Explaining Tree Models

Bernhard Jaeger

University of Tübingen

Tübingen, Germany
bernhard.jaeger@student.uni-tuebingen.de

Abstract—Understanding the decisions made by machine learning models can be challenging due to their black box nature. We investigate the additive feature attribution method SHAP (SHapley Additive exPlanations) that addresses this problem [2]. While SHAP can be used to explain the decisions of any model, the generic KernelSHAP algorithm for it can be intractable for larger datasets. For tree models there exists a specialized algorithm (Tree SHAP) that can compute exact SHAP values in polynomial time [1]. We use the SHAP framework to investigate the relationship between Decision Trees and Hoeffding Trees [3]. Theory tells us that a Hoeffding Tree should converge towards a Decision Tree when trained. In our experiments however we could not observe convergence. The reason for this remains unclear.

Index Terms—Tree SHAP, SHAP, Decision Tree, Hoeffding Tree

I. Introduction

This . This and [3] document is a model and instructions for LATEX. Please observe the conference page limits.

II. ADDITIVE FEATURE ATTRIBUTION METHODS

Modern models of Machine Learning have become increasingly complex making it hard to explain their decisions. To address this challenge we can go one layer of abstraction further and make a model of the model which we want to be simple enough to be interpretable again. In [2] they coined the term explanation model for this approach of using an interpretable approximation of the original model. When viewed trough this lens multiple of the current explanation methods can be categorized in the class of **Additive Feature Attribution methods**. In [2] they defined this as methods having an explanation model that is a linear function of binary variables:

$$g(z') = \phi_0 + \sum_{i=1}^{M} \phi_i z_i' \tag{1}$$

Where g is the explanation model, $z' \in \{0,1\}^M$, $\phi \in \mathbb{R}$. Local methods like this first approximate their model f(x) using simplified inputs x' where $x = h_x(x')$.

The objective is then to ensure $g(z') \approx f(h_x(z'))$ whenever $z' \approx x'$.

 ϕ_i is then called the **effect** of feature i and summing up all effects approximates the output of the model f(x) we wish to explain. Note that these *explanation models* are now easily interpretable. We can for a prediction f(x) given input x say what influence or effect each component x_i had on the final

decision.

Methods falling in the category of Additive Feature Attribution methods include LIME [4], DeepLIFT [5], layerwise relevance propagation [6], Quantitive Input Influence [7], Shapley sampling values [8] and SHAP [2].

Additive Feature Attribution methods can have 3 desirable theoretical properties [2]:

Local Accuracy:

$$f(x) = g(x')whenx = h_x(x')and\phi_0 = f(h_x(0))$$
 (2)

The intuition being that the explanation model should match the original model for the simplified input (notice x'=z' here).

Missingness:

$$x_i' = 0 \to \phi_i = 0 \tag{3}$$

The intuition is that feature missing in the original input may have no impact even if they are present in the simplified version. (Notice that even if x' = 0, z' does not necessarily have to be 0).

Consistency:

 $f_x(z') := f(h_x(z'))$, and let $z' \setminus i$ be $z'_i = 0$ For any two models f and f', if:

$$f_x'(z') - f_x'(z' \setminus i) \ge f_x(z') - f_x(z' \setminus i) \tag{4}$$

for all inputs $z' \in 0, 1^M$.

Meaning that the model changes in a way that some simplified input's contribution becomes larger.

Then: $\phi_i(f', x) \ge \phi_i(f, x)$

Meaning that it's inputs attribution should not become smaller.

Now it turns out that the only possible features for an Additive Feature attribution method that satisfies all 3 properties are the Shapley values defined as:

$$\phi_i(f, x) = \sum_{z' \subseteq x'} \frac{|z'|!(M - |z'| - 1)!}{M!} [f_x(z') - f_x(z' \setminus i)]$$
(5)

 $z' \subseteq x'$ are all z' vectors where the non-zero entries are a subset of the non-zero entries in x'.

|z'| represents the number of non-zero entries in z'.

This means that at least in theory Additive Feature Attribution methods using Shapley Values as effects are to be preferred over other methods. In practice methods using shapely values can be intractable for larger sets.

In the next section we will introduce the SHAP framework which tries to unify these measures of feature importance.

III. SHAP VALUES

IV. DECISION AND HOEFFDING TREES

A. Abbreviations and Acronyms

Define abbreviations and acronyms the first time they are used in the text, even after they have been defined in the abstract. Abbreviations such as IEEE, SI, MKS, CGS, ac, dc, and rms do not have to be defined. Do not use abbreviations in the title or heads unless they are unavoidable.

B. Equations

Number equations consecutively. To make your equations more compact, you may use the solidus (/), the exp function, or appropriate exponents. Italicize Roman symbols for quantities and variables, but not Greek symbols. Use a long dash rather than a hyphen for a minus sign. Punctuate equations with commas or periods when they are part of a sentence, as in:

$$a + b = \gamma \tag{6}$$

C. ET_FX-Specific Advice

Please use "soft" (e.g., \eqref{Eq}) cross references instead of "hard" references (e.g., (1)). That will make it possible to combine sections, add equations, or change the order of figures or citations without having to go through the file line by line.

D. Figures and Tables

a) Positioning Figures and Tables: Place figures and tables at the top and bottom of columns. Avoid placing them in the middle of columns. Large figures and tables may span across both columns. Figure captions should be below the figures; table heads should appear above the tables. Insert figures and tables after they are cited in the text. Use the abbreviation "Fig. 1", even at the beginning of a sentence.

TABLE I TABLE TYPE STYLES

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Sample of a Table footnote.

Fig. 1. Example of a figure caption.

V. METHODOLOGY VI. EVALUATION VII. CONCLUSION

VIII. REPRODUCIBILITY CONSIDERATIONS

A. Software Libraries:

The software library versions we used (read out using pip -freeze) are documented in table II.

All experiments were conducted on a single personal computer. The hardware specs can be found in table III.

TABLE II SOFTWARE LIBRARY VERSIONS

| Software library | Version |
|------------------------|-------------|
| Python | 3.7.4 |
| anaconda-client | 1.7.2 |
| anaconda-navigator | 1.9.7 |
| anaconda-project | 0.8.3 |
| conda | 4.7.12 |
| conda-build | 3.18.9 |
| conda-package-handling | 1.6. |
| 0 conda-verify | 3.4.2 |
| ipykernel | 5.1.2 |
| ipython | 7.8.0 |
| ipython-genutils | 0.2.0 |
| jupyter | 1.0.0 |
| jupyter-client | 5.3.3 |
| jupyter-console | 6.0.0 |
| jupyter-core | 4.5.0 |
| jupyterlab | 1.1.4 |
| jupyterlab-server | 1.0.6 |
| matplotlib | 3.1.1 |
| notebook | 6.0.1 |
| numpy | 1.16.5 |
| pandas | 0.25.1 |
| scikit-image | 0.15.0 |
| scikit-learn | 0.21.3 |
| scikit-multiflow | 0.5.0 |
| scipy | 1.3.1 |
| shap | 0.35.0 |
| sklearn | 0.0 |
| torch | 1.5.0+cu101 |
| torchvision | 0.6.0+cu101 |

ACKNOWLEDGMENT

The preferred spelling of the word "acknowledgment" in America is without an "e" after the "g". Avoid the stilted expression "one of us (R. B. G.) thanks ...". Instead, try "R. B. G. thanks...". Put sponsor acknowledgments in the unnumbered footnote on the first page.

TABLE III HARDWARE SPECIFICATIONS:

| Component | Model |
|------------------|---------------------------------------|
| Processor | Intel Core i7-6700 CPU |
| RAM | 16 GB Corsair Vengeance LPX DDR4-2400 |
| GPU | NVIDIA GeForce GTX 980 |
| Motherboard | ASUS Z170 Pro Gaming |
| Operating system | Microsoft Windows 10 Education N |
| Hard Drive | SSD Crucial MX200 |

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