On Explaining Random Forests with SAT

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Abstract

Random Forests (RFs) are among the most widely used Machine Learning (ML) classifiers. Even though RFs are not interpretable, there are no dedicated non-heuristic approaches for computing explanations of RFs. Moreover, there is recent work on polynomial algorithms for explaining ML models, including naive Bayes classifiers. Hence, one question is whether finding explanations of RFs can be solved in polynomial time. This paper answers this question negatively, by proving that deciding whether a set of literals is a PI-explanation of an RF is D^{P}-complete. Furthermore, the paper proposes a propositional encoding for computing explanations of RFs, thus enabling finding PI-explanations with a SAT solver. This contrasts with earlier work on explaining boosted trees (BTs) and neural networks (NNs), which requires encodings based on SMT/MILP. Experimental results, obtained on a wide range of publicly available datasets, demonstrate that the proposed SAT-based approach scales to RFs of sizes common in practical applications. Perhaps more importantly, the experimental results demonstrate that, for the vast majority of examples considered, the SAT-based approach proposed in this paper significantly outperforms existing heuristic approaches.

1 Introduction

The recent successes of Machine Learning (ML), and the forecast continued growth of ML-enabled applications, including applications that impact human beings or that are even safety critical, has raised the need for identifying explanations for the predictions made by ML models. As a result, recent years witnessed the rapid growth of the field of explainable Artificial Intelligence (XAI) (see e.g. [Guidotti *et al.*, 2019; Li *et al.*, 2018; Montavon *et al.*, 2018; Shih *et al.*, 2018; Shih *et al.*, 2019; Ribeiro *et al.*, 2016; Ribeiro *et al.*, 2018; Ignatiev *et al.*, 2019; Ignatiev, 2020; Audemard *et al.*, 2020; Ignatiev *et al.*, 2020; Ignatiev and Marques-Silva, 2021; Marques-Silva *et al.*, 2021]). Unfortunately, the most promising ML models, including neural networks or ensembles of classifiers, due to their size and intrinsic complexity, are generally accepted to be non-interpretable (or black-box), with the understanding that the predictions made by such black-box models cannot be understood by human decision makers.

A large body of work on XAI is based on heuristic approaches [Ribeiro *et al.*, 2016; Lundberg and Lee, 2017; Ribeiro *et al.*, 2018], offering no formal guarantees regarding computed explanations[1]. In contrast, recent work focused on non-heuristic approaches which offer formal guarantees with respect to computed explanations [Shih *et al.*, 2018; Ignatiev *et al.*, 2019; Shih *et al.*, 2019; Ignatiev, 2020; Darwiche and Hirth, 2020; Audemard *et al.*, 2020; Marques-Silva *et al.*, 2020; Ignatiev *et al.*, 2020; Ignatiev and Marques-Silva, 2021; Marques-Silva *et al.*, 2021].

Approaches to explainability can also be characterized as being model-agnostic or model-precise[2]. Model-agnostic approaches do not require information about the ML model representation, thus allowing the explanation of any class of ML models. In contrast, in model-precise approaches, some representation of the concrete ML model is reasoned about, and so these are characterized by being model-specific. Whereas model-agnostic approaches are in general heuristic, model-precise approaches can either be non-heuristic [Shih *et al.*, 2018; Ignatiev *et al.*, 2019; Shih *et al.*, 2019; Ignatiev, 2020; Darwiche and Hirth, 2020; Audemard *et al.*, 2020; Marques-Silva *et al.*, 2020; Ignatiev *et al.*, 2020; Ignatiev and Marques-Silva, 2021; Marques-Silva *et al.*, 2021] or heuristic [Zhao *et al.*, 2019; Petkovic *et al.*, 2018; Mollas *et al.*, 2020]. For model-precise non-heuristic approaches different solutions have been investigated. [Shih *et al.*, 2018] propose an approach for explaining Bayesian network classifiers, which is based on compiling such classifiers into Ordered Decision Diagrams representing all prime implicants of the boolean function representing the target class predictions. These represent the so-called PI-explanations (which we revisit in Section 2). A different approach, based on abductive reasoning [Ignatiev *et al.*, 2019; Ignatiev, 2020], exploits automated reasoning tools (e.g. SMT, MILP, etc.) with explanations being com-

[1]For example, an explanation E, for an input I_1 resulting in prediction A, can also be consistent with input I_2 resulting in prediction $B \neq A$ [Ignatiev, 2020]. Such *loose* explanations inevitably raise concerns in applications where safety is critical.

[2]Orthogonal to the goals of the paper is the classification of explanations as *local* or *global* [Guidotti *et al.*, 2019].

puted on demand. In abductive reasoning approaches, the ML model is represented as a set of constraints and, given some target instance, a prime implicant is computed, which represents a minimal set of feature-value pairs that is sufficient for the prediction. Earlier work investigated encodings of neural networks [Ignatiev *et al.*, 2019] and of boosted trees [Ignatiev, 2020].

This paper extends earlier work on model-precise non-heuristic explainability. Concretely, the paper proposes a novel approach for computing PI (or abductive) explanations (AXps) of Random Forest classifiers [Breiman, 2001; Yang *et al.*, 2020; Zhang *et al.*, 2019; Gao and Zhou, 2020; Feng and Zhou, 2018; Zhou and Feng, 2017]. Random Forests (RFs) represent a widely used tree ensemble ML model, where each RF ML model is composed of a number of decision trees (DTs). (The importance of RFs is further illustrated by recent proposals for implementing deep learning (DL) with RFs [Zhou and Feng, 2017; Zhang *et al.*, 2019; Feng and Zhou, 2018].)

In contrast with earlier work [Ignatiev, 2020], we show that in the case of RFs it is possible to devise a purely propositional encoding. In turn, this enables achieving very significant performance gains. Concretely, the experimental results show that our approach is able to compute explanations of realistically-sized RFs most often in a fraction of a second. The experiments also show that our approach is on average more than one order of magnitude faster than a state of the art model-agnostic heuristic approach [Ribeiro *et al.*, 2018].

Recent work on model-precise non-heuristic explainability has shown that some ML models can be explained in polynomial time [Audemard *et al.*, 2020; Marques-Silva *et al.*, 2020]. In contrast, this paper proves that it is D^{P}-complete to decide whether a set of literals is a PI-explanation (AXp) of an RF, thus making it unlikely that RFs can be explained in polynomial time.

The paper is organized as follows. Section 2 covers the preliminaries. Section 3 proves the complexity of deciding whether a set of literals is an explanation for an RF. Section 4 proposes a propositional encoding for computing one AXp of an RF. Section 5 presents the experimental results. Finally, Section 6 concludes the paper.

2 Preliminaries

ML Classification. We consider a machine learning classification problem, defined by a set of features $\mathcal{F} = \{1, \ldots, m\}$, and by a set of classes $\mathcal{K} = \{c_1, c_2, \ldots, c_K\}$. Each feature $j \in \mathcal{F}$ takes values from a domain $\mathbb{D}_i$. (Domains may correspond to Boolean, Categorical or Continuous data.) Thus, feature space is defined as $\mathbb{F} = \mathbb{D}_1 \times \mathbb{D}_2 \times \ldots \times \mathbb{D}_m$. To refer to an arbitrary point in feature space we use the notation $\mathbf{x} = (x_1, \ldots, x_m)$, whereas to refer to a specific point in feature space we use the notation $\mathbf{v} = (v_1, \ldots, v_m)$, with $v_i \in \mathbb{D}_i$, $i = 1, \ldots, m$. An *instance* (or example) denotes a pair $(\mathbf{v}, c)$, where $\mathbf{v} \in \mathbb{F}$ and $c \in \mathcal{K}$. An ML classifier is characterized by a classification function τ that maps the feature space $\mathbb{F}$ into the set of classes $\mathcal{K}$, i.e. $\tau : \mathbb{F} \to \mathcal{K}$. To learn a classifier, a set of instances $\{(\mathbf{v}_1, c_1), \ldots, (\mathbf{v}_k, c_k)\}$ is used as training data by a learning algorithm that returns a function with a best fit on the training data.

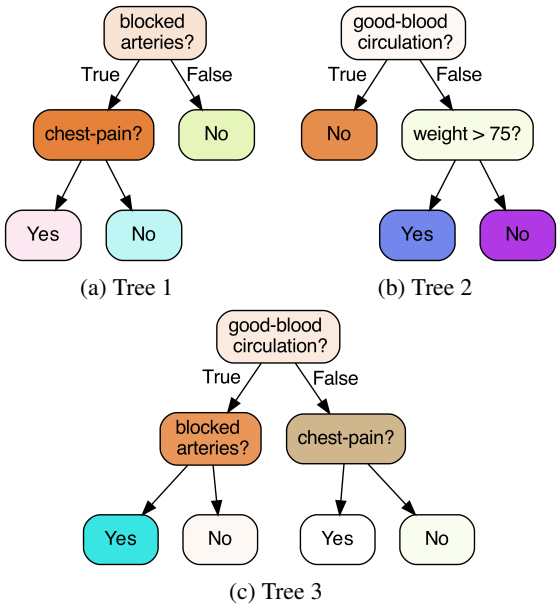
Decision Tree and Random Forest Classifiers. Decision trees rank among the most widely-used techniques ML models [Breiman *et al.*, 1984; Quinlan, 1993]. Formally, a decision tree $\mathcal{T} = (V_{\mathcal{T}}, E_{\mathcal{T}})$ is a directed acyclic graph, where the root node has no incoming edges, and every other node has exactly one incoming edge. The nodes of a tree are partitioned into terminal (V_T) and non-terminal (V_{NT}) nodes. Terminal nodes denote the leaf nodes, and have no outgoing edges (i.e. children). Non-terminal nodes denote the internal nodes, and have outgoing edges. Each terminal node $j \in V_T$ is associated with a class taken from $\mathcal{K}$. We define a map $\kappa : V_T \to \mathcal{K}$ to represent the class associated with each terminal node. Each non-terminal node is associated with a feature taken from a set of features $\mathcal{F}$. Given a feature $j \in \mathcal{F}$ associated with a non-terminal node l, each outgoing edge represents a literal of the form $x_j \bowtie S_j$, where either $S_j \in \mathbb{D}_j$ or $S_j \subseteq \mathbb{D}_j$ [3]. Each path in $\mathcal{T}$ is associated with a consistent conjunction of literals, denoting the values assigned to the features so as to reach the terminal node in the path. We will represent the set of literals of some tree path R_k by $\mathcal{L}(R_k)$.

A well-known drawback of decision trees is overfitting with respect to the training data. In contrast, tree ensembles such as Random Forests (RFs) [Breiman, 2001] combine several tree-based models, which allows for improved accuracy and ability to generalize beyond the training data. More formally, an RF $\mathfrak{F}$ is a collection of decision trees (DTs) $\mathfrak{F} = \{\mathcal{T}_1, \mathcal{T}_2, \ldots, \mathcal{T}_M\}$. Each tree $\mathcal{T}_i \in \mathfrak{F}$ is trained on a subsample of the training dataset so as the trees of the RF are not correlated. The prediction function in RF works by majority vote, that is each tree votes for a class and the most voted class is picked. (In case of ties, for simplicitly we will pick the lexicographically smallest class.)

Running Example. Let us assume a simple binary classification problem for predicting whether or not a patient has a heart disease. The class variables are: *Yes* and *No* (*Yes* to classify the patient as suffering from heart disease and *No* to classify the patient as without heart disease.) and a set of features in the following order: *blocked-arteries*, *good-blood-circulation*, *chest-pain*, and *weight*, where features 1, 2 and 3 represent Boolean variables, and feature 4 represents an ordinal variable. Let the set of trees, shown in Figure 1, be the tree ensemble of an RF classifier $\mathfrak{F}$ trained on the heart disease problem and τ its classification function. There are 3 trees in the forest and each tree has a maximum depth of 2. Assume we have an instance $\mathbf{v} = (1, 0, 1, 70)$, namely, *blocked-arteries* = 1, *good-blood-circulation* = 0, *chest-pain* = 1, *weight* = 70. Hence, Trees 1 and 3 vote for *Yes* and Tree 2 votes for *No*. As the majority votes go for *Yes*, then the classifier will return *Yes* for $\mathbf{v}$, i.e. $\tau(\mathbf{v}) =$ *Yes*.

Boolean satisfiability (SAT). The paper assumes the notation and definitions standard in SAT [Biere *et al.*, 2021], i.e. the decision problem for propositional logic, which is known to be NP-complete [Cook, 1971]. A propositional

[3] Features are either categorical (including boolean) or real- or integer-valued ordinal, and $\bowtie \in \{=, \in\}$. (Observe that these operators allow for intervals to be represented.)



(a) Tree 1 (b) Tree 2

(c) Tree 3

Figure 1: Running example.

formula φ is defined over a finite set of Boolean variables $X = \{x_1, x_2, \ldots, x_n\}$. Formulas are most often represented in *conjunctive normal form* (CNF). A CNF formula is a conjunction of clauses, a clause is a disjunction of literals, and a literal is a variable (x_i) or its negation ($\neg x_i$). Whenever convenient, a formula is viewed as a set of sets of literals. A Boolean interpretation μ of a formula φ is a total mapping of X to $\{0, 1\}$ (0 corresponds to *False* and 1 corresponds to *True*). Interpretations can be extended to literals, clauses and formulas with the usual semantics; hence we can refer to $\mu(l)$, $\mu(\omega)$, $\mu(\varphi)$, to denote respectively the value of a literal, clause and formula given an interpretation. Given a formula φ, μ is a *model* of φ if it makes φ *True*, i.e. $\mu(\phi) = 1$. A formula φ is *satisfiable* ($\varphi \not\models \bot$) if it admits a model, otherwise, it is *unsatisfiable* ($\varphi \models \bot$). Given two formulas φ and ψ, we say that φ *entails* ψ (denotes $\varphi \models \psi$) if all models of φ are also models of ψ. φ and ψ are equivalent (denoted $\varphi \equiv \psi$) if $\varphi \models \psi$ and $\psi \models \varphi$.

Abductive explanations. The paper uses the definition of *PI-explanation* [Shih *et al.*, 2018] (also referred to as *abductive explanation* (AXp) in [Ignatiev *et al.*, 2019]) [4], based on prime implicants of some decision function (related with the predicted class). Let us consider a given ML model, computing a classification function τ on feature space $\mathbb{F}$, a point $\mathbf{v} \in \mathbb{F}$, with prediction $c = \tau(\mathbf{v})$, with $\mathbf{v} = (v_1, \ldots, v_m)$. A PI-explanation (AXp) is any minimal subset $\mathcal{X} \subseteq \mathcal{F}$ such that:

$$\forall(\mathbf{x} \in \mathbb{F}). \left[\bigwedge\nolimits_{i \in \mathcal{X}} (x_i = v_i)\right] \rightarrow (\tau(\mathbf{x}) = c) \qquad (1)$$

In a similar vein, we consider contrastive explanations (CXps) [Miller, 2019]. A formal definition of contrastive explanation is proposed in recent work [Ignatiev *et al.*, 2020].

[4]Throughout the paper we will use both terms *PI-explanation* and *abductive explanation* (AXp) interchangeably.

Contrastive explanations. Contrastive explanation can be defined as a minimal subset $\mathcal{Y} \subseteq \mathcal{F}$ that suffice to changing the prediction if features of $\mathcal{Y}$ are allowed to take some arbitrary value from their domain. Given $\mathbf{v} = (v_1, \ldots, v_m) \in \mathbb{F}$ with $\kappa(\mathbf{v}) = c$, a CXp is any minimal subset $\mathcal{Y} \subseteq \mathcal{F}$ such that,

$$\exists(\mathbf{x} \in \mathbb{F}). \bigwedge\nolimits_{j \in \mathcal{F} \setminus \mathcal{Y}} (x_j = v_j) \land (\kappa(\mathbf{x}) \neq c) \qquad (2)$$

Building on the results of R. Reiter in model-based diagnosis [Reiter, 1987], [Ignatiev *et al.*, 2020] proves a minimal hitting set (MHS) duality relation between AXps and CXps, i.e. AXps are MHSes of CXps and vice-versa.

Example 1. *Consider the binary classifier $\mathfrak{F}$ of the running example. and the instance $(\mathbf{v} = (1, 0, 1, 70), Yes)$. If the features good-blood-circulation and weight are allowed to take any possible value from their domain, and the values of the features blocked-arteries and chest-pain are kept to their values in $\mathbf{v}$, then the prediction is still Yes. This means that the features good-blood-circulation and weight can be deemed irrelevant for the prediction of Yes given the other feature values in $\mathbf{v}$. Moreover, by allowing either blocked-arteries or chest-pain to take any value, prediction will change to No. Hence, $\{$blocked-arteries, chest-pain$\}$ is a subset-minimal set of features sufficient for predicting $\tau(\mathbf{v}) =$ Yes, that is a PI-explanation (AXp). Additionally, setting the value of blocked-arteries to 0 suffices to changing the prediction of $\mathbf{v}$ (i.e. $\tau(0, 0, 1, 70) =$ No), thus $\{$blocked-arteries$\}$ is a CXp.*

3 Complexity of AXps for RFs

Recent work identified classes of classifiers for which one AXp can be computed in polynomial time [Audemard *et al.*, 2020; Marques-Silva *et al.*, 2020]. These classes of classifiers include those respecting specific criteria of the knowledge compilation map [Audemard *et al.*, 2020][5], but also Naive Bayes and linear classifiers (resp. NBCs and LCs) [Marques-Silva *et al.*, 2020]. (In the case of NBCs and LCs, enumeration of AXps was shown to be solved with polynomial delay.) One question is thus whether there might exist a polynomial time algorithm for computing one computing AXp of an RF. This section shows that this is unlikely to be the case, by proving that deciding whether a set of features represents an AXp is D^{P}-complete[6].

Let $\mathfrak{F}$ be an RF, with classification function τ, and let $\mathbf{v} \in \mathbb{F}$, with prediction $\tau(\mathbf{v}) = c \in \mathcal{K}$. τ is parameterized with c, to obtain the boolean function τ_c, s.t. $\tau_c(\mathbf{x}) = 1$ iff $\tau(\mathbf{x}) = c$. A set of literals $I_{\mathbf{v}}$ is associated with each $\mathbf{v}$. Let ρ be a subset of the literals associated with $\mathbf{v}$, i.e. $\rho \subseteq I_{\mathbf{v}}$. Hence,

Theorem 1. *For a random forest $\mathfrak{F}$, given an instance $\mathbf{v}$ with prediction c, deciding whether a set of literals is an AXp is D^{P}-complete.*

[5]The knowledge compilation map was first proposed in 2002 [Darwiche and Marquis, 2002].

[6]The class D^{P} [Papadimitriou, 1994] is the set of languages defined by the intersection of two languages, one in NP and one in coNP.

Proof. Given an instance $\mathbf{v}$ and predicted class c, deciding whether a set of literals ρ is an AXp of an RF $\mathfrak{F}$ is clearly in D^{P}. We need to prove that $\rho \models \tau_c$, which is a problem in coNP. We also need to prove that a set of literals ρ', obtained by the removal of any single literal from ρ (and there can be at most m of these), is such that $\rho \not\models \tau_c$, a problem in NP. To prove that the problem is hard for D^{P}, we reduce the problem of computing a prime implicant of a DNF, which is known to be complete for D^{P} [Umans *et al.*, 2006], to the problem of computing a PI-explanation of an RF $\mathfrak{F}$.

Consider a DNF $\phi = t_1 \lor \cdots \lor t_n$, where each term t_i is a conjunction of literals defined on a set $X = \{x_1, \ldots, x_m\}$ of boolean variables. Given ϕ, we construct an RF $\mathfrak{F}$, defined on a set $\mathcal{F}$ of m features, where each feature i is associated with an x_i element of X, and where $D_i = \{0, 1\}$. Moreover, $\mathfrak{F}$ is such that $\phi(\mathbf{x}) = 1$ iff $\tau_1(\mathbf{x}) = 1$. $\mathfrak{F}$ is constructed as follows.

i. Associate a decision tree (DT) $\mathcal{T}_i$ with each term t_i, such that the assignment satisfying t_i yields class 1, and the other assignments yield class 0. Clearly, the size of the DT $\mathcal{T}_i$ is linear on the size of t_i, since each literal not taking the value specified by the term will be connected to a terminal node with prediction 0.
ii. Create $(n-1)$ additional trees, each having exactly one terminal node and no non-terminal nodes. Moreover, associate class 1 with the terminal node.

Next, we prove that $\phi(\mathbf{x}) = 1$ iff $\tau_1(\mathbf{x}) = 1$.

i. Let $\mathbf{x}$ be such that $\phi(\mathbf{x}) = 1$. Then, there is at least one term t_j, such that $t_j(\mathbf{x}) = 1$. As a result, the corresponding tree $\mathcal{T}_j$ in the RF will predict class 1. Hence, at least n trees predict class 1, and at most $n-1$ trees predict class 0. As a result, the predicted class is 1, and so $\tau_1(\mathbf{x}) = 1$.
ii. Let $\mathbf{x}$ be such that $\tau_1(\mathbf{x}) = 1$. This means that at least one of the trees associated with the terms t_i must predict value 1. Let such tree be $\mathcal{T}_j$, associated with term t_j. For this tree to predict class 1, then $t_j(\mathbf{x}) = 1$, and so $\phi(\mathbf{x}) = 1$.

Now, let ρ be a conjunction of literals defined on X. Then, we must have $\rho \models \phi$ iff $\rho \models \tau_1$. Every model of ρ is also a model of ϕ, and so it must also be a model of τ_1. Conversely, every model of ρ is also a model of τ_1, and so it must also be a model of ϕ. □

4 AXps for Random Forests

This section outlines the computation of PI-explanations (AXps) for RFs. We first present the algorithm's organization. The algorithm requires a logical encoding of RFs, which are presented next.

Computing AXps. A minimal set of features $\mathcal{X} \in \mathcal{F}$ is an AXp if (1) holds. Clearly, this condition holds iff the following formula is unsatisfiable,

$$\left[\bigwedge\nolimits_{i \in \mathcal{X}} (x_i = v_i)\right] \land \mathsf{Enc}(\tau(\mathbf{x}) \neq c)$$

The previous formula has two components $\langle \mathcal{H}, \mathcal{S} \rangle$. $\mathcal{H}$ represents the set of hard clauses, encoding the representation of the ML model and also imposing a constraint on the predicted class, i.e. $\mathsf{Enc}(\tau(\mathbf{x}) \neq c)$. $\mathcal{S}$ represents the unit (*soft*) clauses, each capturing a literal $(x_i = v_i)$. Since the clauses in $\mathcal{S}$ are *soft*, they can be *dropped* (thus allowing x_i to take any value) while searching for a minimal subset of $\mathcal{E}$ of $\mathcal{S}$, such that,

$$\left[\bigwedge\nolimits_{(x_1 = v_i) \in \mathcal{E}} (x_i = v_i)\right] \land \mathsf{Enc}(\tau(\mathbf{x}) \neq c)$$

is unsatisfiable. Our goal is to find a minimal set $\mathcal{S}$ such that the pair $\langle \mathcal{H}, \mathcal{S} \rangle$ remains unsatisfiable (where $\mathcal{S}$ can be viewed as the background knowledge against which the clauses in $\mathcal{S}$ are inconsistent). This corresponds to finding a minimal unsatisfiable subset (MUS) of $\langle \mathcal{H}, \mathcal{S} \rangle$, and so any off-the-shelve MUS extraction algorithm can be used for computing an AXp (as noted in earlier work [Ignatiev *et al.*, 2019]).

Clearly, adapting the descibed procedure above of computing one AXp to one that computes a CXp is straightforward. That is, the minimal set $\mathcal{Y}$ of $\mathcal{S}$ to search is, such that,

$$\left[\bigwedge\nolimits_{(x_1 = v_i) \in \mathcal{S} \setminus \mathcal{Y}} (x_i = v_i)\right] \land \mathsf{Enc}(\tau(\mathbf{x}) \neq c)$$

is satisfiable. Further, hitting set duality between AXps and CXps allows to exploit any algorithm for computing MUSes/MCSes[7] to enumerate both kinds of explanations (AXps and CXps). (Recent work [Ignatiev *et al.*, 2020; Marques-Silva *et al.*, 2021; Ignatiev and Marques-Silva, 2021] exploits the MUS/MCS enumeration algorithm MARCO [Liffiton *et al.*, 2016] for enumerating AXps/CXps.)

We detail next how to encode an RF, while requiring some prediction not to hold. We start with a simple encoding of an RF into an SMT formula, and then we detail a purely propositional encoding, which enables the use of SAT solvers.

SMT Encoding. Several encodings of tree ensemble models, such as Boosted Trees (BTs), have been proposed and they are essentially based on SMT/MILP (see e.g. [Chen *et al.*, 2019; Einziger *et al.*, 2019; Ignatiev, 2020], etc). Hence, it is natural to follow prior work and propose a straightforward encoding of RFs in SMT. Intuitively, the formulation of RFs into SMT formulas is as follows. We encode every single DT of an RF as a set of implication rules. That is, a DT path (classification rule) is interpreted as a rule of the form *antecedent* $\rightarrow$ *consequent* where the *antecedent* is a conjunction of predicates encoding the non-terminal nodes of the path and the *consequent* is a predicate representing the class associated with the terminal node of the path. Next, we aggregate the prediction (votes) of the DTs and count the prediction score for each class. This can be expressed by an arithmetic function that calculates the sum of trees predicting the same class. Lastly, a linear inequality checks which class has the largest score.

The implementation of the encoding above resulted in performance results comparable to those of BTs [Ignatiev, 2020]. However, in the case of RFs it is possible to devise a purely propositional encoding, as detailed below.

[7] An MCS is a minimal set of clauses to remove from an unsatisfiable CNF formula to recover consistency . It is well-known that MCSes are minimal hitting sets of MUSes and vice-versa [Reiter, 1987; Birnbaum and Lozinskii, 2003].

SAT Encoding. Our goal is to represent the structure of an RF with a propositional formula. This requires abstracting away what will be shown to be information used by the RF that is unnecessary for finding an AXp. Concretely, and as shown below, the actual values of the features used as literals in the RF need not be considered when computing one AXp. We start by detailing how to encode the nodes of the decision trees in an RF. This is done such that the actual values of the features are abstracted away. Then, we present the encoding of the RF classifier itself, including how the majority voting is represented.

To encode a terminal node of a DT, we proceed as follows. Given a set of classes $\mathcal{K} = \{c_1, c_2, \ldots, c_K\}$, a terminal node t labeled with one class of $\mathcal{K}$. Then, we define for each $c_j \in \mathcal{K}$ a variable l_j and represent the terminal node t with its corresponding label class c_j, i.e. $\kappa(t) = c_j$.

Moreover, the encoding of a non-terminal node of a DT is organized as follows. Given a feature $j \in \mathcal{F}$ associated with a non-terminal node l, with a domain $\mathbb{D}_j$, each outgoing edge of l is represented by a literal l_j of the form $x_j \bowtie S_j$ s.t. $x_j \in \mathcal{F}$ is the variable of feature j, $S_j \bowtie \mathbb{D}_j$ and $\bowtie \in \{=, \subseteq, \in\}$. Hence we distinguish three cases for encoding $x_j \bowtie S_j$. For the first case, feature j is binary, and so the literal l_j is True if $x_j = 1$ and False if $x_j = 0$. For the second case, feature j is categorical, and so we introduce a Boolean variable z_i for each value $v_i \in \mathbb{D}_j$ s.t. $z_i = 1$ iff $x_j = v_i$. Assume $S_j = \{v_1, \ldots, v_n\}$, then we connect l_j to variables $z_i, i = 1, \ldots, n$ as follows: $l_j \leftrightarrow (z_1 \vee \ldots \vee z_n)$ or $\neg l_j \leftrightarrow (z_1 \vee \ldots \vee z_n)$, depending on whether the current edge is going to left or right child-node. Finally, for the third case, feature j is real-valued. Thus, S_j is either an interval or a union of intervals. Concretely, we consider all the splitting thresholds of the feature j existing in the RF and we generate (in order) all the possible intervals. Each interval $I_i \subseteq \mathbb{D}_j$ is denoted by a Boolean variable z_i. Let us assume $S_j = I_1 \cup \ldots \cup I_n$ and $z_1, \ldots, z_n$ are variables associated with $I_1 \cup \ldots \cup I_n$, then we have $l_j \leftrightarrow (z_1 \vee \ldots \vee z_n)$ or $\neg l_j \leftrightarrow (z_1 \vee \ldots \vee z_n)$. Moreover, this encoding can be reduced into a more compact set of constraints (that also improves propagation in the SAT solver). Indeed, if the number of intervals is large the encoding will be as well. Hence, we propose to use auxiliary variables in the encoding. Assume $\mathbb{D}_j = I_1 \cup I_2 \cup I_3$, nodes l and l' s.t. $\neg l_j \leftrightarrow z_1$, $\neg l_j \leftrightarrow (z_1 \vee z_2 \vee z_3)$, $\neg l'_j \leftrightarrow (z_1 \vee z_2)$, $l'_j \leftrightarrow z_3$, then this can be re-written as: $\neg l_j \leftrightarrow z_1$, $l_j \leftrightarrow (z_2 \vee l'_j)$, $\neg l'_j \leftrightarrow (z_2 \vee \neg l_j)$, $l'_j \leftrightarrow z_3$.

The next step is to encode the RF classifier. Given an RF $\mathfrak{F}$ formed by a set of M DTs, i.e. $\mathfrak{F} = \{\mathcal{T}_1, \mathcal{T}_2, \ldots, \mathcal{T}_M\}$, and τ the classification function of $\mathfrak{F}$. For every DT $\mathcal{T}_i \in \mathfrak{F}$, we encode the set of paths $\mathcal{R}_i$ of $\mathcal{T}_i$ as follows:

$$\bigwedge\nolimits_{R_k \in \mathcal{R}_i} \left(\left(\bigwedge\nolimits_{l_j \in \mathcal{L}(R_k)} l_j \right) \rightarrow l_{ij} \right) \tag{3}$$

where l_{ij} is a literal associated with $\mathcal{T}_i$ in which the voted class is $c_j \in \mathcal{K}$.

For every DT $\mathcal{T}_i \in \mathfrak{F}$, and every path $R_k \in \mathcal{R}_i$, we enforce the condition that exactly one variable l_{ij} is *True* in $\mathcal{T}_i$ [8]. This can be expressed as[9]:

$$\left(\bigvee\nolimits_{j=1}^{K} l_{ij} \right) \wedge \sum\nolimits_{j=1}^{K} l_{ij} \leq 1 \tag{4}$$

Finally, for capturing the majority voting used in RFs, we need to express the constraint that the counts (of individual tree selections) for some class $c_k \neq c_j$ have to be large enough (i.e. greater than, or greater than or equal to) when compared to the counts for class c_j. We start by showing how cardinality constraints can be used for expressing such constraints. The proposed solution requires the use of $K - 1$ cardinality constraints, each comparing the counts of c_j with the counts of some other c_k. Afterwards, we show how to reduce to 2 the number of cardinality constraints used.

Let $c_j \in \mathcal{K}$ be the predicted class. The index j is relevant and ranges from 1 to $K = |\mathcal{K}|$. Moreover, let $1 \leq k < j \leq K$. Class c_k is selected over class c_j if:

$$\sum\nolimits_{i=1}^{M} l_{ik} > \sum\nolimits_{i=1}^{M} l_{ij} \Leftrightarrow \sum\nolimits_{i=1}^{M} l_{ik} + \sum\nolimits_{i=1}^{M} \neg l_{ij} \geq M \tag{5}$$

Similarly, let $1 \leq j < k \leq K$. Class c_k is selected over class c_j if:

$$\sum\nolimits_{i=1}^{M} l_{ik} > \sum\nolimits_{i=1}^{M} l_{ij} \Leftrightarrow \sum\nolimits_{i=1}^{M} l_{ik} + \sum\nolimits_{i=1}^{M} \neg l_{ij} \geq M + 1 \tag{6}$$

(A simple observation is that these constraints can be optimized for the case $|\mathcal{K}| = 2$.)

It is possible to reduce the number of cardinality constraints as follows. Let us represent (5) and (6), respectively, by $\mathsf{Cmp}_{\prec}(z_1^{\prec}, \ldots, z_M^{\prec})$ and $\mathsf{Cmp}_{\succ}(z_1^{\succ}, \ldots, z_M^{\succ})$. (Observe that the encodings of these constraints differ (due to the different RHSes).) Moreover, in (5) and (6) we replace $(z_1^{\prec}, \ldots, z_M^{\prec})$ and $(z_1^{\succ}, \ldots, z_M^{\succ})$ resp. by $l_{1k}, \ldots, l_{Mk}$, for some k. The idea is that we will *only* use two cardinality constraints, one for (5) and one for (6).

Let $p_k = 1$ iff k is to be compared with j. In this case, $\mathsf{Cmp}_{\bowtie}(z_1^{\bowtie}, \ldots, z_M^{\bowtie})$ (where $\bowtie$ is either $\prec$ or $\succ$) is comparing the class counts of c_j with the class counts of some c_k. Let us use the constraint $p_k \rightarrow (z_i^{\bowtie} \leftrightarrow l_{ik})$, with $k \in \{1, \ldots, K\} \setminus \{j\}$, and $1 \leq i \leq M$. This serves to allow associating the (free) variables $(z_1^{\bowtie}, \ldots, z_M^{\bowtie})$ with some set of literals $(l_{1k}, \ldots, l_{Mk})$. Moreover, we also let $p_0 \rightarrow (z_i^{\bowtie} \leftrightarrow 1)$ and $p_j \rightarrow (z_i^{\bowtie} \leftrightarrow 1)$, i.e. we allow p_0 and p_j to pick *guaranteed winners*, and such that $\neg p_0 \vee \neg p_j$. Essentially, we allow for a guaranteed winner to be picked below j or above j, but not both. Clearly, we must pick one k, either below or above j, to pick a class c_k, when comparing the counts of c_k and c_j. We do this by picking two winners, one below j and one above j, and such that at most one is allowed to be a guaranteed winner (either 0 or j):

$$\left(\sum\nolimits_{r=0}^{j-1} p_r = 1 \right) \wedge \left(\sum\nolimits_{r=j}^{K} p_r = 1 \right)$$

Observe that, by starting the sum at 0 and j, respectively, we allow the picking of one guaranteed winner in each summation, if needed be. To illustrate the described encoding above we consider again the running example.

[8] Only one class is returned by $\mathcal{T}_i$.

[9] We use the well-known cardinality networks [Asín *et al.*, 2011] for encoding all the cardinality constraints of the proposed encoding.

Dataset	(#F	#C	#I)	RF			CNF		SAT oracle				AXp (RFxpl)				Anchor	
				D	#N	%A	#var	#cl	MxS	MxU	#S	#U	Mx	m	avg	%w	avg	%w
ann-thyroid	(21	3	718)	4	2192	98	17 854	29 230	0.12	0.15	2	18	0.36	0.05	0.13	96	0.32	4
appendicitis	(7	2	43)	6	1920	90	5181	10 085	0.02	0.02	4	3	0.05	0.01	0.03	100	0.48	0
banknote	(4	2	138)	5	2772	97	8068	16 776	0.01	0.01	2	2	0.03	0.02	0.02	100	0.19	0
biodegradation	(41	2	106)	5	4420	88	11 007	23 842	0.31	1.05	17	22	2.27	0.04	0.29	97	4.07	3
ecoli	(7	5	66)	5	3860	90	20 081	34 335	0.10	0.09	4	2	0.21	0.05	0.10	98	0.38	2
glass2	(9	2	66)	6	2966	90	7303	15 194	0.04	0.03	5	4	0.09	0.02	0.03	100	0.61	0
heart-c	(13	2	61)	5	3910	85	5594	11 963	0.04	0.02	6	7	0.07	0.01	0.04	100	0.85	0
ionosphere	(34	2	71)	5	2096	87	7174	14 406	0.02	0.02	22	11	0.11	0.02	0.03	100	12.43	0
iris	(4	3	60)	6	1446	93	16 346	25 603	0.02	0.01	2	2	0.05	0.02	0.03	100	0.21	0
karhunen	(64	10	200)	5	6198	91	36 708	70 224	1.06	1.41	35	29	14.64	0.65	2.78	100	28.15	0
letter	(16	26	398)	8	44 304	82	28 991	68 148	1.97	3.31	8	8	6.91	0.24	1.61	70	2.48	30
magic	(10	2	381)	6	9840	84	29 530	66 776	0.51	1.84	6	4	2.13	0.07	0.14	99	0.91	1
mofn-3-7-10	(10	2	128)	6	8776	92	2926	8646	0.00	0.01	3	7	0.02	0.01	0.01	100	0.29	0
new-thyroid	(5	3	43)	5	1766	100	17 443	28 134	0.03	0.01	3	2	0.08	0.03	0.05	100	0.36	0
pendigits	(16	10	220)	6	12 004	95	30 522	59 922	2.40	1.32	10	6	4.11	0.14	0.94	96	3.68	4
phoneme	(5	2	540)	6	8962	82	21 899	49 840	0.09	0.07	3	2	0.22	0.05	0.09	98	0.37	2
ring	(20	2	740)	6	6188	89	19 114	42 362	0.27	0.44	11	9	1.25	0.05	0.25	92	7.25	8
segmentation	(19	7	42)	4	1966	90	21 288	35 381	0.11	0.17	8	10	0.53	0.11	0.31	100	4.13	0
shuttle	(9	7	1160)	3	1460	99	18 669	29 478	0.11	0.08	2	7	0.34	0.05	0.14	99	0.42	1
sonar	(60	2	42)	5	2614	88	9938	20 537	0.04	0.06	36	24	0.43	0.04	0.09	100	23.02	0
spambase	(57	2	442)	5	4614	92	13 055	28 284	0.07	0.06	18	37	0.50	0.05	0.11	100	6.18	0
spectf	(44	2	54)	5	2306	88	6707	13 449	0.07	0.06	20	24	0.34	0.02	0.07	100	8.12	0
texture	(40	11	550)	5	5724	87	34 293	64 187	0.79	0.63	23	17	3.24	0.19	0.93	100	28.13	0
threeOf9	(9	2	103)	3	920	100	2922	4710	0.00	0.00	1	8	0.01	0.00	0.01	100	0.14	0
twonorm	(20	2	740)	5	6266	94	21 198	46 901	0.08	0.08	12	8	0.28	0.06	0.10	100	5.73	0
vowel	(13	11	198)	6	10 176	90	44 523	88 696	1.66	2.11	8	5	4.52	0.15	1.15	66	1.67	34
waveform-21	(21	3	500)	5	6238	84	29 991	57 515	0.68	0.54	10	11	2.27	0.09	0.34	100	5.86	0
waveform-40	(40	3	500)	5	6232	83	30 438	58 380	0.50	0.86	15	25	7.07	0.11	0.88	100	11.93	0
wdbc	(30	2	114)	4	2028	96	7813	15 742	0.06	0.02	12	18	0.13	0.03	0.05	100	10.56	0
wine-recog	(13	3	72)	3	1188	97	17 718	28 421	0.04	0.04	5	8	0.13	0.04	0.07	100	1.46	0
wpbc	(33	2	78)	5	2432	76	9078	18 675	1.00	1.53	20	13	5.33	0.03	0.65	79	3.91	21
xd6	(9	2	172)	6	8288	100	2922	8394	0.00	0.00	3	6	0.02	0.01	0.01	100	0.57	0

Table 1: Performance evaluation of the RF explainability tool (RFxpl), and comparison with Anchor. The table shows results for 32 datasets, i.e. those for which test data accuracy is no less than 76%. Columns **#F**, **#C** and **#I** report, respectively, the number of features, classes and tested instances, in the dataset. Columns **D**, **#N** and **%A** show, respectively, each tree's max. depth, total number of nodes and test accuracy of an RF classifier. Columns **#var** and **#cl** show the number of variables and clauses of a CNF formula encoding an RF classifier along with any instance to analyze. Column **MxS** (resp. **MxU**) reports the maximum runtime of a SAT call (UNSAT call, resp.) and column **#S** (**#U**, resp.) reports the average number of SAT calls (resp. UNSAT calls) performed to extract an AXp. Column **avg** (**Mx** and **m**, resp.) shows the average (max. and min., resp.) runtime for extracting an explanation. The percentage of won instances is given as **%w**.

Example 2. *Consider again the RF $\mathfrak{F}$ of the running example and the instance $\mathbf{v} = (1, 0, 1, 70)$, giving the prediction Yes. Let us define the Boolean variables x_1, x_2 and x_3 associated with the binary features blocked-arteries, good-blood-circulation, chest-pain, resp. and variables w_1 and w_2 representing $(weight > 75)$ and $(weight \leq 75)$ resp. and an auxiliary variable w. Also, to represent the classes No and Yes, we associate variables denoting the classes for each tree: $\{l_{11}, l_{12}\}$ for $\mathcal{T}_1$, $\{l_{21}, l_{22}\}$ for $\mathcal{T}_2$ and $\{l_{31}, l_{32}\}$ for $\mathcal{T}_3$. Hence, the corresponding set of encoding constraints is: $\{x_1 \wedge x_3 \rightarrow l_{12}$, $x_1 \wedge \neg x_3 \rightarrow l_{11}$, $\neg x_1 \rightarrow l_{11}$, $x_2 \rightarrow l_{21}$, $\neg x_2 \wedge w \rightarrow l_{22}$, $\neg x_2 \wedge \neg w \rightarrow l_{21}$, $x_2 \wedge x_1 \rightarrow l_{32}$, $x_2 \wedge \neg x_1 \rightarrow l_{31}$, $\neg x_2 \wedge x_3 \rightarrow l_{32}$, $\neg x_2 \wedge \neg x_3 \rightarrow l_{31}$, $w \leftrightarrow w_1$, $\neg w \leftrightarrow w_2$, $(l_{11} + l_{21} + l_{31}) \geq 2$, x_1, $\neg x_2$, x_3, $w_2\}$. Observe that $\{x_1, \neg x_2, x_3, w_2\}$ denotes the set of the soft constraints whereas the remaining are the hard constraints.*

5 Experimental Results

This section assess the performance of our approach to compute PI-explanations (AXps) for RFs and also compares the results with an heuristic explaining model Anchor [Ribeiro *et al.*, 2018][10] The assessment is performed on a selection of 32 publicly available datasets, which originate from *UCI Machine Learning Repository* [Dua and Graff, 2017] and *Penn Machine Learning Benchmarks* [Olson *et al.*, 2017]. Benchmarks comprise binary and multidimensional classification datasets. The number of classes in the benchmark suite varies from 2 to 26. The number of features (resp. data samples) varies from 4 to 64 (106 to 58000, resp.) with the average being 21.9 (resp. 5131.09). When training RF classifiers for

[10]Anchor computes heuristic *local* explanations and not PI-explanations (AXp). Also, we do not consider other tools, such as LIME [Ribeiro *et al.*, 2016] or SHAP [Lundberg and Lee, 2017], as these learn a simpler ML model as an explanation and not a set of literals.

the selected datasets, we used 80% of the dataset instances (20% used for test data). For assessing explanation tools, we randomly picked fractions of the dataset, depending on the dataset size. Concretely, for datasets containing, resp., less than 200, 200–999, 1000–9999 and 10000 or more, we randomly picked, resp., 40%, 20%, 10% and 2% of the instances to analyze. The number of trees in each RF is set to 100 while tree depth varies between 3 and 8. (Note that we have tested other values for the number of trees ranging from 30 to 200, and we fixed it to 100 since with 100 trees RFs achieve the best train/test accuracies.) As a result, the accuracy of the trained models varies between 76% to 100%. We use the scikit-learn ML tool to train RF models. Note that, scikit-learn can only handle binary and ordinal features in the case of RFs. Accordingly, the experiments focus on binary and continuous data and do not include categorical features. In addition, we have overridden the implemented RF learner in sciki-learn so that it reflects the original algorithm described in [Breiman, 2001] [11]. Furthermore, PySAT [Ignatiev *et al.*, 2018] is used to instrument incremental SAT oracle calls.

The experiments are conducted on a MacBook Pro with a Dual-Core Intel Core i5 2.3GHz CPU with 8GByte RAM running macOS Catalina. Table 1 summarizes the results of assessing the performance of our RF explainer tool (`RFxpl`) on the selected datasets. (The table's caption also describes the meaning of each column.) As can be observed, and with three exceptions, the average running time of `RFxpl` is less than 1sec. per instance. In terms of the largest running times, there are a few outliers (this is to be expected since we are solving a D^P-hard problem), and these occur when the number of classes is large. To assess the scalability of `RFxpl`, we compared `RFxpl` with the well-known heuristic explainer Anchor [Ribeiro *et al.*, 2018]. (Clearly, the exercise does not aim to compare the explanation accuracies of Anchor and `RFxpl`, but only to assess how scalable it is in practice to solve a D^P-complete explainability problem with a propositional encoding and a SAT oracle.) Over all datasets, `RFxpl` outperforms Anchor on more than 96% of the instances (i.e. 8438 out of 8746). In terms of average running time per instance, `RFxpl` outperforms Anchor by more than 1 order of magnitude, concretely the average run time of Anchor is 14.22 times larger than the average runtime of `RFxpl`.

6 Conclusion

This paper proposes a novel approach for explaining random forests. First, the paper shows that it is D^P-complete to decide whether a set of literals is a PI-explanation (AXp) for a random forest. Second, the paper proposes a purely propositional encoding for computing PI-explanations (AXps) of random forests. The experimental results allow demonstrating that the proposed approach not only scales to realistically sized random forests, but it is also significantly more efficient that a state of the art model-agnostic heuristic approach. Given the practical interest in RFs [Zhou and Feng, 2017], finding AXps represents a promising new application area of SAT solvers.

Two extensions of the work can be envisioned. One extension is to improve further the propositional encoding proposed in this paper, aiming at eliminating the very few cases where heuristic approaches are more efficient. Another extension is to exploit the proposed model (and any of its future improvements) to explain deep random forests [Zhou and Feng, 2017].

[11] The RF model implemented by scikit-learn uses probability estimates to predict a class, whereas in the original proposal for RFs [Breiman, 2001], the prediction is based on majority vote.

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