Exploring Local Explanations of Non-linear Models Using Animated Linear Projections

Abstract

The increased predictive power comes at the cost of interpretability, which has led to the emergence of eXplainable AI (XAI). XAI attempts to shed light on how models are using predictors, to arrive at a prediction, with a point estimate of the linear variable importance in the vicinity of each observation. These can be considered to be linear projections, and as such can be further explored interactively to better understand the interaction between variables used to make predictions, across the predictive model surface. Here we describe interactive linear interpolation used for exploration at any observation, and illustrate with examples with categorical (penguin species, chocolate types) and quantitative (football salaries, house prices) response variables. The methods are implemented in the **R** package **cheem**, available on CRAN.

1 Introduction

There are different reasons and emphases to fit a model. Breiman (2001), reiterated by Shmueli (2010), taxonomizes modeling based on its purpose; explanatory modeling is done for some inferential purpose, while predictive modeling focuses more on the predictions of out-of-sample observations. The intended use has important implications for model selection and development. In explanatory modeling, interpretability is vital for drawing inferential conclusions. While predictive modeling may opt for more accurate non-linear models. The use of black-box models is becoming increasingly common, but not without their share of controversy (O'Neil 2016; Kodiyan 2019). However, the loss of interpretation presents a challenge.

Interpretability is vital for exploring and protecting against potential biases (e.g. sex (Dastin 2018; Duffy 2019), race (Larson et al. 2016), and age (Díaz et al. 2018)) in any model. For instance, models regularly pick up on biases in the training data that have observed influence on the response (output) variable, which is then built into the model. Variable-level (feature-level) interpretability of models is essential in the evaluation models for such biases. It is also generally important for many problems, where it is not enough to accurately predict accurately but one must be able to explain which predictors are most responsible in generating a response value.

Another concern is that of data drift, which is a shift in support or domain of the explanatory variables (feature or predictors). Non-linear models are typically more sensitive, and do not extrapolate well outside of the training data domain. Better interpretability of the model means that there is more transparency where models' predictions may be plausible or completely unreliable.

Explainable Artificial Intelligence (XAI) is an emerging field of research that tries to increase the interpretability of black-box models. A common approach is to use *local explanations*, which attempt to approximate linear variable importance at the location of each observation (instance), or the predictions at a specific point in the data domain. Because these are point specific, a challenge is visualizing them to more comprehensively understand a model.

In multivariate data visualization, a *tour* (Asimov 1985; Buja and Asimov 1986; S. Lee et al. 2021) is a sequence of linear projections of data onto a lower-dimensional space. Tours are viewed as an animation over minor changes to the projection basis. Structure in a projection can then be explored visually to see which variables contribute to the formation of that structure. The intuition is similar to watching the shadow of a hidden 3D object change as the object is rotated; watching the shape of the shadow change conveys information of the structure and features of the object.

There are various types of tours distinguished by the generation of projection bases. In a manual tour (Cook and Buja 1997; Spyrison and Cook 2020), the path is defined by changing the contribution of a selected variable. Applying tours to models has been done in a couple of contexts. Specifically for exploring various statistical model fits and classification boundaries (Wickham, Cook, and Hofmann 2015), and using tree- and forest-based approaches as a projection pursuit index to generate a tour basis paths (Y. D. Lee et al. 2013; da Silva, Cook, and Lee 2021).

In our proposed approach we use the radial manual tour to scrutinize a local explanation. Additional interactivity allows the user to identify an observation of interest, then explore its local explanation by changing variable contribution with the radial tour. The methods are implemented in R package **cheem**. Example datasets are provided to illustrate usage for classification and regression tasks.

Using a radial tour can be considered similar to counterfactual, what-if analysis, such as *ceteris paribus* (Biecek 2020). This phrase, Latin for "other things held constant" or "all else unchanged", shows how an observation's prediction would change from a marginal change in one explanatory variable given that other variables are held constant. It ignores correlations of the variables and imagines a case that was not observed. In contrast, our approach is a geometric explanation of the factual; it varies contributions of the variables by rotating the basis, a reorientation of the data object. A constraint in our approach is that the basis must remain orthonormal. That means, when the contribution of one variable decreases, the contributions of others necessarily increase such that there is a complete component in that direction. This also ensures that what is seen is strictly a low-dimensional projection from high-dimensions, and is thus an interpretable visualisation.

The remainder of this paper is organized as follows. The following Section, 2 covers the background of the local explanation, and the traditional visuals produced. Section ?? explains the animations of continuous linear projections. Section 4 discusses the visual layout in the interactive interface, how they facilitate analysis, data preprocessing, and package infrastructure. Then Section @ref(#sec:casestudies) illustrates the application to supervised learning with categorical and quantitative response variables. We conclude with Section 6 of the insights gained and directions that might be explore in the future.

2 Local explanations

Consider a highly non-linear model. It can be hard to determine whether small changes in a variable's value will make a class prediction change group or identify which variables contribute to an extreme residual. Local explanations shed light on these situations by approximating linear variable importance in the vicinity of a single observation or point.

A comprehensive summary of the taxonomy and literature of explanation techniques is provided in Figure 6 of Arrieta et al. (2020). It includes a large number of model-specific explanations such as deepLIFT (Shrikumar et al. 2016; Shrikumar, Greenside, and Kundaje 2017), a popular recursive method for estimating importance in neural networks. There are fewer model-agnostic explanations, of which LIME (Ribeiro, Singh, and Guestrin 2016) SHAP (Lundberg and Lee 2017), and their variants are popular.

These instance-level explanations are used in various ways depending on the data. In image classification, where pixels would correspond to predictors, saliency maps overlay or offset a heatmap indicating important pixels (Simonyan, Vedaldi, and Zisserman 2014). For instance, pixels corresponding to snow may be highlighted when distinguishing if a picture contains a wolf or husky. In text analysis, word-level contextual sentiment analysis can be used to highlight the sentiment and magnitude of influential words (Vanni et al. 2018). In the case of numeric regression, they are used to explain variable additive contributions from the model intercept to the observation's prediction (Ribeiro, Singh, and Guestrin 2016).

SHaply Additive exPlanations (SHAP) approximates the variable importance in the vicinity of one observation conceptually by examining the effect of other variables on the contribution of the variable of interest on predicting the response. This explanations almost all point to Shapley (1953)'s method to evaluate an individual's contribution to cooperative games by permuting the players that contribute to the score. Strumbelj and Kononenko (2010) introduced the use of SHAP for local explanations in ML models. While the models themselves are invariant to the order of the predictors, the additive explanations are not. The

SHAP values are the mean contributions over some subset these permutations. This is also related to partial dependence plots (Molnar 2020), used to explain the effect of a variable by predicting the response for a range of values on this variable, after fixing the value of all other variables to their mean. Partial dependence plots are a global approximation of the variable importance, while SHAP is specific to one instance. It could also be considered to be similar to examining the coefficients from all subsets regression, as described in Wickham, Cook, and Hofmann (2015), which helps to understand the relative importance of each variable in the context of all other candidate variables.

For our application, we use *tree SHAP*, a variant of SHAP enjoys a lower computational complexity (Lundberg, Erion, and Lee 2018). Instead of aggregating over permutations of the variable order, tree SHAP approximates instance level feature importance by exploring the stucture of the decision trees. Tree SHAP is only compatible with tree-based models; we illustrate random forests. The following section will use normalized explanations as the starting projection basis (call this the *attribution projection*) to further scrutinize the explanation.

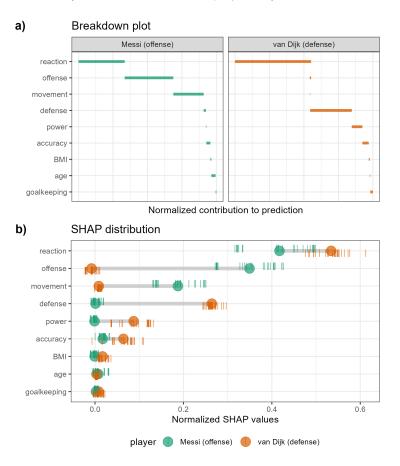


Figure 1: Illustration of the use of SHAP values for a random forest model for salaries of FIFA 2020 players based on nine predictors corresponding to different skills. A star offensive and densive player, Messi and a defensive player are compared, L. Messi and V van Dijk respectively. Plot a) is the break-down plot showing one additive variable-attributution. These attributions are sensitive to the order of the variables. Plot b) shows the distribution of attribution for each variable across 25 such permutation of the order of predictors, with the mean displayed as a dot, for each players. Offense and movement are important for Messi but not van Dijk, and conversely defense and power are important for van Dijk but not Messi.

Following the use case *Explanatory Model Analysis* (Biecek and Burzykowski 2021), we use FIFA data to illustrate the use of SHAP. Consider soccer data from the FIFA 2020 season (Leone 2020). There are 5000 observations of 9 skill measures (after aggregating highly correlated variables). A random forest model is fit regressing wages [2020 Euros], from the skill measures. We then extract the SHAP values of a star offensive

player (L. Messi) and defensive player (V. van Dijk). The results are displayed in Figure 1. We expect to see a difference in the attribution of the variable importance across the two positions of the players, which would be interpreted as how the player's salary depends on this combination of skill sets. Plot (b) is a modified breakdown plot (Gosiewska and Biecek 2019) where the order of variables is fixed, so the two observations can be more easily compared.

In summary, these plots highlight how local explanations bring interpretability to a model, at least in the vicinity of their observations. In this instance, two players with different positions receive different profiles of variable importance to explain the prediction of their wages.

3 Tours and the radial tour

A tour enables viewing of high-dimensional data by animating many linear projections with small incremental changes. It is achieved by following a path of linear projections (bases) of high-dimensional space. One of the features of the tour is the object permanence of the data points; one can track the relative change of observations in time, and as such gain information about the relationships between points across multiple variables. There are various types of tours that are distinguished by how the paths are generated (S. Lee et al. 2021; Cook et al. 2008).

The manual tour (Cook and Buja 1997) defines its path by changing a selected variable's contribution to a basis, to allow the variable to contribute more or less to the projection. The contribution of all other variables is constrained by the requirement that a basis needs to be orthonormal (column correspond to vectors, with unit length, and orthogonal to each other). The manual tour is primarily used to assess the importance of a variable to structure visible in a projection. It also lends itself to pre-computation to be queued in advance or computed on-the-fly for human-in-the-loop analysis (Karwowski 2006).

A version of the manual tour called a *radial tour* is implemented in Spyrison and Cook (2020) and forms the basis of the new work. In a radial tour, the selected variable is allowed to change its magnitude of contribution but not its angle; it must move along the direction of its original contribution. The implementation allows for pre-computation and also interactive re-calculation to focus on a different variable.

4 The cheem viewer

To explore the local explanations, an ensemble of plots (Unwin and Valero-Mora 2018) is provided, called the *cheem viewer*. There are two primary plots: the global view to give the context of all of the SHAP values, and the radial tour view to explore the local explanations with user-controlled rotation. In addition, there are numerous user inputs, including variable selection for the radial tour, and instance selection for making comparisons. Figures 2 and 3 contain screenshots showing the cheem viewer for the two primary tasks classification (categorical response) and regression (quantitative response).

4.1 Global view

The global view provides the context of all observations and facilitates the exploration of the separability of the data- and attribution-spaces. Both of these spaces are of dimension $n \times p$, where n is the number of observations and p is the number of predictors. The attribution space corresponds to the local explanations for each observation, which will have p values for each observation.

A visualisation of these spaces is provided by the first two principal components of their respective spaces. In addition, a plot observed by predicted response is also provided. In both PCA plots the orientation and magnitude of the variables are inscribed on a unit circle, similar to a biplot (Gabriel 1971). A single 2D projection will not encompass all of the structure of higher-dimensional space, but it is generally a useful visual summary. For classification tasks, misclassified observations are circled in red if applicable. Linked brushing between the plots is provided and a tabular display of selected points helps to facilitate exploration of the spaces and the model.

While the comparison of these spaces is interesting, a main purpose of the global view is to enable the selection of observations, from which to explore the local explanations.

4.2 Radial tour

The global view facilitated the selection of a primary and optional comparison observation. The variable-level attribution of the primary observation is normalized and used as the initial 1D basis in a radial tour. This is an approximation of the contributions of the linear variables that best explain the difference between the model intercept and an observation's prediction, not the local shape of the model surface.

The initial frame is the normalized SHAP values of the primary observation. The current projection basis is depicted as the width of a bar, the variable's contribution to the horizontal axis. The normalized values of all observations are shown as vertical parallel coordinate plots.

The radial tour creates a basis path by varying the contribution of a selected variable, fully into and out of a projection frame. Doing so tests an individual variable's sensitivity to the structure identified by the local explanation. The default variable selected has the largest discrepancy between the attribution of primary and comparison observations. The following sections elaborate on the takeaways from applying this approach in classification and regression tasks. Now that we have introduced the global view and corresponding cheem radial tour, let us discuss the differences between the classification and regression cases.

4.3 Classification task

Typically we select a misclassified observation compared to a correctly classified point nearby in data space. The model infomation in the global view is a depiction of the model conmfusion matrix. The radial tour is 1D, with density display, while the goal of the tour; exploring the sensitivity of each variable to structure identified by the local explanation, evaluating the support or robustness of the prediction.

4.4 Regression task

In the regression case, the global view can be colored on a statistic to highlight the explanation space's structure. For this purpose, we include residuals, log Mahalanobis distance of data space (a measure of outlyingness), and the correlation of the attribution projection with the observed response. In the radial tour, the horizontal positions are the same, the basis projection of the radial tour. The vertical position is fixed to the observed response variable and residuals in the middle and right panels. Correspondingly, the display changes from univariate density to 2D scatterplot. The basis is still one component (horizontal) independent of the vertical position.

4.5 Interactive features

The application has several reactive inputs that affect the data used, aesthetic display, and tour manipulation. These reactive inputs make the software flexible and extensible. The application also has more exploratory interactions to help link points across displays and reveal structure found in different spaces.

A tooltip displays observation number/name and classification information while the cursor hovers over a point. Linked brushing allows the selection of points (left click and drag) where those points will be highlighted across plots. The information corresponding to the selected points is populated on a dynamic table. These interactions aid exploration of the spaces and, finally, identification of a primary and comparison observation.

4.6 Preprocessing

It is vital to mitigate the render time of visuals, especially when users may want to iterate many times. All computational operations should be prepared before runtime. The work remaining when an application is ran is solely reacting to inputs and rendering of visuals and tables. Below we discuss the steps and details of the reprocessing.



Figure 2: Overview of the cheem viewer for classification tasks. Plots are colored on predicted class, and red circles indicate misclassified observations. Model visual is essentially a representation of the confusion matrix of the model. The radial tour is a 1D projection starting the attribution projection. The first frame is the linear variable importances that best describe the observation's prediction. We probe the support of variable contributions by selecting a variable and use the radial tour to vary its coefficient.

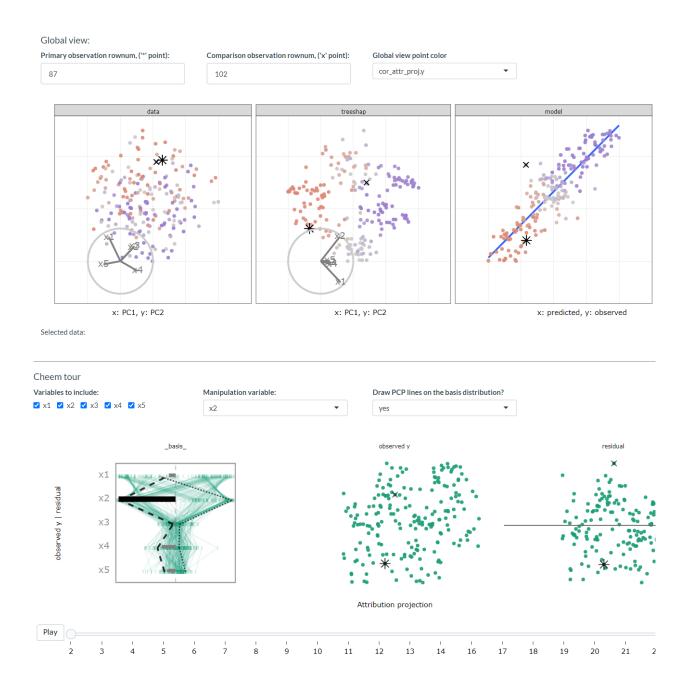


Figure 3: Overview of the cheem viewer for regression tasks. The global view can be colored on the correlation between the projection of the data generated by the local explanation and the observed response. In the radial tour, the horizontal values are the same as the classification case; the projection through the basis. The vertical position is now mapped to the observed y and residuals.

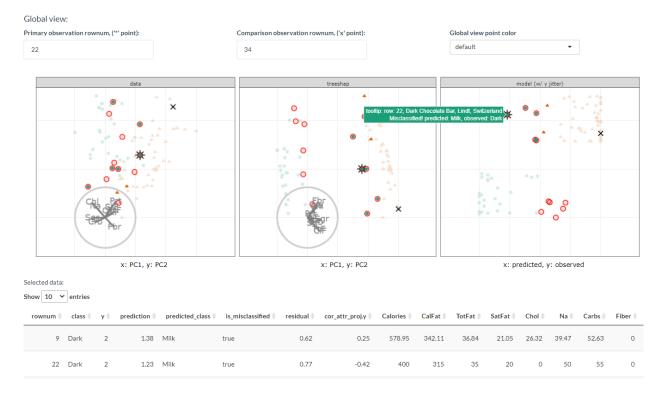


Figure 4: Illustration of data explorations interactions in the global view. This view has linked brushing, where observations selected in one facet are highlighted in the other facets and populate an interactive tabular display below. Tooltips display when hovering over an observation.

- Data: predictors and response are unscaled complete numerical matrix. Most models and local
 explanations are scale invariant.
- Model and explanation: any model can be used with this method. Currently, we apply random forest models via the package randomForest [Liaw and Wiener (2002)], compatibility tree SHAP. We use modest hyperparameters, namely: 125 trees, number variables randomly sampled at each split, $\text{mtry} = \sqrt{p}$ or p/3 for classification and regression, and minimum size of terminal nodes max(1, n/500) or max(5, n/500) for classification and regression. Tree SHAP is calculated for each observation using the package treeshap Kominsarczyk et al. (2021). This implementation aggregates over exhaustively over the attribution of all trees and we opt to not to fit interactions of features.
- Cheem view: after the model and full explanation space are calculated we scale each feature by standard deviations away from the mean to achieve a common support for visuals. Statistics for mapping to color are calculated on the scaled spaces. Interactive tabular display reports the original values.

The time to preprocess the data will vary significantly with the model and local explanation. For reference, the FIFA data, 5000 observations of nine explanatory variables, took 2.5 seconds to fit a random forest model of modest hyperparameters. Extracting the tree SHAP values of each observation took 270 seconds combined. PCA and statistics of the variables and attributions took 2.8 seconds. These runtimes were from a non-parallelized R session on a modern laptop, but suffice to say that the bulk of the time will be spent on the local attribution. An increase in model complexity or data dimensionality will quickly become an obstacle. With its reduced computational complexity, this makes tree SHAP a good candidate to start with. Alternatively, the package **fastshap** (Greenwell 2020) claims extremely low runtimes, which are attributed to fewer calls to the prediction function, partial implementation in C++, and efficient use of logical subsetting.

4.7 Package infrastructure

The above-described method and application are implemented as an open-source **R** package, **cheem** available on **CRAN**. Preprocessing was facilitated with models created via **randomForest** (Liaw and Wiener 2002), and explanations calculated with **treeshap** (Kominsarczyk et al. 2021). The application was made with **shiny** (Chang et al. 2021). The tour visual is built with **spinifex** (Spyrison and Cook 2020). Both views are created first with first with **ggplot2** (Wickham 2016) and then rendered as interactive HTML widgets with **plotly** (Sievert 2020). **DALEX** (Biecek 2018) and the free ebook, *Explanatory Model Analysis* (Biecek and Burzykowski 2021) were a huge boon to understanding local explanations and how to apply them.

4.8 Installation and getting started

The following \mathbf{R} code will help getting up and running:

```
## Download the package
install.packages("cheem", dependencies = TRUE)

## Restart the R session so the IDE has the correct directory structure
restartSession()

## Load cheem into session
library("cheem")

## Try the app
run_app()

# Processing your data

## Install treeshap from github, to use as a local explainer
remotes::install_github('ModelOriented/treeshap') ## Local

## Follow the examples in cheem_ls()
?cheem_ls
```

5 Case studies

To illustrate the use of the cheem method, we apply it to modern datasets, two classification examples and then two of regression.

5.1 Palmer penguin, species classification

The Palmer penguins data (Gorman, Williams, and Fraser 2014; Horst, Hill, and Gorman 2020) was collected on three species of penguins foraging near Palmer Station, Antarctica. The data was publicly available to be a substitute for the overly-used iris data, and is quite similar in form. There are 330 observations and we will use the four physical measurements, bill_length_mm (b_1), bill_depth_mm (b_d), flipper_length_mm (f_1), body_mass_g (wgt), for this illustration. A random forest model was fitted with species as the response variable.

Figure 5 shows plots from the cheem viewer for exploring the random forest model on the penguins data. Plot (a) shows the global view, and plot (b) shows several 1D projections generated with the radial tour. Penguin 124, an Adelie (green), is the observation of interest because it has been misclassified as a Chinstrap (orange).

There is more separation visible in the attribution space than the data space, as would be expected. The observed vs predicted plot reveals a handful of misclassified observations. A misclassified point (represented by the asterisk in the global view, and as a dashed vertical line in the tour view) is contrasted with a correctly classified point (represented by an \times and vertical dotted line).

The radial tour starts from the attribution projection of the misclassified observation (left plot). The important variables identified by SHAP in the (wrong) prediction for this observation is mostly b_d with smaller contributions of f_1 and wgt. This projection is a view where the Gentoo (purple) penguins are most distinguished from Adelie and Chinstrap. For this observation we would like to know why an Adelie has

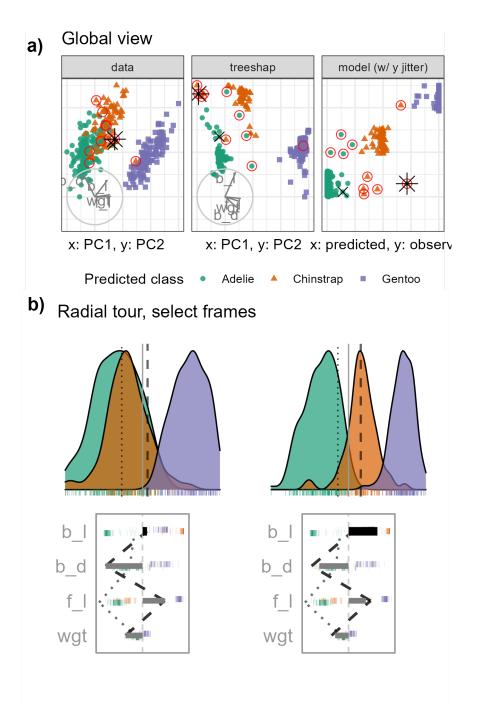


Figure 5: Examining the SHAP values for a random forest model classifying Palmer penguin species. The observation of interest is an Adelie (green) penguin that is misclassified as a Chinstrap (orange), marked as an asterisk in (a), and the dashed vertical line in (b). XXX needs fixing Starting from the attribution projection the contribution of b_1 is varied. This explanation is not supported sense by the time there is moderate contribution. The current basis is fairly close to the regularly attribution to other chinstrap penguins aside from the sign on flipper length being flipped. It feels odd that SHAP has identified a profile where chinstrap and adelie penguins are hard to distinguish when there are separating orientations that should be found within 125 trees. The .mp4 animation of this tour can be found at shorturl.at/hFHNS

been wrongly labelled a Chinstrap, so this combination of variables is not particularly useful. To explore this we use the radial tour to vary the contribution of bill length (b_1). The more b_1 contributes to the the projection the more this penguin looks like a Chinstrap, that it is mislabelled as. This suggests that b_1 should have been an important variable for explaining the (wrong) prediction.

5.2 Chocolates, milk/dark chocolate classification

The chocolates dataset consists of 88 observations of ten nutritional measurements from their labels. Each of which was labeled as being either milk or dark chocolates. We can see if a manufacturer accurately portrays the chocolate with this data. We are curious to see if chocolates that nutritionally look like milk chocolates are labeled as dark chocolates, which may hold a higher market value. We should note that not all chocolates consist wholly of chocolate. The addition of other ingredients will decrease the predictive power of the model nutritional explanatory variable. A random forest model is fit classifying the type of chocolate. We selected a chocolate labeled dark, through predicted to be milk chocolate compared with a chocolate labeled 85% cocoa.

Figure 6 similarly shows that attribution-space is more separable than data-space. Interestingly, the class imbalance that we suspected was not observed; there are only six chocolates labeled as dark and predicted as milk, while eight of the inverse case. We look at one extreme instance and vary the contribution of sugar. We see notice 2 instances that have clearly well within the milk chocolate dispite being observed as dark chocolate on their product label. While conjector, there are plausible reasons that a manufacturer has incentives to cut corners and label their products different than what they are. This feels related a measurement theory problem.

5.3 FIFA, wage regression

The 2020 season FIFA data (Leone 2020; Biecek 2018) contains many skill measurements of soccer/football players and wage information. After aggregation of the skill measurements, we regress player wages [2020 euros] given just the skill aggregates. The model was fit from 5000 observations of the nine skill aggregates before being thinned to 500 players to mitigate occlusion and render time. We compare a leading offensive fielder (L. Messi) with that of a top defensive fielder (V. van Dijk), the same observations were used in figure

With figure 7, we will test the premise of the local explanation. While offense and reaction skills both crutial to the explaintion of a star offensive player. We increase the contribution of denfensive skills and Messi is no longer separated from the group while van Dijk and other defensive players are better explained in this case.

5.4 Ames housing 2018, sales price regression

Ames 2018, housing data was subset to North Ames (the neighborhood with the most house sales). The remaining are 338 house sales across nine variables. Using interaction from the global view, we select a house with an extreme negative residual and an accurate observation close to it in the data.

Figure 8 shows the global view and extrema of the tour. The horizontal distance in the tour did not show a significant disparity between our selected points. This is not particularly surprising as most variables have a sizable contribution. Rotating any one variable out of the frame will rotate other vital variables into the frame, preserving most of the distance from intercept to prediction. However, the tour has revealed an interesting feature worth discussing. Notice that the observations pivot about the origin, the basis roughly halfway between bases in frames one and two of panel b) the data is near a singular profile. This means that there is a basis orthogonal to this point that describes sizable variation. Knowing these singular bases can point toward others with meaningful data variation.

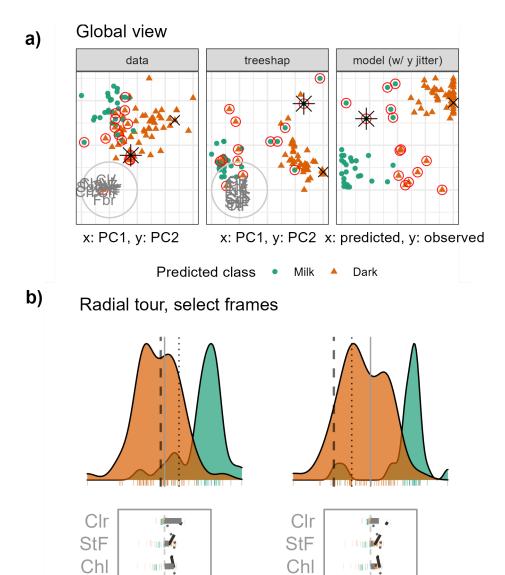


Figure 6: Chocolates data type classification (milk or dark). We select a chocolate labeled as dark though a random forest model predicts it to be milk chocolate from the values on the nutritional label. The attribution projection already looks more like a dark chocolate than milk. We remove a 4 variables with the lowest contribution for the selected instance and vary the contribution of Sugar. The misclassification of two instances seems improbable when sugar is near max contribution. Animated tour can be found at shorturl.at/dBE28.

Na

Fbr

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Global view model data treeshap x: PC1, y: PC2 x: PC1, y: PC2 x: predicted, y: observed Predicted class **FALSE** b) Radial tour, select frames basis observed y residual **BMI** rct off def mvm pwr residual basis observed **BMI** rct off

Figure 7: FIFA 2020 data, a random forest model regresses wages [2020 Euros] from nine aggregated of skill measurements. The primary observation is a star offensive player (L. Messi) compared with a top defensive player (V. van Dijk). We remove three variables with low attribution from both players. The attribution projection starts with selected instance on the right. We vary the contribution from defense, the star offensive player is not distinguished in the horizontal direction. At this point defensive players have been rotated to the highest horizonatal value. The animate radial tour can be found at shorturl.at/ICK26

def mvm pwr

Global view treeshap model data x: PC1, y: PC2 x: PC1, y: PC2 x: predicted, y: observed Predicted class **FALSE** b) Radial tour, select frames basis observed y residual LtA Qlt LvA Rms **GYB** GrA

Figure 8: Ames housing 2018 regressing sales price [2018 USD]. The primary observation is a house that a large lot area (LtA), but small living area (LvA). The comparison instance is in the opposite; a large house on a relatively small lot. Similar to the soccer players, these house sale have diverging attribution to better predict their sales prices. Varying the contribution living area the separation between these house sales crosses when there is a low contribution which is so important to explaining their prediction though in differet ways. The corresponding animation is at shorturl.at/oqyDU

observed y

basis

LtA Qlt LvA Rms GYB GrA residual

6 Discussion

The need to maintain the interpretability of black-box models is evident. One aspect uses local explanations of the model in the vicinity of an observation. Local explanations approximate the linear variable importance to the model. Our contribution is to assess explanations by examining the support by varying the contributions with a radial tour. First, a global view visualizes approximations of the data space, explanation space, model predictions side-by-side, using dynamic interaction to compare and contrast and identify primary and comparison observations of interest. The normalized linear importance from the explanation of the primary observation becomes the feature of interest to further explore with the radial tour. The tours explore the variable sensitivity to the structure identified in the explanation.

We have illustrated this method on random forest models using the tree SHAP local explanation, while it could be generally used with any compatible model-explanation pairing. We apply it to the classification and regression tasks. We have created an open-source **R** package **cheem**, available on **CRAN**, to facilitate preprocessing and exploration with the described interactive application. Toy and real data are provided, or upload your data after preprocessing.

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The namesake, Cheem, refers to a fictional race of humanoid trees from Doctor Who lore. **DALEX** pulls on from that universe, and we initially apply tree SHAP explanations specific to tree-based models.

References

- Arrieta, Alejandro Barredo, Natalia Díaz-Rodríguez, Javier Del Ser, Adrien Bennetot, Siham Tabik, Alberto Barbado, Salvador García, Sergio Gil-López, Daniel Molina, and Richard Benjamins. 2020. "Explainable Artificial Intelligence (XAI): Concepts, Taxonomies, Opportunities and Challenges Toward Responsible AI." Information Fusion 58: 82–115.
- Asimov, Daniel. 1985. "The Grand Tour: A Tool for Viewing Multidimensional Data." SIAM Journal on Scientific and Statistical Computing 6 (1): 128–43. https://doi.org/https://doi.org/10.1137/0906011.
- Biecek, Przemyslaw. 2018. "DALEX: Explainers for Complex Predictive Models in R." The Journal of Machine Learning Research 19 (1): 3245–49.
- ——. 2020. ceteris Paribus: Ceteris Paribus Profiles. https://CRAN.R-project.org/package=ceterisParibus. Biecek, Przemyslaw, and Tomasz Burzykowski. 2021. Explanatory Model Analysis: Explore, Explain, and Examine Predictive Models. CRC Press.
- Breiman, Leo. 2001. "Statistical Modeling: The Two Cultures (with Comments and a Rejoinder by the Author)." Statistical Science 16 (3): 199–231.
- Buja, Andreas, and Daniel Asimov. 1986. "Grand Tour Methods: An Outline." In *Proceedings of the Seventeenth Symposium on the Interface of Computer Sciences and Statistics on Computer Science and Statistics*, 63–67. New York, NY, USA: Elsevier North-Holland, Inc. http://dl.acm.org/citation.cfm?id=26036.26046.
- Chang, Winston, Joe Cheng, JJ Allaire, Carson Sievert, Barret Schloerke, Yihui Xie, Jeff Allen, Jonathan McPherson, Alan Dipert, and Barbara Borges. 2021. Shiny: Web Application Framework for r. https://CRAN.R-project.org/package=shiny.
- Cook, Dianne, and Andreas Buja. 1997. "Manual Controls for High-Dimensional Data Projections." *Journal of Computational and Graphical Statistics* 6 (4): 464–80. https://doi.org/10.2307/1390747.
- Cook, Dianne, Andreas Buja, Eun-Kyung Lee, and Hadley Wickham. 2008. "Grand Tours, Projection Pursuit Guided Tours, and Manual Controls." In *Handbook of Data Visualization*, 295–314. Berlin, Heidelberg: Springer Berlin Heidelberg. https://doi.org/10.1007/978-3-540-33037-0 13.

- da Silva, Natalia, Dianne Cook, and Eun-Kyung Lee. 2021. "A Projection Pursuit Forest Algorithm for Supervised Classification." *Journal of Computational and Graphical Statistics*, 1–21.
- Dastin, Jeffrey. 2018. "Amazon Scraps Secret AI Recruiting Tool That Showed Bias Against Women." Reuters, October. https://www.reuters.com/article/us-amazon-com-jobs-automation-insight-idUSKCN1MK08G.
- Díaz, Mark, Isaac Johnson, Amanda Lazar, Anne Marie Piper, and Darren Gergle. 2018. "Addressing Age-Related Bias in Sentiment Analysis." In *Proceedings of the 2018 Chi Conference on Human Factors in Computing Systems*, 1–14.
- Duffy, Claire. 2019. "Apple Co-Founder Steve Wozniak Says Apple Card Discriminated Against His Wife." CNN, November. https://www.cnn.com/2019/11/10/business/goldman-sachs-apple-card-discrimination/index.html.
- Gabriel, Karl Ruben. 1971. "The Biplot Graphic Display of Matrices with Application to Principal Component Analysis." *Biometrika* 58 (3): 453–67.
- Gorman, Kristen B., Tony D. Williams, and William R. Fraser. 2014. "Ecological Sexual Dimorphism and Environmental Variability Within a Community of Antarctic Penguins (Genus Pygoscelis)." *PloS One* 9 (3): e90081.
- Gosiewska, Alicja, and Przemyslaw Biecek. 2019. "IBreakDown: Uncertainty of Model Explanations for Non-Additive Predictive Models." arXiv Preprint arXiv:1903.11420.
- Greenwell, Brandon. 2020. Fastshap: Fast Approximate Shapley Values. https://CRAN.R-project.org/package=fastshap.
- Horst, Allison Marie, Alison Presmanes Hill, and Kristen B. Gorman. 2020. "Palmerpenguins: Palmer Archipelago (Antarctica) Penguin Data." https://allisonhorst.github.io/palmerpenguins/.
- Karwowski, Waldemar. 2006. International Encyclopedia of Ergonomics and Human Factors, -3 Volume Set. CRC Press.
- Kodiyan, Akhil Alfons. 2019. "An Overview of Ethical Issues in Using AI Systems in Hiring with a Case Study of Amazon's AI Based Hiring Tool." Researchgate Preprint.
- Kominsarczyk, Konrad, Pawel Kozminski, Szymon Maksymiuk, and Przemyslaw Biecek. 2021. "Treeshap." Model Oriented. https://github.com/ModelOriented/treeshap.
- Larson, Jeff, Surya Mattu, Lauren Kirchner, and Julia Angwin. 2016. "How We Analyzed the COMPAS Recidivism Algorithm." *ProPublica*, May. https://www.propublica.org/article/how-we-analyzed-the-compas-recidivism-algorithm?token=RPR1E2qtzJltfJ0tS-gB_41kmfoWZAu4.
- Lee, Stuart, Dianne Cook, Natalia da Silva, Ursula Laa, Nicholas Spyrison, Earo Wang, and H. Sherry Zhang. 2021. "The State-of-the-Art on Tours for Dynamic Visualization of High-Dimensional Data." WIREs Computational Statistics n/a (n/a): e1573. https://doi.org/10.1002/wics.1573.
- Lee, Yoon Dong, Dianne Cook, Ji-won Park, and Eun-Kyung Lee. 2013. "PPtree: Projection Pursuit Classification Tree." *Electronic Journal of Statistics* 7: 1369–86.
- Leone, Stefano. 2020. "FIFA 20 Complete Player Dataset." https://kaggle.com/stefanoleone992/fifa-20-complete-player-dataset.
- Liaw, Andy, and Matthew Wiener. 2002. "Classification and Regression by randomForest." R News 2 (3): 18-22.
- Lundberg, Scott M., Gabriel G. Erion, and Su-In Lee. 2018. "Consistent Individualized Feature Attribution for Tree Ensembles." arXiv Preprint arXiv:1802.03888.
- Lundberg, Scott M., and Su-In Lee. 2017. "A Unified Approach to Interpreting Model Predictions." In Proceedings of the 31st International Conference on Neural Information Processing Systems, 4768–77.
- Molnar, Christoph. 2020. Interpretable Machine Learning. Lulu. com. christophm.github.io/interpretable-ml-book/.
- O'Neil, Cathy. 2016. Weapons of Math Destruction: How Big Data Increases Inequality and Threatens Democracy. Crown.
- Ribeiro, Marco Tulio, Sameer Singh, and Carlos Guestrin. 2016. ""Why Should I Trust You?": Explaining the Predictions of Any Classifier." In *Proceedings of the 22nd ACM SIGKDD International Conference on Knowledge Discovery and Data Mining*, 1135–44. KDD '16. New York, NY, USA: Association for Computing Machinery. https://doi.org/10.1145/2939672.2939778.
- Shapley, Lloyd S. 1953. A Value for n-Person Games. Princeton University Press.
- Shmueli, Galit. 2010. "To Explain or to Predict?" Statistical Science 25 (3): 289–310.
- Shrikumar, Avanti, Peyton Greenside, and Anshul Kundaje. 2017. "Learning Important Features Through

- Propagating Activation Differences." In *International Conference on Machine Learning*, 3145–53. PMLR. Shrikumar, Avanti, Peyton Greenside, Anna Shcherbina, and Anshul Kundaje. 2016. "Not Just a Black Box: Learning Important Features Through Propagating Activation Differences." *arXiv Preprint arXiv:1605.01713*.
- Sievert, Carson. 2020. Interactive Web-Based Data Visualization with R, Plotly, and Shiny. Chapman; Hall/CRC. https://plotly-r.com.
- Simonyan, Karen, Andrea Vedaldi, and Andrew Zisserman. 2014. "Deep Inside Convolutional Networks: Visualising Image Classification Models and Saliency Maps." In *In Workshop at International Conference on Learning Representations*. Citeseer.
- Spyrison, Nicholas, and Dianne Cook. 2020. "Spinifex: An R Package for Creating a Manual Tour of Low-Dimensional Projections of Multivariate Data." *The R Journal* 12 (1): 243. https://doi.org/10.32614/RJ-2020-027.
- Strumbelj, Erik, and Igor Kononenko. 2010. "An Efficient Explanation of Individual Classifications Using Game Theory." The Journal of Machine Learning Research 11: 1–18.
- Unwin, Antony, and Pedro Valero-Mora. 2018. "Ensemble Graphics." *Journal of Computational and Graphical Statistics* 27 (1): 157–65. https://doi.org/10.1080/10618600.2017.1383264.
- Vanni, Laurent, Mélanie Ducoffe, Carlos Aguilar, Frédéric Precioso, and Damon Mayaffre. 2018. "Textual Deconvolution Saliency (TDS): A Deep Tool Box for Linguistic Analysis." In *Proceedings of the 56th Annual Meeting of the Association for Computational Linguistics (Volume 1: Long Papers)*, 548–57.
- Wickham, Hadley. 2016. *Ggplot2: Elegant Graphics for Data Analysis*. Springer-Verlag New York. https://ggplot2.tidyverse.org.
- Wickham, Hadley, Dianne Cook, and Heike Hofmann. 2015. "Visualizing Statistical Models: Removing the Blindfold." Statistical Analysis and Data Mining: The ASA Data Science Journal 8 (4): 203–25. https://doi.org/10.1002/sam.11271.