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shapr: An R package for explaining machine learning models with dependence-aware Shapley values

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Summary

A common task within machine learning is to train a model which is able to predict an unknown outcome (response variable) based on a set of known input variables/features. When using such models for real life applications, it is often crucial to understand why a certain set of features lead to exactly a specific prediction. Most machine learning models are however so complicated and hard to understand that they are often viewed as "black-boxes" producing output when provided some input.

Shapley values (Shapley (1953)) is a concept from cooperative game theory used to fairly distribute a joint payoff among the cooperating players. Štrumbelj & Kononenko (2010) and later Lundberg & Lee (2017) proposed to use the Shapley value framework to explain predictions by distributing the prediction value on the input features. Established methods and implementations for explaining predictions with Shapley values like Shapley Sampling Values (Štrumbelj & Kononenko (2014)), SHAP/Kernel SHAP (Lundberg & Lee (2017)), and to some extent TreeSHAP (Lundberg, Erion, & Lee (2018)), assume that the features are independent when approximating the Shapley values for prediction explanation. The `R`-package `shapr` implements the methodology proposed by Aas, Jullum, & Løland (2019), where predictions are explained while accounting for the dependence between the features, resulting in significantly more accurate approximations to the Shapley values.

Implementation

`shapr` implements a variant of the Kernel SHAP (Lundberg & Lee (2017)) methodology for efficiently dealing with the combinatorial problem related to the Shapley value formula. The main methodological contribution of Aas et al. (2019) is three different methods to estimate certain conditional expectation quantities, referred to as the `empirical`, `gaussian` and `copula` approach. Additionaly, the user has the option of combining the three approaches. The implementation supports explanation of the following models natively: `stats::lm`, `stats::glm`, `ranger::ranger`, `mgcv::gam` and `xgboost::xgboost/xgboost::xgb.train`. Moreover, the package supports explanation of custom models by supplying two simple additional class functions.

For reference, the package also includes a benchmark implementation of the original (independence assuming) version of Kernel SHAP (Lundberg & Lee (2017)), providing identical results to the "official" Kernel SHAP `Python` package `shap` (Lundberg (2019)). This allows the user to easily see the effect and importance of accounting for the feature dependence.

The user interface in the package has largely been adopted from the `R`-package `lime`

(Pedersen & Benesty (2019)). The user first sets up the explainability framework for the model to explain with the `shapr` function. Then the output from `shapr` is provided to the `explain` function, along with the data to explain the prediction for and which method should be used to estimate the aforementioned conditional expectations.

The majority of the code is plain `R` (R Core Team (2019)), while the most time consuming operations has been coded in `C++` through the `Rcpp` package (Eddelbuettel & François (2011)) for computational speed up. For RAM efficiency and computational seed up of typical bookeeping operations in `R`, we utilize the `data.table` package (Dowle & Srinivasan (2019)) which does operations "by reference", i.e. without memory copies.

For a detailed description of the underlying methodology of the package, we refer to the paper (Aas et al. (2019)). For getting started with the package, we recommend the user to go through the package vignette and introductory examples available at the package's pkgdown site.

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