Updates on the Complexity of SHAP Scores

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Abstract

SHAP scores represent one of the most widely used methods of explainability by feature attribution, as illustrated by the explainable AI tool SHAP. A number of recent works studied the computational complexity of the exact computation of SHAP scores, covering a comprehensive range of families of classifiers. This paper refines some of the existing complexity claims, including families of classifiers for which the computation of SHAP scores is computationally hard and those for which there exist polynomial-time algorithms.

1 Introduction

Shapley values [Shapley, 1953; Roth, 1988] are widely used as a method for explaining the prediction of machine learning (ML) models by feature attribution [Molnar, 2020], being referred to as SHAP scores [Strumbelj and Kononenko, 2010; Strumbelj and Kononenko, 2014; Datta *et al.*, 2016; Lundberg and Lee, 2017b; Van den Broeck *et al.*, 2021; Arenas *et al.*, 2021; Rozemberczki *et al.*, 2022; Van den Broeck *et al.*, 2022; Arenas *et al.*, 2023].

The computational complexity of computing SHAP scores has been studied in recent years [Van den Broeck *et al.*, 2021; Arenas *et al.*, 2021; Van den Broeck *et al.*, 2022; Arenas *et al.*, 2023], and the existing intractability results justify the use of incomplete methods for approximating the SHAP scores [Lundberg and Lee, 2017b] for most families of classifiers. There are however exceptions, i.e. there exist families of classifiers for which the computation of SHAP scores has been shown or claimed to be tractable. One well-known example are deterministic decomposable negation normal forms (d-DNNFs),[1] for which polynomial-time algorithms have been devised [Arenas *et al.*, 2021]. Subsequent work generalized those algorithms to classifiers with non-binary discrete features [Arenas *et al.*, 2023]. Furthermore, independent work [Van den Broeck *et al.*, 2021; Van den Broeck *et al.*, 2022] claimed a number of additional (and related) tractability results, namely: (i) *Linear regression models*; (ii) *Decision and regression trees*; (iii) *Random forests or additive tree ensembles*; (iv) *Factorization machines, regression circuits*; (v) *Boolean functions in d-DNNF, binary decision diagrams*; and (vi) *Bounded-treewidth Boolean functions in CNF*. Regarding random forests (and tree ensembles), similar claims have been made in a growing number of works by other authors [Lundberg and Lee, 2017a; Lundberg *et al.*, 2018; Lundberg *et al.*, 2020; Campbell *et al.*, 2022; Muschalik *et al.*, 2024].

As this paper demonstrates, claim (iii) does not hold true when random forests (or tree ensembles) are used for classification, and when class selection is implemented by weighted or majority voting, as is the case with most publicly available implementations. Moreover, this paper proves that the computational complexity of SHAP scores is #P-hard for these widely used families of random forest (RF) classifiers. In order to prove this result, this paper proposes rigorous formalizations of different types of random forests and tree ensembles. More importantly, proposed implementations [Lundberg and Lee, 2017a; Lundberg *et al.*, 2018; Lundberg *et al.*, 2020] are necessarily problematic in the case of RFs/TEs used in practice; otherwise, it would be the case that #P $=$ FP [2] and therefore P $=$ NP [Arora and Barak, 2009].

Furthermore, the paper proposes a generalization of the polynomial-time algorithms for computing SHAP scores proposed in earlier work [Arenas *et al.*, 2021; Arenas *et al.*, 2023], for boolean classifiers defined on binary and non-binary discrete features, and represented with (non-binary) d-DNNFs. Concretely, the paper extends these algorithms for computing SHAP scores to the case of non-boolean classes, i.e., discrete classifiers, provided the classifiers are represented as generalized d-DNNFs. An immediate consequence of this result is that SHAP scores can also be computed for discrete classifiers represented as read-once decision trees.

The paper is organized as follows. Section 2 introduces the definitions and notation used throughout the paper, including the computation of SHAP scores. Section 3 briefly overviews existing complexity results regarding the computation of SHAP scores. Section 4 formally defines random

[1]Which include binary decision trees and free binary decision diagrams [Wegener, 2000; Darwiche and Marquis, 2002].

[2]The paper assumes basic knowledge of computational complexity. The complexity classes mentioned in the paper are standard in reference texts [Arora and Barak, 2009].

forests and tree ensembles, and proves basic relationships between different families of tree ensembles. Section 5 proves that computing SHAP scores for the simplest model of random forest is #P-hard. Section 6 shows how to generalize existing polynomial-time algorithms for (binary) d-DNNFs defined on non-binary features [Arenas *et al.*, 2023] to the case of non-boolean classifiers. Section 7 summarizes the paper's contributions.

2 Preliminaries

Classification problems. Let $\mathcal{F} = \{1, \ldots, m\}$ represent a set of features and $\mathcal{K} = \{c_1, \ldots, c_K\}$ represent a set of classes. Each feature i takes values from a domain $\mathbb{D}_i$. If feature i is binary, then $\mathbb{D}_i = \mathbb{B} = \{0, 1\}$. Similarly, if the classification problem is boolean, then $\mathcal{K} = \mathbb{B}$. Both the features' domains and the classes are assumed to be numeric. Given the features' domains, feature space $\mathbb{F}$ is defined by $\mathbb{F} = \mathbb{D}_1 \times \mathbb{D}_2 \times \cdots \times \mathbb{D}_m$. A classification function κ maps each point in feature space $\mathbb{F}$ to a class in $\mathcal{K}$. One often assumes that κ is non-constant, but this will not be imposed in this paper. A classifier is a tupple $\mathcal{M} = (\mathcal{F}, \mathbb{F}, \mathcal{K}, \kappa)$. An instance is a tuple $(\mathbf{v}, c)$, with $\mathbf{v} \in \mathbb{F}$ representing the *input*, and $c \in \mathcal{K}$, representing the computed *output*, $c = \kappa(\mathbf{v})$. Most of the results in Sections 3 and 5 consider binary features and a boolean classification problem. The other sections consider the more general setting where features and classes are non-binary but discrete.

Finally, the goal of explainability is to find explanations given some instance $(\mathbf{v}, c)$. An explanation problem is a tuple $\mathcal{E} = (\mathcal{M}, (\mathbf{v}, c))$. The paper considers explanations by feature attribution [Molnar, 2020], with another alternative being explanations by feature selection [Molnar, 2020].

Decision trees & ensembles. A decision tree $\mathcal{T}$ is a directed acyclic graph composed of a set V of n nodes $N = \{1, \ldots, n\}$ and a set of $n-1$ edges $E = \{e_1, \ldots, e_{n-1}\}$, where each $e_i \in N \times N$. By convention, the root node is assigned node number 1, and has no input edges. All other nodes have exactly one input edge. V is partitioned into a set N of non-terminal nodes and a set T of terminal nodes. Each terminal node has no output edges, whereas non-terminal nodes have 2 or more output edges. Each terminal node is associated with a class $c \in \mathcal{K}$. Moreover, each non-terminal node $p \in N$ is associated with a feature $i \in \mathcal{F}$, such that each of the output edges is ascribed a literal (i.e. $x_i = v_i$), and while guaranteeing that the literals of the output edges partition the domain of feature i associated with node p. A decision tree $\mathcal{T}$ is *read-once* if along any path of $\mathcal{T}$ a feature is associated with at most one node.

Moreover, tree ensembles (TEs) are aggregations of decision trees, equipped with a mechanism for selecting a class for each assignment to the features and given the individual predictions of the decision trees. One example of a widely used mechanism is majority voting [Breiman, 2001; Zhou, 2012]. TEs are discussed in greater detail in Section 4.

Example 1. *Fig. 1 shows the running example of a random forest with* majority voting *[Breiman, 2001; Zhou, 2012]. For each input, each tree selects the class consistent with the input. The choices of all trees are then combined, and the class selected by most trees is output. The example RF $\mathbb{T}$ consists of 3 decision trees $\mathcal{T}_1$, $\mathcal{T}_2$ and $\mathcal{T}_3$, and captures a classification function defined on the $\mathcal{F} = \{1, 2, 3\}$ with $\mathbb{D}_i = \{0, 1, 2\}, i \in \{1, 2, 3\}$ and $\mathcal{K} = \{0, 1, 2\}$. For the input $\mathbf{v} = (0, 1, 1)$, tree $\mathcal{T}_1$ selects class 2, tree $\mathcal{T}_2$ selects class 1, tree $\mathcal{T}_3$ selects class 2. Since class 2 is the most selected, then it is the class that is output. The highlighted edges in Fig. 1 indicate the prediction of each tree.*

SHAP scores. Methods of eXplainable AI (XAI) can be broadly categorized as those based on feature selection, e.g. Anchors [Ribeiro *et al.*, 2018], and those based on feature attribution, e.g. LIME [Ribeiro *et al.*, 2016] and SHAP [Lundberg and Lee, 2017b]. At present, SHAP and its variants are one of the most widely used explainability approaches.

SHAP is based on the computation of SHAP scores, which represent Shapley values [Shapley, 1953] in the context of explainability [Strumbelj and Kononenko, 2010; Strumbelj and Kononenko, 2014; Lundberg and Lee, 2017b]. We briefly overview the computation of *exact* SHAP scores, and adopt the formalization of SHAP scores used in recent work [Arenas *et al.*, 2021; Arenas *et al.*, 2023].

Given a point $\mathbf{v}$ in feature space $\mathbb{F}$, we define $\Upsilon : 2^{\mathcal{F}} \to 2^{\mathbb{F}}$ as follows,

$$\Upsilon(\mathcal{S}) := \{\mathbf{x} \in \mathbb{F} \mid \wedge_{i \in \mathcal{S}} x_i = v_i\} \tag{1}$$

i.e. for a given set $\mathcal{S} \subseteq \mathcal{F}$, and parameterized by the point $\mathbf{v}$ in feature space,[3] $\Upsilon(\mathcal{S})$ denotes all the points $\mathbf{x} = (x_1, \ldots, x_m) \in \mathbb{F}$ that have in common with $\mathbf{v} = (v_1, \ldots, v_m) \in \mathbb{F}$ the values of the features specified by $\mathcal{S}$.

Using the proposed definition for Υ, we introduce $\phi : 2^{\mathcal{F}} \to \mathbb{R}$ as follows,

$$\phi(\mathcal{S}) := \frac{1}{|\Upsilon(\mathcal{S})|} \sum\nolimits_{\mathbf{x} \in \Upsilon(\mathcal{S})} \kappa(\mathbf{x}) \tag{2}$$

As a result, and given a set $\mathcal{S}$ of selected features, $\phi(\mathcal{S})$ represents the expected value of the classifier over the points of feature space represented by $\Upsilon(\mathcal{S})$. The formulation presented in earlier work [Arenas *et al.*, 2021; Arenas *et al.*, 2023] allows for different input distributions when computing the expected values. For the purposes of this paper, it suffices to consider solely uniform input distributions, and so the dependency on the input distribution is not accounted for.

To simplify the notation, the following definitions are used,

$$\Delta(i, \mathcal{S}) := (\phi(\mathcal{S} \cup \{i\}) - \phi(\mathcal{S})) \tag{3}$$

$$\varsigma(\mathcal{S}) := {}^{|\mathcal{S}|!(|\mathcal{F}| - |\mathcal{S}| - 1)!}/_{|\mathcal{F}|!} \tag{4}$$

Finally, let $\mathsf{Sc} : \mathcal{F} \to \mathbb{R}$, i.e. the SHAP score for feature i, be defined by,

$$\mathsf{Sc}(i) := \sum\nolimits_{\mathcal{S} \subseteq (\mathcal{F} \setminus \{i\})} \varsigma(\mathcal{S}) \times \Delta(i, \mathcal{S}) \tag{5}$$

Given an instance $(\mathbf{v}, c)$, the SHAP score assigned to each feature measures the *contribution* of that feature with respect to the prediction [Strumbelj and Kononenko, 2010].

[3]Throughout the paper, all parameterizations are elided for simplicity; these are always clear from the context.

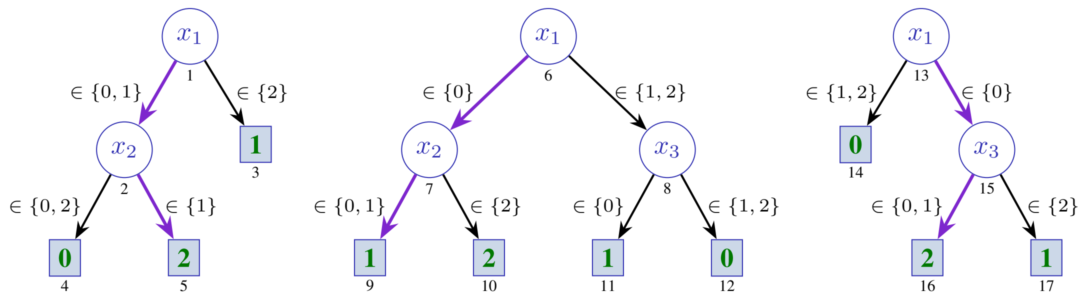


Fig. 1: Random Forest with majority voting, and class selection for the input $(0, 1, 1)$.

As proved in earlier work [Arenas *et al.*, 2021; Arenas *et al.*, 2023], the definition of SHAP scores (5) can be rewritten as follows:

$$\mathsf{Sc}(i) := \sum_{k=0}^{m-1} \sum_{\substack{\mathcal{S}\subseteq\mathcal{F}\setminus\{i\}\\|\mathcal{S}|=k}} \varsigma(k) \times \Delta(i, \mathcal{S}) \qquad (6)$$

where, with a slight abuse of notation, we define $\varsigma(k) = {}^{k!(m-k-1)!}/_{m!}$. (6) differs from (5) in that the computation of the SHAP score is organized by different values of k. This modification is instrumental for devising polynomial-time algorithms for computing SHAP scores in the case of d-DNNFs [Arenas *et al.*, 2021; Arenas *et al.*, 2023].

Finally, SHAP_Scores denotes the function problem of computing the SHAP scores, given some explanation problem, i.e. a tuple $(\mathcal{M}, (\mathbf{v}, c))$, representing a classifier $\mathcal{M}$ and an instance.

3 Complexity of Computing SHAP Scores

Tractable cases. For d-DNNFs, it has been shown that SHAP scores can be computed in polynomial-time for binary classifiers defined on binary features [Arenas *et al.*, 2021]. More recently, this result has been extended to discrete non-binary features [Arenas *et al.*, 2023]. The downsides of this work are: (i) it applies only to binary classifiers, i.e. classifiers for which the set of classes is $\{0, 1\}$; (ii) the circuits are read-once, i.e. in the case of DTs, a feature is tested at most once in each path; and (iii) features are discrete.

Independent work proved that SHAP scores can be computed in polynomial-time for the following families of models [Van den Broeck *et al.*, 2021; Van den Broeck *et al.*, 2022]:

i. *Linear regression models*;
ii. *Decision and regression trees*;
iii. *Random forests or additive tree ensembles*;
iv. *Factorization machines, regression circuits*;
v. *Boolean functions in d-DNNF, binary decision diagrams*; and
vi. *Bounded-treewidth Boolean functions in CNF*.

Regarding claim iii. above (which is taken from [Van den Broeck *et al.*, 2021; Van den Broeck *et al.*, 2022]), for random forests and/or additive tree ensembles, the proof of polynomial-time computation of SHAP scores hinges solely on the linearity of expectation [Van den Broeck *et al.*, 2022], and the proof implicitly assumes a regression setting. Unfortunately, and for classification problems, the best-known and most widely used mechanisms for class selection do not respect linearity (see Section 4).[4] Thus, as shown in Section 5, by considering variants of RFs widely used in practice [Breiman, 2001; Pedregosa *et al.*, 2011], the computation of SHAP scores is shown be #P-hard. In turn, this implies that is would be extremely unlikely that the computation of SHAP scores might be polynomial in the case of realistic RFs/TEs classifiers.

Intractable cases. For most families of models it is known that the computation of SHAP scores is intractable, being #P-hard [Van den Broeck *et al.*, 2021; Van den Broeck *et al.*, 2022]:

i. *Logistic regression models*;
ii. *Neural networks with sigmoid activation functions*;
iii. *Naive Bayes classifiers, logistic circuits*; and
iv. *Boolean functions in CNF or DNF*.

4 Random Forests & Tree Ensembles

In order to prove complexity results regarding random forests (RF) and tree ensembles (TE) classifiers, we must first define rigorously how these families of classifiers are organized.

Random forests were originally proposed by Breiman [Breiman, 2001], and targeted the selection of a class by selecting the most voted class from a number of decision trees, each of which built by random selecting the features to consider. More recently, random forests implement a more general organization, in which each tree votes not only a class but assigns a weight to its vote. This weighted voting approach is used for example in Scikit-learn [Pedregosa *et al.*, 2011].

In a more general setting, tree ensembles,[5] capture a fairly general mechanism of aggregating weak classifiers (often decision trees) into a single (stronger) classifier. In general, tree ensembles comprise different families of random forests [Breiman, 2001; Pedregosa *et al.*, 2011], boosted trees

[4]It should be underlined that both random forests and other tree ensembles are ubiquitous in classification [Breiman, 2001; Zhou, 2012; Delgado *et al.*, 2014; Sagi and Rokach, 2018].

[5]Ensembles of classifiers have been studied extensively over the years [Schapire, 1990; Freund, 1995; Breiman, 1996; Freund and Schapire, 1996; Freund and Schapire, 1997; Opitz and Maclin, 1999; Zhou, 2012; Sagi and Rokach, 2018].

(BTs) [Friedman, 2001; Chen and Guestrin, 2016], among many others [Zhou, 2012; Sagi and Rokach, 2018].

This section formalizes TE, BT and different types of RF classifiers. In addition, this section also proves some of their relationships.

General case for TEs. A TE $\mathcal{E}$ represents a set of decision trees $\mathbb{T}(\mathcal{E}) = \{\mathcal{T}_1, \ldots, \mathcal{T}_k\}$. Each tree $\mathcal{T}_j$ consists of a set of paths $\{P_{1,j}, \ldots, P_{r_j,j}\}$ such that for each input $\mathbf{x} \in \mathbb{F}$, exactly one path is consistent with $\mathbf{x}$. Moreover, for each input $\mathbf{x} \in \mathbb{F}$, each $\mathcal{T}_j$ tree outputs a class $c(\mathcal{T}_j, \mathbf{x}) \in \mathcal{K}$ and a weight $w(\mathcal{T}_j, \mathbf{x}) \in \mathbb{R}$, to be assigned to the picked class c. By summing up the weights of each class over all trees, the class with the largest sum of weights is the predicted class.

For each class $c_r \in \mathcal{K}$, its assigned weight is defined as follows:

$$W(c_r, \mathbf{x}) := \sum\nolimits_{j=1}^{k} \mathrm{ITE}(c_r = c(\mathcal{T}_j, \mathbf{x}), w(\mathcal{T}_j, \mathbf{x}), 0) \quad (7)$$

where ITE denotes the if-then-else operator. Finally, the picked class, given the input $\mathbf{x}$ is given by,

$$c_p(\mathbf{x}) := \underset{c_r \in \mathcal{K}}{\mathrm{argmax}}\{W(c_r, \mathbf{x})\} \quad (8)$$

Boosted trees [Chen and Guestrin, 2016]. Boosted tree (BTs) are a special case of a TE such that each decision tree $\mathcal{T}_j$ is associated with a pre-defined class $c(\mathcal{T}_j) \in \mathcal{K}$. In addition, for each input $\mathbf{x} \in \mathbb{F}$, each tree $\mathcal{T}_j$ outputs a weight $w(\mathcal{T}_j, \mathbf{x})$, to be associated with the class $c(\mathcal{T}_j)$. Given the definition of class and weight associated with the tree, it is plain to redefine (7) and (8) in the case of BTs. Furthermore, it is immediate that a BT is a special case of a TE, and so it is the case that,

Proposition 1. *Any BT is a TE.*

Proof. We reduce a BT to a TE as follows. For any $\mathbf{x} \in \mathbb{F}$ and any $\mathcal{T}_j \in \mathbb{T}$, set $c(\mathcal{T}_j, \mathbf{x}) = c(\mathcal{T}_j)$. It is then immediate to compute $W(c_r, \mathbf{x})$ given (7), and pick the resulting class using (8). □

RFs with weighted voting [Pedregosa *et al.*, 2011]. *Random forest with weighted voting* (RFwv) output a class and an associated weight for each tree. The selected class is the class with the largest sum over all trees. As can be concluded, each RFwv is a TE and vice-versa.

Proposition 2. *Any RFwv is a TE (and vice-versa).*

RFs with majority voting [Breiman, 2001]. *Random forests with majority voting* (RFmv) are based on a fairly restricted model, in that for each point $\mathbf{x} \in \mathbb{F}$, each decision tree $\mathcal{T}_j$ chooses a class $c(\mathcal{T}_j, \mathbf{x}) \in \mathcal{K}$, and the picked class is the class chosen by the majority of the decision trees. Thus, we can rewrite (7) as follows:

$$W(c_r, \mathbf{x}) := \sum\nolimits_{j=1}^{k} \mathrm{ITE}(c_r = c(\mathcal{T}_j, \mathbf{x}), 1, 0) \quad (9)$$

Moreover, (8) is also used to pick the selected class in the case of RFmv. Despite the relative simplicity, majority voting ranks as one of the most popular voting methods [Zhou, 2012].

Given the above definition of RFmv, we now prove that,

Proposition 3. *The following holds:*

1. *Any RFmv is a BT;*
2. *Any RFmv is a RFwv; and*
3. *Any RFmv is a TE.*

Proof. We analyze each case separately.

1. Any RFmv is a BT:
   Given a RFmv, we replace each tree $\mathcal{T}_j$ by $|\mathcal{K}|$ copies. For each class $c_r \in \mathcal{K}$, copy $\mathcal{T}_{j,r}$ outputs weight 1 if the predicted class if c_r; otherwise it outputs weight 0.
2. Any RFmv is a RFwv:
   The reduction mimics the one for the general case below.
3. Any RFmv is a TE:
   From each tree $\mathcal{T}_j$, we construct a modified decision tree as follows. Each leaf in the original DT $\mathcal{T}_j$, with output class c_r, will output a pair $(c_r, 1)$ in the resulting TE. □

Complexity-wise, Proposition 3 can be used to prove hardness results for BTs, RFwvs and TEs, by proving instead hardness results for RFmvs.

Furthermore, it is plain to conclude that this section covers a rather wide range of possible definitions of RFs, and also of their generalizations, i.e. BTs and TEs. It is also plain that the best-known and the most widely used definitions of RFs are covered by the cases studied in this section [Zhou, 2012; Sagi and Rokach, 2018].

Additional variants. Additional mechanisms for creating ensembles include different variants of bagging and boosting [Schapire, 1990; Freund, 1995; Breiman, 1996; Freund and Schapire, 1996; Freund and Schapire, 1997; Bauer and Kohavi, 1999; Friedman, 2001; Zhou, 2012; Sagi and Rokach, 2018]. For classification problems, all such variants must adopt a mechanism to combine results, and select one of the possible classes [Zhou, 2012]. In the case of using decision trees as the basic (weak) classifier, it is plain that any of these ensemble variants can be cast as special cases of the general tree ensemble framework detailed above.

5 Updates on Intractable Cases

This section proves that computing SHAP scores for *any* of the TE classifiers discussed in Section 4 (including RFwvs and RFmvs) is #P-hard. Unless P = #P (a very unlikely result), the results in this section challenge recent claims that computing SHAP scores for RF is in P (see Corollary 4 of [Van den Broeck *et al.*, 2021] or Corollary 5 of [Van den Broeck *et al.*, 2022]). This section only analyzes in detail the hardness of computing SHAP scores for RFmvs. However, due to Propositions 1 to 3, any hardness result for RFmvs is also a hardness result for any of the other cases of TEs studied in Section 4.

The decision problem for RFmvs is NP-complete. We start by showing a tight connection between the CNFSAT problem and the problem of deciding prediction 1 for a boolean classifier represented with a RFmv.

Definition 1. *The decision problem for an ML classifier is to decide the existence of a point* $\mathbf{x}$ *in feature space such that a* *target class is predicted, i.e. given $c \in \mathcal{K}$, the goal is to decide whether $\mathbf{x} \in \mathbb{F}$ exists such that $\kappa(\mathbf{x}) = c$.*

When referring to the different types of RFs/TEs, we will qualify the different decision problems, e.g. the RFmv decision problem refers to RFs with majority voting.

Proposition 4. *The decision problem for RFmvs is NP-complete.*

Proof. Clearly, the decision problem is in NP, i.e. given some input, we can decide in polynomial-time whether the prediction is the target one.
Next, we reduce the CNFSAT problem to the problem of deciding whether an RFmv predicts a concrete class.
Let $\varphi = \varsigma_1 \wedge \varsigma_2 \wedge \cdots \wedge \varsigma_t$ be a CNF formula. For each clause ς_q in φ, create one tree than predicts 1 iff the clause satisfied, i.e. if any of its literals is satisfied, the prediction is 1; otherwise the prediction for the tree is 0. In addition, create $t-1$ trees, each with a single terminal node 0.
Clearly, if all of the t clauses are satisfied, then the RF picks 1, since t trees have picked 1, and only $t-1$ can pick 0. Conversely, if at least one clause is falsified, the RF picks 0, since now at least t trees pick 0, and at most $t-1$ trees pick 1.
It is plain that the reduction is polynomial on the number of literals of φ. □

The construction used in the above proof is illustrated by the following example.

Example 2. *Consider the conjunctive normal form (CNF) formula $\varphi = (x_1 \vee \neg x_2 \vee x_3) \wedge (\neg x_1 \vee x_2 \vee \neg x_3) \wedge (x_1 \vee x_2 \vee x_3)$. As illustrated in the proof of Proposition 4, we create one DT for each clause, i.e. three DTs in total. In addition, we create two DTs that just predict 0. As one might antecipate, Fig. 2 represents the reduction of φ to the RF decision problem. Concretely, the formula φ is satisfiable iff there exists a point in feature space for which the prediction is 1.*

A possible criticism of the proposed reduction is that the classifier is *non-constant* iff the formula is satisfiable. (And as noted in Section 2, it is convenient to require the classifier not to be constant.) Nevertheless, one can devise a different reduction, that circumvents this minor issue.

Proposition 5. *One can reduce a CNF formula to a non-constant RFmv classifier such that the predicted class is 1 iff the CNF formula is satisfiable.*

Proof. We use classes 0, 1 and 2. Moreover, we add an additional feature x_{m+1}. The semantics becomes as follows:

1. If $x_{m+1} = 1$, then all DTs are instrumented to output class 2, and so the predicted class is 2. In practice, all the trees above are changed to have a non-terminal root node, that checks the value of x_{m+1}, it picks class 2 if $x_{m+1} = 1$, and otherwise, it replicates each of the trees detailed above.
2. Clearly, if $x_{m+1} = 0$, then the RF behaves as detailed above.
3. Moreover, the predicted class is 1 iff φ is satisfiable. □

The construction used in the above proof is illustrated by the following example.

Example 3. *We consider again the CNF formula φ from Example 2. Define $\mathcal{F} = \{1,2,3,4\}$ with $\mathbb{D}_i = \mathbb{B}, i \in \{1,2,3,4\}$, $\mathcal{K} = \{0,1,2\}$. As a result, we construct a random forest with majority voting $\mathbb{T} = \{\mathcal{T}_1, \mathcal{T}_2, \mathcal{T}_3, \mathcal{T}_4, \mathcal{T}_5\}$, as shown in Fig. 3.*

SHAP_Scores for RFmvs is not in P, unless P = NP. We now exploit well-known properties of SHAP scores, used for example in [Van den Broeck *et al.*, 2022], to disprove a claim also included in [Van den Broeck *et al.*, 2022].

Proposition 6. *SHAP_Scores for RFmvs is not in P, unless P = NP.*

Proof. It is known [Strumbelj and Kononenko, 2014; Van den Broeck *et al.*, 2022] that the following holds for SHAP scores:

$$\sum\nolimits_{i=1}^{m} \mathsf{Sc}(i) + \phi(\emptyset) = \kappa(\mathbf{v}) \tag{10}$$

We show that, if one could compute SHAP scores in polynomial-time for RFmv classifiers, then one could decide SAT in polynomial-time. We proceed as follows:

1. Pick any point $\mathbf{z}$ in feature space with $z_{m+1} = 0$. Then, the predicted class is either 0 or 1. If it is 1, then we are done.
2. Otherwise, the prediction is $\kappa(\mathbf{z}) = 0$, i.e. the predicted class is 0. Let $\phi_{x_i}(\emptyset), \phi_{\neg x_i}(\emptyset)$ denote, respectively, the average value given the assignments $x_i = 1, x_i = 0$. Hence, for any (binary) feature i, it holds that $\phi(\emptyset) = \frac{\phi_{x_i}(\emptyset)+\phi_{\neg x_i}(\emptyset)}{2}$. Concretely, for $i = m+1$, we have $\phi_{x_i}(\emptyset) = 2$, since $\kappa(\mathbf{x}) = 2$ for any point $\mathbf{x}$ with $x_{m+1} = 1$. Hence, we get $\phi(\emptyset) = \frac{2}{2} + \frac{\phi_{\neg x_{m+1}}}{2}$, and so from (10), we have,
$$\phi_{\neg x_{m+1}} = 2 \times \left(0 - \sum\nolimits_{i=1}^{m} \mathsf{Sv}(i) - 1\right)$$
3. Clearly, $\phi_{\neg x_{m+1}} = 0$ iff the prediction is *never* 1. Hence, the original formula is satisfiable iff $\phi_{\neg x_{m+1}} \neq 0$, and this we can compute in polynomial-time as long as the SHAP scores can be computed in polynomial-time.
4. The previous arguments prove that, if we could compute the SHAP scores of RFs in polynomial-time, then we could decide the satisfiability of a CNF formula in polynomial-time, and so P = NP. □

SHAP_Scores for RFmvs is #P-hard. As an alternative to the arguments above, we now provide another argument to disprove the claim that SHAP scores for RFmvs is in polynomial-time.

Proposition 7. *SHAP_Scores is #P-hard.*

Proof. From Theorem 3 of [Van den Broeck *et al.*, 2022], it is known that computing the SHAP scores is polynomially equivalent to computing the expected value of a classifier. Furthermore, for a binary classifier, computing the expected value is polynomially equivalent to counting the number of assignments yielding prediction 1.
Now, from the proof of Proposition 4, we observe that for any point $\mathbf{x} \in \mathbb{F}$, $\varphi(\mathbf{x}) = 1$ iff $\kappa_{RFmv}(\mathbf{x}) = 1$. Hence, the

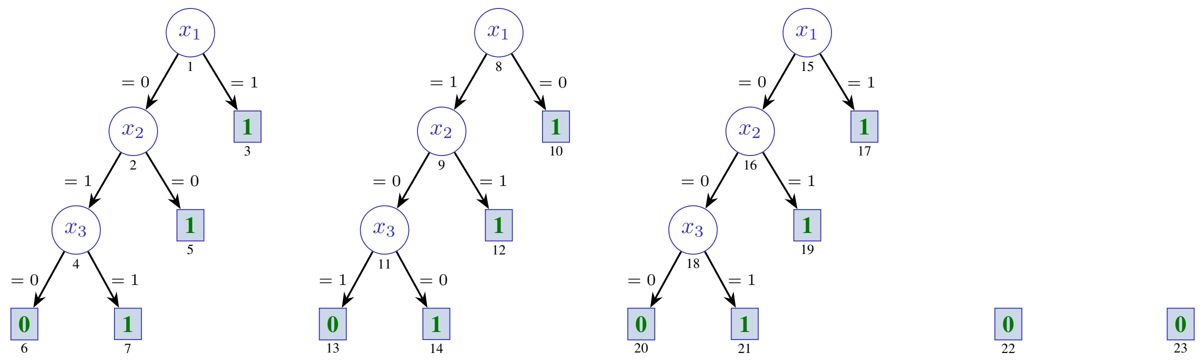


Fig. 2: Random forest obtained from reducing CNFSAT to the RFmv decision problem.

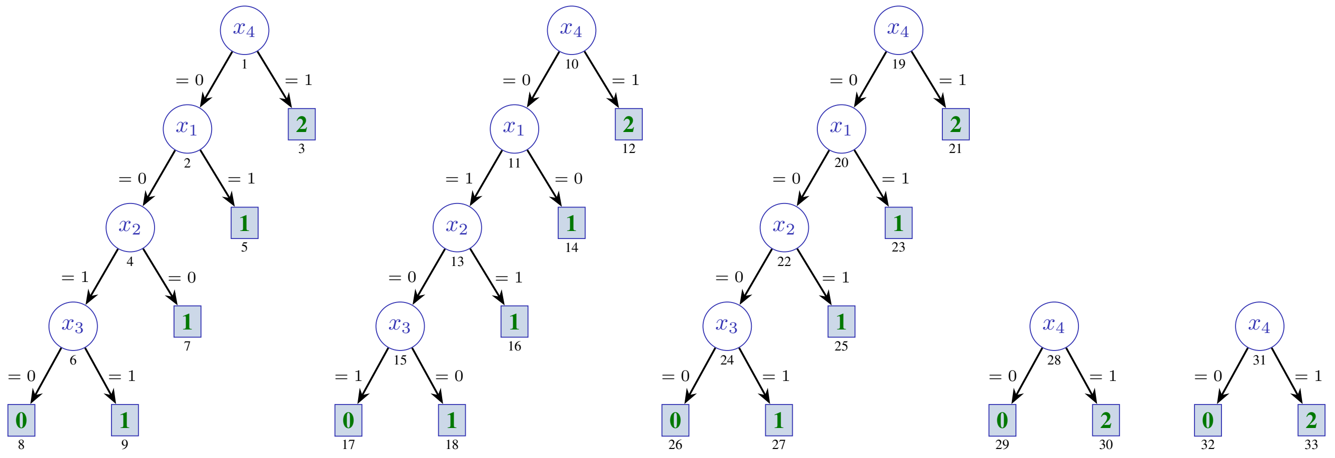


Fig. 3: A different reduction from CNFSAT to the RFmv decision problem.

number of models of φ is the same as the number of points in feature space for which the RF prediction is 1. Thus, if we could count the number of assignments with prediction 1, then we could count the models of a CNF formula, and so SHAP_Scores is #P-hard. □

SHAP_Scores for BTs, RFwvs and TEs are #P-hard. The hardness of computing SHAP scores for BTs, RFwvs and TEs are immediate results given Propositions 1 to 3 and 7.

The corollary of the results in this section is that computing SHAP scores for all of the most widely used TE classifiers (including the simplest type of RF classifiers [Breiman, 2001]) is #P-hard. This means that, for these types of RF and TE classifiers it is extremely unlikely that computing SHAP scores might be in P, as claimed in earlier work, concretely in Corollary 4 of [Van den Broeck *et al.*, 2021] and Corollary 5 of [Van den Broeck *et al.*, 2022]. Similar claims have been made or implied in other works [Lundberg and Lee, 2017a; Lundberg *et al.*, 2018; Lundberg *et al.*, 2020; Campbell *et al.*, 2022; Muschalik *et al.*, 2024], which are also disproved by the results in this section.

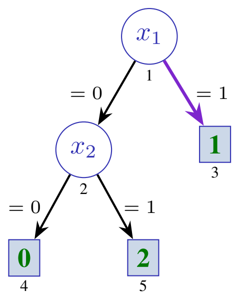
6 Update on Tractable Cases

To the best of our knowledge, the only polynomial-time algorithms for computing SHAP scores were proposed for d-DNNFs [Arenas *et al.*, 2021] and later extended to d-DNNFs with non-binary features [Arenas *et al.*, 2023].[6] In the case of DTs, non-binary d-DNNFs encompass read-once binary decision trees where features can take discrete values. Furthermore, one could conceptually extract an algorithm for a broader range of DTs, by adapting the proof of polynomial-time computation of SHAP scores for decision trees in [Van den Broeck *et al.*, 2021; Van den Broeck *et al.*, 2022]. However, the algorithm extracted from the proof would require solving a system of m equations, which is $\mathcal{O}(m^3)$. In addition, the algorithms proposed in earlier work [Arenas *et al.*, 2021; Arenas *et al.*, 2023] exploit (6) to avoid enumerating all possible sets of fixed features. The purpose of this section is to propose two simple generalizations to the earlier algorithms [Arenas *et al.*, 2021; Arenas *et al.*, 2023], thereby ensuring polynomial-time (and efficient) solutions for computing SHAP scores in the case of d-DNNFs. These generalizations are discussed in the remainder of this section.

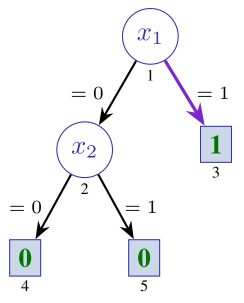
6.1 d-DNNF Replication

The first solution consists of analyzing a polynomial number of modified copies of the classifier, each represented by a dis-

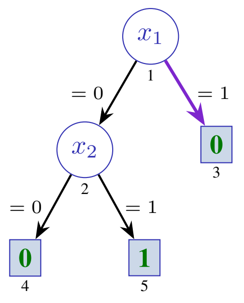
[6]As proved elsewhere [Van den Broeck *et al.*, 2021; Van den Broeck *et al.*, 2022], other earlier attempts [Lundberg *et al.*, 2020] resulted in unsound algorithms.



(a) Non-binary DT



(b) DT for $\kappa_{c=1}$, $\lambda_{c=1} = 1$



(c) DT for $\kappa_{c=2}$, $\lambda_{c=2} = 2$

Function	$\mathsf{Sc}(1)$	$\mathsf{Sc}(2)$	$\lambda_{c=c_l}$
$\kappa_{c=1}$	$1/2$	0	1
$\kappa_{c=2}$	$-3/4$	$1/4$	2
κ	$-1/4$	$1/4$	

(d) SHAP scores

Fig. 4: Example of computing SHAP scores for DT, with $(\mathbf{v}, c) = ((1, 1), 1)$.

tinct d-DNNF.

Let $\gamma(\mathbf{x}) = \sum_l \lambda_l \kappa_l(\mathbf{x})$. A well-known result of SHAP scores (e.g. see eq. (4) in [Van den Broeck *et al.*, 2022]) is that,

$$\mathsf{Sc}_\gamma(i) = \sum\nolimits_l \lambda_l \mathsf{Sc}_{\kappa_l}(i) \tag{11}$$

Thus, for a classifier with classes $\mathcal{K} = \{c_1, \ldots, c_K\}$, we create K copies of the classifier where, for each copy l, the only non-zero prediction is c_l, which we set to 1. This becomes function κ_l and we set $\lambda_l = c_l$. Moreover, one then constructs the d-DNNF for the classifier κ_l, and compute the SHAP scores. Finally, we use (11) to compute the SHAP scores of the original classifier. We refer to this approach as *d-DNNF replication*.

Example 4. *For the example DT in Fig. 4a, $\mathcal{F} = \{1, 2, 3\}$, with $\mathbb{D}_i = \mathbb{B}, i = 1, 2, 3$ and $\mathcal{K} = \{0, 1, 2\}$. The target instance is $(\mathbf{v}, c) = ((1, 1, 1), 1)$. As noted above, the algorithms proposed in earlier work [Arenas* et al.*, 2021; Arenas* et al.*, 2023] cannot be used for this DT, because $\mathcal{K} \neq \mathbb{B}$. Also, as proposed above, for each $c_l \in \mathcal{K}$ with $c_l \neq 1$, we create a new d-DNNF representing a classifier for which the only non-zero prediction is for class c_l, which we convert to class 1. After computing the SHAP scores, these are multiplied by c_l. For the example DT, this is shown in Figs. 4b and 4c. Using Eq.* (11)*, the final computed SHAP scores are obtained by summing over all individual d-DNNFs (DTs in the example), as shown in Fig. 4d.*

The discussion above confirms the following result.

Proposition 8. *For a classification function $\gamma : \mathbb{F} \to \mathcal{K}$ that can be expressed as a linear combination of classifiers defined by a linear combination of non-binary but boolean classifiers, each of which represented by a d-DNNF, then the computation of SHAP scores is polynomial-time.*

6.2 Non-Binary Non-Boolean d-DNNFs for DTs

The second solution consists of generalizing the non-binary d-DNNFs studied in earlier work [Arenas *et al.*, 2023], to allow for non-binary inputs but also non-boolean classes (NB2) in the concrete case of read-once DTs. The basic algorithm of [Arenas *et al.*, 2023] is included in Appendix A; a few minor changes are clarified below.

We recall that the translation from read-once DTs to d-DNNFs is well-known [Arenas *et al.*, 2023]; essentially each non-terminal node is replaced by the encoding of an ITE (if-then-else) operator. Concretely, given a node g testing a literal l_j, such that the input value is $\nu_{g,0}$ when l_j is false and $\nu_{g,1}$ when l_j is true, the output of the node is $\text{ITE}(l_j, \nu_{g,1}, \nu_{g,0})$, which is encoded in d-DNNFs as $\text{OR}(\text{AND}(l_j, \nu_{g,1}), \text{AND}(\neg l_j, \nu_{g,0}))$.

In contrast to earlier work [Arenas *et al.*, 2021; Arenas *et al.*, 2023], the insight is to allow constant nodes to take *any* value, subject to constraints on how the d-DNNFs can be organized. In the case of NB2 DTs, $\neg$-gates are only allowed to have variable nodes as inputs. Moreover, $\land$-gates are modified to compute numerical values, given one boolean input and one non-boolean input, i.e. if the boolean input takes value 0, the output is 0, and if the boolean input takes value 1, the output replicates the non-boolean input. Finally, because the d-DNNFs is deterministic, $\lor$-gates are guaranteed to have at most one input with a non-zero value; this value is replicated to the output. With these restrictions, the algorithms described in earlier work [Arenas *et al.*, 2021; Arenas *et al.*, 2023] can be used without additional changes.

7 Conclusions

This paper revisits recent complexity results regarding the computation of SHAP scores for ML classifiers. The first result proves that an often heralded claim [Lundberg and Lee, 2017a; Lundberg *et al.*, 2018; Lundberg *et al.*, 2020; Van den Broeck *et al.*, 2021; Campbell *et al.*, 2022; Van den Broeck *et al.*, 2022; Muschalik *et al.*, 2024] that SHAP scores for Random Forest (and also Additive Tree Ensemble) classifiers can be computed in polynomial-time does not hold for the most commonly used RF (and TE) classifiers, i.e. those with decision mechanisms based on voting. Concretely, the paper proves that, even for very simple, but realistic, models of RF/TE classifiers, the computation of SHAP scores is #P-hard. A second result refines the class of classifiers for which SHAP scores can be computed in polynomial time. A corollary is that for read-once multi-valued decision trees, the computation of SHAP scores is also polynomial time. A topic of research for decision trees that do not respect the read-once condition is whether SHAP scores can be computed more efficiently than what the proof of membership in P [Van den Broeck *et al.*, 2022] suggests.

Algorithm 1 Computation of SHAP scores for non-boolean DTs

```
Input: Feature $i$, Smoothed d-DNNF $D$ with output $g_{out}$
Parameters: Explanation problem $\mathcal{E}$
Output: SHAP score $\mathsf{Sc}(i)$

1: function SHAP_SCORES($i, D; \mathcal{E}$)
2:     for $g \in D$, by bottom-up induction on $D$ do
3:         $r \leftarrow |\text{var}(g) \setminus \{i\}|$
4:         if $g$ is a constant gate with label $a$ then          ▷ Constant gate; value of $a$ unrestricted
5:             $(\gamma_g^0, \delta_g^0) \leftarrow (a, a)$
6:         else if $g$ is a variable gate with var$(g) = i$ then          ▷ Variable gate associated with feature $i$
7:             $(\gamma_g^0, \delta_g^0) \leftarrow (1, 0)$
8:         else if $g$ is a variable gate with var$(g) = j$ and $j \neq i$ then          ▷ Variable gate not associated with feature $i$
9:             $(\gamma_g^0, \delta_g^0) \leftarrow (p(j), p(j))$
10:            $(\gamma_g^1, \delta_g^1) \leftarrow (\nu(j), \nu(j))$
11:        else if $g$ is a $\neg$-gate with input gate $g'$ then
12:            for $l \in \{0, \ldots, r\}$ do          ▷ Analyze $\neg$ gate; input gate $g'$ must be a variable gate
13:                $q \leftarrow \binom{r}{l}$
14:                $\gamma_g^l \leftarrow q - \gamma_{g'}^l$
15:                $\delta_g^l \leftarrow q - \delta_{g'}^l$
16:            end for
17:        else if $g$ is a $\vee$-gate with input gates $g_1, g_2$ then          ▷ Analyze $\vee$ gate, each $\vee$ gate has a fan-in of exactly 2
18:            for $l \in \{0, \ldots, r\}$ do
19:                $\gamma_g^l \leftarrow \gamma_{g_1}^l + \gamma_{g_2}^l$
20:                $\delta_g^l \leftarrow \delta_{g_1}^l + \delta_{g_2}^l$
21:            end for
22:        else if $g$ is a $\wedge$-gate with input gates $g_1, g_2$ then          ▷ Analyze $\wedge$ gate, each $\wedge$ gate has a fan-in of exactly 2
23:            for $l \in \{0, \ldots, r\}$ do
24:                $(r_1, r_2) \leftarrow (|\text{var}(g_1) \setminus \{i\}|, |\text{var}(g_2) \setminus \{i\}|)$
25:                $\gamma_g^l \leftarrow \sum_{l_1 \in \{0,\ldots,\min(l,r_1)\}, l_2 \in \{0,\ldots,\min(l,r_2)\}, l_1+l_2=l} \gamma_{g_1}^{l_1} \cdot \gamma_{g_2}^{l_2}$
26:                $\delta_g^l \leftarrow \sum_{l_1 \in \{0,\ldots,\min(l,r_1)\}, l_2 \in \{0,\ldots,\min(l,r_2)\}, l_1+l_2=l} \delta_{g_1}^{l_1} \cdot \delta_{g_2}^{l_2}$
27:            end for
28:        end if
29:    end for
30:    return $\sum_{k=0}^{m-1} \varsigma(k) \cdot [(\nu(i) - p(i))(\gamma_{g_{out}}^k - \delta_{g_{out}}^k)]$          ▷ Returned value is the SHAP score $\mathsf{Sc}(i)$ for feature $i \in \mathcal{F}$
31: end function
```

A Appendix – SHAP Scores for NB2 DTs

Restriction on d-DNNFs & rationale. We consider d-DNNFs obtained from read-once DTs, where features take discrete values, and classes are numerical and discrete, i.e. non-binary features and non-boolean classes (NB2) DTs. The translation from read-once DTs to d-DNNF is well-known [Arenas *et al.*, 2023]; essentially each non-terminal node is replaced by the encoding of an ITE (if-then-else) operator. Concretely, given a node g testing a literal l_j., such that the input value is $\nu_{g,0}$ when l_j is false and $\nu_{g,1}$ when l_j is true, the output of the node is ITE$(l_j, \nu_{g,1}, \nu_{g,0})$, which is encoded in d-DNNF as OR(AND$(l_j, \nu_{g,1})$, AND$(\neg l_j, \nu_{g,0})$).

Building on earlier work [Arenas *et al.*, 2023] we generalize such d-DNNFs to allow for terminal nodes to be assigned *arbitrary* numerical values. Clearly, the computed value will match the value assigned to the terminal node of the unique path consistent with the input.

Algorithm 1 (see Page 8) summarizes the algorithm for computing SHAP scores for generalized d-DNNFs (e.g. obtained from DTs), which mimics the one proposed in earlier work [Arenas *et al.*, 2023], with minor changes on the requirements on the values of constant nodes. In addition, the algorithm imposes that constant gates must *not* be the input of $\neg$-gates. In addition, the value assigned to constant gates is allowed to be arbitrary (see line 4 of Algorithm 1).

Ethical Statement

There are no ethical issues.

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