Provably Precise, Succinct and Efficient Explanations for Decision Trees

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Abstract

Decision trees (DTs) embody interpretable classifiers. DTs have been advocated for deployment in high-risk applications, but also for explaining other complex classifiers. Nevertheless, recent work has demonstrated that predictions in DTs ought to be explained with rigorous approaches. Although rigorous explanations can be computed in polynomial time for DTs, their size may be beyond the cognitive limits of human decision makers. This paper investigates the computation of $\delta$-relevant sets for DTs. $\delta$-relevant sets denote explanations that are succinct and provably precise. These sets represent generalizations of rigorous explanations, which are precise with probability one, and so they enable trading off explanation size for precision. The paper proposes two logic encodings for computing smallest $\delta$-relevant sets for DTs. The paper further devises a polynomial-time algorithm for computing $\delta$-relevant sets which are not guaranteed to be subset-minimal, but for which the experiments show to be most often subset-minimal in practice. The experimental results also demonstrate the practical efficiency of computing smallest $\delta$-relevant sets.

1 Introduction

Decision trees (DTs) are widely regarded as epitomizing interpretable classifiers in machine learning (ML) [Breiman, 2001; Freitas, 2013; Molnar, 2020]. In a DT, a prediction is associated with a concrete tree path. Such a tree path is expected to be succinct given the number of features, and this is expected to be the case for sparse DTs. Moreover, recent work advocates using DTs (and other interpretable models) in high-risk applications [Rudin, 2019]\textsuperscript{1}, with the main justification being the interpretability of DTs. The perceived importance of DTs has also motivated a growing body of work on learning provably optimal and/or sparse DTs [Bertsimas and Dunn, 2017; Hu et al., 2019; Verhaeghe et al., 2020; Schidler and Szeider, 2021]. DTs have also been proposed for explaining more complex models, including LIME [Ribeiro et al., 2016] or SHAP [Lundberg and Lee, 2017], again due to being interpretable. Nevertheless, the interpretability of DTs has been disputed by recent work [Barceló et al., 2020; Audemard et al., 2021; Huang et al., 2021], concretely when interpretability equates with succinctness of explanations. The main observation, supported by experimental evidence, is that paths in DTs may not be as succinct as rigorously computed explanations. In turn, this implies that predictions of DT classifiers should also be explained. Although computing smallest rigorous explanations for DTs has been shown to be NP-hard [Barceló et al., 2020], it is also the case that a number of relevant queries on DTs has been shown to be tractable [Audemard et al., 2021], including the computation of subset-minimal rigorous explanations [Huang et al., 2021]. As a consequence, the computation of rigorous explanations for DTs was shown to be feasible in practice. Nevertheless, as shown by the experiments in this paper, explanations for DTs can also be too large, exceeding the cognitive limits of human decision makers [Miller, 1956]. One possible alternative is the computation of $\delta$-relevant sets, i.e. approximate explanations that offer strong probabilistic guarantees in terms of precision (i.e. measuring how good the explanation actually is given the function computed by the classifier). However, recent work [Waldchen et al., 2021] proved that, for a general class of classifiers, computing such approximate explanations is hard for $NP^{PP}$. This complexity result hints at the practical infeasibility of exactly computing approximate explanations that offer probabilistic guarantees in terms of precision. This paper shows that the problem is computationally easier in the concrete case of DTs, in theory and in practice.

This paper investigates the computation of approximate explanations that offer probabilistic guarantees in terms of precision, specifically for the concrete case of DTs. First, the paper shows that approximate explanations, which offer strong probabilistic guarantees but which are not guaranteed to be subset-minimal, can be computed in polynomial time. The paper then shows that the decision problem for approximate explanations with a size bound is in NP. This result in-
volves two encodings of the problem of computing a smallest approximate explanation into Satisfiability Modulo Theories (SMT), one involving non-linear arithmetic, and another involving linear arithmetic.

The experimental results demonstrate that computing smallest approximate explanations can be solved efficiently for large size DTs. More importantly, the experimental results suggest that, most often, the polynomial-time algorithm for computing approximate explanations yields explanations that are indeed subset-minimal, with negligible running times. The experimental results also compare the algorithms proposed in this paper, with the well-known model-agnostic explainer Anchor [Ribeiro et al., 2018]. The difference in the quality of computed explanations is conclusive, further validating prior evidence that model-agnostic explainers offer poor guarantees on the precision of computed explanations.

2 Preliminaries

Classification problems. This paper considers classification problems, which are defined on a set of features (or attributes) \( \mathcal{F} = \{1, \ldots, m\} \) and a set of classes \( \mathcal{K} = \{c_1, c_2, \ldots, c_k\} \). Each feature \( i \in \mathcal{F} \) takes values from a domain \( D_i \). In general, domains can be categorical or ordinal, with values that can be boolean, integer or real-valued. Feature space is defined as \( \mathbb{P} = D_1 \times D_2 \times \ldots \times D_m; |\mathbb{P}| \) represents the total number of points in \( \mathbb{P} \). For boolean domains, \( D_i = \{0, 1\}, i = 1, \ldots, m, \) and \( \mathbb{P} = \mathbb{B}^m \). The notation \( x = (x_1, \ldots, x_m) \) denotes an arbitrary point in feature space, where each \( x_i \) is a variable taking values from \( D_i \). The set of variables associated with features is \( \mathcal{X} = \{x_1, \ldots, x_m\} \). Moreover, the notation \( \nu = (v_1, \ldots, v_m) \) represents a specific point in feature space, where each \( v_i \) is a constant representing one concrete value from \( D_i \). An ML classifier \( \mathcal{M} \) is characterized by a (non-constant) classification function \( \kappa \) that maps feature space \( \mathbb{P} \) into the set of classes \( \mathcal{K} \), i.e. \( \kappa : \mathbb{P} \rightarrow \mathcal{K} \). An instance denotes a pair \((\nu, c)\), where \( \nu \in \mathbb{P} \) and \( c \in \mathcal{K} \), with \( c = \kappa(\nu) \).

Decision trees. A decision tree \( T = (V, E) \) is a directed acyclic graph, with \( V = \{1, \ldots, |V|\} \), having at most one path between every pair of nodes. \( T \) has a root node, characterized by having no incoming edges. All other nodes have one incoming edge. We consider univariate decision trees where each non-terminal node is associated with a single feature \( x_i \). Each edge is labeled with a literal, relating a feature (associated with the edge’s starting node) with some values (or range of values) from the feature’s domain. We will consider literals to be of the form \( x_i \in D_i \). \( x_i \) is a variable that denotes the value taken by feature \( i \), whereas \( D_i \subseteq D_i \) is a subset of the domain of feature \( i \) in \( T \). The type of literals used to label the edges of a DT allows the representation of the DTs generated by a wide range of decision tree learners (e.g. [Utgoff et al., 1997]). The set of paths of \( T \) is denoted by \( \mathcal{P} \). \( \Phi(R_k) \) denotes the set of features associated with path \( R_k \in \mathcal{P} \), one per node in the tree, with repetitions allowed. It is assumed that for any \( \nu \in \mathbb{P} \) there exists exactly one path in \( T \) that is consistent with \( \nu \). By consistent we mean that the literals associated with the path are satisfied (or consistent) with the feature values in \( \nu \).

Running example. Figure 1 shows the example DT used throughout the paper. This example DT also illustrates the

![Figure 1: Example DT](image_url)

The notation used to represent DTs. The set of paths \( \mathcal{P} \) is partitioned into two sets \( \mathcal{P} \) and \( \mathcal{Q} \), such that the paths in \( \mathcal{P} = \{p_1, p_2, p_3\} \) yield a prediction of 1, and such that the paths in \( \mathcal{Q} = \{q_1, q_2\} \) yield a prediction of 0. (In general, \( \mathcal{P} \) denotes the paths with prediction \( c \), and \( \mathcal{Q} \) denotes the paths with prediction other than \( c \), in \( \mathcal{K} \setminus \{c\} \).)

Formal explanations. We now define formal explanations. In contrast with the well-known model-agnostic approaches to XAI [Ribeiro et al., 2016; Lundberg and Lee, 2017; Ribeiro et al., 2018; Guidotti et al., 2019], formal explanations are model-precise, i.e. their definition reflects the model’s computed function. Prime implicant (PI) explanations [Shih et al., 2018] denote a minimal set of literals (relating a feature value \( x_i \) and a constant \( v_i \in D_i \)) that are sufficient for the prediction. PI-explanations are related with abduction, and so are also referred to as abductive explanations (AXp) [Ignatiev et al., 2019]. More recently, PI-explanations have been studied in terms of their computational complexity [Barcelò et al., 2020; Audemard et al., 2021]. Recent work on formal explanations includes for example [Mafra et al., 2021; Izza and Marques-Silva, 2021; Boumazouza et al., 2021].

Formally, given \( \nu = (v_1, \ldots, v_m) \in \mathbb{P} \) with \( \kappa(\nu) = c \), an AXp is any minimal subset \( \mathcal{X}' \subseteq \mathcal{F} \) such that,

\[
\forall (\nu \in \mathbb{P}). \left( \bigwedge_{i \in \mathcal{X}'} (x_i = v_i) \right) \rightarrow (\kappa(\nu) = c) \tag{1}
\]

i.e. the features in \( \mathcal{X}' \) are sufficient for the prediction when these take the values dictated by \( \nu \) and \( \mathcal{X}' \) is irreducible. Also, a non-minimal set such that (1) holds is a WeakAXp. AXp’s can be viewed as answering a ‘Why?’ question, i.e. why is some prediction made given some point in feature space. Contrastive explanations [Miller, 2019] offer a different view of explanations, but these are beyond the scope of the paper.

Example 1. The computation of WeakAXp’s and AXp’s is illustrated with the DT from Figure 1. The instance considered throughout is \( \nu = (v_1, v_2, v_3) = (4, 4, 2) \), with \( c = \kappa(\nu) = 1 \). The point \( \nu \) is consistent with \( P_2 \) and \( \Phi(P_3) = \{1, 2, 3\} \). Table 1 (columns 1 to 4) analyzes three sets of features \( \{1, 2, 3\}, \{1, 3\} \) and \( \{3\} \) in terms of being a WeakAXp or an AXp. The decision on whether each set is a WeakAXp or an AXp can be obtained by analyzing all the 32 points in feature space, or by using an off-the-shelf algorithm.

(Analysis of all points in feature space is omitted for brevity.)
Relevant sets. δ-relevant sets were proposed in more recent work [Wäldchen et al., 2021] as a generalized formalization of explanations. δ-relevant sets can be viewed as probabilistic Pls, with AXp’s representing 1-relevant sets, i.e. probabilistic Pls that are actual Pls. We briefly overview the definitions related with relevant sets. The assumptions regarding the probabilities of logical propositions are those made in earlier work [Wäldchen et al., 2021]. Let \( \text{Pr}_x(A(x)) \) denote the probability of some proposition \( A \) defined on the vector of variables \( x = (x_1, \ldots, x_m) \), i.e.

\[
\begin{align*}
\text{Pr}_x(A(x)) &= \frac{|\{x \in F : A(x) = 1\}|}{|\{x \in F : A(x) = 1\}|} \\
\text{Pr}_x(A(x) | B(x)) &= \frac{|\{x \in F : (A(x) = 1) \land B(x) = 1\}|}{|\{x \in F : B(x) = 1\}|}
\end{align*}
\] (2)

(Similar to earlier work, it is assumed that the features are independent and uniformly distributed [Wäldchen et al., 2021]. Moreover, the definitions above can be adapted in case some of the features are real-valued. To keep the notation simple, the paper studies only categorical and integer-valued features.)

Definition 1 (δ-relevant set [Wäldchen et al., 2021]). Consider \( \kappa : \mathbb{B}^m \to \mathcal{K} = \mathbb{B} \mathcal{V} \in \mathbb{B}^m \), \( \kappa(v) = c \in \mathbb{B} \), and \( \delta \in [0, 1] \). \( S \subseteq \mathcal{F} \) is a δ-relevant set for \( \kappa \) and \( v \) if,

\[
\text{Pr}_x(\kappa(x) = c | x_S = v_S) \geq \delta
\] (3)

(where the restriction of \( x \) to the variables with indices in \( S \) is represented by \( x_S = (x_i)_{i \in S} \)).

(Observe that \( \text{Pr}_x(\kappa(x) = c | x_S = v_S) \) is often referred to as the precision of \( S \) [Ribeiro et al., 2018; Narodytska et al., 2019].) Thus, a δ-relevant set represents a set of features which, if fixed to some pre-defined value (taken from a reference vector \( v \)), ensure that the probability of the prediction being the same as the one for \( v \) is no less than \( \delta \).

Definition 2 (Min-δ-relevant set). Given \( \kappa, v \in \mathbb{B}^m \), and \( \delta \in [0, 1] \), find the smallest \( k \), such that there exists \( S \subseteq \mathcal{F} \), with \(|S| = k\), and \( S \) is a δ-relevant set for \( \kappa \) and \( v \).

With the goal of proving the computational complexity of finding a minimum-size set of features that is a δ-relevant set, earlier work [Wäldchen et al., 2021] restricted the definition to the case where \( \kappa \) is represented as a boolean circuit.

Related work. Besides δ-relevant sets, there is work that also offers strong probabilistic guarantees by implicitly learning DTs [Blanc et al., 2021]. As argued in this and earlier work [Barceló et al., 2020; Huang et al., 2021; Audemard et al., 2021], learning a DT may not suffice to reveal logically sound explanations. There is work [Wang et al., 2021] that can be related with δ-relevant sets, but it opts instead for exploiting heuristic methods for computing explanations.

| \( S \) | \( \mathcal{U} \) | WeakAXp? | AXp? | \( \text{Pr}_x(\kappa(x) = c | x_S = v_S) \) | WeakPAXp? | PAXp? | \#(\( P_1 \)) | \#(\( P_2 \)) | \#(\( P_3 \)) | \#(\( Q_1 \)) | \#(\( Q_2 \)) |
|---|---|---|---|---|---|---|---|---|---|---|---|
| \( \{1, 2, 3\} \) | \emptyset | Yes | No | \( 1 \geq \delta \) | Yes | No | 1 | 0 | 0 | 1 | 0 | 0 |
| \( \{1, 3\} \) | \( \{2\} \) | Yes | Yes | \( 1 \geq \delta \) | Yes | No | 4 | 0 | 1 | 3 | 0 | 0 |
| \( \{3\} \) | \( \{1, 2\} \) | No | \( \geq 15/16, 0.9375 \geq \delta \) | Yes | Yes | 16 | 3 | 3 | 9 | 1 | 0 |

Table 1: Examples of sets of fixed features given \( v = (4, 2, 3) \) and \( \delta = 0.93 \)

3 δ-Relevant Sets for Decision Trees

Observe that Definition 2 imposes no restriction on the representation of the classifier that is assumed in earlier work [Wäldchen et al., 2021], i.e. the logical representation of \( \kappa \) need not be a boolean circuit. As a result, we extend Definition 2, as detailed below.

3.1 Generalizations

A weak probabilistic AXp (WeakPAXp) is a pick of fixed features for which the conditional probability of predicting the correct class \( c \) exceeds \( \delta \), given \( c = \kappa(v) \). (The classifier is only required to compute function \( \kappa \)). Thus, \( S \subseteq \mathcal{F} \) is a WeakPAXp if,

\[
\text{WeakPAXp}(S; \mathcal{F}, \kappa, v, \delta) := \text{Pr}_x(\kappa(x) = c | x_S = v_S) \geq \delta \] (4)

\[
:= \frac{|\{x \in F : \kappa(x) = c \land (x_S = v_S)\}|}{|\{x \in F : x_S = v_S\}|} \geq \delta
\]

which means that the fraction of the number of models predicting the target class and consistent with the fixed features (represented by \( S \)), given the total number of points in feature space consistent with the fixed features, must exceed \( \delta \). (Observe that the difference to (3) is solely that features and classes are no longer required to be boolean.) Moreover, a probabilistic AXp (PAXp) \( \mathcal{X} \) is a WeakPAXp that is also subset-minimal,

\[
\text{PAXp}(\mathcal{X}; \mathcal{F}, \kappa, v, \delta) := \begin{cases} 
\text{WeakPAXp}(\mathcal{X}; \mathcal{F}, \kappa, v, \delta) \land & (5) \\
\text{WeakPAXp}(\mathcal{X}'; \mathcal{F}, \kappa, v, \delta) \land \forall(\mathcal{X}' \subseteq \mathcal{X}) & (6)
\end{cases}
\]

Minimum-size PAXp’s (MinPAXp) generalize Min-δ-relevant sets in Definition 2.

Example 2. Table 1 summarizes the values of \( \text{Pr}_x(\kappa(x) = c | x_S = v_S) \) (column 5) for the sets \( \{1, 2, 3\} \), \{1, 3\} and \( \{3\} \). The table also includes information on whether each set is a WeakPAXp or a PAXp (columns 6 and 7).

We recall that the goal of our work is to efficiently compute precise and succinct explanations. However, in case of probabilistic AXp’s a critical observation is that WeakPAXP is a non-monotone predicate; hence standard algorithms for computing a subset-minimal set are not guaranteed to yield subset-minimal sets [Marques-Silva et al., 2017]. The results in Section 4 validate this observation.

3.2 Computing Path Probabilities

This section investigates how to compute, in the case of DTs, the conditional probability,

\[
\text{Pr}_x(\kappa(x) = c | x_{\mathcal{X}} = v_{\mathcal{X}})
\] (6)

where \( \mathcal{X} \) is a set of fixed features (whereas the other features are not fixed, being deemed universal), and (\( v, c \)) is an instance. (Also, note that (6) is the left-hand side of (3)). To
motivate the proposed approach, let us first analyze how can we compute \( \Pr_{\mathcal{X}}(\kappa(x) = c) \), where \( \mathcal{P} \subseteq \mathcal{R} \) is the set of paths in the DT with prediction \( c \). Let \( \Lambda(R_k) \) denote the set of literals (each of the form \( x_i \in \mathcal{E}_i \)) in path \( R_k \in \mathcal{R} \). If a feature \( i \) is tested multiple times along path \( R_k \), then \( \mathcal{E}_i \) is the intersection of the sets in each of the literals on \( i \). The number of values of \( \mathcal{D}_i \) consistent with literal \( x_i \in \mathcal{E}_i \) is \( |\mathcal{E}_i| \). Finally, the features not tested along \( R_k \) are denoted by \( \Psi(R_k) \). For path \( R_k \), the probability that a randomly chosen point in feature space is consistent with \( R_k \) (i.e. the path probability of \( R_k \)) is given by,

\[
\Pr(R_k) = \left[ \prod_{x_i \in \mathcal{E}_i \in \Lambda(R_k)} |\mathcal{E}_i| \right] / |\mathcal{P}|
\]

As a result, we get that,

\[
\Pr_{\mathcal{X}}(\kappa(x) = c) = \sum_{R_k \in \mathcal{P}} \Pr(R_k)
\]

Given an instance \( (v, c) \) and a set of fixed features \( \mathcal{X} \) (and so a set of universal features \( \mathcal{F} \setminus \mathcal{X} \)), we now detail how to compute (3). Since some features will now be declared universal, multipaths with possibly different conditions can become consistent. For example, in Figure 1 if feature 1 and 2 are declared universal, then (at least) paths \( P_1, P_2 \) and \( Q_1 \) are consistent with some of the possible assignments. Although universal variables might seem to complicate the computation of the conditional probability, this is not the case.

A key observation is that the feature values that make a path consistent are disjoint from the values that make other paths consistent. This observation allows us to compute the models consistent with each path and, as a result, to compute (3). Let \( n_{ik} \) represent the (integer) number of assignments to feature \( i \) that are consistent with path \( R_k \in \mathcal{R} \), given \( v \in \mathcal{F} \) and \( \mathcal{X} \subseteq \mathcal{F} \). The value of \( n_{ik} \) is defined as follows:

1. If \( i \) is fixed:
   
   a). If \( i \) is tested along \( R_k \) and the value of \( x_i \) is inconsistent with \( R_k \), i.e. there exists a literal \( x_i \in \mathcal{E}_i \) \( \in \Lambda(R_k) \) and \( \{v_i\} \cap \mathcal{E}_i = \emptyset \), then \( n_{ik} = 0 \);
   
   b). If \( i \) is tested along \( R_k \) and the value of \( x_i \) is consistent with \( R_k \), then \( n_{ik} = 1 \);
   
   c). If \( i \) is not tested along \( R_k \), then \( n_{ik} = 1 \).

2. Otherwise, \( i \) is universal:
   
   a). If \( i \) is tested along \( R_k \), with some literal \( x_i \in \mathcal{E}_i \), then \( n_{ik} = |\mathcal{E}_i| \);
   
   b). If \( i \) is not tested along \( R_k \), then \( n_{ik} = |\mathcal{D}_i| \).

Using the definition of \( n_{ik} \), we can then compute the number of assignments consistent with \( R_k \) as follows:

\[
\#(R_k; v, \mathcal{X}) = \prod_{x_i \in \mathcal{F} \setminus \mathcal{X}} n_{ik}
\]

Finally, (6) is given by,

\[
\Pr_{\mathcal{X}}(\kappa(x) = c | x_{\mathcal{X}} = v_{\mathcal{X}}) = \frac{\sum_{R_k \in \mathcal{P}} \#(R_k; v, \mathcal{X}) / \sum_{R_k \in \mathcal{R}} \#(R_k; v, \mathcal{X})}{\sum_{R_k \in \mathcal{R}} \#(R_k; v, \mathcal{X})}
\]

As can be concluded for the case of \( \mathcal{X} \), both \( \Pr_{\mathcal{X}}(\kappa(x) = c | x_{\mathcal{X}} = v_{\mathcal{X}}) \) and \( \text{WeakPAXp}(\mathcal{X}; \mathcal{F}, v, \kappa, \delta) \) are computed in polynomial time on the size of the DT.

**Example 3.** With respect to the DT in Figure 1, and given the instance \((4, 4, 2, 1)\), the number of models for each path is shown in Table 1. For example, for set \( \{3\} \), we immediately get that \( \Pr_{\mathcal{X}}(\kappa(x) = c | x_{\mathcal{X}} = v_{\mathcal{X}}) = \frac{1}{15/15+1} = 15/16 \).

3.3 Refining Weak \( \delta \)-Relevant Sets

Recent work showed that, for DTs, one AXP can be computed in polynomial time [Huang et al., 2021]. A simple polynomial-time algorithm can be summarized as follows. The AXP \( \mathcal{X} \) is initialized to all the features in \( \mathcal{F} \). Pick the path consistent with a given instance \((v, c)\). The features not in the path are removed from \( \mathcal{X} \). Then, iteratively check whether \( \mathcal{X} \setminus \{i\} \) guarantees that all paths to a prediction in \( \mathcal{K} \setminus \{c\} \) are still inconsistent. If so, then update \( \mathcal{X} \). We can use a similar approach for computing one approximate probabilistic AXP: an ApproxPAXp \( \mathcal{X} \) is a WeakPAXp such that the removal of any single feature \( i \) from \( \mathcal{X} \) will falsify WeakPAXp\((\mathcal{X} \setminus \{i\}; \mathcal{F}, v, c, \delta)\) (see (4)). To compute an ApproxPAXp, we start from \( \mathcal{F} \) and remove features while it is safe to do so, i.e. while (4) holds for the resulting set. The algorithm runs in polynomial time. Thus, by construction, the resulting ApproxPAXp is an over-approximation of a PAXp. However, due to non-monotonicity of WeakPAXp, an ApproxPAXp may not be subset-minimal and so not a PAXp.

3.4 Computing MinPAXp’s

For computing a smallest PAXp, we propose two SMT encodings, thus showing that the decision problem is in NP, and that finding a smallest set requires a logarithmic number of calls to an NP-oracle. Regarding the two SMT encodings, one involves the multiplication of integer variables, and so it involves non-linear arithmetic. Given the structure of the problem, we also show that linear arithmetic can be used, by proposing a (polynomially) larger encoding.

A multiplication-based SMT encoding. Taking into account the definition of path probabilities (see Section 3.2), we now devise a model that computes path probabilities based on the same ideas. Let \( n_{ijk} \) denote the number of elements in \( \mathcal{D}_j \) consistent with path \( R_k \) (for simplicity, we just use the path index \( k \)). If \( j \) is not tested along path \( R_k \), then if \( j \) is fixed, then \( n_{ijk} = 1 \). If not, then \( n_{ijk} = |\mathcal{D}_j| \). Otherwise, \( j \) is tested along path \( R_k \), \( n_{ijk} = 0 \) if \( j \) is fixed (i.e. \( u_j = 0 \)) and inconsistent with the values of \( \mathcal{D}_j \) allowed for path \( R_k \). \( n_{ijk} = 1 \) if \( j \) is fixed and consistent with the values of \( \mathcal{D}_j \) allowed for path \( R_k \). If \( j \) is not fixed (i.e. it is universal), the \( n_{ijk} \) denotes the number of domain values of \( j \) consistent with path \( R_k \). Let the fixed value of \( n_{jk} \) be \( n_{0jk} \) and the universal value of \( n_{jk} \) be \( n_{1jk} \). Thus, \( n_{jk} \) is defined as follows,

\[
n_{jk} = \text{ite}(u_j, n_{1jk}, n_{0jk})
\]

Moreover, let \( \eta_k \) denote the number of models of path \( R_k \). Then, \( \eta_k \) is defined as follows:

\[
\eta_k = \prod_{i \in \Psi(k)} n_{ik}
\]

If the domains are boolean, then we can use a purely boolean formulation for the problem. However, if the domains are multi-valued, then we need this formulation.

Recall what we must ensure that (4) holds true. In the case of DTs, since we can count the models associated with each path, depending on which features are fixed or not, then the previous constraint can be translated to:

\[
\sum_{R_k \in \mathcal{P}} \eta_k \geq \delta \times \sum_{R_k \in \mathcal{P}} \eta_k + \delta \times \sum_{R_k \in \mathcal{Q}} \eta_k
\]

Recall that \( \mathcal{P} \) are the paths with the matching prediction, and \( \mathcal{Q} \) are the rest of the paths.

Finally, the soft constraints are of the form \((u_i)\), one for each feature \( i \in \mathcal{F} \setminus \Psi(R_k) \). (For each \( i \in \Psi(R_k) \) we enforce that the feature is universal by adding a hard clause \((u_i)\).) The solution to the optimization problem will then be a smallest
| Feature | Attr. | $P_1$ | $P_2$ | $P_3$ | $Q_1$ | $Q_2$ |
|---------|-------|-------|-------|-------|-------|-------|
| 1       | $n_{01k}$ | 0     | 1     | 1     | 0     | 1     |
|         | $n_{11k}$ | 1     | 3     | 3     | 1     | 3     |
|         | $n_{1k}$ | $n_{1k} = \text{ite}(u_1, n_{11k}, n_{01k})$ |       |       |       |       |
| 2       | $n_{02k}$ | 1     | 0     | 1     | 0     | 1     |
|         | $n_{22k}$ | 3     | 3     | 1     | 3     | 1     |
|         | $n_{2k}$ | $n_{2k} = \text{ite}(u_2, n_{12k}, n_{02k})$ |       |       |       |       |
| 3       | $n_{03k}$ | 1     | 1     | 1     | 0     |       |
|         | $n_{33k}$ | 2     | 2     | 1     | 2     | 1     |
|         | $n_{3k}$ | $n_{3k} = \text{ite}(u_3, n_{13k}, n_{03k})$ |       |       |       |       |

Table 2: Concrete values for the multiplication-based encoding for the case $X = \{3\}$, i.e. $u_1 = u_2 = 1$ and $u_3 = 0$. We accept as well a PAXp. (The minimum-cost solution is well-known to be computed with a worst-case logarithmic number of calls (on the number of features) to an SMT solver.)

Example 4. For the running example, let us consider $X = \{3\}$. This means that $u_1 = u_2 = 1$. As a result, given the instance and the proposed encoding, we get Table 2 and Table 3. Finally, by plugging into (11) the values from Tables 2 and 3, we get: $15 \geq 0.93 \times (15 + 1)$. Thus, $\mathcal{X}$ is a WeakPAXp, and we can show that it is both a PAXp and a MinPAXp. Indeed, with $\mathcal{Y} = \emptyset$, we get $Pr_{\mathcal{X}}(v(x) = c | x_\mathcal{Y} = v_\mathcal{Y}) = 21/32 = 0.65625 < \delta$. Hence, $\mathcal{X} = \{3\}$ is subset-minimal. Since there can be no PAXp’s of smaller size, then $\mathcal{X}$ is also a MinPAXp.

An additional addition-based SMT encoding. A possible downside of the SMT encoding described above is the use of multiplication of variables in (10); this causes the SMT problem formulation to involve different theories (which may turn out to be harder to reason about in practice). Given the problem formulation, we can use an encoding that just uses linear arithmetic. This encoding is organized as follows. Let the domain of features be: $\{1, 2, \ldots, \mathcal{m}\}$. Define $n_{j,k}$ as the sum of models of path $R_k$ taking into account features $1$ up to $j$, with $n_{0,k} = 1$. Given $n_{j-1,k}, n_{j,k}$ is computed as follows:

- Let the domain of feature $j$ be $D_j = \{v_{j1}, \ldots, v_{jr}\}$, and let $s_{j,l,k}$ denote the number of models taking into account features $1$ up to $j - 1$ and domain values $v_{jl}$ up to $v_{j-1}$. Also, let $s_{j,0,k} = 0$.
- For each value $v_{jl}$ in $D_j$, for $l = 1, \ldots, r$:
  - If $j$ is not tested along path $R_k$: (i) If $v_{jl}$ is inconsistent with path $R_k$, then $s_{j,l,k} = s_{j,l-1,k}$; (ii) If $v_{jl}$ is consistent with path $R_k$ and with $v$, then $s_{j,l,k} = s_{j,l-1,k} + n_{j-1,k}$; (iii) If $v_{jl}$ is consistent with path $R_k$ but not with $v$, or if feature $j$ is not tested in path $R_k$, then $s_{j,l,k} = s_{j,l-1,k} + \text{ite}(u_j, n_{j-1,k}, 0)$.
  - Finally, define $n_{j,k} = s_{j,j,k}$.

If $j$ is not tested along path $R_k$: (i) If $v_{jl}$ is consistent with $v$, then $s_{j,l,k} = s_{j,l-1,k} + n_{j-1,k}$; (ii) Otherwise, $s_{j,l,k} = s_{j,l-1,k} + \text{ite}(u_j, n_{j-1,k}, 0)$.

After considering all the features in order, $n_{m,k}$ represents the number of models for path $R_k$ given the assignment to the $u_j$ variables. As a result, we can re-write (11) as follows:

$$\sum_{R_k \in \mathcal{P}} n_{m,k} \geq \delta \times \sum_{R_k \in \mathcal{P}} n_{jm,k} + \delta \times \sum_{R_k \in \mathcal{Q}} n_{jm,k}$$

(12)

As with the multiplication-based encoding, the soft clauses are of the form $(u_i) \in F$.

3.5 Deciding if an ApproxPAXp is a PAXp

Deciding whether a set of features $\mathcal{X}$, representing an ApproxPAXp, is subset-minimal can be achieved by using one of the models above, keeping the features that are already universal, and checking whether additional universal features can be made to exist. In addition, we need to add constraints forcing universal features to remain universal, and at least one of the currently fixed features to also become universal. Thus, if $X$ is the set of fixed features, the SMT models proposed in earlier sections is extended with the following constraints:

$$\bigwedge_{j \in \mathcal{X} \setminus \{u\}} (u_j) \land \left( \bigvee_{j \in \mathcal{X} \setminus \{u\}} (-u_j) \right)$$

(13)

which allow checking whether some set of fixed features can be declared universal while respecting the other constraints.

4 Experimental Results

This section evaluates the algorithms proposed for computing MinPAXp and ApproxPAXp. The evaluation includes a comparison with the model-agnostic explainer Anchor [Ribeiro et al., 2018], aiming at assessing not only the succinctness and precision of computed explanations but also the scalability of our solution.

Prototype implementation. A prototype implementation of the proposed algorithms is developed in Python; whenever necessary, it instruments oracle calls to well-known SMT solver z3 $^3$ [de Moura and Bjørner, 2008] as described in Section 3. Hence, the prototype implements the ApproxPAXp procedure outlined in Section 3.5 and augmented with a heuristic that orders the features in $\mathcal{X}$. The idea consists in computing the precision loss of the over-approximation of each $\mathcal{X} \setminus \{j\}$ and then sorting the features from the less to the most important one. This strategy often allows obtaining the closest superset to a PAXp, in contrast to the simple lexicographic order applied over $\mathcal{X}$. (Recall that $\mathcal{X}$ is initialized to the set of features involved in the decision path.) Algorithm MinPAXp outlined in Section 3.4 implements the two (multiplication- and addition-based) SMT encodings. Nevertheless, preliminary results show that both encodings perform similarly, with some exceptions where the addition-based encoding is much larger and slower. Therefore, the results reported below refer only to the multiplication-based encoding.

Experimental setup. The experiments are conducted on a MacBook Air with a 1.1GHz Quad-Core Intel Core i5 CPU with 16 Gbyte RAM running macOS Monterey. The benchmarks used in the experiments comprise publicly available

$^3$https://github.com/Z3Prover/z3/
Table 4: Assessing explanations of MinPAXp, ApproxPAXp, and Anchor. (For each dataset, we run the explainers on 500 samples randomly picked from the training data or all training samples if there are less than 500.) In column DT, N and A denote, resp., the number of nodes and the training accuracy of the DT. Column δ reports in (%) the value of the threshold δ. In column Path, avg (resp. M and m) denotes the average (resp. max. and min.) depth of paths consistent with the instances. In column Length, avg (resp. M and m) denotes the average (resp. max. and min.) length of the explanations; and F$_{gp}$avg denotes the avg. % of features in Anchors that do not belong to the consistent paths. Precision reports in (%) the average precision (defined in (3)) of resulting explanations. m$_\infty$ shows the number in (%) of ApproxPAXp’s that are subset-minimal, i.e. PAXp’s. Time reports (in seconds) the average runtime to compute an explanation. Finally, D indicates which distribution is applied on data given to Anchor: either data distribution (denoted by d) or uniform distribution (denoted by u).

| Dataset       | DT N A | Path M m avg | δ % | MinPAXp Length N m avg | Prec m avg | Time M m avg | ApproxPAXp Length N m avg | Prec m avg | Time M m avg | Anchor Length N m avg | Prec m avg | F$_{gp}$avg | Time M m avg |
|---------------|--------|--------------|-----|------------------------|-----------|--------------|--------------------------|-----------|--------------|----------------------|-----------|-----------|--------------|
| adult         | 1241   | 89 14 3 10.7 | 10 11 | 6.8 100 | 2.34 | 11 3 | 6.9 100 | 0.00 | 12 2 | 7.0 26.8 | 76.8 | 0.96 |
| dermatology   | 71     | 100 13 1 5.1 | 95 11 | 6.2 98.4 | 5.36 | 11 3 | 6.3 98.6 | 0.01 | 13 3 | 10.0 29.4 | 93.7 | 2.20 |
| kr-vs-kp      | 231    | 100 14 3 6.6 | 90 10 | 5.6 94.6 | 4.64 | 11 2 | 5.8 95.2 | 0.01 |
| letter        | 3261   | 93 14 4 11.8 | 100 12 | 4.4 100 | 0.35 | 12 1 | 4.4 100 | 0.00 | 31 0 | 1.0 58.1 | 32.9 | 3.10 |
| soybean       | 219    | 100 16 3 7.3 | 90 12 | 4.0 98.8 | 0.35 | 11 1 | 4.0 98.8 | 0.00 |
| spambase      | 141    | 99 14 3 8.5 | 90 12 | 3.2 95.4 | 0.92 | 10 2 | 3.3 95.4 | 0.00 |
| texture       | 257    | 100 13 3 6.6 | 90 12 | 3.9 98.1 | 0.97 | 11 2 | 4.0 98.1 | 0.00 |

Table: Assessing explanations of MinPAXp, ApproxPAXp, and Anchor. (For each dataset, we run the explainers on 500 samples randomly picked from the training data or all training samples if there are less than 500.) In column DT, N and A denote, resp., the number of nodes and the training accuracy of the DT. Column δ reports in (%) the value of the threshold δ. In column Path, avg (resp. M and m) denotes the average (resp. max. and min.) depth of paths consistent with the instances. In column Length, avg (resp. M and m) denotes the average (resp. max. and min.) length of the explanations; and F$_{gp}$avg denotes the avg. % of features in Anchors that do not belong to the consistent paths. Precision reports in (%) the average precision (defined in (3)) of resulting explanations. m$_\infty$ shows the number in (%) of ApproxPAXp’s that are subset-minimal, i.e. PAXp’s. Time reports (in seconds) the average runtime to compute an explanation. Finally, D indicates which distribution is applied on data given to Anchor: either data distribution (denoted by d) or uniform distribution (denoted by u).

and widely used datasets that originate from UCI ML Repository [UCI, 2020]. All the DTs are trained using the learning tool IAI (Interpretable AI) [Bertsimas and Dunn, 2017; IAI, 2020]. The maximum depth parameter in IAI is set to 16. As the baseline, we ran Anchor with the default explanation precision of 0.95. Two assessments are performed with Anchor: (i) with the original training data3 that follows the data distribution; (ii) with using sampled data that follows a uniform distribution. Our setup assumes that the training data is available. For the majority of tested instances across all datasets, noticeably shorter than consistent-path explanations. More importantly, the computed explanations are trustworthy and show good quality precision, e.g. dermatology, soybean and texture show avg. precisions greater than 98% for all values of δ. Additionally, the results clearly demonstrate that our proposed SMT encoding scales for deep DTs with runtimes on avg. less than 20 sec for the largest encodings while the runtimes of ApproxPAXp are negligible, never exceeding 0.01 sec. Also, observe that the lion’s share of over-approximations computed by ApproxPAXp are often subset-minimal PAXp’s, mostly as short as computed MinPAXp’s. This demonstrates empirically the advantage of the algorithm, i.e. in practice one may rely on the computation of ApproxPAXp’s, which pays off in terms of (1) performance, (2) sufficiently high probabilistic guarantees of precision, and (3) good quality over-approximation of subset-minimal PAXp’s. In contrast, Anchor is unable to provide precise and succinct explanations in both settings of data and uniform distribution. Moreover, we observe that Anchor’s explanations often include features that are not involved in the consistent path, e.g. for texture less than 20% of an explanation is shared with the consistent path. (This trend was also pointed out by [Ignatiev, 2020].) In terms of average runtime, Anchor is overall slower, being outperformed by the computation of ApproxPAXp by several orders of magnitude.

Focusing solely on large PAXp’s of size greater than 7, Table 5 reports the detailed results of ApproxPAXp and MinPAXp tested with probabilities δ ∈ {0.9, 0.95, 1.0}. (Note that these results are included in summarized results in Table 4 shown in the paper.) Hence, the purpose is to

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3The same training set used to learn the model.
Abductive explanations are guaranteed to be sufficient for computing provably succinct explanations when the instances to explain match very large tree paths and AXp’s are also large (exceeding the computational limits of human decision makers [Miller, 1956]). As can be seen from the table, both methods deliver shorter explanations, with allowing to drop a small threshold probability of the precision (i.e. $1 - \delta$). For example, the average size of computed PAXp’s in spambase decreases from 10 features to 5 features while respecting a precision greater than $0.95$.

Overall, the experiments demonstrate that our approach efficiently computes succinct and provably precise explanations for large DTs. The results also substantiate the limitations of model-agnostic explainers, both in terms of explanation quality and computation time.

### 5 Conclusions

Abductive explanations are guaranteed to be sufficient for the prediction while being subset-minimal [Shih et al., 2018; Ignatiev et al., 2019; Darwiche and Hirth, 2020]. However, the size of abductive explanations may be beyond the cognitive reach of human decision makers [Miller, 1956]. Recent work proposed $\delta$-relevant sets [Waldchen et al., 2021]. The downside of this earlier work is the practically prohibitive computational complexity of deciding whether a set of features is such an approximate explanation. Building on recent work on explaining decision trees [Barceló et al., 2020; Huang et al., 2021; Audemard et al., 2021], this paper shows that computing a smallest WeakPAXp (which generalizes smallest $\delta$-relevant sets) can be solved with a logarithmic number of calls to an NP oracle in the concrete case of DTs. Furthermore, the paper argues that existing algorithms for finding subset-minimal sets will yield tight over-approximations (ApproxPAXp’s) of subset-minimal sets when used for refining a given WeakPAXp. The experimental results demonstrate that the proposed SMT encodings scale in practice, and that the computation of ApproxPAXp’s most often yields WeakPAXp’s that are indeed subset-minimal, i.e. a PAXp. Furthermore, the paper offers additional evidence to the poor quality of explanations computed by state of the art model-agnostic explainers [Ribeiro et al., 2018].

### Acknowledgments

This work was supported by the AI Interdisciplinary Institute ANITI, funded by the French program “Investing for the Future – PIA3” under Grant agreement no. ANR-19-PI3A-0004, and by the H2020-ICT38 project COALA “Cognitive Assisted agile manufacturing for a Labor force supported by trustworthy Artificial intelligence”.

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