard-to-interpret black-box models. In such models, increased predictive power comes at the cost of opaque factor analysis, which has led to the field of explainable AI (XAI). XAI attempts to shed light on these models, one such approach is the use of local explanations. A local explanation of a model give a point-estimate of linear variable importance in the vicinity of one observation. We extract explanations for each observation, and approximate data and this attribution space side-by-side with linked brushing. After identifying an observation of interest its local explanation is used as a 1D projection basis. We then manipulate the magnitude of the variable contributions with a technique called the tour. This tour animates many projections over small changes in the projection basis. Doing so allows a user to visually explore the data space through the lens of this local explanation and interrogate its variable importance. The implementation of our framework is available as an R package called cheem available at github.com/nspyrison/cheem.

1 Introduction

Mathematically rigorous approaches to predictive modeling are attributed to the method of least squares, over two centuries ago by Legendre and Gauss in 1805 and 1809 respectively. In 1886 Francis Galton coined the term *regression* to refer to continuous, quantitative predictions. While *classification* refers discretion predictions as introduced by Fisher in 1936.

Breiman and Shmueli Shmueli (2010) introduce the idea of distinguishing modeling based on its purpose; *explanatory* modeling is done for some inferential purpose such as hypothesis testing, while *predictive* modeling is performed for to predict new or future out-of-sample observations. This distinction draws attention to the divide between interpretable models and black-box models. In explanatory modeling the interpretable is a key feature for drawing inferential conclusions. While predictive modeling may opt for potentially more accurate black-box models. The intended use of a model has important implications for which methods are used and the development of those models.

Predictive model and black box modeling is becoming increasingly common, but not without controversy and issues Kodiyan (2019). Applications have been known to reflect common biases against sex Duffy (2019), race (Larson et al. 2016), and age (Díaz et al. 2018). This is a common issue stemming from biases the in sample data are violate ethical principals. Another issue is that of data-drift, when new data is outside the support of latent or exogenous explanatory variables. Data-drift can lead to worse predictions Salzberg (2014). Such issues highlight the need to make models fair, accountable, ethical, and transparent which has led to the movement of XAI Arrieta et al. (2020).

One branch of XAI is local explanations, which take a variable attribution approach to bring transparency to a model. Local explanations attempt to approximate a linear variable importance at the location of one observation. There are many such local explanations, any of which is works with our approach (assuming model-explanation compatibility).

However, to illustrate our work we apply the model-agnostic explanation SHAP Štrumbelj and Kononenko (2014). The exact details of SHAP are tangent to the ideas of this work, but suffice it to say that SHAP approximates variable importance by taking the median importance over permutations of the explanatory variables. To be exact we apply a variant that enjoys a lower computational complexity, known as tree SHAP (S. M. Lundberg, Erion, and Lee 2018).

In multivariate data visualization a *tour* S. Lee et al. (2021) is a sequence of linear projections of data onto a lower dimensional space, typically 1-3D. Tours are viewed as an animation over small changes to a projection basis. Structure in a projection can then be explored visually to see which variables contribute to the formation of the structure. The intuition is similar to watching the shadow of hidden 3D object change as the object is rotated; watching the structural shape of the shadow change gleans insight into the shape and features of the object. There are various types of tours, which are distinguished be the generation of sequence of projection bases. In a *manual* tour Spyrison and Cook (2020) this path is defined by changing the contribution of a selected variable. Applying tours in conjunction with models has been previously done, *ie* for exploring various statistical model fits (Wickham, Cook, and Hofmann 2015), and using tree- and forest-based approaches as a projection pursuit index to generate a tour basis path Silva, Cook, and Lee (2021).

The approach purposed below is to use the manual tour as means to interrogate a local explanation; it see if its variable importance are good explanation for the model predictions. We make R package `cheem` with an interactive application to facilitate analysis. By viewing approximations of data- and attribution-space side-by-side, with linked brushing an analyst can identify observations of interest whose explanations are then rendered at the initial projection basis and explored with a manual tour to further interpret the variable importance of the local explanation. We give case studies of toy and modern datasets for both classification and regression tasks.

The rest of paper is organized as follows. The next section SHAP covers the background of the local explanation SHAP and the traditional visuals produced from it. The section Application Design discusses the layout of the application, how it facilitates analysis. Following that, Software Instructure discusses the backend details of the package and preprocessing. The section Case Studies illustrates several applications of this method. We conclude with Discussion of the insights we draw from classification and regression tasks.

2 SHAP local explanation

SHaply Additive exPlanations, or SHAP (S. Lundberg and Lee 2017) approximates the variable importance in the vicinity of one observation by taking the median importance of a subset of permutations in the explanatory variables. This idea stems from the field of game theory where Shapley devised a method to evaluate individual's contribution to cooperative games by permuting the players contributing to the score (Shapley 1953).

TO illustrate SHAP and its original use we use soccer data from FIFA 2020 season (Leone 2020). We have 5000 observations of 9 aggregated skill measures and use a use a random forest model to regress the wages, in 2020 Euros, from the skill measures. We then extract the SHAP values of a star offensive player (Messi) and defensive player (van Dijk). We expect to see a difference in attribution of the variable importance across the two positions of the players.

Figure 1 illustrates the SHAP values of these players. Panel b) shows the underlying distribution of the SHAP attributions while permuting the explanatory variables, with the medians being the SHAP values. In the light of the player position, the difference in the variable importance makes sense; offensive and movement are more important for the offensive player, while defensive and power skills are more important to the model for explaining the the prediction of the defensive player. We would likewise expect the profile of variable importance to be unique for star players of other positions as well, such as goalkeepers or middle fielders. Panel c) shows a simplified breakdown plot (Gosiewska and Biecek 2019), where a local explanation is used to additively explain the difference from the intercept to the observations prediction. Such additive approaches will show an asymmetry with respect to the variable ordering, so we opt to fix the order to that of panel b), namely, by decreasing sum of the SHAP values.

In summary, this highlights how local explanations bring transparency to a model at least in the vicinity of their observations. In this instance we showed how two very different soccer players receive different profiles of variable importance to explain the the prediction of their wages. In the following section we will be using normalized explanations as the starting projection basis to interrogate the explanation further.

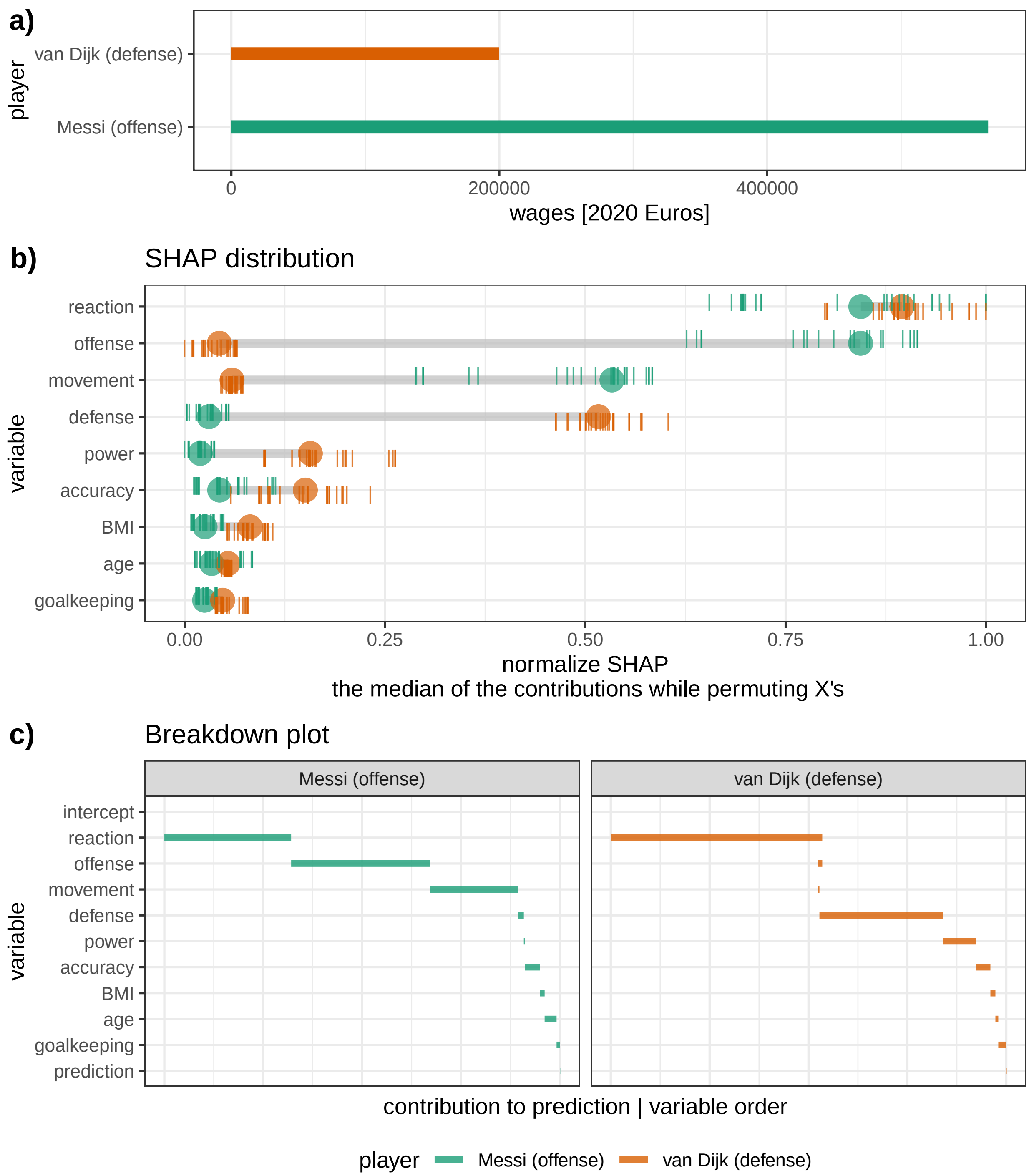

Figure 1: Illustration of the distribution of SHAP attributions, the SHAP values, and a breakdown plot, the typical visual of SHAP local explanations. For FIFA 2020 data, of a random forest model regressing wages from 9 skill attributes for a star offensive and defensive player. a) The players have very different wages. b) Shows the distributions of the attributions permuting over 25 permutations in the explanatory variables. The median of these distributions are the final SHAP values, notice that that the variable importance differs across the exogenous information of player position. These explanations make sense; the variable importances make sense in light of the position of the player. c) Breakdown plots of the observations the explanation used to additively explain the difference beween the intercept and prediction

3 Application Design

Below we illustrate the two primary displays of the application: the global view and the tour view. Then we'll cover what we takeaway from the classification and regression tasks. Lastly, we discuss the preprocessing that needs to be done before display.

3.1 Global view

3.2 Cheem tour

3.3 Classifcation task

3.4 Regression task

3.5 Preprocessing

The benefit of having dynamic interaction with data is predicated on a reasonably small render time. The it is important to preprocess as much work as possible so that application resources can be used efficiently. Below we discuss the steps and details of the reprocessing.

- **Data:** a complete numerical matrix; explanatory and response variable, an optional aesthetic (color/shape) variable can be mapped typically a categorical variable exogenous to the model.
- **Model:** any model can be used with this method. Currently we apply random forest models via the package **randomForest** (Liaw and Wiener 2002) to mitigate the runtime of our local explanation which requires tree-based models.
- **Local explanation:** any model-compatible linear explanation could be used. We apply tree SHAP, a more computationally efficient variant of SHAP applicable to tree-based models. This is done with the package **treeshap** (Kominsarczyk et al. 2021), hosted on GitHub only]. The global view shows all observations in attribution space requiring that we must extract the variable weightings from *all* observations rather than just one.
- **Global view:** The data- and attribution-spaces are approximated as their the first two principal components. The within class separability of points can also optionally be displayed as QQ plots of the Mahalanobis distances within those spaces.

The time to preprocess the data will vary significantly with the choice of model and local explanation. However, for reference the FIFA data, 5000 observation of 9 explanatory variable, took 1.5 seconds to create PCA and Mahalanobis distances for both the data and attribution spaces. On the same data, a modestly hyper-parametered random forest model fit in 2.6 seconds, while extracting the tree SHAP values of each observation took 278 seconds combined. These time were from a non-parallelized R session on a modern laptop, but suffice it to say that the bulk of the run time will be spent on the local attribution. This makes tree SHAP a good candidate to start with. The package **fastshap** (Greenwell 2020) claims extremely low runtimes that are attributed to fewer calls to the prediction function, partial implementation in C++, and efficient use of logical subsetting.

The work remaining at runtime consists mostly in rendering the frames of the tour as specified by the selection of the parameters. The application is made with **shiny** (Chang et al. 2021). The global view is created first with **ggplot2** (Wickham 2016) which is then rendered to an interactive html widget with **plotly** (**sievet_interactive_2020?**). The tour view is created in **spinifex** (Spyrison and Cook 2020), which creates the manual tour basis array, and facilitates similar rendering to html widget.

4 Software Infrastructure

4.1 Extend spinifex, consume DALEX & treeshap

4.2 Preprocess

4.3 Runtime rendering

5 Case Studies

5.1 1) Penguins speicies classification

5.2 2) FIFA wage regression

5.3 3)?

5.4 4)?

6 Discsussion

7 Acknoledgements

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