Logic-Based Explainability in Machine Learning

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Abstract. The last decade witnessed an ever-increasing stream of successes in Machine Learning (ML). These successes offer clear evidence that ML is bound to become pervasive in a wide range of practical uses, including many that directly affect humans. Unfortunately, the operation of the most successful ML models is incomprehensible for human decision makers. As a result, the use of ML models, especially in high-risk and safety-critical settings is not without concern. In recent years, there have been efforts on devising approaches for explaining ML models. Most of these efforts have focused on so-called model-agnostic approaches. However, all model-agnostic and related approaches offer no guarantees of rigor, hence being referred to as non-formal. For example, such non-formal explanations can be consistent with different predictions, which renders them useless in practice. This paper overviews the ongoing research efforts on computing rigorous model-based explanations of ML models; these being referred to as formal explanations. These efforts encompass a variety of topics, that include the actual definitions of explanations, the characterization of the complexity of computing explanations, the currently best logical encodings for reasoning about different ML models, and also how to make explanations interpretable for human decision makers, among others.

Keywords: Explainable AI · Formal explanations · Automated reasoning
# Table of Contents

1  Introduction .................................................. 4

2  Preliminaries .................................................. 8
   2.1 Logic Foundations ........................................ 8
       2.1.1 Propositional Logic & Boolean Satisfiability ........ 8
       2.1.2 First Order Logic .................................. 15
       2.1.3 Encodings & Interfacing Reasoners .................. 16
   2.2 Classification Problems .................................. 16
       2.2.1 Examples of Classifiers ............................. 17
       2.2.2 Running Examples ................................. 20
   2.3 Non-Formal Explanations ................................. 24

3  Formal Explainability ........................................ 26
   3.1 Abductive Explanations .................................. 26
   3.2 Contrastive Explanations ................................ 28
   3.3 Global Abductive Explanations & Counterexamples ....... 29
   3.4 Duality Results ......................................... 30
   3.5 Additional Notes ........................................ 31
   3.6 A Timeline for Formal Explainability .................. 33

4  Computing Explanations ...................................... 34
   4.1 Progress in Computing Explanations ...................... 34
   4.2 General Oracle-Based Approach ......................... 34
   4.3 Explaining Decision Lists ............................... 38
   4.4 From DLs to DTs & DSs .................................. 41
   4.5 Explaining Neural Networks ............................ 42
   4.6 Other Families of Classifiers .......................... 43
   4.7 An Alternative – Compilation-Based Approaches ....... 44

5  Tractable Explanations ....................................... 44
   5.1 Decision Trees ........................................... 44
   5.2 Monotonic Classifiers .................................... 48
   5.3 Other Families of Classifiers ........................... 49

6  Explainability Queries ........................................ 50
   6.1 Enumeration of Explanations ............................. 50
   6.2 Explanation Membership .................................. 52
   6.3 Additional Explainability Queries ....................... 54

7  Probabilistic Explanations .................................. 56
   7.1 Problem Formulation ....................................... 56
   7.2 Probabilistic Explanations for Decision Trees ........ 57
   7.3 Additional Results ........................................ 58
8  Input Constraints & Distributions ................................ 59
9  Formal Explanations with Surrogate Models ..................... 60
10  Additional Topics & Extensions .................................. 61
11  Future Research & Conclusions .................................. 62
   11.1  Research Directions ....................................... 63
   11.2  Concluding Remarks ....................................... 64
References ................................................................. 65
1 Introduction

Recent years witnessed remarkable advancements in artificial intelligence (AI), concretely in machine learning (ML) [49,143,217,222]. These advancements have triggered an ever-increasing range of practical applications [142]. Some of these applications often impact humans, with credit worthiness representing one such application, among many others [116]. Unfortunately, the most promising ML models are inscrutable in their operation, with the term black-box being often ascribed to such ML models. Black-box ML models cause distrust, especially when their operation is difficult to understand or it is even incorrect, not to mention situations where the operation of ML models is the likely cause for events with disastrous consequences [82,104,183], but also the case of unfairness and bias [292,334]. (The issues caused by AI systems are illustrated by an ever-increasing list of incidents [6,252].) Moreover, recent work argues [53] that Perrow’s framework of normal accidents [284] (which has been used to explain the occurrence of catastrophic accidents in the past) also applies to AI systems, thereby conjecturing that such (catastrophic) accident(s) in AI systems should be expected in the near future. Motivated by this state of affairs, but also by recent regulations and recommendations [115,156,277], and by existing proposals of regulation of AI/ML systems [7,116,338], there is a pressing need for building trust into the operation of ML models. The demand for clarifying the operation of black-box decision making has motivated the rapid growth of research in the general theme of explainable AI (XAI). XAI can be viewed as the process of aiding human decision makers to understand the decisions made by AI/ML systems, with the purpose of delivering trustworthy AI. The importance of both trustworthy AI and XAI is illustrated by recent guidelines, recommendations and regulations put forward by the European Union (EU), the United States government, the Australian government, the OECD and UNESCO [7,30,31,93,115–117,156,157,273,277,338], among others. Motivated by the above, there have been calls for the use of formal methods in the verification of systems of AI and ML [315], with explainability representing a key component [242]. There have also been efforts towards developing an understanding of past incidents in AI systems [251–253,285,360,361].

Well-known explainability approaches include so-called model-agnostic methods [235,301,302] and, for neural networks, approaches based on variants of saliency maps [263,309,322]. Unfortunately, the most popular XAI approaches proposed in recent years are marred by lack of rigor, and provide explanations that are often logically unsound [170,180,272]. (One illustrative example is that of an explanation consistent both with a declined bank loan application and with an approved bank loan application [242].) The drawbacks of these (non-formal) XAI approaches raise important concerns in settings that impact humans. Example settings include those referred to as high-risk and safety-critical\(^1\). The use

\(^1\) The definition of high-risk in this proposal is aligned with recent EU documentation [116]. Concrete examples include the management and operation of critical infrastructure, credit worthiness, law enforcement, among many others [116]. Some
of unsound explainability methods in either high-risk or safety-critical could evidently have catastrophic consequences. (And there are unfortunately too many examples of bugs having massive economic cost, or that resulted in the loss of lives [3, 39, 133, 223, 254, 311].)

A more recent alternative XAI approach offers formal guarantees of rigor, it is logic-based, and it is in most cases based on efficient automated reasoning tools. This document offers an overview of the advancements made in the general field of formal explainability in AI (FXAI).

A brief history of FXAI. The recent work on formal explainability in machine learning finds its roots in the independent efforts of two research teams [178, 320]. The initial goals of this earlier work seemed clear at the outset: to propose a formal alternative to the mostly informal approaches to explainability that were being investigated at the time. Nevertheless, the experimental results in these initial works also raised concerns about the practical applicability of formal explanations. However, it soon became clear that there was much more promise to formal explainability than what the original works anticipated. Indeed, we claim that it is now apparent that formal explainability represents an emerging field of research, and one of crucial importance. A stream of results in recent years amply support this claim [11–13, 19, 21, 22, 24–29, 38, 40, 59–61, 64, 65, 84, 85, 96–99, 101, 122, 145, 163–168, 170–172, 174, 177–180, 185, 186, 187, 189–192, 219, 232, 233, 237, 239, 240, 242, 272, 297, 298, 319–321, 354, 355, 362, 367, 368]. Among these, several results are significant. It has been shown that computing one explanation is tractable for a number of classifiers [84, 99, 165, 166, 186, 187, 239, 240]. Different duality results have been obtained [177, 179], which relate different kinds of explanations. Practically efficient logic encodings have been devised for computing explanations for a number of families of classifiers [28, 170, 172, 174, 180, 191]. Compilation approaches for explainability have been studied in a number of recent works [96, 97, 99, 101, 320, 321]. A number of computational complexity results, that cover the computation of one explanation but also other queries, have been proved [25, 166, 174, 191, 240]. Different explainability queries have been studied [25, 29, 166]. The size of formal explanations have been addressed by considering probabilistic explanations [22, 189, 190, 354, 355]. The effect of input constraints on explainability, that restrict the points in feature space to consider, has been studied in recent works [145, 367]. The use of surrogate models

authors refer to high-stakes when addressing related topics [304]. By safety-critical, we take the meaning that is common in formal methods [211], namely settings where errors are unacceptable, e.g. where human lives are at risk. There is growing interest in deploying ML-enabled systems in safety-critical applications (e.g. [91]).

It should be noted that efforts towards explaining the operation of systems of artificial intelligence (AI) can be traced back to at least the late 70s [331], with follow up work since then [14–16, 111, 118, 119, 128, 175, 283, 308, 313, 317, 332]. Nevertheless, the interest in formalizing explanations is documented in much earlier work [153]. A distinctive aspect of recent work is not only the focus on ML models, namely classifiers, but also the research on novel topics, e.g. contrastive and probabilistic explanations, which we will define later.
for computing formal explanations of complex models has been proposed [65]. Formal explanations have been applied in different application domains [237]. Furthermore, initial links between explainability and fairness, robustness and model learning have been uncovered [171, 179]. Given the above, the purpose of this document is to offer an account of what we feel have been the most important results in this novel field of research, up until the time of writing.

Main goals. The paper aims to offer a high-level comprehensive overview of the emerging field of formal explainability. The paper starts by covering existing formal definitions of explanations. One class of explanations answers a **Why?** question; these are referred to as abductive explanations. Another class of explanations answers a **Why not?** question; these are referred to as contrastive explanations. Then, the paper builds on the rigorous definitions of explanations to study how formal explanations can be computed in practice, highlighting some of the algorithms used. The paper uses running examples to illustrate how such explanations are computed in practice. Moreover, the paper also overviews families of classifiers for which computing one explanation is tractable. These include decision trees and naive bayes classifiers, among several others. Furthermore, the paper summarizes recent progress along a number of lines of research, which aim at making formal explainability a practical option of choice. Concrete examples of lines of research include: i) answering a growing number of explainability queries, e.g. enumeration of explanations; ii) computing probabilistic explanations, which trade-off explanation size for rigor; iii) taking into account input constraints and distributions, since not all inputs may be possible for an ML model; and also iv) approximating complex ML models with simpler models, which are easier to explain. The paper also overviews a number of additional topics of research in the general area of formal explainability. Since the paper aims at offering a broad overview of the field, some more technical aspects are omitted, and left to the existing references.

Additional goals. This document also takes the opportunity to deconstruct a number of misconceptions that pervade Machine Learning research. One unfortunately common misconception is that logic is inadequate for reasoning about ML models. This paper, but also a growing list of references (see above), offer ample evidence that this is certainly not the case. For example, formal explanations for random forests [191] were shown to be more efficient to compute than those obtained with heuristic methods. Another common misconception is that computationally hard (e.g. NP-hard, DP-hard, etc.) problems are intractable, and so large-scale problems cannot be solved in practice. By now, there are more than two decades of comprehensive experimental evidence that attests to the contrary [55, 131]. In many practical settings, automated reasoners are often (and sometimes most often) remarkably efficient at solving computationally hard problems of very large scale [131, 342, 343]. Boolean satisfiability (SAT) solvers (but also mixed integer linear programming (MILP) solvers) are prime examples of the progress that has been observed in improving, sometimes dramatically, the
practical efficiency of automated reasoners \cite{55,57,58,81,212}. The bottom line is that some of these computational problems may be intractable in theory, but in practice that is hardly ever the case \cite{131,343}. Another quite common misconception is the existence of so-called interpretable models, e.g., decision trees, lists and sets, but even linear classification models. For example, some of the best known model agnostic (and so non-formal) explainability approaches \cite{235,301} learn a simple interpretable model as the explanation for a more complex model. Some other authors propose the use of interpretable models as the explanation itself \cite{262,304,305}, specially in high-risk and safety-critical settings. There is by now comprehensive evidence \cite{166,174,186,187,239} that even these so-called interpretable models can provide explanations that are arbitrarily redundant. Therefore, even so-called interpretable models ought to be explained with the methods described in this paper\footnote{More importantly, the growing evidence on the need to explain “interpretable” models \cite{166,174,186,187,239} justifies wondering, in hindsight, about the practical relevance of learning (quasi-)optimal interpretable models \cite{4,5,10,17,18,32,33,43,51,52,78,105,136–138,161,162,173,181,196,220,228,238,255,271,275,276,280,306,312,314,318,346–349,352,353,356,358,365,366]. It should be clarified that SAT, MILP and SMT automated reasoners and their variants solve their target problems exactly, provided such reasoners are given enough time \cite{55,57,58,81,212}. Nevertheless, these automated reasoners should not be confused with the burgeoning field of exact exponential and parameterized algorithms \cite{90,125}. The former, i.e., automated reasoners, are without exception extensively validated and evaluated in practical settings, being applied to large-scale problem-solving \cite{55,81}; regarding the latter, decades of research have resulted in significant theoretical advances, but these have not been matched by practical impact.}\footnote{It should be clarified that SAT, MILP and SMT automated reasoners and their variants solve their target problems exactly, provided such reasoners are given enough time \cite{55,57,58,81,212}. Nevertheless, these automated reasoners should not be confused with the burgeoning field of exact exponential and parameterized algorithms \cite{90,125}. The former, i.e., automated reasoners, are without exception extensively validated and evaluated in practical settings, being applied to large-scale problem-solving \cite{55,81}; regarding the latter, decades of research have resulted in significant theoretical advances, but these have not been matched by practical impact.}

**Organization.** The paper is organized in two main parts. The first part introduces a number of well-established topics. Section 2 introduces the definitions and notation used throughout the paper. Section 3 introduces the formal definitions of explanations that have been studied in recent years. Based on the proposed definitions of explanations, Section 4 studies algorithms for the computation of explanations. In addition, as shown in Section 5, for some families of classifiers, there are polynomial-time algorithms for computing one explanation. The rest of the document covers the second part of the paper, and targets topics related with ongoing research. Thus, this second part is presented with less detail. Section 6 goes beyond computing one explanation, and delves into explainability queries, that include enumeration of explanations and deciding feature inclusion in explanations. Section 7 addresses the size of explanations, and proposes probabilistic explanations as a mechanism to reduce explanation size. Section 8 overviews approaches for accounting for input constraints and distributions. Section 9 overviews work on approximating complex ML models with surrogate (or distilled) simpler models, which are easier to explain. Section 10 summarizes a number of additional topics of research. Finally, Section 11 identifies some directions of research, and concludes the paper.
2 Preliminaries

Computational Complexity

The paper addresses a number of well-known classes of decision and function (or search) problems. For decision problems, these include P, NP, D^P, \Sigma^P_2, among others. For function problems, we will also consider standard classes, including FP, FNP, among others. (The interested reader is referred to a standard reference on computational complexity [23].)

2.1 Logic Foundations

Throughout this section, we adopt notation and definitions from standard references [45, 55, 66, 81, 87, 281].

2.1.1 Propositional Logic & Boolean Satisfiability. This section studies the decision problem for propositional logic, also referred to as the Boolean Satisfiability (SAT) problem [55]. (The presentation follows standard references, e.g. [55, 87, 210].) SAT is well-known to be an NP-complete [83] decision problem, with algorithm implementations that can be traced to the early 1960s [102, 103].

Syntax – well-formed propositional formulas. We consider a set of propositional atoms \( X = \{x_1, \ldots, x_n\} \) (these are also most often referred to as boolean variables), and associate an index with each atom, i.e. \( i \) with \( x_i \), \( i = 1, \ldots, n \), represented as the set \( X \). A (well-formed) propositional formula, or simply a formula, is defined inductively as follows:

1. An atom \( x_i \) is a formula.
2. If \( \varphi \) is a formula, then \( \neg \varphi \) is a formula. (The logic operator \( \neg \) is referred to as negation.)
3. If \( \varphi_1 \) and \( \varphi_2 \) are formulas, then \( \varphi_1 \lor \varphi_2 \) is a formula. (The logic operator \( \lor \) is referred to as disjunction.)
4. If \( \varphi \) is a formula, then \( (\varphi) \) is a formula.

A literal is an atom \( x_i \) or its negation \( \neg x_i \). We can use additional logic operators, defined in terms of the basic operators above. Well-known examples include:

1. \( \varphi_1 \land \varphi_2 \) represents the formula \( \neg (\neg \varphi_1 \lor \neg \varphi_2) \). (The logic operator \( \land \) is referred to as conjunction.)
2. \( \varphi_1 \rightarrow \varphi_2 \) represents the formula \( \neg \varphi_1 \lor \varphi_2 \). (The logic operator \( \rightarrow \) is referred to as implication.)
3. \( \varphi_1 \leftrightarrow \varphi_2 \) represents the formula \( (\varphi_1 \rightarrow \varphi_2) \land (\varphi_2 \rightarrow \varphi_1) \). (The logic operator \( \leftrightarrow \) is referred to as equivalence. Also, we use \( \rightarrow \) in the definition for simplicity, and could just use the initial logic operators.)

Parentheses are used to enforce precedence between operators. Otherwise, the precedence between operators is: \( \neg, \land, \lor, \rightarrow, \leftrightarrow \). A clause is a disjunction of literals. A term is a conjunction of literals. For both clauses and terms, we will disallow having either clauses or terms defined using an atom and its negation,
or repetition of literals. This is formalized as follows. Given $A, B \subseteq X$, with $A \cap B = \emptyset$, a clause is defined by,
\[
\omega_{A,B} \triangleq (\lor_{i \in A} x_i \lor \lor_{i \in B} \neg x_i)
\]
and a term is defined by,
\[
\tau_{A,B} \triangleq (\land_{i \in A} x_i \land \land_{i \in B} \neg x_i)
\]
when clear from the context, we will drop the subscript from $\omega_{A,B}$ and $\tau_{A,B}$.

\[\mathbb{W}\] denotes the set of all possible clauses defined on the set of atoms $X$. Similarly, $\mathbb{T}$ denotes the set of all possible terms defined on the set of atoms $X$. A conjunctive normal form (CNF) formula is a conjunction of clauses. A disjunctive normal form (DNF) formula is a disjunction of terms.

To simplify some of the subsequent definitions in this section, clauses and terms will also be viewed as sets of literals, each CNF formula as a set of clauses, and each DNF formula as a set of terms.

Semantics – assignments & valuations. An assignment is any point in $u \in \{0,1\}^n$. (Throughout, we associate 0 with both \textit{false} and $\bot$, and 1 with both \textit{true} and $\top$.) The actual value ascribed to a propositional formula is derived from the assignment of propositional values to the formula’s atoms. Each such complete assignment is referred to as an \textit{interpretation}. Given a formula $\varphi$, and an assignment $u \in \{0,1\}^n$, the valuation of $\varphi$ given $u$ is represented by $\varphi^u$, and it is defined inductively as follows:

1. $\varphi^u = 1$ if $\varphi = x_i$ and $u_i = 1$ or $\varphi = \neg x_i$ and $u_i = 0$.
2. $\varphi^u = 0$ if $\varphi = x_i$ and $u_i = 0$ or $\varphi = \neg x_i$ and $u_i = 1$.
3. $\varphi^u = \neg(\psi^u)$, if $\varphi = \neg\psi$.
4. $\varphi^u = \psi^u_1 \lor \psi^u_2$, if $\varphi = \psi_1 \lor \psi_2$.
5. $\varphi^u = (\psi^u)$, if $\varphi = (\psi)$.

Clearly, for any $u \in \{0,1\}^n$, $\varphi^u \in \{0,1\}$. Also, it is plain to extend the semantics to the other logic operators: $\land$, $\rightarrow$, $\leftrightarrow$. A propositional formula $\varphi$ can also be viewed as representing a boolean function that maps $\{0,1\}^n$ to $\{0,1\}$. The same symbol will be used to refer to both formula and function, i.e. $\varphi : \{0,1\}^n \rightarrow \{0,1\}$. Given some assignment $u \in \{0,1\}^n$, it is the case that $\varphi(u) = \varphi^u$.

Given a formula $\varphi$, $u \in \{0,1\}$ is a \textit{model} of $\varphi$ if it makes $\varphi$ \textit{true}, i.e. $\varphi^u = 1$. A formula $\varphi$ is \textit{satisfiable} or \textit{consistent} (represented by $\varphi \models \bot$) if it admits a model; otherwise, it is \textit{unsatisfiable} or \textit{inconsistent} (represented by $\varphi \nvdash \bot$).

Practical reasoners for the SAT problem represent a success story of Computer Science \[131,342\]. Modern conflict-driven clause learning (CDCL) SAT reasoners routinely decide formulas with millions of variables and tens of millions of clauses \[55, Chapter 4\]. (This success hinges on the paradigm of learning clauses from search conflicts \[247,248\].) Furthermore, SAT reasoners are the underlying engine used to achieve significant performance gains in different areas of automated reasoning, including different boolean optimization problems \[55, Chapters 23, 24, 28\], answer-set programming \[134\], constraint programming \[278\].
quantified boolean formulas [55, Chapters 30, 31], but also for reasoners for fragments of first order logic [55, Chapter 33] and theorem proving [132,213,214,351]. SAT reasoners are often publicly available and their performance improvements are regularly assessed\(^5\). There exist publicly available toolkits that streamline prototyping with SAT reasoners. At the time of writing, the reference example is PySAT [176].

It should be noted that the high performance reasoners mentioned above most often require logic formulas represented in CNF (or in clausal form). There are well-known, efficient, procedures for converting arbitrary (non-clausal) logic formulas into clausal form [286,336]. Given a propositional formula \(\varphi\), defined on a set of propositional atoms \(X\), \(\psi = \llbracket\varphi\rrbracket\) is the clausification of \(\varphi\), such that \(\psi\) is defined on a set of atoms \(X \cup A\), where \(A\) denotes additional auxiliary atoms.

One important result is that \(\varphi\) and \(\psi\) are equisatisfiable, i.e. \(\varphi\) is satisfiable iff \(\psi\) is satisfiable. Encodings are detailed further in Section 2.1.3.

Entailment and equivalence. Given two formulas \(\varphi\) and \(\tau\), we say that \(\tau\) entails \(\varphi\), denoted by \(\tau \models \varphi\), if,

\[
\forall (u \in \{0, 1\}^n). [\tau^u \rightarrow \varphi^u]
\]

which serves to indicate that any model of \(\tau\) is also a model of \(\varphi\). We say that \(\varphi_1 \equiv \varphi_2\) iff \(\varphi_1 \models \varphi_2\) and \(\varphi_2 \models \varphi_1\).

Let \(\tau_{A,B}\) and \(\tau_{C,D}\) be terms, with both \(A, B\) and \(C, D\) representing disjoint pairs of subsets of \(X\). Then, we have that,

**Proposition 1.** \(\tau_{A,B} \equiv \tau_{C,D}\) iff \(A = C\) and \(B = D\).

**Proposition 2.** If \(\tau_{A,B} \models \tau_{C,D}\) and \(\tau_{A,B} \not\equiv \tau_{C,D}\), then \(C \subseteq A\) and \(D \subseteq B\).

Clearly, similar results can be stated for clauses.

**Example 1.** The terms \(x_1 \land \neg x_2 \land x_3\) and \(x_1 \land \neg x_2\) are represented, respectively, by \(\tau_{A,B}\) and \(\tau_{C,D}\), with \(A = \{1, 3\}\), \(B = \{2\}\), \(C = \{1\}\) and \(D = \{2\}\). It is the case that \(x_1 \land \neg x_2 \land x_3 \models x_1 \land \neg x_2\). As can be concluded, \(C \subseteq A\) and \(D \subseteq B\).

Prime implicants and implicates. Let \(\varphi\) represent a propositional formula, and let \(\tau_{A,B}\) represent a term. \(\tau_{A,B}\) is a prime implicant of \(\varphi\) if,

1. \(\tau_{A,B} \models \varphi\).
2. For any other term \(\tau_{C,D}\), such that \(\tau_{A,B} \models \tau_{C,D}\) and \(\tau_{A,B} \not\equiv \tau_{C,D}\), then \(\tau_{C,D} \not\models \varphi\).

Whenever the first condition holds (i.e. \(\tau_{A,B} \models \varphi\)), then we say that \(\tau_{A,B}\) is an implicant of \(\varphi\).

\(^5\) http://www.satcompetition.org/.
Example 2. Consider the terms $\tau_{A,B} = x_1 \land x_2$ and $\tau_{C,D} = x_1$. (Note that $A = \{1, 2\}, B = \emptyset, C = \{1\}, D = \emptyset$.) Let $\varphi = (x_1 \land x_2 \land x_3) \lor (x_1 \land x_2 \land \neg x_3)$. Clearly, for any assignment $u \in \{0, 1\}^3$ to $x_1, x_2, x_3$, if $x_1 = x_2 = 1$, then $\tau_{A,B} = 1$ and also $\varphi = 1$, independently of the value of $x_3$. Hence, $\tau_{A,B} \models \varphi$. However, $\tau_{C,D} \not\models \varphi$, in that there are assignments $u$ to $x_1, x_2, x_3$ such that $\tau^{u}_{C,D} = 1$ but $\varphi^{u} = 0$. For example, whenever $x_2 = 0$, then $\varphi$ takes value 0, and that is not necessarily the case with $\tau_{C,D}$. Proving that $\tau_{A,B}$ is a prime implicant of $\varphi$ would apparently require proving that any term with literals that are a proper subset of $\tau_{A,B}$ are not implicants of $\varphi$. As discussed below, in practice one can devise more efficient algorithms.

For completeness, we also mention prime implicates. Let $\varphi$ be a propositional formula, and let $\omega_{A,B}$ be a clause. $\omega_{A,B}$ is a prime implicate of $\varphi$ if,

1. $\varphi \models \omega_{A,B}$.
2. For any other clause $\omega_{C,D}$, such that $\omega_{C,D} \models \omega_{A,B}$ and $\omega_{A,B} \not\models \omega_{C,D}$, then $\varphi \not\models \tau_{C,D}$.

Whenever the first condition holds (i.e. $\varphi \models \omega_{A,B}$), then we say that $\omega_{A,B}$ is an implicate of $\varphi$.

A well-known result (which can be traced to [307]) is that, for a propositional formula $\varphi$, prime implicants are minimal hitting sets (MHSes) of the prime implicates and vice-versa.\(^6\) This result is at the core of recent algorithms for enumerating prime implicants and implicates of a propositional formula $\varphi$ [288].

Given a propositional formula $\varphi$ and a term $\tau$, with $\tau \models \varphi$, a prime implicant $\pi$, with $\pi \models \pi$, can be computed with at most a linear number of calls to an NP oracle [67, 288, 337]. (The same observations apply to the case of prime implicates.) In Section 4, we will revisit some of these results when computing formal explanations.

**Reasoning about inconsistency.** In many situations, there is the need to reason about inconsistent formulas [246]. For example, we may be interested in explaining the reasons of inconsistency, but we may also be interested in identifying which clauses to ignore (or equivalently to remove from the formula) so as to restore consistency\(^7\). The general setting is to consider a set of clauses $\mathcal{B}$. $\mathcal{B}$ represents some background knowledge base, and so it is assumed to be consistent. We say that $\mathcal{B}$ contains the hard clauses (or in general the hard constraints). A clause is hard when it cannot be removed (from the set of clauses) to recover consistency. Furthermore, we also consider a set clauses $\mathcal{S}$, such that $\varphi_{B,S} = \mathcal{B} \cup \mathcal{S} \models \bot$, and $\varphi_{B,S}$ is the formula (or set of constraints) we want to reason about. The clauses in $\mathcal{S}$ represent the soft clauses (or constraints), and these can be removed to restore consistency. (In the rest of this document, we

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\(^6\) Recall that a set $\mathcal{H}$ is a hitting set of a set of sets $\mathcal{S} = \{S_1, \ldots, S_k\}$ if $\mathcal{H} \cap S_i \neq \emptyset$ for $i = 1, \ldots, k$. $\mathcal{H}$ is a minimal hitting set of $\mathcal{S}$, if $\mathcal{H}$ is a hitting set of $\mathcal{S}$, and there is no proper subset of $\mathcal{H}$ that is also a hitting set of $\mathcal{S}$.

\(^7\) This paragraph aims at brevity. However, there are recent up-to-date treatments of these topics [246].
will just refer to \( \varphi \), being implicit that \( \varphi \) is characterized by the background knowledge \( B \) and by the soft clauses \( S \).)

**Definition 1 (MUS).** Let \( \varphi = B \cup S \) be an inconsistent set of clauses (or constraints), i.e. \( \varphi \models \bot \). \( M \subseteq S \) is a Minimal Unsatisfiable Subset (MUS) if \( B \cup M \models \bot \) and \( \forall M' \subseteq M, B \cup M' \not\models \bot \).

Informally, an MUS provides some irreducible information that suffices to be added to the background knowledge \( B \) to attain an inconsistent formula; thus, an MUS represents an explanation for the causes of inconsistency. Alternatively, one might be interested in correcting the formula, removing some clauses to achieve consistency.

**Definition 2 (MCS).** Let \( \varphi = B \cup S \) be an inconsistent set of clauses (\( \varphi \models \bot \)). \( C \subseteq S \) is a Minimal Correction Subset (MCS) if \( B \cup S \setminus C \not\models \bot \) and \( \forall C' \subseteq C, B \cup S \setminus C' \models \bot \).

With each MCS \( C \), one associates a Maximal Satisfiable Subset (MSS), given by \( S \setminus C \).

**Example 3.** Let \( c_1 = (x_1), c_2 = (x_2), c_3 = (x_3), c_4 = (\neg x_1 \lor \neg x_2), \) and \( c_5 = (\neg x_1 \lor \neg x_3) \). Moreover, let \( \varphi = B \cup S \), with \( B = \{c_4, c_5\} \) and \( S = \{c_1, c_2, c_3\} \). Hence, it is simple to conclude that an example of an MUS is \( \{c_1, c_2\} \), an example of an MCS is \( \{c_1\} \), and an example of an MSS is \( \{c_2, c_3\} \).

Let \( \text{MUS} \), be a predicate, \( \text{MUS} : 2^S \to \{0, 1\} \), such that \( \text{MUS}(M) = 1 \) iff \( M \subseteq S \) is an MUS of \( \varphi = B \cup S \). Moreover, let \( \text{MCS} \), be a predicate, \( \text{MCS} : 2^S \to \{0, 1\} \), such that \( \text{MCS}(C) = 1 \) iff \( C \subseteq S \) is an MCS of \( \varphi = B \cup S \). Furthermore, we define,

\[
\text{MU}(\varphi) = \{ M \subseteq S \mid \text{MUS}(M) \} \\
\text{MC}(\varphi) = \{ C \subseteq S \mid \text{MCS}(C) \}
\]

Moreover, there exists a well-known (subset-)minimal hitting set relationship between MUSes and MCSes:

**Proposition 3.** Given \( \varphi = B \cup S \), and \( M \subseteq S, C \subseteq S \), then

1. \( M \) is an MUS iff it is a minimal hitting set of the MCSes in \( \text{MC} \);
2. \( C \) is an MCS iff it is a minimal hitting set of the MUSes in \( \text{MU} \).

The MHS relationship between MUSes and MCSes was first demonstrated in the context of model-based diagnosis [300] and later investigated for propositional formulas in clausal form [56]. As immediate from the original work [300], the MHS relationship applies in general to systems of constraints, where each is represented as a first-order logic statement.

**Example 4.** For the formula from Example 3, it is immediate to conclude that,

\[
\text{MU}(\varphi) = \{ \{c_1, c_2\}, \{c_1, c_3\} \} \\
\text{MC}(\varphi) = \{ \{c_1\}, \{c_2, c_3\} \}
\]

Moreover, one can observe that each MUS is an MHS of the MCSes, and that each MCS is an MHS of the MUSes.
Complexity-wise, deciding whether a set of clauses is an MUS is known to be $D^p$-complete [281, 282]. It is also well-known that an MUS can be computed with at most a number of calls to an NP-oracle that grows linearly with the number of clauses in the worst-case [79]. MUSes and MCSes are tightly related with optimization problems [246]. For example, if each soft constraint is assigned a unit cost, then solving the maximum satisfiability problem (MaxSAT) corresponds to finding a maximum cost MSS [55, 264]. Under the assumption of a unit cost assigned to each clause, then an MCS can be computed with a logarithmic number of calls to an NP-oracle, e.g. by solving (unweighted) MaxSAT. (If non-unit costs are assumed, then a worst-case linear number of calls to an NP-oracle is required.) However, in practice there are more efficient algorithms that may require in the worst-case a number of calls to an NP-oracle larger than logarithmic [241, 256, 257]. There have been very significant improvements in the practical performance of MaxSAT solvers in recent years [55, Chapters 23, 24, 28]. A number of solvers for MaxSAT and related problems are publicly available [8, https://maxsat-evaluations.github.io/ and http://www.cril.univ-artois.fr/PB16/http://www.satcompetition.org/2011/ (MUS track)].

Quantification problems. It is often of interest to quantify some of the variables in a propositional formula (by default it is assumed that all variables are existentially quantified). This is achieved by using two more logic operators, namely $\forall$ for universal quantification and $\exists$ for existential quantification. QBF (Quantified Boolean Formulas) is the problem of deciding whether a quantified propositional formula is true or false. The problem of deciding QBF is PSPACE-complete [23]. In this paper, we will briefly study quantified problems with two levels of quantifier alternation, concretely $\exists\forall$, which is a well-known $\Sigma_2^p$-complete decision problem. There have been very significant improvements in the practical performance of QBF solvers in recent years [55, Chapters 30, 31]. A number of solvers for QBF are publicly available [9, http://www.qbflib.org/].

Logic-based abduction. Abductive reasoning can be traced to the work of C. Peirce [152], with its first uses in artificial intelligence in the early 1970s [266, 287]. Logic-based abduction can be viewed as the problem of finding a (minimum or minimal) subset of hypotheses, which is consistent with some background theory, and such that those hypotheses are sufficient for some manifestation. A propositional abduction problem (PAP) is represented by a 5-tuple $P = (X, H, M, T, \varsigma)$ [175, 308]. $X$ is a finite set of atoms. $H$, $M$ and $T$ denote propositional formulas representing, respectively, the set of hypotheses, the set of manifestations, and the background theory. ($H$ is further constrained to be a set of clauses.) $\varsigma$ is a function that associates a cost with each clause of $H$, $\varsigma : H \to \mathbb{R}_+^*$. Given the background theory $T$, a set $E \subseteq H$ of hypotheses is an explanation (for the manifestations) if: (i) $E$ entails the manifestations $M$ (given $T$), i.e. $T \land E \models M$; and (ii) $E$ is consistent (given $T$), i.e. $T \land E \not\models \bot$.

\[\begin{align*}
8 & \text{https://maxsat-evaluations.github.io/ and http://www.cril.univ-artois.fr/PB16/}
\text{http://www.satcompetition.org/2011/ (MUS track).}
9 & \text{http://www.qbflib.org/}.
\end{align*}\]
The propositional abduction problem is usually defined as computing a minimum cost (or cardinality minimal) explanation for the manifestations subject to the background theory. Moreover, one can consider explanations of (subset-)minimal cost. The complexity of logic-based abduction has been studied in the past [73, 111]. There are also recent practical algorithms for propositional abduction [175, 308].

The computation of a prime implicant of some propositional formula \( \varphi \), defined on atoms \( X \), can be formulated as a problem of abduction. Let \( u \) be an assignment to the atoms of \( \varphi \), such that \( \varphi^u = 1 \). Given \( u \), construct the set \( \mathcal{H} \) of hypotheses as follows: if \( u_i = 1 \), then add \( x_i \) to \( \mathcal{H} \), otherwise add \( \neg x_i \) to \( \mathcal{H} \). We let \( \mathcal{T} = \emptyset \) and \( M = \varphi \). Given the definition of \( \mathcal{H} \), then a (subset-)minimal set \( \mathcal{E} \subseteq \mathcal{H} \) is a prime implicant if, (i) \( \mathcal{E} \models \varphi \); and (ii) \( \mathcal{E} \not\models \bot \). Observe that, by hypothesis, condition (ii) is trivially satisfied. Hence, a prime implicant of \( \varphi \) (given \( \mathcal{H} \)) is a subset-minimal set of literals \( \mathcal{E} \subseteq \mathcal{H} \) such that \( \mathcal{E} \models \varphi \).

In practice, when \( \varphi \) is non-clausal, deciding entailment is somewhat more complicated. In these cases, and as mentioned earlier, most often one needs to clausify \( \varphi \), so that it can be reasoned about. A difficulty with efficient clausification procedures is that these introduce auxiliary variables. As a result, we need to follow a different approach for computing a prime implicant.

Let \( \psi = [\varphi]_V \) be the propositional clausal representation of \( \varphi \), given some logic theory \( V \), which uses additional auxiliary atoms represented as set \( A \). (Section 2.1.3 details further the use of logic encodings.) We distinguish an auxiliary propositional atom \( t \in A \), such that \( t = 1 \) for the assignments to \( X \) and \( A \) which satisfy \( \psi \) (and so \( \varphi \)). In this new setting, we let \( \mathcal{T} = \psi \) and \( M = (t) \). Given a (consistent) set of literals \( \mathcal{H} \), representing a satisfying assignment to the atoms of \( \varphi \), then a (subset-)minimal set \( \mathcal{E} \subseteq \mathcal{H} \) is a prime implicant if, (i) \( \psi \land \mathcal{E} \models t \); and (ii) \( \mathcal{E} \not\models \bot \). As before, condition (ii) is trivially satisfied. Hence, a prime implicant of \( \varphi \) (given \( \mathcal{H} \)) is a subset-minimal set of literals \( \mathcal{E} \subseteq \mathcal{H} \) such that \( \psi \land \mathcal{E} \models t \).

Propositional Languages. A propositional language represents a subset of the set of propositional formulas, and several such subsets have been extensively studied [94, 95, 100]. One well-known example is negation normal form (NNF), representing a directed-acyclic graph of \( \land \) and \( \lor \) operators, where the leaves are atomic propositions or their negation. Other well-known examples are DNF and CNF formulas. By imposing additional constraints on the \( \lor \) and \( \land \) nodes of NNF formulas, one can devise classes of propositional languages that exhibit important tractability properties. A detailed analysis of propositional languages is available in [100]. Some results on formal explainability have been derived for propositional languages in recent years [25, 29, 97, 165, 320].

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10 For brevity, we will not delve into defining propositional languages and queries/transformations of interest. The interested reader is referred to the bibliography [100].
2.1.2 First Order Logic. This section briefly mentions one well-known extension of propositional logic, namely first order logic (FOL). FOL extends propositional logic with predicates, functions, constants and quantifiers, and such that variables are allowed to take values from arbitrary domains. In contrast with propositional logic, where an interpretation is an assignment of values to the formula’s atoms, in the case of FOL, an interpretation must ascribe a meaning to predicates, functions and constants. Whereas validity in FOL is undecidable [45], one can reason in concrete theories, with a well-known example being satisfiability modulo theories.

Satisfiability modulo theories (SMT). By providing first order logic with concrete theories, e.g. integer arithmetic, real arithmetic or mixed integer-real arithmetic, among many other possibilities, one obtains decidable fragments, for which practically efficient reasoners have been developed over the last two decades. (There exist undecidable theories in SMT [218], but that is beyond the goals of this document. SMT solvers generalize SAT to reason with fragments of first order logic [55, 81, 218]. Throughout this paper, we will use SMT reasoners solely as an alternative for mixed-integer linear programming reasoners (see below), even though SMT reasoners allow for significantly more general fragments of FOL. Similar to the case of SAT, we can solve optimization problems over SMT formulas (MaxSMT), and we can also reason about inconsistency. Previous definitions (see Section 2.1.1) also apply in this setting.

Mixed integer linear programming (MILP). MILP can be formulated as a first-order logic theory (e.g. [66], where variables can take values from boolean, integer and real domains, and where the allowed binary functions are + and −, with their usual meanings, and the allowed binary predicates are = and ≤, also with their usual meanings. We will also allow a countable number of unary constant functions $b$, with $b \in \mathbb{R}$ (thus accounting for the other possible cases of $\mathbb{B}$ and $\mathbb{Z}$), and where each $b$ represents a coefficient. Starting from a set $V$ of (variable) numbers, i.e. $V = \{1, \ldots, m\}$, we consider a partition of $V$ into $B$, $I$ and $R$. The general MILP formulation is thus:

\[
\begin{align*}
\min & \quad \sum_{j=1}^{n} c_j x_j \\
\text{s.t.} & \quad \sum_{j=1}^{n} a_{ij} x_j \leq b_i, \, i = 1, \ldots, r \\
& \quad x_j \in \{0, 1\}, \, j \in B \\
& \quad x_j \in \mathbb{Z}, \, j \in I \\
& \quad x_j \in \mathbb{R}, \, j \in R \\
& \quad a_{ij}, b_i \in \mathbb{R}
\end{align*}
\]

Several proprietary and publicly available MILP solvers are available\(^\text{11}\), with significant performance gains reported over the years [57, 58, 212].

\(^{11}\) For example, https://www.ibm.com/ae-en/analytics/cplex-optimizer, https://www.gurobi.com/, https://sourceforge.net/projects/lpsolve/.
**Additional definitions.** The definitions introduced in the propositional logic case can be generalized to the case of FOL, SMT, MILP, etc. These generalizations include entailment, prime implicants and implicants, but also the definitions associated with reasoning about inconsistency. A discussion of some of these concepts beyond propositional logic is available for example in [246].

### 2.1.3 Encodings & Interfacing Reasoners.

Throughout the document, we will extensively refer to SAT, SMT and MILP reasoners. Consistency checking with a reasoner for theory $T$ on a $T$-theory formula $\varphi_T$ is represented by $\text{CO}(\varphi_T; T)$, and denotes whether $\varphi_T$ has at least one model (given $T$), i.e. an interpretation that satisfies $\varphi_T$. For simplicity, the parameterization on $T$ is omitted, and so we use $\text{CO}(\varphi_T)$ instead. These theory reasoners operate on formulas of a suitable logic language. Given some logic formula $\varphi$, $\llbracket \varphi \rrbracket_T$ denotes the encoding of $\varphi$ in a representation suitable for reasoning by a decision oracle for theory $T$. (For simplicity, we just use $\llbracket \varphi \rrbracket$.) As shown below, the computation of formal explanations assumes the existence of a reasoner that decides the satisfiability (or consistency) of a statement expressed in theory $T$.

For the case of propositional theories, SAT reasoners most often work with clausal representations. As noted earlier, there exist procedures for converting arbitrary (non-clausal) logic formulas into clausal form [286, 336], which require the use of additional propositional atoms. There are also well-known encodings of constraints into clausal form [55, Chapters 02, 28]. Examples include cardinality constraints, e.g. AtMost$K$ (i.e. $\sum_i x_i \leq K$, with boolean $x_i$) or AtLeast$K$ (i.e. $\sum_i x_i \geq k$, with boolean $x_i$) constraints, and pseudo-boolean constraints ($\sum_i a_i x_i \leq b$, also with boolean $x_i$), among many others.

### 2.2 Classification Problems

Classification problems in ML 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 or integer. (Although real-valued could be considered for some of the classifiers studied in the paper, we opt not to specifically address real-valued features.) The set of domains is represented by $\mathcal{D} = (D_1, \ldots, D_m)$. Feature space is defined as $\mathcal{F} = D_1 \times D_2 \times \ldots \times D_m$; $|\mathcal{F}|$ represents the total number of points in $\mathcal{F}$. For boolean domains, $D_i = \{0, 1\} = \mathcal{B}$, $i = 1, \ldots, m$, and $\mathcal{F} = \mathcal{B}^m$. 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 $X = \{x_1, \ldots, x_m\}$. Moreover, the notation $v = (v_1, \ldots, v_m)$ represents a specific point in feature space, where each $v_i$ is a constant representing one concrete value from $D_i$. With respect to the set of classes $\mathcal{K}$, the size of $\mathcal{K}$ is assumed to be finite; no additional restrictions are imposed on $\mathcal{K}$. Nevertheless, with the goal of simplicity, the paper considers examples where $|\mathcal{K}| = 2$, concretely $\mathcal{K} = \{0, 1\}$, or alternatively $\mathcal{K} = \{\bot, \top\}$.

An ML classifier $\mathcal{M}$ is characterized by a (non-constant) classification function.
\( \kappa \) that maps feature space \( \mathcal{F} \) into the set of classes \( \mathcal{K} \), i.e. \( \kappa : \mathcal{F} \rightarrow \mathcal{K} \). Each classifier \( \mathcal{M} \) is represented unambiguously by the tuple \( (\mathcal{F}, \mathcal{D}, \mathcal{F}, \mathcal{K}, \kappa) \). (With a mild abuse of notation, we also write \( \mathcal{M} = (\mathcal{F}, \mathcal{D}, \mathcal{F}, \mathcal{K}, \kappa) \).) An instance (or observation) denotes a pair \((v, c)\), where \( v \in \mathcal{F} \) and \( c \in \mathcal{K} \), with \( c = \kappa(v) \).

The classifier decision problem (CDP) is to decide whether the logic statement \( \exists (x \in \mathcal{F}).(\kappa(x) = c) \), for \( c \in \mathcal{K} \), is true. Given some target class \( c \in \mathcal{K} \), the goal of CDP is to decide whether there exists some point \( x \) in feature space for which the prediction is \( c \). For example, for a neural network or a random forest, it is easy to prove that CDP is NP-complete. In contrast, for univariate decision trees, CDP is in P. This is further discussed in the next section.

### 2.2.1 Examples of Classifiers.

This paper studies decision trees (DTs), decision sets (DSs) and decision lists (DLs) in greater detail. Nevertheless, formal explainability has been studied in the context of several other well-known families of classifiers, including naive bayes classifiers (NBCs) [239], decision diagrams and graphs [166], tree ensembles [170,172,180,191], monotonic classifiers [84,240], neural networks [178], and bayesian network classifiers [320,321]. Additional information can be found in the cited references.

#### Decision trees (DTs).

DTs are among the still most widely used family of classifiers, with applications in both ML and data mining (DM) [70,124,293,294,363]. A decision tree is a directed acyclic graph, with one root node that has no incoming edges, and the remaining nodes having exactly one incoming edge. Terminal nodes have no outgoing edges, and non-terminal nodes have two or more outgoing edges. Each terminal node is associated with a class, i.e. the predicted class for the node. Each non-terminal node is associated with exactly one feature\(^{12}\). Each outgoing edge is associated with a literal defined using the values of the feature, and such that any value of the feature domain is consistent with exactly one of the literals of the outgoing edges. A tree path \( P \) connects the root node with one of the tree’s terminal nodes. Common (implicit) assumptions of DTs are that: (i) all paths in a DT are consistent; and (ii) for each point \( v \) in feature space, there exists exactly one path \( P \) that is consistent with \( v \). (Observe that (ii) requires that the branches at each node capture all values in the domain of the tested feature and that the branches’ conditions be mutually disjoint.) Given these assumptions of DTs, it is easy to see that CDP is in P.

One simply picks the target class and a terminal node predicting the class, and reconstructs the path to the root; a procedure that runs in linear time on the size of the tree. An example of a DT is shown in Figure 2a. (This example will be analyzed in greater detail below.)

\(^{12}\) Thus, this paper only considers univariate DTs, for which where each non-terminal node test a single feature. In contrast, for multivariable DTs [71], we assume that each non-terminal node can test arbitrary functions of the features. For ordinal features, multivariate DTs are also referred to as oblique [267].
Decision lists (DLs) and sets (DSs). DLs and DSs also find a wide range of applications [17, 18, 80, 124, 220]. DLs and DSs represent, respectively, ordered and unordered rule sets. There exist in-depth studies of DLs [303], but in contrast DSs are less well-understood. Each rule is of the form:

\[ R_j: \text{IF} \ (\tau_j) \ \text{THEN} \ d_j \]

where \( \tau_j \) represents a boolean expression defined on the features and their domains, and \( d_j \in K \). We say that the rule fires if its literal \( \tau_j \) is consistent (or holds true). For DLs, and with the exception of the first rule, all other rules are of the form:

\[ R_l: \text{ELSE IF} \ (\tau_l) \ \text{THEN} \ d_l \]

For the last (default) rule, it is required that \( \tau_l \) is a tautology, i.e. the rule always fires if all others do not. (This basically corresponds to solely having ELSE as the rule’s condition.) The default rule is marked as \( R_{\text{def}} \). An example of a DL is shown in Figure 1a. An example of a DS would be the same DL, but without the ELSE’s, i.e. there would be no order among the listed rules. (The DL example will be analyzed in greater detail below.) In contrast with DLs, the lack of order of rules in DSs raises a number of issues [181]. One issue is overlap, i.e. two or more rules predicting different classes may fire on the same point of feature space. A second issue is coverage, i.e. without a default rule, it may happen that no rule fires on some points of feature space. It is conjectured that is is \( \Sigma_2^p \)-hard to learn DSs that ensure both no overlap and ensuring coverage of all points in feature space [181].

Neural networks (NNs). We consider a simple architecture for an NN, concretely feed-forward NNs, which we refer to as NNs. (A comprehensive treatment of NNs can be found elsewhere [142].) An NN is composed of a number of layers of neurons. The output values of the neurons in a given layer \( x^l \) are computed given the output values of the neurons in the previous layer \( x^{l-1} \), up to a number \( L \) of layers, and such that the inputs represent layer 0. Furthermore, each neuron computes an intermediate value given the output values of the neurons in the previous layer, and the weights of the connections between layers. For each layer, the intermediate computed values are represented by \( y^l \). The output value of each neuron is the result of applying a non-linear activation function on the values of \( y^l \), thus obtaining \( x^l \). Assuming a ReLU [269] activation function, one obtained the following:

\[
\begin{align*}
y^l &= A^l \cdot (x^{l-1})^T \\
x^l &= \max(y^l, 0)
\end{align*}
\]

where \( x^0 \) denote the input values, \( x^L \) denotes the output values, and \( A^l \) denotes the weights matrix (that also accounts for a possible bias vector, by including a variable \( x^{l-1}_0 = 1 \)). For classification problems, there are different mechanisms to predict the actual class associated with the computed output values. One option is to have each output represent a class. Another option is to pick the class
depending on the range of values taken by the output variable. This alternative is illustrated with the running example presented later in this section.

A recent alternative to NNs, namely binarized neural networks (BNNs) [169] has also been investigated from the perspective of explainability [272].

**Monotonic classifiers.** Monotonic classifiers find a number of important applications, and have been studied extensively in recent years [120, 231, 324, 364]. Let \( \preceq \) denote a partial order on the set of classes \( \mathcal{K} \). For example, we assume \( c_1 \preceq c_2 \preceq \ldots \preceq c_K \). Furthermore, we assume that each domain \( D_i \) is ordered such that the value taken by feature \( i \) is between a lower bound \( \lambda(i) \) and an upper bound \( \mu(i) \). Given \( \mathbf{v}_1 = (v_{11}, \ldots, v_{1i}, \ldots, v_{1m}) \) and \( \mathbf{v}_2 = (v_{21}, \ldots, v_{2i}, \ldots, v_{2m}) \), we say that \( \mathbf{v}_1 \preceq \mathbf{v}_2 \) if, \( \forall (i \in \mathcal{F}). v_{1i} \leq v_{2i} \). Finally, a classifier is monotonic if whenever \( \mathbf{v}_1 \preceq \mathbf{v}_2 \), then \( \kappa(\mathbf{v}_1) \preceq \kappa(\mathbf{v}_2) \).

**Additional families of classifiers.** Formal explainability has been studied in the context of other families of classifiers, including random forests (RFs) [65, 191], boosted trees (BTs) [170, 172, 180], tree ensembles (TEs, which include both RFs and BTs) [172], decision graphs (DGs) & diagrams [166], naive bayes classifiers (NBCs) [239], monotonic classifiers [240], propositional language classifiers [165], and bayesian network classifiers [320, 321]. Most of these classifiers are covered in standard references on ML [124, 142, 316].

A random forest is represented by a set of decision trees, each tree trained from a random sample of the original dataset. In the originally proposed formulation of RFs [68], the selected class is picked by majority voting among all trees. As an example, we show that CDP for RFs is NP-complete.

**Proposition 4.** For RFs, CDP is NP-complete.

*Proof.* The decision problem is clearly in NP. Simply pick a point in feature space, and then compute in polynomial time the prediction of the RF, the decision problem answers \textbf{true} if the prediction is \( c \), and it answers \textbf{false} if the prediction is other than \( c \).

To prove NP-hardness, we reduce the decision problem for propositional formulas represented in CNF, a problem well-known to be complete for NP. Let \( \psi \) be a CNF formula with \( m \) propositional variables and \( n \) clauses, \( \varsigma_1, \ldots, \varsigma_n \):

- Create \( n \) decision trees, one for each clause \( \varsigma_j \), and such that DT \( j \) predicts 1 if at least one literal of \( \varsigma_j \) is satisfied, and 0 if all literals of \( \varsigma_j \) are falsified.
- Also, create \( n-1 \) decision trees, each with a single terminal node with prediction 0.

Clearly, the reduction runs in polynomial time. Moreover, it is immediate that the RF picks class 1 if and only if the formula is satisfied. Let the assignment to \( \psi \) be such that \( \psi(x_1, \ldots, x_m) \) is satisfied. In this case, each DT associated with a clause will predict 1 and the other \( n-1 \) DTs will predict 0; hence the prediction will be 1. Furthermore, for the prediction to be 1, it must be the case that the \( n \) DTs associated with the clauses must predict 1, since one must offset the \( n-1 \) trees that guaranteeedly predict 0. \( \square \)
A simpler argument could be used to prove that CDP for multivariate decision trees is also NP-complete. As an example, the CNF formula could be tested on a single tree node.

### 2.2.2 Running Examples

Throughout the paper, the following running examples will be used to illustrate some of the main results.

**Example 5 (DL).** The first running example is a simple DL, that is adapted from [124, Section 6.1]. (The original classification problem is to decide whether some animal is a dolphin. The features have been numbered, respectively 1 is Gills, 2 is Teeth, 3 is Beak, and 4 is Length. Moreover, the feature values have been replaced by numbers. These changes are meant to facilitate the logical analysis of the classifier, and do not affect in any way the computed explanations.) As a result, $F_1 = \{1, 2, 3, 4\}$, $D_{1i}, i = 1, 2, 3$, $D_{14} = \{0, 1, 2\}$, $K_1 = \{0, 1\}$, and $\kappa_1$ is defined by Figure 1a. Clearly, $F = \{0, 1\} \times \{0, 1\} \times \{0, 1\} \times \{0, 1, 2\}$. Moreover, the target instance is $(v, c) = ((0, 0, 1, 2), 1)$. Each of the rules $R_1$, $R_2$, and $R_3$ tests a single literal, and a final default rule $R_{\text{def}}$ fires on the points in feature space inconsistent with the other rules. Finally, Table 1 lists the class predicted by the DL for every point in feature space.

![Decision list and classification problem](image)

![Mapping of features](image)
| Entry | $x_1$ | $x_2$ | $x_3$ | $x_4$ | Rule | $\kappa_1(x_1, x_2, x_3, x_4)$ |
|-------|-------|-------|-------|-------|------|-------------------------------|
| 00    | 0     | 0     | 0     | 0     | $R_{\text{DEF}}$ | 1 |
| 01    | 0     | 0     | 0     | 1     | $R_3$ | 0 |
| 02    | 0     | 0     | 0     | 2     | $R_{\text{DEF}}$ | 1 |
| 03    | 0     | 0     | 1     | 0     | $R_{\text{DEF}}$ | 1 |
| 04    | 0     | 0     | 1     | 1     | $R_3$ | 0 |
| 05    | 0     | 0     | 1     | 2     | $R_{\text{DEF}}$ | 1 |
| 06    | 0     | 1     | 0     | 0     | $R_2$ | 1 |
| 07    | 0     | 1     | 0     | 1     | $R_2$ | 1 |
| 08    | 0     | 1     | 0     | 2     | $R_2$ | 1 |
| 09    | 0     | 1     | 1     | 0     | $R_2$ | 1 |
| 10    | 0     | 1     | 1     | 1     | $R_2$ | 1 |
| 11    | 0     | 1     | 1     | 2     | $R_2$ | 1 |
| 12    | 1     | 0     | 0     | 0     | $R_1$ | 0 |
| 13    | 1     | 0     | 0     | 1     | $R_1$ | 0 |
| 14    | 1     | 0     | 0     | 2     | $R_1$ | 0 |
| 15    | 1     | 0     | 1     | 0     | $R_1$ | 0 |
| 16    | 1     | 0     | 1     | 1     | $R_1$ | 0 |
| 17    | 1     | 0     | 1     | 2     | $R_1$ | 0 |
| 18    | 1     | 1     | 0     | 0     | $R_1$ | 0 |
| 19    | 1     | 1     | 0     | 1     | $R_1$ | 0 |
| 20    | 1     | 1     | 0     | 2     | $R_1$ | 0 |
| 21    | 1     | 1     | 1     | 0     | $R_1$ | 0 |
| 22    | 1     | 1     | 1     | 1     | $R_1$ | 0 |
| 23    | 1     | 1     | 1     | 2     | $R_1$ | 0 |

Table 1: Truth table for Example 5, where the target instance $(v, c) = ((0, 0, 1, 2), 1)$ corresponds to entry 05.

**Example 6 (DT).** The second running example is the decision tree shown in Figure 2. (This DT is adapted from [162] by replacing the names of the features and renaming the binary domains to boolean. The original DT was produced with the tool OSDT (optimal sparse decision trees) [162] for this DT classifier (see Figure 2b), $\mathcal{F}_2 = \{1, 2, 3, 4, 5\}$, $\mathcal{D}_2 = \{0, 1\}$, $i = 1, \ldots, 5$, $\mathcal{K}_2 = \{0, 1\}$, and $\kappa_2$ is captured by the DT shown in the Figure 2a. As can be observed, the DT has 15 nodes, with the non-terminal nodes being $N = \{1, 2, 4, 5, 7, 8, 10\}$ and the terminal nodes being $T = \{3, 6, 9, 11, 12, 13, 14, 15\}$. Each non-terminal node is associated with a feature from $\mathcal{F}$ (we assume univariate DTs), and each outgoing edge tests one or more values from the feature’s domain. For example, the edge
(2, 4) is associated with the literal $x_2 = 0$, being consistent with points in feature space where $x_2$ takes value 0. Each terminal node is associated with a prediction from $K$. The set of paths is $\mathcal{R}$. Throughout the paper, $\mathcal{R}$ is partitioned into two sets, namely $\mathcal{P}$ associated with prediction 1, and $\mathcal{Q}$ associated with prediction 0. (The split of $\mathcal{R}$ serves to aggregate paths according to their prediction, but the naming is arbitrary, and we could consider other splits, e.g. $\mathcal{P}$ for prediction 0, and $\mathcal{Q}$ for prediction 1.) Moreover, $\mathcal{P} = \{P_1, P_2, P_3, P_4, P_5\}$, with $P_1 = \{1, 2, 4, 7, 10, 15\}$, $P_2 = \{1, 2, 4, 7, 11\}$, $P_3 = \{1, 2, 5, 8, 13\}$, $P_4 = \{1, 2, 5, 9\}$, and $P_5 = \{1, 3\}$. Similarly, $\mathcal{Q} = \{Q_1, Q_2, Q_3\}$, with $Q_1 = \{1, 2, 4, 6\}$, $Q_2 = \{1, 2, 4, 7, 10, 14\}$, and $Q_3 = \{1, 2, 5, 8, 12\}$. Furthermore, the target instance we will study is $(v, c) = ((0, 0, 1, 0, 1), 1)$, being consistent with path $P_1$ and so with prediction 1. Finally, Table 2 shows parts of the truth table of the example DT, that will be used later when analyzing the instance $(v, c) = ((0, 0, 1, 0, 1), 1)$.

Example 7 (NN). The third running example is an NN, as shown in Figure 3. For this example, $F_3 = \{1, 2\}$, $D = \{D_{31}, D_{32}\}$, with $D_{31} = D_{32} = \{0, 1\}$, and so $F_3 = \{0, 1\}^2$, $K = \{0, 1\}$, and $\kappa_3(x_1, x_2) = (\max(x_1 + x_2 - 0.5, 0) > 0)$. We also have, from (3):

$$A^1 = \begin{bmatrix} -0.5 & +1 & +1 \end{bmatrix}$$
$$x^0 = \begin{bmatrix} 1 & x_1^0 & x_2^0 \end{bmatrix}$$
$$y^1 = \begin{bmatrix} y_1^1 \end{bmatrix} = A^1 \cdot (x^0)^T$$
Table 2: Partial truth tables of $\kappa_2$. These serve to analyze the values taken by $\kappa_2(x_1, x_2, x_3, x_4, x_5)$ for different combinations of feature values, starting from $x = (0, 0, 1, 0, 1)$.

(a) With $x_3 = x_5 = 1$, it is the case that $\kappa_2(x_1, x_2, x_3, x_4, x_5) = 1$, independently of the values of the other features

(b) With $x_1 = x_2 = x_4 = 0$, it is the case that $\kappa_2(x_1, x_2, x_3, x_4, x_5)$ can take a value other than 1, depending on the values assigned to $x_3$ and $x_5$.

(a) With $x_3 = x_5 = 1$, it is the case that $\kappa_2(x_1, x_2, x_3, x_4, x_5) = 1$, independently of the values of the other features

(b) With $x_1 = x_2 = x_4 = 0$, it is the case that $\kappa_2(x_1, x_2, x_3, x_4, x_5)$ can take a value other than 1, depending on the values assigned to $x_3$ and $x_5$.

Example 8 (Monotonic classifier). The fourth and final running example is a monotonic classifier, adapted from [240]. The goal is to predict a student’s grade given the grades on the different components of assessment. The different grading components have domain $\{0, \ldots, 10\}$. It is also the case that $F \preceq E \preceq D \preceq C \preceq B \preceq A$, where the operator $\preceq$ is used to represent the order between different
### (a) Features and domains

| Feature id | Feature variable | Feature name | Domain       |
|------------|------------------|--------------|--------------|
| 1          | Q                | Quiz         | {0, ..., 10} |
| 2          | X                | Exam         | {0, ..., 10} |
| 3          | H                | Homework     | {0, ..., 10} |
| 4          | R                | Project      | {0, ..., 10} |

### (b) Definition of \( \kappa_4 \)

\[
M = \text{ite}(S \geq 9, A, \text{ite}(S \geq 7, B, \text{ite}(S \geq 5, C, \text{ite}(S \geq 4, D, \text{ite}(S \geq 2, E, F)))))
\]

\[
S = \max[0.3 \times Q + 0.6 \times X + 0.1 \times H, R]
\]

Also, it is clearly the case that, \( \kappa_4(x_1) \ll \kappa_4(x_2) \) if \( x_1 \leq x_2 \), and so the classifier is monotonic.

#### 2.3 Non-Formal Explanations

As observed in Section 1, most of past work on XAI has studied non-formal explainability approaches. We will briefly summarize the main ideas. The interested reader is referred to the many surveys on the topic [1, 149, 159, 160, 263, 299, 309, 310, 335]. There is a burgeoning and fast growing body of work on non-formal approaches for computing explanations. The best known approaches offer no guarantees of rigor, and include model-agnostic approaches or solutions based on saliency maps for neural networks.

**Model-agnostic methods.** The most visible approaches for explaining ML models are model-agnostic methods [235, 301, 302]. These can be organized into methods that learn a simpler interpretable model, e.g. a linear model or a decision tree. This is the case with LIME [301] and SHAP [235]. The difference between LIME and SHAP is the approach used to learn the model, with LIME being based on iterative sampling, and SHAP based on the *approximate* computation...
of Shapley values. (It should be underscored that the Shapley values in SHAP are not computed exactly, but only approximated. Indeed, the complexity of exactly computing Shapley values is unwieldy [20,72], with one exception being a fairly restricted form of boolean circuits [20], referred to as deterministic, decomposable boolean circuits [100], and which capture binary decision trees. These model agnostic methods can also be viewed as associating a measure of relative importance to each features, being often referred to as feature attribution methods. One alternative model-agnostic approach is to identify which features are the most relevant for the prediction. We refer to such approaches as feature selection methods. One concrete example is Anchor [302]. Similar to other model agnostic approaches, Anchor is based on sampling. It should be noted that model-agnostic approaches exhibit a number of important drawbacks, the most critical of which is unsoundness [170,180,272]. Despite critical limitations, including the risk of unsound explanations, the impact of these tools can only be viewed as impressive.

Neural networks & saliency maps. In the concrete case of neural networks, past work proposed the use of variants of saliency maps [263,309,310,322], that give a graphical interpretation of a prediction. One popular approach is based on so-called layerwise relevancy propagation [36]. However, recent work has revealed important drawbacks of these approaches [2,209,325,350].

Intrinsic interpretability. Some authors have advocated the use of so-called interpretable ML models, for which the explanation is the model itself [43,77,230,262,304,305,314,357]. For example, it is widely accepted that decision trees are interpretable. Claims about the interpretability of decision trees go back at least until the early 2000s [69, Sec. 9, Page 206]. Motivated by their interpretability, decision trees have been applied to a wide range of domains, including the medical domain [224,333,340]. Unfortunately, recent results [187] demonstrate that decision trees cannot be deemed interpretable, at least as long as interpretability correlates with the succinctness of explanations. Interpretability of decision lists and sets is at least as problematic as it is for decision trees. If that were not the case, then one would be able to just represent DTs as DLs or DSs [303]. The bottom line is that even interpretable ML models should be explained, as the comprehensive results in earlier work [187] demonstrate.

Assessment. A number of additional limitations of non-formal explanations have been reported in recent years [75,108,135,189,216,221,326]. Furthermore, a number of authors have raised concerns about the current uses of XAI and its technology [199,268,274], with examples of misuse also reported [184].

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13 Earlier work [234] also investigated the exact computation of Shapley values for decision trees. However, issues about the proposed algorithm have been raised by more recent work [20,72].

14 See for example https://bit.ly/3eXIiNU, https://bit.ly/3BJL4z7, and https://bit.ly/3djA1Do.
3 Formal Explainability

Formal explanation approaches have been studied in a growing body of research in recent years [11–13, 19, 21, 22, 24–29, 38, 40, 59–61, 64, 65, 84, 85, 96–99, 101, 122, 145, 163–168, 170–172, 174, 177–180, 185, 186, 187, 189–192, 219, 232, 233, 237, 239, 240, 242, 272, 297, 298, 319–321, 354, 355, 362, 367, 368]. This section introduces formal explanations and describes some of their properties.

**Explanation problems.** Given a classifier \( \mathcal{M} = (\mathcal{F}, \mathcal{D}, \mathcal{F}, \mathcal{K}, \kappa) \), we consider two explanation problems. First, we mostly study a given local explanation problem \( \mathcal{E}_L = (\mathcal{M}, \mathbf{v}, \mathbf{c}) \), with \( \mathbf{v} \in \mathcal{F} \), \( \mathbf{c} \in \mathcal{K} \) and \( \mathbf{c} = \kappa(\mathbf{v}) \), which respects a concrete point in feature space, i.e. a concrete prediction. Second, we will also consider a global explanation problem \( \mathcal{E}_G = (\mathcal{M}, \mathbf{c}) \), with \( \mathbf{c} \in \mathcal{K} \), which respects solely a concrete prediction \( \mathbf{c} \), that can be predicted in many points of feature space.

As a result, a tuple \((\mathcal{M}, (\mathbf{v}, \mathbf{c}))\) will allow us to unambiguously represent the classification problem \( \mathcal{M} \) for which we want to compute the local AXp’s and CXp’s given the instance \((\mathbf{v}, \mathbf{c})\). Similarly, \((\mathcal{M}, \mathbf{c})\) also unambiguously represents the classification problem for which we want to compute the global AXp’s given the prediction \( \mathbf{c} \).

3.1 Abductive Explanations

This paper uses the definition of abductive explanation [178] (AXp), which corresponds to a PI-explanation [320] in the case of boolean classifiers. AXp’s represent prime implicants of the discrete-valued classifier function (which computes the predicted class)\(^{15}\). AXp’s can also be viewed as an instantiation of logic-based abduction \([73, 111, 128, 313]\). Throughout this paper we will opt to use the acronym AXp to refer to abductive explanations.

Let us consider a given classifier, computing a classification function \( \kappa \) on feature space \( \mathcal{F} \), a point \( \mathbf{v} \in \mathcal{F} \), with prediction \( \mathbf{c} = \kappa(\mathbf{v}) \), and let \( \mathcal{X} \) denote a subset of the set of features \( \mathcal{F} \), \( \mathcal{X} \subseteq \mathcal{F} \). \( \mathcal{X} \) is a weak AXp for the instance \((\mathbf{v}, \mathbf{c})\) if,

\[
\text{WeakAXp}(\mathcal{X}) := \forall (\mathbf{x} \in \mathcal{F}) : [\bigwedge_{i \in \mathcal{X}} (x_i = v_i)] \rightarrow (\kappa(\mathbf{x}) = c)
\]

(We could highlight that \( \text{WeakAXp} \) is parameterized on \( \kappa \), \( \mathbf{v} \) and \( \mathbf{c} \), but opt not to clutter the notation, and so these dependencies will be left implicit.) Thus, given an instance \((\mathbf{v}, \mathbf{c})\), a (weak) AXp is a subset of features which, if fixed to the values dictated by \( \mathbf{v} \), then the prediction is guaranteed to be \( \mathbf{c} \), independently of the values assigned to the other features.

\(^{15}\) There exist also standard references with detailed overviews of the uses of prime implicants in the context of boolean functions \([87, 151]\). Generalizations of prime implicants beyond boolean domains have been considered before \([249]\). Prime implicants have also been referred to as minimum satisfying assignments in first-order logic (FOL) \([107]\), and have been studied in modal and description logics \([54]\).
Example 9. With respect to the DL of Figure 1, it is apparent that $X = \{1, 4\}$ is a (weak) abductive explanation for the instance $(v, c) = ((0, 0, 0, 1, 2), 1)$. Indeed, if $(x_1 = 0) \land (x_4 = 2)$, then the prediction will be 1, independently of the values taken by the other features. This can easily be concluded from Table 1; if $x_1$ and $x_4$ are fixed, then the possible entries are 02, 05, 08 and 11, all with prediction 1. Hence, we can write that,

$$
\forall(x \in F_1). [(x_1 = 0) \land (x_4 = 2)] \rightarrow (\kappa_1(x) = 1)
$$

Observe that any set $Z$, with $X \subseteq Z \subseteq F$, is also a weak AXp. ✡

Moreover, $X \subseteq F$ is an AXp if, besides being a weak AXp, it is also subset-minimal, i.e.

$$
AXp(X) := \text{WeakAXp}(X) \land \forall(X' \subseteq X). \neg\text{WeakAXp}(X')
$$

(5)

Example 10. From Table 1, and given the weak AXp $\{1, 4\}$ (see Example 9) it is also possible to conclude that if either $x_1$ or $x_4$ are allowed to change their value, then the prediction can be changed. Hence, $X = \{1, 4\}$ is effectively an AXp. ✡

Observe that an AXp can be viewed as a possible irreducible answer to a “Why?” question, i.e. why is the classifier’s prediction $c$? It should be plain in this work, but also in earlier work, that the representation of AXp’s using subsets of features aims at simplicity. The sufficient condition for the prediction is evidently the conjunction of literals associated with the features contained in the AXp.

The following example demonstrates the importance of explaining decision trees, even if these are most often deemed interpretable.

Example 11. We consider the DT from Figure 2, and the instance $((0, 0, 0, 1, 2), 1)$. Intrinsic interpretability [262, 304] would argue that the explanation for this instance is the path consistent with the instance. Hence, we would claim that,

$$
\text{IF } [(x_1 = 0) \land (x_2 = 0) \land (x_3 = 1) \land (x_4 = 0) \land (x_5 = 1)] \text{ THEN } 1
$$

However, Table 2 clarifies that, as long as features 3 and 5 are assigned the same value, then the prediction remains unchanged. Hence, a far more intuitive explanation would be,

$$
\text{IF } [(x_3 = 1) \land (x_5 = 1)] \text{ THEN } 1
$$

Clearly, the (only) AXp for the given instance is exactly that one, i.e. $X = \{3, 5\}$, and we can state,

$$
\forall(x \in F_2). [(x_3 = 1) \land (x_5 = 1)] \rightarrow (\kappa_2(x) = 1)
$$

✡
Example 11 illustrates important limitations of DTs in terms of interpretability, and justifies recent work on explaining DTs [186–188]. More importantly, it has been shown that the redundancy in tree paths (i.e., features unnecessary for the prediction) can be arbitrarily large on the number of features [187]. Given the recent efforts on learning optimal (and quasi-optimal) “interpretable” models [4, 5, 10, 17, 18, 32, 33, 51, 52, 78, 105, 106, 136–138, 161, 162, 173, 181, 196, 220, 228, 238, 255, 271, 275, 276, 280, 306, 312, 318, 346–349, 352, 353, 356, 358, 365, 366], that include learning optimal decision trees and sets, recent results demonstrate [174, 187] that even such optimal and interpretable models should be explained.

3.2 Contrastive Explanations

Similarly to the case of AXp’s, one can define (weak) contrastive explanations (CXp’s) [177, 261]. \( \mathcal{Y} \subseteq \mathcal{F} \) is a weak CXp for the instance \((v, c)\) if,

\[
\text{WeakCXp}(\mathcal{Y}) := \exists (x \in \mathcal{F}), \left[ \bigwedge_{i \in \mathcal{Y}} (x_i = v_i) \right] \land (\kappa(x) \neq c) \tag{6}
\]

(As before, for simplicity we keep the parameterization of WeakCXp on \( \kappa, v \) and \( c \) implicit.) Thus, given an instance \((v, c)\), a (weak) CXp is a subset of features which, if allowed to take any value from their domain, then there is an assignment to the features that changes the prediction to a class other than \( c \), this while the features not in the explanation are kept to their values (ceteris paribus).

Example 12. For the DT of Figure 2, and the instance \((v, c) = ((0, 0, 1, 0, 1), 1)\), it is the case that \( \mathcal{Y} = \{3\} \) is a (weak) contrastive explanation. Indeed, if we allow the value of feature 3 to change, then there exists some point in feature space, e.g., \((0, 0, 0, 0, 1)\), for which the remaining features take the values in \( v \), and such that the prediction changes to 0. Hence, we can write,

\[\exists (x \in \mathcal{F}_2), (x_1 = 0) \land (x_2 = 0) \land (x_4 = 0) \land (x_5 = 1) \land (\kappa_2(x) \neq 1)\]

Intuitively, we are saying that it suffices to change the value of feature 3 to get a different prediction. \( \triangleright \)

Furthermore, a set \( \mathcal{Y} \subseteq \mathcal{F} \) is a CXp if, besides being a weak CXp, it is also subset-minimal, i.e.

\[
\text{CXp}(\mathcal{Y}) := \text{WeakCXp}(\mathcal{Y}) \land \forall (\mathcal{Y}' \subseteq \mathcal{Y}). \neg \text{WeakCXp}(\mathcal{Y}') \tag{7}
\]

Example 13. For the DL of Figure 1, it is plain that if \( x_1 \) is allowed to change value (i.e., entry 14 of Table 1) or if \( x_4 \) is allowed to change value (i.e., entry 01 of Table 1), then the prediction will change. Hence, either \{1\} or \{4\} are weak contrastive explanations for the given instance. Furthermore, both weak CXp’s are irreducible, and so both are effectively CXp’s. \( \triangleright \)
A CXp can be viewed as a possible irreducible answer to a “Why Not?” question, i.e., why isn’t the classifier’s prediction a class other than \( c \)? A different perspective for a contrastive explanation is as the answer to a How? question, i.e., how to change the features so as to change the prediction. In recent literature this alternative view has been investigated under the name actionable recourse \([200, 201, 339, 345]\). It should be underlined that whereas AXp’s correspond to prime implicants of the boolean function \( (\kappa(x) = c) \) that are consistent with some point \( v \in F \), CXp’s are not prime implicates of function \( (\kappa(x) = c) \). Nevertheless, the concept of counterexample studied in formal explainability \([178]\) corresponds to prime implicants of the function \( (\kappa(x) = c) \) (which are not restricted to be consistent with some specific point \( v \in F \)).

One important observation is that, independently of what \( \kappa \) represents, the WeakAXp and WeakCXp predicates (respectively defined using (4) and (6)) are monotone\(^{16}\). This means that the tests for minimality (i.e., respectively (5) and (7)) can be simplified to:

\[
\text{AXp}(\mathcal{X}) := \text{WeakAXp}(\mathcal{X}) \land \forall (t \in \mathcal{X}). \neg \text{WeakAXp}(\mathcal{X} \setminus \{t\})
\]

and,

\[
\text{CXp}(\mathcal{Y}) := \text{WeakCXp}(\mathcal{Y}) \land \forall (t \in \mathcal{Y}). \neg \text{WeakCXp}(\mathcal{Y} \setminus \{t\})
\]

Observe that, instead of considering all possible subsets of \( \mathcal{X} \) (resp. \( \mathcal{Y} \)), it suffices to consider the subsets obtained by removing a single element from \( \mathcal{X} \) (resp. \( \mathcal{Y} \)). This observation is at the core of the algorithms proposed in recent years for computing AXp’s and CXp’s of a growing range of families of classifiers \([164, 166, 174, 178, 179, 186, 191, 237, 239, 240, 272]\). As will be clarified in Section 4, the computation of AXp’s can be related with MUS extraction, and the computation of CXp’s can be related with MCS extraction.

Given a local explanation problem \( \mathcal{E} \), the sets of AXp’s and CXp’s are defined as follows,

\[
\mathcal{A}(\mathcal{E}) = \{ \mathcal{X} \subseteq F \mid \text{AXp}(\mathcal{X}) \}\]

\[
\mathcal{C}(\mathcal{E}) = \{ \mathcal{Y} \subseteq F \mid \text{CXp}(\mathcal{Y}) \}\]

### 3.3 Global Abductive Explanations & Counterexamples

The definition of AXp’s considered until now is localized, in that it takes a concrete point \( v \) into account. However, abductive explanations can be defined only with respect to the class, and ignore concrete points in feature space; these are referred to as global AXp’s. Following \([179]\), let \( \pi : F \rightarrow \{0, 1\} \), represent a term that is a prime implicant of the predicate \( [\kappa(x) = c] \), i.e.,

\[
\forall (x \in F). \pi(x) \rightarrow (\kappa(x) = c)
\]

\(^{16}\) Clearly, from the definition of WeakAXp (resp. WeakCXp), if WeakAXp(\( \mathcal{Z} \)) (resp. WeakCXp(\( \mathcal{Z} \))) holds, then WeakAXp(\( \mathcal{Z}' \)) (resp. WeakCXp(\( \mathcal{Z}' \))) also holds for any superset \( \mathcal{Z}' \) of \( \mathcal{Z} \). If WeakAXp(\( \mathcal{Z} \)) (resp. WeakCXp(\( \mathcal{Z} \))) does not hold, then WeakAXp(\( \mathcal{Z}' \)) (resp. WeakCXp(\( \mathcal{Z}' \))) also does not hold for any subset \( \mathcal{Z}' \) of \( \mathcal{Z} \).
Table 3: Global abductive explanations and counterexamples for the DL of Figure 1a.

| Global AXp’s         | \{x_1 = 1\}, \{x_2 = 0, x_4 = 1\} |
|----------------------|-----------------------------------|
| Counterexamples      | \{x_1 = 0, x_2 = 1\}, \{x_1 = 0, x_4 = 0\} |

(Each literal will be of the form \(x_i = u_i\), where \(u_i\) is taken from \(D_i\).) The set of literals of \(\pi\) is a global abductive explanation of the prediction \(c\).

We are also interested in the prime implicates of the predicate \([\kappa(x) = c]\), which will be convenient to represent by \(\neg \eta\), where \(\eta\) is a term \(\eta : F \to \{0, 1\}\),

\[
\forall (x \in F). (\kappa(v) = c) \rightarrow [\neg \eta(x)]
\]

This statement can be rewritten as follows,

\[
\forall (x \in F). \eta(x) \rightarrow (\kappa(v) \neq c)
\]

The set of literals in \(\eta\) is referred to as a counterexample (CEx) for the prediction \(c\), and represents the negation of a prime implicate for the predicate \([\kappa(x) = c]\). Clearly, both global AXp’s and CEx’s are irreducible (and so subset-minimal).

Example 14. For the DL of Figure 1a, let \(c = 0\), i.e. the predicted class is 0. It is plain that the predicted class is 0 whenever \(x_1 = 1\). Thus, \(\{(x_1 = 1)\}\) is a global abductive explanation for class \(c = 0\). Similarly, if \(x_2 = 0\) and \(x_4 = 1\), then the predicted class is again guaranteed to be 0. Thus, the other global abductive explanation is \(\{(x_2 = 0), (x_4 = 1)\}\). We could use minimal hitting set duality between prime implicants and implicates [307] to list the counterexamples. However, we can also directly reason in terms of the DL to uncover the CEx’s, as shown in Table 3.

(Local) AXp’s, CXp’s and global AXp’s and CEx’s reveal important relationships between prime implicants and implicates, as discussed later in Section 3.5.

3.4 Duality Results

This section overviews duality results in formal explainability, which have been established in recent years [177, 179].

Duality between AXp’s and CXp’s. Given the definition of sets of AXp’s and CXp’s (see (10) and (11)), and by building on Reiter’s seminal work [300], recent work [177] proved the following duality between minimal hitting sets:

Proposition 5 (Minimal hitting-set duality between AXp’s and CXp’s). Given a local explanation problem \(\mathcal{E}\), we have that,

1. \(\mathcal{X} \subseteq \mathcal{F}\) is an AXp (and so \(\mathcal{X} \in \mathcal{A}(\mathcal{E})\)) iff \(\mathcal{X}\) is an MHS of the CXp’s in \(\mathcal{C}(\mathcal{E})\).
2. \( \mathcal{Y} \subseteq \mathcal{F} \) is a CXp (and so \( \mathcal{X} \in \mathbb{C}(\mathcal{E}) \)) iff \( \mathcal{Y} \) is an MHS of the AXp’s in \( \mathbb{A}(\mathcal{E}) \).

We refer to Proposition 5 as MHS duality between AXp’s and CXp’s. The previous result has been used in more recent papers for enabling the enumeration of explanations [166,174,240].

**Example 15.** For the DL of Example 5, and the instance \((v, c) = ((0, 0, 1, 2), 1)\), we have argued (see Examples 9, 10 and 13) that an AXp is \( \{1, 4\} \) and that \( \{1\} \) and \( \{4\} \) are CXp’s. Clearly, the AXp is a MHS of the CXp’s and vice-versa. Hence, we have listed all the AXp’s and CXp’s for this instance. △

Furthermore, a consequence of Proposition 5 is the following result:

**Proposition 6.** Given a classifier function \( \kappa : \mathcal{F} \to \mathcal{K} \), defined on a set of features \( \mathcal{F} \), a feature \( i \in \mathcal{F} \) is included in some AXp iff \( i \) is included in some CXp.

**Duality between global AXp’s and counterexamples [179].** Another minimal hitting-set duality result, different from Proposition 5, was investigated in earlier work [179], and relates global AXp’s (i.e. not restricted to be consistent with a specific point \( v \in \mathcal{F} \)) and counterexamples (see also Page 29). Given the definition of (global) AXp’s and CEx’s (see Section 3.3), we say that two sets of literals break each other if these have inconsistent literals. Furthermore, [179] proves the following result,

**Proposition 7.** For a global explanation problem, every CEx breaks every global AXp and vice-versa.

**Example 16.** From Example 14, it is plain to conclude (see Table 3) that each global abductive explanation breaks each counterexample and vice-versa. △

### 3.5 Additional Notes

**Relationship with non-formal explainability.** Past work has shown how formal explanations can serve to assess the quality or rigor of non-formal explanations [170,180,272]. For example, a non-formal explanation can be corrected and made subset-minimal, using the non-formal explanation as a starting point for the computation of some other, formal, explanations [170,180]. Moreover, some authors have recently noticed what is referred to as the disagreement problem in XAI [216]. From the perspective of formal explainability, differences in explanations just represent different AXp’s, which can exist. More important, as discussed in Section 6, it is conceptually feasible, and often practically efficient, to navigate the space of explanations.
Literals based on the equality operator. As can be observed, both running examples use literals of the form \((x_i = u_i)\). The same applies to the definitions of (weak) AXp’s and CXp’s. This need not be the case, as discussed elsewhere [187]. In the case of DTs, more general literals have been associated with explanations [187], e.g. by describing literals using set membership. Nevertheless, and for simplicity, in this document we will use literals that use solely the equality operator.

Prime implicants & implicates vs. MUSes & MCSes. For global abductive explanations, the duality result established in earlier work [179] essentially relates prime implicants and implicates of some boolean function \(\varsigma : \mathbb{F} \to \{0, 1\}\), with \(\varsigma(x) = (\kappa(x) = c)\). In contrast, the duality results established in more recent work [177] relate localized AXp’s and CXp’s, and can instead be viewed as relating MUSes and MCSes of some inconsistent formula (see Section 4 for additional detail). These results reveal a more fine-grained relationship between prime implicants and prime implicates, than what is proposed in earlier work [288, 307].

Formal explainability and model-based diagnosis. Although we approach formal explainability as a problem of abduction, there are other possible ways to represent the problem of explainability. One well-known example is model-based diagnosis (MBD) [300]. We consider a system description SD consisting of a set of first-order logic statements, and a set of constants Comp, representing the system’s components. Each component may or may not be operating correctly, and we use a predicate \(\text{Ab}\) to indicate whether the component \(C_j\) is operating incorrectly (i.e. \(\text{Ab}(C_j)\) holds, denoting abnormal behavior), or correctly (i.e. \(\neg\text{Ab}(C_j)\) holds, denoting normal behavior). Furthermore, we also assume some observation Obs about the system’s expected behavior. In a diagnosis scenario, where Obs disagrees with expected result, it is the case that,

\[
SD \cup \{\neg\text{Ab}(C_1), \neg\text{Ab}(C_2), \ldots, \neg\text{Ab}(C_n)\} \cup \text{Obs} \models \bot \tag{12}
\]

A conflict set is a (subset)-minimal set CS of Comp such that,

\[
SD \cup \{\neg\text{Ab}(C_i) \mid C_i \in \text{CS}\} \cup \text{Obs} \models \bot \tag{13}
\]

A diagnosis is a subset-minimal set \(\Delta\) of Comp such that,

\[
SD \cup \{\neg\text{Ab}(C_i) \mid C_i \in \text{Comp} \setminus \Delta\} \cup \text{Obs} \not\models \bot \tag{14}
\]

A simple reduction of the problem of finding abductive explanations to model based diagnosis, can be organized as follows:

1. SD is given by, \(\llbracket \land_{i \in \mathcal{X}}[(x_i = v_i) \lor \text{Ab}(i)] \rrbracket\), where \(\llbracket \cdot \rrbracket\) denotes a logic encoding in a suitable logic theory.
2. Obs is given by \(\llbracket \kappa(x) \neq c \rrbracket\).

Clearly, if all components operate correctly, then the system description is inconsistent with the stated observation, as expected. (And in this case the stated
3.6 A Timeline for Formal Explainability

Figure 5 depicts the evolution in time of the main areas of research in formal explainability. The initial focus (in 2019-2020) was on the definition of explanations, duality results, but also approaches for the computation of explanations. The next major effort (in 2020-2021) was on classifiers exhibiting tractable computation of one explanation. This was soon followed by efforts on the efficient computation of explanations even when the computation of explanations was computationally hard (in 2021-2022). More recently, there has been research on addressing different explainability queries (in 2021-2022), tackling input distributions (started in 2022), and computing probabilistic explanations in practice (also started in 2022). There are additional topics of research, which are also
discussed in this document. Although there is ongoing research in most areas of research shown in Figure 5, it is also the case that the most recent topics exhibit more open research questions. The rest of this paper, overviews the areas of research in formal explainability shown in Figure 5.

4 Computing Explanations

This section covers the computation of explanations, both abductive and contrastive. The focus are on families of classifiers for which computing one explanation is computationally hard. The next section covers families of classifiers for which there exist polynomial-time algorithms for computing one abductive/contrastive explanation.

4.1 Progress in Computing Explanations

Since 2019, there has been steady progress in the practical efficiency of computing formal explanations. Figure 6 summarizes the observed progress. For some families of classifiers, including decision trees, graphs and diagrams, naive bayes classifiers, monotonic classifiers, restricted propositional language classifiers and others, it has been shown that computing one AXp is tractable \[84, 165, 166, 186, 188, 239, 240\]. For some other families of classifiers, e.g. decision lists and sets, random forests and tree ensembles, it has been established the computational hardness of computing one AXp \[174, 191\]. However, and also for these families of classifiers, existing logical encodings enable the efficient computation of one AXp \[170, 172, 174, 180, 191\] in practice. Finally, for a few other families of classifiers \[178, 320\], computing one AXp is not only computationally hard, but existing algorithms are not efficient in practice, at least for large scale ML models. The next sections analyze some of these results in more detail.

4.2 General Oracle-Based Approach

The main approach for computing explanations is based on exploiting automated reasoners (e.g. SAT, SMT, MILP, etc.) as oracles. We start by analyzing how to decide whether a subset \(X\) of features is a weak AXp. From (4), negating twice, we get:

\[
\neg \exists (x \in \mathbb{F}). \left[ \bigwedge_{i \in X} (x_i = v_i) \right] \land (\kappa(x) \neq c)
\]

This corresponds to deciding the consistency of a logic formula, as follows:

\[
\neg \text{CO} \left( \left[ \bigwedge_{i \in X} (x_i = v_i) \right] \land (\kappa(x) \neq c) \right)
\]

The computation of a single AXp or a single CXp can be achieved by adapting existing algorithms provided a few requirements are met. First, reasoning in theory \(\mathcal{T}\) is required to be monotone, i.e. inconsistency is preserved if constraints are added to a set of constraints, and consistency is preserved if constraints are
removed from a set of constraints. Second, for computing one AXp, the predicate to consider is:

$$P_{axp}(S; T, F, \kappa, v) \triangleq \neg CO \left( \left[ \left( \bigwedge_{i \in S} (x_i = v_i) \right) \land (\kappa(x) \neq c) \right] \right) \quad (15)$$

and for computing one CXp, the predicate to consider is:

$$P_{cxp}(S; T, F, \kappa, v) \triangleq CO \left( \left[ \left( \bigwedge_{i \in F \setminus S} (x_i = v_i) \right) \land (\kappa(x) \neq c) \right] \right) \quad (16)$$

where, the starting set $S$ can be any set that respects the invariant of the predicate for which it serves as an argument. For example, for computing a AXp, $S$ can represent any weak AXp, and for computing a CXp, $S$ can represent any weak CXp. (Similar to the case of CO, $P_{axp}$ and $P_{cxp}$ are parameterized by $T$, $F$, $\kappa$, $v$, and also $c = \kappa(v)$. For simplicity, this parameterization will be left implicit when convenient. Also, the parameterization on $c = \kappa(v)$, given the ones on $\kappa$ and $v$.) Observe that, since (4) and (6) are monotone, then $P_{axp}$ and $P_{cxp}$ are also monotone with respect to set $S$. Moreover, the monotonicity of $P_{axp}$
Algorithm 1 Finding one AXp/CXp

**Input:** Seed $S \subseteq \mathcal{F}$, parameters $\mathbb{P}, \mathcal{T}, \mathcal{F}, \kappa, v$

**Output:** One XP $W$

1: procedure oneXP($S, \mathbb{P}, \mathcal{T}, \mathcal{F}, \kappa, v$)
2: $W \leftarrow S$ \hspace{1em} \triangleright Initialization: $\mathbb{P}(W)$ holds
3: for $i \in S$ do
4: \hspace{1em} if $\mathbb{P}(W \setminus \{i\}; \mathcal{T}, \mathcal{F}, \kappa, v)$ then
5: \hspace{2em} $W \leftarrow W \setminus \{i\}$ \hspace{1em} \triangleright Update $W$ only if $\mathbb{P}(W \setminus \{i\})$ holds
6: return $W$ \hspace{1em} \triangleright Returned set $W$: $\mathbb{P}(W)$ holds

and $\mathbb{P}_{\text{exp}}$ enables adapting standard algorithms for computing one explanation. Algorithm 1 illustrates one possible approach\(^\text{17}\). For computing one AXp or one CXp, the initial seed set $S$ of Algorithm 1 is set to $\mathcal{F}$. However, as long as the precondition $\mathbb{P}(S)$ holds, then any set $S \subseteq \mathcal{F}$ can be considered.

**Example 17.** We consider the DT of Figure 2, and both the computation of one AXp and one CXp when $S = \{3, 4, 5\}$. For the AXp, it is plain that if features $\{3, 4, 5\}$ are fixed, then the prediction does not change (as shown in Table 2a).

Table 4 summarizes the execution of Algorithm 1 when computing one AXp and one CXp, starting from a set of literals (i.e. the seed) $S = \{3, 4, 5\}$. (Without additional information, we would start from $S = \mathcal{F}$, and so the table would include a few more lines.) The difference between the two executions is the result of the predicate used.

In some settings, it may be relevant to compute one smallest AXp or one smallest CXp. Computing one CXp can be achieved by computing a smallest(-cost) MCS. Hence, a MaxSAT/MaxSMT reasoner can be used in this case. For AXp’s, and given their relationship with MUSes, a different approach needs to be devised. For a given theory $\mathcal{T}$, let

$$\text{Decide}(\mathcal{A}) := \text{CO}(\left[ \left( \bigwedge_{i \in \mathcal{A}} (x_i = v_i) \right) \land (\kappa(x) \neq c) \right]_\mathcal{T})$$

(17)

Furthermore, we assume that $\text{Decide}(\mathcal{A})$ returns a pair $(\text{outc}, \mu)$, indicating whether the formula is indeed consistent and, if it is, the computed assignment. Algorithm 2 illustrates the use of dualization for computing one smallest AXp, and builds on earlier work on computing smallest MUSes [182]. Any minimum-size hitting set such that the picked (fixed) features represent a weak AXp must be a smallest AXp.

---

\(^{17}\) This algorithm is referred to as the *deletion-based* algorithm [79], but it can be traced back to the work of Valiant [341] (and some authors [197] argue that it is implicit in works from the 19th century [259]). Although variants of Algorithm 1 are most often used in practical settings, there are several alternative algorithms that can also be used, including QuickXplain [198], Progression [243], or even insertion-based [323], among others [34, 44]. As illustrated by Algorithm 1, it is now known that most of these algorithms can be formalized in an abstract way, thus allowing them to be used to solve subset-minimal problems when these problems can be represented by...
Table 4: Computation of 1 AXp and 1 CXp starting from seed \( S = \{3, 4, 5\} \). The partial truth tables in Tables 2a and 2b can be used for computing both \( \mathcal{P}_{axp} \) and \( \mathcal{P}_{cxp} \). Table 2a serves to validate whether the prediction remains unchanged. Table 2b serves to assess whether there are points in feature space for which the prediction changes.

Algorithm 2 Finding one smallest AXp

\begin{algorithm}
\caption{Finding one smallest AXp}
\begin{algorithmic}[1]
\Procedure{minXP}{ } 
\State \( \mathcal{H} \leftarrow \emptyset \)
\While{true}
\State \( \mathcal{M} \leftarrow \text{MinimumHS}(\mathcal{H}) \)
\State \((\text{outc}, \mu) \leftarrow \text{Decide}(\mathcal{M}; \mathcal{T}, \mathcal{F}, \kappa, \nu)\)
\If{not outc}
\State return \( \mathcal{M} \)
\Else
\State \( \mathcal{L} \leftarrow \text{PickFalseLits}(\mathcal{F} \setminus \mathcal{M}, \mu) \)
\State \( \mathcal{H} \leftarrow \mathcal{H} \cup \mathcal{L} \)
\EndIf
\EndWhile
\EndProcedure
\end{algorithmic}
\end{algorithm}

Relationship with MUSes & MCSes. We can relate the computation of AXp’s and CXp’s respectively with the extraction of MUSes and MCSes. We construct a formula \( \varphi = \mathcal{B} \cup \mathcal{S} \) in some theory \( \mathcal{T} \) where the background knowledge \( \mathcal{B} \) corresponds to,

\[
\mathcal{B} \triangleq \llbracket \kappa(x) \neq c \rrbracket \mathcal{T}
\]  

and the soft constraints \( \mathcal{S} \) correspond to,

\[
\mathcal{S} \triangleq \{ \llbracket x_i = v_i \rrbracket \mathcal{T} \mid i \in \mathcal{F} \}
\]  

Clearly, \( \varphi = \mathcal{B} \cup \mathcal{S} \) is inconsistent, i.e. if all features are fixed, then the prediction must be \( c \). As a result, an MUS \( \mathcal{U} \) of \( \mathcal{B} \cup \mathcal{S} \) (i.e. a subset of \( \mathcal{U} \) of \( \mathcal{S} \)) is such that \( \mathcal{U} \cup \mathcal{S} \) is inconsistent. Thus, \( \mathcal{U} \) represents a subset-minimal set of features which, monotonic predicates [245]. As argued earlier, predicates \( \mathcal{P}_{axp} \) (see Equation (15)) and \( \mathcal{P}_{cxp} \) (see Equation (16)) are both monotonic.
if fixed, ensure inconsistency (and so the prediction must be \( c \)); hence, \( \mathcal{U} \) is an AXp. Similarly, an MCS \( \mathcal{C} \) of \( \mathcal{B} \cup \mathcal{S} \) (i.e. a subset of \( \mathcal{C} \) of \( \mathcal{S} \)) is such that \( \mathcal{B} \cup (\mathcal{S} \setminus \mathcal{C}) \) is consistent. Thus, \( \mathcal{C} \) represents a subset-minimal set of features which, if allowed to change their, ensure consistency (and so the prediction can be different from \( c \)); hence, \( \mathcal{C} \) is a CXp.

### 4.3 Explaining Decision Lists

This section details the computation of AXp’s/CXp’s in the case of DLs. Furthermore, it is briefly mentioned the relationship with computing explanations for DSs and DTs.

**Explaining DLs.** The computation of AXp’s has been shown to be computationally hard, both for DLs and DSs [174]. As a result, the solution approach is to follow the general approach detailed in Section 4.2. However, we will devise a propositional encoding and use SAT solvers as NP oracles.

To illustrate the computation of explanations (both AXp’s and CXp’s), we consider a DL with the following structure:

\[
R_1: \quad \text{IF} \quad \tau_1 \quad \text{THEN} \quad d_1 \\
R_2: \quad \text{ELSE IF} \quad \tau_2 \quad \text{THEN} \quad d_2 \\
\quad \ldots \\
R_j: \quad \text{ELSE IF} \quad \tau_j \quad \text{THEN} \quad d_j \\
\quad \ldots \\
R_n: \quad \text{ELSE IF} \quad \tau_n \quad \text{THEN} \quad d_n \\
R_{\text{DEF}}: \quad \text{ELSE} \quad \text{THEN} \quad d_{n+1}
\]

where \( d_r \in \mathcal{K}, r = 1, \ldots, n + 1 \), and \( \tau_j \) is a conjunction of literals, or in general some logic formula.

Let \( [\phi]_T \) denote the propositional CNF encoding of \( \phi \). This encoding can introduce not only a number of additional clauses, but also fresh propositional variables. The resulting formula will be represented by \( \mathcal{E}_\phi(z_1, \ldots) \), where \( z_1 \) is a propositional variable taking value 1 iff \( \phi \) takes value 1. To develop a propositional CNF encoding, we let \( \mathcal{E}_{\tau_j}(t_j, \ldots) \) represent the clauses associated with \( [\tau_j]_T \), i.e. the propositional CNF encoding of \( \tau_j, j = 1, \ldots, n \), and where \( t_j \) represents a new propositional variable that takes value 1 only in points of feature space where \( \tau_j \) is true. (Additional propositional variables may be used, and these are represented by \( \ldots \) at this stage.) Let the target class be \( c \) and define the propositional constant \( e_j \) to be 1 iff \( d_j \) matches \( c \).

Moreover, since literals may require propositional encodings, let \( \mathcal{E}_{x_i = v_i}(l_i, \ldots) \) represent the clauses associated \( [x_i = v_i]_T, i = 1, \ldots, m \), and where \( l_i \) represents a new propositional variable that takes value 1 only in points of feature space where \( x_i = v_i \). (Additional propositional variables may be used, and these are represented by \( \ldots \) at this stage. Also, we can envision re-using and sharing common encodings; this will be discussed in Example 18 below.)
Clearly, for some point \( x \) in feature space, the prediction changes if it is the case that,

1. For \( \tau_j \), with \( e_j = 0 \) and \( 1 \leq j \leq n \), it is the case that \( \tau_j \) is true, and for any \( 1 \leq k < j \), with \( e_k = 1 \), \( \tau_k \) is false:

\[
[f_j \leftrightarrow (t_j \land \bigwedge_{1 \leq k < j, e_k = 1} \neg t_k)]
\]

where \( f_j \) is a new propositional variable, denoting that rule \( j \) with a different prediction would fire (and so it would flip its previous status). (Clearly, if some other rule \( R_r, \tau_r \) with \( r < j \) and \( e_r = 0 \), fires then the prediction will also change as intended, and this is covered by some other constraint. Hence, there is no need to account for such rules.)

2. Moreover, we require that at least one \( f_j \), with \( e_j = 0 \) and \( 1 \leq j \leq n \), to be true:

\[
\left( \bigvee_{1 \leq j \leq n, e_j = 0} f_j \right)
\]

Given the above, we now organize the propositional encoding in two components, one composed of soft clauses and the other composed of hard clauses:

- The set of soft clauses is given by:

\[
S \triangleq \{(l_i), i = 1, \ldots, m\}
\]  \hspace{1cm} (20)

- The set of hard clauses is given by:

\[
B \triangleq \bigwedge_{1 \leq i \leq m} \mathbf{c}_{x_i = v_i}(l_i, \ldots) \land \bigwedge_{1 \leq j \leq n} \mathbf{c}_{\tau_j}(t_j, \ldots) \land \\
\bigwedge_{1 \leq j \leq n, e_j = 0} \left( f_j \leftrightarrow (t_j \land \bigwedge_{1 \leq k < j, e_k = 1} \neg t_k) \right) \land \\
\left( \bigvee_{1 \leq j \leq n, e_j = 0} f_j \right)
\]  \hspace{1cm} (21)

It is plain that \( B \cup S \) represents an inconsistent propositional formula. Any MUS of \( B \cup S \) is a subset of \( S \), and represents one AXp. Moreover, any MCS is also a subset of \( S \), and represents one CXp. As argued earlier, AXp’s are MHSes of CXp’s and vice-versa \([56, 177, 300]\). This observation also means that we can use any algorithm for MUS/MCS extraction/enumeration for computing explanations of DLs \([246]\).

Finally, the propositional encoding proposed above differs slightly from the one proposed in earlier work \([174]\), offering a more streamlined encoding.

**Example 18.** Let us investigate how we can encode the computation of one AXp for the DL running example (see Figure 1). The soft clauses are given by,

\[
S = \{l_1, l_2, l_3, l_4\}
\]

where \( l_i \) is associated with \([x_i = v_i]_T\), i.e. it is one of the variables used in \( \mathbf{c}_{x_i = v_i} \). For simplicity, there is no need to encode \( x_i = v_i \) for \( i = 1, 2, 3 \), with
\[v = (0, 0, 1, 2),\] and so we let \(l_1 \leftrightarrow \neg x_1, l_2 \leftrightarrow \neg x_2,\) and \(l_4 \leftrightarrow x_3.\) However, for \(x_4 = 2,\) a dedicated propositional encoding is required. Hence, we use three propositional variables, \(\{x_{41}, x_{42}, x_{43}\},\) and pick a one-hot encoding to get \(\mathcal{E}_{\tau_j}(l_4, \ldots) \triangleq l_4 \leftrightarrow x_{43} \land \text{EqualsOne}(x_{41}, x_{42}, x_{43}),\) where \(x_{43} = 1\) iff \(x_4 = 1.\) There are many propositional encodings for \(\text{EqualsOne}(x_{41}, x_{42}, x_{43})\) [55] constraints. One simple solution is,

\[
(\neg x_{41} \lor \neg x_{42}) \land (\neg x_{41} \lor \neg x_{43}) \land (\neg x_{42} \lor \neg x_{43}) \land (x_{41} \lor x_{42} \lor x_{43})
\]

For each rule we need to encode \(\tau_j.\) It is immediate to get \(t_1 \leftrightarrow x_1\) for \(\tau_1,\)

\[
\begin{align*}
f_1 & \leftrightarrow t_1 \\
f_3 & \leftrightarrow (t_3 \land \neg t_2)
\end{align*}
\]

indicating that the prediction changes if either \(t_1\) is true (i.e. rule \(R_1\) fires), or \(t_3\) is true and \(t_2\) is false (i.e. rule \(R_3\) fires and rule \(R_2\) does not fire, and earlier rules are already covered by other constraints). Finally, we need the constraint \((f_1 \lor f_3),\) to enforce that a change of prediction will take place.

Given the above, we get that,

\[
\mathcal{B} = (l_1 \leftrightarrow \neg x_1) \land (l_2 \leftrightarrow \neg x_2) \land (l_3 \leftrightarrow x_3) \land (l_4 \leftrightarrow x_{43}) \land \\
\text{EqualsOne}(x_{41}, x_{42}, x_{43}) \land \\
(t_1 \leftrightarrow x_1) \land (t_2 \leftrightarrow x_2) \land (t_3 \leftrightarrow x_{42}) \land \\
(f_1 \leftrightarrow t_1) \land (f_3 \leftrightarrow (t_3 \land \neg t_2)) \land (f_1 \lor f_3)
\]

Moreover, and by inspection, the tuple \((\mathcal{S}, \mathcal{B})\) can be simplified to,

\[
\mathcal{S} = \{\neg x_1, \neg x_2, x_3, x_{43}\}
\]

and,

\[
\mathcal{B} = \text{EqualsOne}(x_{41}, x_{42}, x_{43}) \land (f_1 \leftrightarrow x_1) \land (f_3 \leftrightarrow (x_{42} \land \neg x_2)) \land (f_1 \lor f_3)
\]

It is apparent that \(\mathcal{B} \cup \mathcal{S}\) is inconsistent. Finally, we can also observe that for tuple \((\mathcal{S}', \mathcal{B})\) with,

\[
\mathcal{S}' = \{\neg x_1, x_{43}\}
\]

\[
\mathcal{B} = \text{EqualsOne}(x_{41}, x_{42}, x_{43}) \land (f_1 \leftrightarrow x_1) \land (f_3 \leftrightarrow (x_{42} \land \neg x_2)) \land (f_1 \lor f_3)
\]

\(\mathcal{B} \cup \mathcal{S}'\) is still inconsistent. Thus, \(\mathcal{S}' = \{\neg x_1, x_{43}\}\) is an unsatisfiable subset (which we can prove to be irreducible), and so \(\mathcal{X} = \{1, 4\}\) is a weak \(\text{AXp}\) (which we can prove to be an \(\text{AXp}\)).

Existing results indicate that the computation of explanations for DLs is very efficient in practice [174].
4.4 From DLs to DTs & DSs

Explaining DTs as DLs. A conceptually straightforward approach for explaining DTs is to represent a DT as a DL. Hence, the propositional encoding proposed above for explaining DLs can also be used for explaining DTs. Nevertheless, as argued in Section 5.1, in the case of DTs there are polynomial time algorithms for computing one abductive explanation, and there are polynomial time algorithms for enumerating all the contrastive explanations.

The case of DSs. The fact that DSs are unordered raises a number of technical difficulties, including the fact that, if there can be rules that predict different classes and fire on the same input, then the classifier does not compute a function. This is referred to as overlap [181]. If the rules predicting each class are represented as a DNF, then one call to an NP oracle suffices to decide whether overlap exists.

Let a DS be represented by a set of DNF formulas, one for each class in \( \mathcal{K} \). Moreover, let \( z_r \) represent the value computed for DNF \( r \), which predicts class \( c_r \in \mathcal{K} \). There exists no overlap is the following condition does not hold:

\[
\sum_{r=1}^{K} z_r > 1
\]

If we also want to ensure that there is a prediction for any point in feature space, then we can instead require that the following constraint is inconsistent:

\[
\sum_{r=1}^{K} z_r \neq 1 \tag{22}
\]

i.e. we want the sum to be equal to 1 on each point of feature space. (Clearly, the constraint above must be inconsistent given the logic encoding of the classifier. The actual encoding of each \( z_r \) will depend on how the DNFs are represented, and there is no restriction of considering purely boolean classifiers.)

Under the standard assumption that (22) is inconsistent, then the encoding proposed for DLs can be adapted to the case of DSs. We will have to encode each term (i.e. each unordered rule), and then encode the disjunction of terms for each DNF. We will briefly outline a propositional encoding for computing abductive (and contrastive) explanations. The approach differs from the DL case since we do not have order in the rules. Hence, each class is analyzed as a DNF. As usual, we consider an instance \( (v, c_s) \), where \( c_s \in \mathcal{K} \) is the predicted class. The constraints for the encodings are organized as follows:

1. The DNF \( r \) of class \( c_r \in \mathcal{K} \), it is a disjunction of \( n_r \) terms \( \tau_{rj}, r = 1, \ldots, n_r \).
2. Each term \( \tau_{rj} \) is encoded into \( E_{\tau_{rj}}(t_{rj}, \ldots) \), such that \( t_{rj} = 1 \) iff the term \( \tau_{rj} \) takes value 1.
3. The literals of the form \( (x_i = v_i) \) will be encoded into the clauses \( E_{x_i=v_i}(l_1, \ldots) \).
   (As mentioned earlier in this section in the case of DLs, the encoding from the original feature variables to propositional variables is assumed in all these encodings.)
4. The soft clauses will be \( (l_i), i = 1, \ldots, m \).
5. A class \( c_r \) is picked iff \( p_r = 1 \), where \( p_i \) is a fresh propositional variable. Hence, we define \( p_r \), for class \( c_r \) as follows: \( p_r \leftrightarrow (\lor_{j=1}^{n_r} t_{rj}) \)

6. The prediction changes if \( p_s = 0 \).

(Observe that we could instead introduce another propositional variable \( s \), defined as follows \( s \leftrightarrow \lor_{c_r \in \mathcal{K}\setminus\{c_s\}} p_r \), such that \( s = 1 \) would mean that the prediction changes. However, this is unnecessary.)

Given the above, we can write down a propositional encoding for a DS classifier which respects (22). The set of soft clauses is given by:

\[
\mathcal{S} \triangleq \{(l_i), i = 1, \ldots, m\} \tag{23}
\]

The set of hard clauses is given by:

\[
\mathcal{B} \triangleq \bigwedge_{1 \leq i \leq m} e_{x_i = v_i}(l_i, \ldots) \land \bigwedge_{1 \leq r \leq K} \bigwedge_{1 \leq j \leq n_r} e_{t_{rj}}(t_{rj}, \ldots) \land \\
\bigwedge_{1 \leq j \leq K} p_r \leftrightarrow (\lor_{j=1}^{n_r} t_{rj}) \tag{24}
\]

### 4.5 Explaining Neural Networks

To illustrate the modeling flexibility of the approach proposed in the previous section, let us develop an MILP/SMT encoding for the problem of computing one AXp for a neural network. The encoding to be used is based on the MILP representation of NNs proposed in earlier work [123] and is illustrated with the NN running example of Figure 3. The MILP encoding is shown in Figure 7a.

To decide whether a set \( \mathcal{X} \subseteq \mathcal{F} \) is a weak AXp, we would have to decide the inconsistency of (adapted from Figure 7a):

\[
\bigwedge_{i \in \mathcal{X}} (x_i = v_i) \land [ (x_1 + x_2 - 0.5 = t_1 - s_1) \land (z_1 = 1 \rightarrow t_1 \leq 0) \land (z_1 = 0 \rightarrow s_1 \leq 0) \land (o_1 = (t_1 > 0)) \land (t_1 \geq 0) \land (s_1 \geq 0) ] \land [(o_1 \neq 1)] \tag{25}
\]

where \( \mathcal{D}_{x_1} = \mathcal{D}_{x_2} = \mathcal{D}_{z_1} = \mathcal{D}_{s_1} = \{0, 1\} \) and \( \mathcal{D}_{t_1} = \mathcal{D}_{o_1} = \mathbb{R} \). (The definition of domains introduces a mild abuse of notation, since the indices used are the names of feature variables and not the names of features. However, the meaning is clear.)

**Example 19.** To compute an AXp for the NN running example, we could iteratively call an MILP solver on (25), starting from \( \mathcal{F} \) and iteratively removing features (see Algorithm 1). However, the very simple encoding for the example NN allows us to analyze the constraints without calling an MILP reasoner. The analysis is summarized in Figure 7. We first consider allowing \( x_1 \) to take any value. In this case, this means allowing \( x_1 \) to take value 0 (besides the value 1 it is assigned to). As can be observed (see Figure 7b), the prediction is allowed to change (actually, in this case it is forced to change). Hence, the feature 1 must be included in the AXp. In contrast, by changing \( x_2 \) from 0 to 1, the prediction...
\[ x_1 + x_2 - 0.5 = t_1 - s_1 \]
\[ z_1 = 1 \Rightarrow t_1 \leq 0 \]
\[ z_1 = 0 \Rightarrow s_1 \leq 0 \]
\[ o_1 = (t_1 > 0) \]
\[ x_1, x_2, z_1, o_1 \in \{0, 1\} \]
\[ t_1, s_1 \geq 0 \]

(a) Logic representation [123]

\[ x_1 = 1, x_2 = 0, z_1 = 0, o_1 = 1 \]
\[ t_1 = 0, s_1 = 0 \]

(b) Instance \((x, c) = ((1, 0), 1)\)

\[ 0 + 0 - 0.5 = 0 - 0.0 \]
\[ 0 \lor 0 \leq 0 \]
\[ 1 \lor 0.5 \leq 0 \]
\[ 0 = (0 > 0) \]
\[ x_1 = 0, x_2 = 0, z_1 = 1, o_1 = 0 \]
\[ t_1 = 0, s_1 = 0.5 \]

(c) Checking \((x_1, x_2) = (0, 0)\)

\[ 1 + 0 - 0.5 = 0.5 - 0 \]
\[ 1 \lor 0.5 \leq 0 \]
\[ 0 \lor 0 \leq 0 \]
\[ 1 = (0.5 > 0) \]
\[ x_1 = 1, x_2 = 1, z_1 = 0, o_1 = 1 \]
\[ t_1 = 1.5, s_1 = 0 \]

(d) Checking \((x_1, x_2) = (1, 1)\)

Fig. 7: Computing one AXp with an NN

cannot change (see Figure 7d). This means that, if the other features remain unchanged, the prediction is 1, no matter the value taken by \(x_2\). Hence, the feature 2 is dropped from the working set of features. As a result, the AXp in this case is \(X' = \{1\}\). ⋄

The computation of AXp’s in the case of NNs was investigated in earlier work on computing formal explanations [178]. However, and in contrast with the families of classifiers studied earlier in this section, the computation of AXp’s/CXp’s in the case of NNs scales up to a few tens of neurons. It is plain that the ability to efficiently compute AXp’s/CXp’s for NNs will track the ability to reason efficiently about NNs. Although there have been steady improvements on reasoners for NNs [202, 203, 229], it is also the case that scalability continues to be a challenge.

4.6 Other Families of Classifiers

**Tree ensembles (TEs).** Based on the general approach detailed in Section 4.2, there have been proposals for computing explanations for boosted trees (BTs) [170, 172, 180], and random forests (RFs) [65, 191]. For RFs, it has been shown that the decision problem of computing one AXp is complete for \(D^p [191]\). Nevertheless, the proposed encodings [191], which are purely propositional, enable computing AXp’s/CXp’s for RFs with thousands of nodes. At present, such RF sizes are representative of what is commonly deployed in practical applications. It should
be noted that the existing propositional encodings consider the organization of RFs as proposed originally [69], i.e. the class is picked by majority voting. For other ways of selecting the chosen class, the encoding is not purely propositional. For BTs, the most recent results also confirm the scalability to classifiers deployed in practical settings.

**Bayesian network classifiers.** The explanations of Bayesian network classifiers (BNCs) have been studied since 2018 [320, 321]. Whereas in the case of NNs, SMT and MILP solvers were used, and followed the approach outlined in Section 4.2, in the case of BNCs, explanations are computed using compilation into a canonical representation (see Section 4.7 below). However, and similarly to NNs, scalability is currently a challenge.

4.7 An Alternative – Compilation-Based Approaches

One alternative to the computation of AXp’s and CXp’s as proposed in the previous sections is to compile the explanations into some canonical representation, from which the explanations can then be queried for. Such compilation-based approaches have been studied in a number of works [96–99, 319–321]. Past work has focused on binary classification with binary features. The extension to non-binary classification and non-binary features raises a number of challenges. Another limitation is that canonical representations are worst-case exponential, and the worst-case behavior is commonly observed. For example, the performance gap between the two approaches in solving related problems is often significant [99, 187].

5 Tractable Explanations

Since 2020, several tractability results have been established in formal explainability [84, 165, 166, 186, 187, 239, 240]. Most of these tractability results concern the computation of one explanation, and apply both to computing one AXp or one CXp [84]. However, there are examples of families of classifiers for which there exist polynomial delay algorithms for enumeration of explanations [239], or even for computing all (contrastive) explanations [166, 187].

5.1 Decision Trees

Given a classification problem for a DT, and an instance \((v, c)\), a set of literals is consistent with \(c\) as long there is at least one inconsistent literal for any path that predicts a class other than \(c\).

**Abductive explanations.** Given the observation above, a simple algorithm for computing one AXp is organized as follows:
1. For each path \(Q_k\) with prediction other than \(c\), let \(I_k\) denote the features which take values inconsistent with the path.
2. Pick a subset-minimal hitting set $H$ of all the sets $I_k$.
3. Clearly, as long as the features in $H$ are fixed, then at least one literal in each path $Q_k$ will be inconsistent, and so the prediction is guaranteed to be $c$.

It is well-known that there exists simple polynomial time algorithms for computing one subset-minimal hitting set $[112]$. Hence, the proposed algorithm runs in polynomial time.

**Example 20.** For the DT of the second running example (see Figure 2a), and instance $(v, c) = ((0, 0, 1, 0, 1), 1)$, we have the following sets:
- $Q_1 = \langle 1, 2, 4, 6 \rangle$, with set $I_1 = \{3\}$.
- $Q_2 = \langle 1, 2, 4, 7, 10, 14 \rangle$, with set $I_2 = \{5\}$.
- $Q_3 = \langle 1, 2, 5, 8, 12 \rangle$, with set $I_3 = \{2, 5\}$.

Clearly, an MHS of $\{I_1, I_2, I_3\}$ is $\{3, 5\}$, which represents a weak AXp for the given instance. It is simple to conclude that it is irreducible, and so it effectively represents an AXp. In addition, it is also plain to establish that there are no other AXp’s. Finally, it should be noted that the abductive explanation computed above concurs with what was presented in Example 11, where a truth-table was used to justify the abductive explanations. (Of course, construction of the truth table would not in general be realistic, whereas the algorithm proposed above runs in linear time on the size of the DT.)

The simple algorithm described above was first proposed in earlier work $[186]$. Nevertheless, one can envision other algorithms, which offer more flexibility $[187]$. (For example, the algorithm described below allows for constraints on the inputs, in cases for which not all points in feature space are possible.)

**Abductive explanations by propositional Horn encoding.** A more flexible approach (see Section 8) is the representation of the problem of computing one AXp as the problem of computing one MUS (or one MCS) of an inconsistent Horn formula$^{18}$. There are simple encodings that are worst-case quadratic on the size of the DT $[187]$. We describe one encoding that is linear on the size of the DT $[187]$.

Let us consider a path $P_k$, with prediction $c \in K$. Moreover, let $Q$ denote the paths yielding a prediction other than $c$. Since the prediction is $c$, then any path in $Q$ has some feature for which the allowed values are inconsistent with $v$. We say that the paths in $Q$ are **blocked**. (To be clear, a path is blocked as long as some of its literals are inconsistent.)

For each feature $i$ associated with some node of path $P_k$, introduce a variable $u_i$. $u_i$ denotes whether feature $i$ is deemed universal, i.e. feature $i$ is not included in the AXp that we will be computing. (Our goal is to find a subset maximal set of features that can be deemed universal, such that all the paths resulting in a prediction other than $c$ remain blocked. Alternatively, we seek to find a

$^{18}$ Since we have tractability, the formulation can be geared towards computing one MUS or instead computing one MCS.
subset-minimal set of features to declare non-universal or fixed, such that paths with a prediction other than $c$ remain blocked. Furthermore, for each DT node $r$, introduce variable $b_r$, denoting that all sub-paths from node $r$ to any terminal node labeled $d \in \mathcal{K} \setminus \{c\}$ must be blocked, i.e. some literal in the sub-path must remain inconsistent. (Our goal is to guarantee that all paths to terminal nodes labeled $d \in \mathcal{K} \setminus \{c\}$ remain blocked even when some variables are allowed to become universal.)

The soft clauses $S$ are given by $\{ (u_i) \mid i \in \mathcal{F} \}$, i.e. one would ideally want to declare universal as many features as possible, thus minimizing the size of the explanation. (As noted above, we will settle for finding subset-maximal solutions.)

We describe next the hard constraints $\mathcal{H}$ for representing consistent assignments to the $u_i$ variables.

We proceed to describe the proposed Horn encoding. Here, we opt to describe first the Horn encoding for computing one AXp. The hard constraints are created as follows:

B1. For the root node $r$, add the constraint $\top \rightarrow b_r$.
(The root node must be blocked.)

B2. For each terminal node $r$ with prediction $c$, add the constraint $\top \rightarrow b_r$.
(Each terminal node with prediction $c$ is also blocked. Also, observe that this condition is on the node, not on the path.)

B3. For each terminal node $r$ with prediction $d \in \mathcal{K} \setminus \{c\}$, add the constraint $b_r \rightarrow \bot$.
(Terminal nodes predicting $d \neq c$ cannot be blocked. Also, and as above, observe that this condition is on the node, not on the path.)

B4. For a node $r$ associated with feature $i$, and connected to the child node $s$, such that the edge value(s) is(are) consistent with the value of feature $i$ in $v$, add the constraint $b_r \rightarrow b_s$.
(If all sub-paths from node $r$ must be blocked, then all sub-paths from node $s$ must all be blocked, independently of the value taken by feature $i$.)

B5. For a node $r$ associated with feature $i$, and connected to the child node $s$, such that the edge value(s) is(are) inconsistent with the value of feature $i$ in $v$, add the constraint $b_r \land u_i \rightarrow b_s$.
(In this case, the blocking condition along an edge inconsistent with the value of feature $i$ in $v$ is only relevant if the feature is deemed universal.)

Example 21. For the running example of Figure 2a, let $(v, c) = ((0, 0, 1, 0, 1), 1)$. As dictated by the proposed Horn encoding, two sets of variables are introduced. The first set represents the variables denoting whether a feature is universal, corresponding to 5 variables: $\{u_1, u_2, u_3, u_4, u_5\}$. The second set represents the variables denoting whether a node is blocked, corresponding to 15 variables: $\{b_1, b_2, b_3, b_4, b_5, b_6, b_7, b_8, b_9, b_{10}, b_{11}, b_{12}, b_{13}, b_{14}, b_{15}\}$. The resulting propositional Horn encoding contains hard ($\mathcal{H}$) and soft ($\mathcal{B}$) constraints, and it is organized as shown in Table 5.

19 As discussed in recent work [187], different types of AXp’s can be computed in the case of DTs; we specifically consider the so-called path-unrestricted AXp’s.
Table 5: Horn clauses for the DT of Figure 2a for computing one AXp with $(v, c) = ((0, 0, 1, 0, 1), 1)$

| Hard constraint type | Horn clauses |
|----------------------|--------------|
| B1                   | $\{(b_1)\}$  |
| B2                   | $\{(b_3), (b_9), (b_{11}), (b_{13}), (b_{15})\}$ |
| B3                   | $\{(-b_6), (-b_{12}), (-b_{14})\}$ |
| B4                   | $\{(b_1 \rightarrow b_2), (b_2 \rightarrow b_4), (b_4 \rightarrow b_7), (b_5 \rightarrow b_8), (b_7 \rightarrow b_{10}), (b_8 \rightarrow b_{13}), (b_{10} \rightarrow b_{15})\}$ |
| B5                   | $\{(b_1 \land u_1 \rightarrow b_3), (b_2 \land u_2 \rightarrow b_5), (b_4 \land u_3 \rightarrow b_6), (b_5 \land u_4 \rightarrow b_9), (b_7 \land u_4 \rightarrow b_{11}), (b_8 \land u_5 \rightarrow b_{12}), (b_{10} \land u_5 \rightarrow b_{14})\}$ |

Soft constraints, $\mathcal{S}$

- $(u_1), (u_2), (u_3), (u_4), (u_5)$

It is easy to see that, if $u_1 = u_2 = u_3 = u_4 = u_5 = 1$, then $\mathcal{B}$ is falsified. Concretely, $(b_1) \land (b_1 \rightarrow b_2) \land (b_2 \rightarrow b_4) \land (u_3) \land (b_4 \land u_3 \rightarrow b_6) \land (\neg b_6) \not\equiv \bot$. The goal is then to find a maximal subset $\mathcal{M}$ of $\mathcal{S}$ such that $\mathcal{M} \cup \mathcal{B}$ is consistent. (Alternatively, the algorithm finds a minimal set $\mathcal{C} \subseteq \mathcal{S}$, such that $\mathcal{S} \setminus \mathcal{C} \cup \mathcal{H}$ is consistent.) For this concrete example, one such minimal set is obtained by picking $u_1 = u_2 = u_4 = 1$ and $u_3 = u_5 = 0$, and by setting $b_1 = b_2 = b_3 = b_4 = b_5 = b_7 = b_8 = b_9 = b_{10} = b_{11} = b_{13} = b_{15} = 1$ and $b_6 = b_{12} = b_{14} = 0$. Hence, all clauses are satisfied, and so $\{3, 5\}$ is a weak AXp. An MCS extractor [241, 256, 257] would confirm that $\{3, 5\}$ is subset-minimal, and so it is an AXp.

**Contrastive explanations.** In the case of DTs, recent work devised efficient polynomial-time algorithms for computing (in fact listing all) contrastive explanations [166]. The main ideas can be summarized as follows:

- For each path $Q_k$ with prediction other than $c$, list the features with literals inconsistent with the instance as set $I_k$.
- Remove any set $I_l$ that is a superset of some other set $I_k$.
- Each of the remaining sets $I_k$ is a CXp.

Since the number of paths is polynomial (in fact linear) on the number of tree nodes, then we have a polynomial time algorithm for listing all contrastive explanations.

**Example 22.** Using the sets $I_k$ computed in Example 20, we observe that $I_3$ is a superset of $I_2$, and so it has to be dropped. As a result, $I_1$ and $I_2$ each represent an CXp. Furthermore, we can confirm again Proposition 5, since the only AXp for this instance, i.e. $\{3, 5\}$ is an MHS of the two CXp’s, i.e. $\{3\}$ and $\{5\}$, and vice-versa.
As noted in recent work, the fact that there exists a polynomial time algorithm to enumerate all CXp’s, implies that are quasi-polynomial algorithms for the enumeration of AXp’s \[166, 187\]. This is discussed in further detail in Section 6.1.

Moreover, and although the Horn encoding proposed earlier for computing one AXp could also be used for computing one CXp, there is no real need for that, given the simplicity of the algorithm for enumerating all CXp’s of a DT.

### 5.2 Monotonic Classifiers

This section illustrates how one AXp (or CXp) can be computed in the case of monotonic classifiers. In the case of classifiers for which computing the prediction runs in polynomial time on the size of the classifier, recent work proved that there exist polynomial time algorithms both for computing one AXp and one CXp \[240\]. The algorithms are dual of each other; as a result, we will just detail the computation of one AXp. Nevertheless, we present the pseudo-code for both algorithms. For computing one AXp, we maintain two vectors, one yielding a lower bound on the computed class, i.e. \(v_L\), and another yielding an upper bound on the computed class, i.e. \(v_U\). In the case of one AXp, the algorithm requires that \(\kappa(v_L) = \kappa(v_U) = \kappa(v)\). The goal is to allow features to take any possible value in their domain, i.e. to make them universal and so we will use an auxiliary function \text{FreeAttr}:

\[
\begin{align*}
\text{v}_L &\leftarrow (v_{L1}, \ldots, \lambda(i), \ldots, v_{LN}) \\
\text{v}_U &\leftarrow (v_{U1}, \ldots, \mu(i), \ldots, v_{UN}) \\
(A, B) &\leftarrow (A \setminus \{i\}, B \cup \{i\}) \\
\text{return } (v_L, v_U, A, B)
\end{align*}
\]

If making a feature universal allows the prediction to change, then the feature must be fixed again (to the value dictated by \(v\)), and for that we use the auxiliary function \text{FixAttr}:

\[
\begin{align*}
\text{v}_L &\leftarrow (v_{L1}, \ldots, v_i, \ldots, v_{LN}) \\
\text{v}_U &\leftarrow (v_{U1}, \ldots, v_i, \ldots, v_{UN}) \\
(A, B) &\leftarrow (A \setminus \{i\}, B \cup \{i\}) \\
\text{return } (v_L, v_U, A, B)
\end{align*}
\]

Given these auxiliary functions, the computation of one AXp is shown in Algorithm 3 (and the computation of one CXp is shown in Algorithm 4).

The algorithm starts from some set \(S \subseteq \mathcal{F}\) (which can be the empty set) of universal features, which is required to ensure that \(\kappa(v_L) = \kappa(v_U) = \kappa(v)\), and iteratively attempts to add features to set \(S\), i.e. to make them universal. Monotonicity of entailment (and the discussion in previous sections) ensures soundness of the algorithm.

**Example 23.** For the monotonic classifier of Figure 4, and instance \(((Q, X, H, R), M) = ((10, 10, 5, 0), A)\), we show how one AXp can be computed. For each feature \(i\), \(1 \leq i \leq 4\), \(\lambda(i) = 0\) and \(\mu(i) = 10\). Moreover, features are analyzed in order: \((1, 2, 3, 4)\); the order is arbitrary. The algorithm’s execution is summarized in Table 6.
Algorithm 3 Computing one AXp for a monotonic classifier

Input: Features $F$, Seed $S \subseteq F$, Point in $F^v$
Output: One AXp $P$

1: procedure oneAXp($F; S, v$)
2:   $v_L \leftarrow (v_1, \ldots, v_N)$
3:   $v_U \leftarrow (v_1, \ldots, v_N)$ \Comment{Ensures: $\kappa(v_L) = \kappa(v_U)$}
4:   $(C, D, P) \leftarrow (F, \emptyset, \emptyset)$
5:   for all $i \in S$ do \Comment{Require: $\kappa(v_L) = \kappa(v_U)$, given $S$}
6:     $(v_L, v_U, C, D) \leftarrow \text{FreeAttr}(i, v, v_L, v_U, C, D)$
7:   for all $i \in F \setminus S$ do \Comment{Loop inv.: $\kappa(v_L) = \kappa(v_U)$}
8:     $(v_L, v_U, C, D) \leftarrow \text{FreeAttr}(i, v, v_L, v_U, C, D)$
9:     if $\kappa(v_L) \neq \kappa(v_U)$ then \Comment{If invariant broken, fix it}
10:    $(v_L, v_U, D, P) \leftarrow \text{FixAttr}(i, v, v_L, v_U, D, P)$
11:   return $P$

Algorithm 4 Computing one CXp for a monotonic classifier

Input: Features $F$, Seed $S \subseteq F$, Point in $F^v$
Output: One CXp $P$

1: procedure oneCXp($F; S, v$)
2:   $v_L \leftarrow \lambda(1), \ldots, \lambda(N))$
3:   $v_U \leftarrow \mu(1), \ldots, \mu(N))$ \Comment{Ensures: $\kappa(v_L) \neq \kappa(v_U)$}
4:   $(C, D, P) \leftarrow (F, \emptyset, \emptyset)$
5:   for all $i \in S$ do \Comment{Require: $\kappa(v_L) \neq \kappa(v_U)$, given $S$}
6:     $(v_L, v_U, C, D) \leftarrow \text{FixAttr}(i, v, v_L, v_U, C, D)$
7:   for all $i \in F \setminus S$ do \Comment{Loop inv.: $\kappa(v_L) \neq \kappa(v_U)$}
8:     $(v_L, v_U, C, D) \leftarrow \text{FixAttr}(i, v, v_L, v_U, C, D)$
9:     if $\kappa(v_L) = \kappa(v_U)$ then \Comment{If invariant broken, fix it}
10:    $(v_L, v_U, D, P) \leftarrow \text{FreeAttr}(i, v, v_L, v_U, D, P)$
11: return $P$

As can be observed, features 1 and 2 are kept as part of the AXp, and features 3 and 4 are dropped from the AXp. Thus, the AXp for the given instance is $\{1, 2\}$, representing the literals $\{Q = 10, X = 10\}$.

Besides monotonic classifiers, recent work that similar ideas have been shown to apply in the case of other (related) families of classifiers [84].

5.3 Other Families of Classifiers

A number of additional tractability results have been uncovered. Recent work [166] showed that the computation of explanations for decision graphs [279], decision diagrams and trees could be unified, and explanations computed in polynomial
Table 6: Execution of algorithm for finding one AXp

| Feat | Initial values | Changed values | Predictions | Dec | Resulting values |
|------|----------------|----------------|-------------|-----|-----------------|
| 1    | (10,10,5,0)   | (10,10,5,0)   | (10,10,5,0) | C   | ✓               |
| 2    | (10,10,5,0)   | (10,10,5,0)   | (10,10,5,0) | E   | ✓               |
| 3    | (10,10,5,0)   | (10,10,0,0)   | (10,10,5,0) | A   | ✗               |
| 4    | (10,10,0,0)   | (10,10,10,0)  | (10,10,10,10)| A   | ✗               |

6 Explainability Queries

Besides the computation of explanations, recent research considered a number of explainability queries [25, 29, 163, 166, 167, 177, 239]. This section considers two concrete queries: enumeration of explanations and feature membership. Additional queries have been investigated in the listed references.

Enumeration addresses a crucial problem in explainability. If a human decision maker does not accept the (abductive or contrastive) explanation provided by an explanation tool, how can one compute some other explanation, assuming one exists? Most non-formal explainability approaches do not propose a solution to this problem. The problem of feature membership is to decide whether some (possibly sensitive) feature is included in some explanation of an instance, among all possible explanations. Feature membership is relevant when assessing whether a classifier can exhibit bias.

6.1 Enumeration of Explanations

Given an explanation problem, and some set of already computed explanations (AXp’s and/or CXp’s), the query of enumeration of explainability is to find one explanation (AXp or CXp) among those that are not included in the set of explanations.

For NBCs, it has been shown that there is a polynomial-delay algorithm for the enumeration AXp’s [239]. A similar approach yields a solution for the enumeration of CXp’s.

For most other families of classifiers, it is conceptually simple to devise algorithms that enumerate CXp’s, without the need of computing or enumerating AXp’s. In contrast, the enumeration of AXp’s is obtained through duality between AXp’s and CXp’s (see Section 3.4 and additional detail in [177]). One
Algorithm 5 Finding all AXp/CXp

**Input:** Parameters $P_{\text{axp}}$, $P_{\text{cxp}}$, $T$, $F$, $\kappa$, $v$

1: $H \leftarrow \emptyset$  \hspace{1cm} $\triangleright$ $H$ defined on set $U = \{u_1, \ldots, u_m\}$
2: repeat
3: \hspace{1cm} $(\text{outc}, u) \leftarrow \text{SAT}(H)$
4: \hspace{1cm} if $\text{outc} = \text{true}$ then
5: \hspace{2cm} $S \leftarrow \{i \in F \mid u_i = 0\}$  \hspace{1cm} $\triangleright$ $S$: fixed features
6: \hspace{2cm} $U \leftarrow \{i \in F \mid u_i = 1\}$  \hspace{1cm} $\triangleright$ $U$: universal features; $F = S \cup U$
7: \hspace{2cm} if $P_{\text{cxp}}(U; T, F, \kappa, v)$ then  \hspace{1cm} $\triangleright$ $U \supseteq$ some CXp
8: \hspace{3cm} $P \leftarrow \text{oneXP}(U; P_{\text{cxp}}, T, F, \kappa, v)$
9: \hspace{3cm} reportCXp($P$)
10: \hspace{2cm} $H \leftarrow H \cup \{(v_i \in P \iff u_i)\}$
11: \hspace{2cm} else  \hspace{1cm} $\triangleright$ $S \supseteq$ some AXp
12: \hspace{3cm} $P \leftarrow \text{oneXP}(S; P_{\text{axp}}, T, F, \kappa, v)$
13: \hspace{3cm} reportAXp($P$)
14: \hspace{2cm} $H \leftarrow H \cup \{(v_i \in P \iff u_i)\}$
15: until $\text{outc} = \text{false}$

Solution for enumerating AXp’s is to compute all CXp’s, and then use hitting set dualization for computing the AXp’s. Unfortunately, the number of CXp’s is often exponential, and this may prevent the enumeration of any AXp. Thus, and building on fairly recent work on the enumeration of MUSes [226], the solution is to iteratively compute AXp’s/CXp’s by exploiting hitting set duality, using a SAT solver for iteratively picking a set of features to serve as a seed for either computing one AXp or one CXp. A number of recent works have reported results on the enumeration of explanations [165, 172, 174, 240]. The query of explanation enumeration has also been studied in terms of its complexity [25, 29]. One important observation is that, for families of classifiers for which computing one explanation is poly-time, then the enumeration of the next explanation (either AXp or CXp) requires a single call to an NP oracle [240].

A general-purpose approach for the enumeration of explanations is shown in Algorithm 5\textsuperscript{20}. Variants of this algorithm have been studied in recent work [165, 166, 172, 174, 177, 240].

\textsuperscript{20} The algorithm mimics the on-demand MUS enumeration algorithm proposed elsewhere [225, 226, 289], which enumerates both MUSes and MCSes. There are several other alternative MUS enumeration algorithms, which could also be considered [34, 35, 37, 46–48, 63, 86, 127, 148, 204–207, 225, 236, 270, 300]. For some of these algorithms, a first required step is the complete enumeration of MCSes, for which a wealth of algorithms also exists [121, 146, 147, 227, 241, 256, 257, 265, 290, 291]. Furthermore, there is a tight relationship between MUS/MCS enumeration and several other computational problems [245, 246], which allows devising generic algorithms for solving families of related problems.
Example 24. For the DT of Figure 2, Tables 7 and 8 show possible executions of the explanation enumeration algorithm. The difference between the two tables is the assignments picked by the SAT solver. (Tables 2a and 2b are used to decide the values of the predicates tested in the algorithm’s execution.) Depending on that assignment \( u \), either there is a pick of features that changes the prediction or there is none. If the prediction can be changed, then one CXp is computed. Otherwise, one AXp is computed. In both cases, Algorithm 1 is used, but a different predicate is considered in each case. The clause added after each AXp/CXp is computed prevents the repetition of explanations. The algorithm terminates when all AXp’s/CXp’s have been enumerated.

As noted in recent work [166, 187], and in the case of DTs, the fact that all CXp’s are computed in poly-time enables using more efficient quasi-polynomial algorithms for the enumeration of AXp’s (e.g. using well-known results in monotone dualization [127]).

6.2 Explanation Membership

The problem of deciding whether a given (possibly sensitive) feature is included in some explanation is referred to as the feature membership problem (FMP) [166].

Definition 3 (FMP). Given an explanation problem \( \mathcal{E}_L = (\mathcal{M}, v, c) \), with \( \mathcal{M} = (\mathcal{F}, \mathcal{D}, \mathcal{P}, \mathcal{K}, \kappa) \), and some target feature \( t \in \mathcal{F} \), the feature membership
problem is to decide whether there exists an AXp (resp. CXp) \( X \subseteq F \) (\( Y \subseteq F \)) such that \( t \in X \) (resp. \( t \in Y \)).

It should be observed that FMP is tightly related with queries in logic-based abduction, namely relevancy/irrelevancy \cite{111, 128, 313}.

Example 25. For the DL of Figure 1a, and the instance \((v, c) = ((0, 0, 1, 2), 1)\), from the list of explanations, \( A = \{\{1, 4\}\} \) (for the AXp’s), and \( C = \{\{1\}, \{4\}\} \) (for the CXp’s), it is plain that features 2 and 3 and not included in any explanation, and 1 and 4 are included in some explanation.

The MHS duality between AXp’s and CXp’s yields the following result:

Proposition 8. Given an explanation problem \( \mathcal{E}_L = (\mathcal{M}, v, c) \), with \( \mathcal{M} = (\mathcal{F}, \mathcal{D}, \mathcal{P}, \mathcal{K}, \kappa) \), and some target feature \( t \in \mathcal{F} \), \( t \) is included in some AXp of \( \mathcal{E}_L \) iff \( t \) is included in some CXp of \( \mathcal{E}_L \).

Hence, when devising algorithms for FMP, one can either study the membership in some AXp or the membership in some CXp.

FMP has a simple QBF formulation:

\[
\exists (X \subseteq \mathcal{F}), [(t \in X) \land AXp(X) \land (\forall (X' \subseteq X).\neg AXp(X'))]
\]

There are several optimizations that can be introduced to this basic QBF formulation, but that is beyond the scope of this document. More importantly, there are some known results about the complexity of FMP. These can be briefly summarized as follows,

Proposition 9 (\cite{166}). FMP for a DNF classifier is \( \Sigma_2^p \)-hard.

Since a DNF classifier can be reduced to more expressive classifiers, like RFs and other tree ensembles like BTs, but also NNs, then we have the following result,

Proposition 10. FMP is \( \Sigma_2^p \)-hard for RFs, BTs and NNs.

One important recent result has been the proof of membership in \( \Sigma_2^p \). As a result, one solution approach for FMP is the use of QBF/2QBF solvers \cite{55}\footnote{There have been observable improvements in the performance of QBF solvers in recent years, which can largely be attributed to the use of abstraction refinement methods \cite{193–195, 295, 296}.}.

Despite the complexity of FMP in general settings, there are families of classifiers for which deciding FMP is in P \cite{166}. An immediate consequence of the fact that CXp’s can be enumerated in polynomial time for DTs is:

Proposition 11 (\cite{166}). FMP for a DT is in P.

More recently, additional results on FMP have been proved,
Proposition 12 ([168]). For a classifier for which it is in P to decide whether a set of features is a WAXp, then deciding FMP is in NP.

Proof. [Sketch] To prove that FMP is in NP in this case, one proceeds as follows. First, one guesses (non-deterministically) a set \( X \) containing the target feature \( t \). By hypothesis, this set is decided to be a weak AXp in poly-time. Next, we show that removing any feature causes the resulting set to no longer represent a weak AXp. Once again, by hypothesis there exists a polynomial time algorithm for deciding whether such a reduced set is a WAXp. Thus, deciding FMP is in P. \( \square \)

6.3 Additional Explainability Queries

A wealth of additional explainability queries have been studied in recent years [25, 29, 101]. Examples include finding mandatory and/or forbidden features, counting and/or enumerating instances, among others. Queries can be broadly categorized as class queries or explanation queries [25, 29]. Examples of class queries include mandatory/forbidden features for a class and necessary features for a class. Examples of explanation queries include finding smallest AXp’s, finding one AXp and finding one CXp. Some of these queries have been studied earlier in this document as well. Complexity-wise, [25] proves the NP-hardness of these queries for the families of classifiers DLs, RFs, BTs, boolean NNs, and binaireized NNs (BNNs). In contrast, and also as shown in this paper, for DTs, most queries can be answered in polynomial time. It should be noted that some of the queries studied in recent work can also be related with queries in logic-based abduction [111, 128, 313], concretely relevancy/irrelevancy but also necessity. More recent work on feature relevancy in explanations includes dedicated algorithms for arbitrary classifiers [167], and NP-hardness proofs for some families of classifiers [163].

Validation of ML models. Recent work [74] illustrates the use of formal explanations for identifying apparent flaws in ML models. For example, the DT shown in Figure 8 has been proposed in the field of medical diagnosis [224], aiming at providing a solution for non-invasive diagnosis of Meningococcal Disease (MD) meningitis. (The actual feature names, and their domains, are shown in Table 9.) Unfortunately, the DT has a number of issues, in that it allows MD meningitis to be diagnosed for patients that exhibit no symptoms whatsoever. The use of formal explanations, namely AXp’s, allows demonstrating these issues.

As one concrete example, the computation of AXp’s allows concluding that MD meningitis will be predicted whenever a patient has more than 5 years of age and lives in a rural area, i.e. without exhibiting any symptoms of the disease, at least among those tested for. To prove that this is the case, one considers the path \( \langle 1, 3, 6, 8, 10, 14 \rangle \), and confirms that there is an explanation that does not include any of the symptoms (i.e. Petechiae, Stiff neck, and Vomiting). Here, the
Fig. 8: Decision tree adapted from [224, Fig. 9]

query is to assess the existence of explanations for which the symptoms need not
be tested for. The conclusion is that one can diagnose MD meningitis without
testing any of the symptoms of meningitis.

As the previous example illustrates, reasoning about formal explanations, in-
cluding different kinds of queries, can serve to help decision makers in assessing
whether an ML model offers sufficient guarantees of quality to be deployed. The
previous example also illustrates the fundamental importance of formal verification of ML models [242, 315] in reduce the likelihood of accidents [53].

7 Probabilistic Explanations

The cognitive limits of human beings are well-known [260]. Unfortunately, it is also the case that formal explanations are often larger than such cognitive limits. One possible solution is to compute explanations that are not as rigorous as AXp’s, but which offer strong probabilistic guarantees of rigor. We refer to these explanations as probabilistic explanations. There is recent initial work on the complexity of computing probabilistic explanations [354, 355], where the name probabilistic prime implicants is used. Following more recent work [185, 189, 190, 192], we will use the term(s) (weak) probabilistic abductive explanations ((W)PAxP’s). To simplify the section contents, features are assumed to be categorical or ordinal, in which case the values are restricted to being boolean or integer.

7.1 Problem Formulation

A probabilistic (weak) AXp generalizes the definition of weak AXp, by allowing the prediction to change in some points of feature space, where a weak AXp would require the prediction not to change, but such that those changes have small probability. One is thus interested in sets $X \subseteq F$ such that,

$$\text{Pr}(\kappa(x) = c \mid x = v, x = v) \geq \delta$$

(26)
where \(0 < \delta \leq 1\) is some given threshold, and \(x_X = v_X\) holds for any point in feature space for which \(\land_{i \in X}(x_i = v_i)\). Clearly, for \(\delta = 1\), (26) corresponds to stating that,
\[
\forall (x \in F). \left[ \land_{i \in X}(x_i = v_i) \right] \rightarrow (\kappa(x) = c) \tag{27}
\]
Recent work [354, 355] established that, for binary classifiers represented by boolean circuits, it is \(\text{NP}^{\text{PP}}\)-complete to decide the existence of a set \(X \subseteq F\), with \(|X| \leq k\), such that (26) holds. Despite this unwieldy complexity, it has been shown that for specific families of classifiers [185, 190, 192], it is computationally easier and practically efficient to compute (approximate) subset-minimal sets such that (26) holds. Concretely, instead of (4), we will instead consider:
\[
\text{WeakPAXp}(X; F, \kappa, v, c, \delta) := \Pr_x(\kappa(x) = c \mid x_X = v_X) \geq \delta \tag{28}
\]
where \(\text{WeakPAXp}\) denotes a weak probabilistic AXp (PAXp). Similarly to the deterministic case, a PAXp is a subset-minimal weak AXp. A set \(X \subseteq F\) such that (28) holds is also referred to as relevant set. In the next section, we will illustrate how PAXp’s are computed in the case of DTs.

### 7.2 Probabilistic Explanations for Decision Trees

**Path Probabilities for DTs.** Next, we investigate how to compute, in the case of DTs, the conditional probability,
\[
\Pr_x(\kappa(x) = c \mid x_X = v_X) \tag{29}
\]
where \(X\) is a set of fixed features (whereas the other features are not fixed, being deemed universal), and \(P_r\) is a path in the DT consistent with the instance \((v, c)\). (Also, note that (29) is the left-hand side of the definition of WeakPAXp in (28) above.) To motivate the proposed approach, let us first analyze how we can compute \(\Pr_x(\kappa(x) = c)\), where \(P \subseteq R\) is the set of paths in the DT with prediction \(c\). Let \(\Lambda(R_k)\) denote the set of literals (each of the form \(x_i \in E_i\)) in some path \(R_k \in R\). If a feature \(i\) is tested multiple times along path \(R_k\), then \(E_i\) is the intersection of the sets in each of the literals of \(R_k\) on \(i\). The number of values of \(D_i\) consistent with literal \(x_i \in E_i\) is \(|E_i|\). 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,
\[
\Pr(R_k) = \left[ \prod_{(x_i \in E_i) \in \Lambda(R_k)} |E_i| \times \prod_{x \in \Psi(R_k)} |D_i| \right] / |F| \tag{30}
\]
As a result, we get that,
\[
\Pr_x(\kappa(x) = c) = \sum_{R_k \in P} \Pr(R_k) \tag{31}
\]
Given an instance \((v, c)\) and a set of fixed features \(X\) (and so a set of universal features \(F \setminus X\)), we now detail how to compute (29). Since some features will
now be declared universal, multiple paths with possibly different conditions can become consistent. 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 (28). Let \( R_k \in \mathcal{R} \) represent some path in the decision tree. (Recall that \( P_i \in \mathcal{P} \) is the target path, which is consistent with \( v \).) Let \( n_{ik} \) represent the (integer) number of assignments to feature \( i \) that are consistent with path \( R_k \). For classifiers represented as boolean circuits, the computation of probabilistic abductive explanations is NP-PP-hard [354, 355]. Motivated by this complexity,

Finally, (29) is given by,

\[
\Pr_{x}(x|\kappa(x) = c| x_{\mathcal{X}} = v_{\mathcal{X}}) = \sum_{p_{k} \in \mathcal{P}} \frac{\#(p_{k};v_{\mathcal{X}})}{\sum_{r_{k} \in \mathcal{R}} \#(r_{k};v_{\mathcal{X}})}
\]

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

**Example 26.** For the DT of Figure 2a, with instance \((v, c) = ((0, 0, 1, 0, 1), 1)\), we know that an AXp is \( \{3, 5\} \). Let \( \delta = 0.85 \), and let us assess whether \( \{5\} \) represents a weak probabilistic explanation. Table 10 shows the path counts given \( \mathcal{X} = \{5\} \) and \( v = (0, 0, 1, 0, 1) \). From the table, we get that,

\[
\Pr_{x}(x|\kappa(x) = c| x_{\mathcal{X}} = v_{\mathcal{X}}) = \sum_{p_{k} \in \mathcal{P}} \frac{\#(p_{k};v_{\mathcal{X}})}{\sum_{r_{k} \in \mathcal{R}} \#(r_{k};v_{\mathcal{X}})} = 14/16 = 0.875
\]

And so, \( \{5\} \) is a weak PAXp.

### 7.3 Additional Results

For classifiers represented as boolean circuits, the computation of probabilistic abductive explanations is NP-PP-hard [354, 355]. Motivated by this complexity,
expected to be beyond the reach of modern reasoners, recent efforts studied specific families of classifiers. In the case of DTs, the approach summarized in the previous section was proposed elsewhere [185, 189, 190], and shown to be effective in practice. Also in the case of DTs, computational hardness results have been proved in more recent work [21, 22]. Furthermore, an approach based on dynamic programming was used for computing probabilistic explanations in the case of NBCs [185, 192].

8 Input Constraints & Distributions

A critical assumption implicit on most work on formal explainability is that all inputs are possible (and equally likely). Unfortunately, this is often not the case. For example, consider a classification problem with features 'order', denoting the animal order, and 'winged', denoting whether the animal has wings. It might be expected that points in feature space having 'order=Proboscidea' (i.e. that includes elephants) and 'winged=true' would be disallowed. In contrast, 'order=Chiroptera' (i.e. that includes bats) and 'winged=true' would be allowed. If such constraints on the features are known a priori, then one can take them into account when computing explanations. However, in most cases, such constraints are unknown. This section summarizes recent work on the general topic of handling of input constraints.

**Constraints on the features.** Let us assume that a given classifier $C$ is characterized by a constraint set $I_C$ capturing the allowed points in feature space. (In general, we view $I_C$ as a predicate, mapping points in feature space into $\{0, 1\}$.) The definition of weak AXp can be adapted to account for such

| Path ($R_k$) | Nodes of $R_k$ | $(R_k; v, X)$ | Obs | Total for $P$ | Total for $Q$ |
|-------------|---------------|--------------|-----|---------------|---------------|
| $P_1$       | $\langle 1, 2, 4, 7, 10, 15 \rangle$ | 1             |     |               |               |
| $P_2$       | $\langle 1, 2, 4, 7, 11 \rangle$     | 1             |     |               |               |
| $P_3$       | $\langle 1, 2, 5, 8, 13 \rangle$     | 2             |     |               |               |
| $P_4$       | $\langle 1, 2, 5, 9 \rangle$         | 2             |     |               |               |
| $P_5$       | $\langle 1, 3 \rangle$               | 8             |     |               |               |
| $Q_1$       | $\langle 1, 2, 4, 6 \rangle$         | 2             |     |               |               |
| $Q_2$       | $\langle 1, 2, 4, 7, 10, 14 \rangle$ | 0             |     |               |               |
| $Q_3$       | $\langle 1, 2, 5, 8, 12 \rangle$     | 0             |     |               |               |

Table 10: Path probabilities for DT of Figure 2a
constraint set as follows,
\[ \forall (x \in F). \left[ \bigwedge_{i \in X} (x_i = v_i) \rightarrow [I_C(x) \rightarrow (\kappa(x) = c)] \right] \]  

(34)

Similarly, the definition of weak CXp can be adapted to account for \( I_C \),
\[ \exists (x \in F). \left[ \bigwedge_{i \notin Y} (x_i = v_i) \land [I_C(x) \land (\kappa(x) \neq c)] \right] \]  

(35)

A number of observations can be made:
1. The definitions of AXp and CXp, given the definitions of input constraint aware weak AXp/CXp’s, remain unchanged.
2. Duality between AXp’s and CXp’s (see Section 3.4) still holds.
3. Depending on the family of classifiers and the representation of the constraints, the complexity of computing one explanation need not change. For example, if the constraints are represented as propositional Horn clauses (and this is the case with propositional rules), then the propositional encoding for computing explanations of DTs will still enable computing explanations in polynomial time.
4. Finally, the same approach can also be used with probabilistic explanations. Given the above, and as long as the allowed points in feature space are represented by a constraint set, then we can take those constraints into account when computing AXp’s and CXp’s. The original ideas on accounting for input constraints were presented in recent work \[145\], and extended more recently for contrastive explanations \[367\]. However, a major difficulty with the handling input constraints is how to infer those input constraints in the first place. A possible solution to this challenge has been proposed in recent work \[367\].

Inferring constraints. When given a dataset and an ML classifier, one can exploit standard ML learning approaches for inferring constraints that are consistent with training data. Recent work studied the learning of rules on the features given the training data \[367\]. The experimental results substantiate the importance of inferring constraints on the features, that also lead to smaller abductive explanations and larger contrastive explanations.

Research directions. Inferring good constraints from training data is a promising direction of research. The goal will be to find the best possible rules, that improve the accuracy of explanations, but that do not impact significantly the performance of formal explainers. Another line of research is to account input distributions when these are either known or can be inferred.

9 Formal Explanations with Surrogate Models

As briefly discussed in Section 2.3, the most visible (non-formal) explainability approaches consist of approximating a complex classifier with a much simpler
classifier (e.g. a linear classifier or a decision tree) which, due to its simplicity, is interpretable and so represents an explanation for the complex classifier [235, 301].

Despite the numerous shortcomings of such line of research (see Section 2.3), it is also the case that approximating complex ML models locally with much simpler (or surrogate) ML models, has been studied in several other works [41, 42, 129]. Furthermore, there has been work on finding surrogate models, that locally approximate a complex ML model, such that computing formal explanations for the surrogate model is efficient in practice [65].

Let \( C \) represent a complex ML model, e.g. a neural network, and let \((v, c)\) represent a target instance. Moreover, let \( A \) represent an approximating (surrogate) ML model, e.g. a random forest, which approximates \( C \) in points of feature space that are sufficiently close to \( v \), i.e. for point \( \mathbf{x} \in F \), with \( ||\mathbf{x} - v|| \leq \epsilon \), for some small \( \epsilon > 0 \), it is the case that \( \kappa_C(\mathbf{x}) \) and \( \kappa_A(\mathbf{x}) \) coincide with high probability. The conjecture out forward in recent work [65] is that a (rigorous) explanation (either \( AXp \) or \( CXp \)) of the instance \((v, c)\) computed for \( A \) is also a sufficiently accurate explanation for \( C \) on the same instance. At present, this novel line of research requires further validation. For example, past work has not shown in practice that formal explanations computed for the surrogate model are sufficiently accurate for the complex model. Although past work considered random forests as the surrogate model, it is plain to conclude that other surrogate models can be considered, e.g. decision trees or NBCs. The reason for considering simpler ML models is that probabilistic explanations can be computed efficiently, and this is not the case with random forests.

10 Additional Topics & Extensions

Links with fairness, robustness, etc. Formal explainability has been related with robustness and fairness. For global explanation problems, it is now known that the minimal hitting sets of abductive explanations (which have been referred to as counterexamples) contain one or more adversarial examples [179]. Moreover, initial links with fairness were investigated in more recent work [171]. Finally, the relationship between model learning and explainability is a topic of future research.

Explanation literals. By definition, the definition of \( AXp \) and \( CXp \) assumes literals based on equality. This is justified by the fact that \( AXp \)'s and \( CXp \)'s are computed with respect to a concrete point in feature space. In some settings, it has been shown that literals based on equality can be generalized to the literals that occur in the model itself. This is the case with decision trees [187], where literals can be defined using the set membership operator, and so explanations can be related with such literals. Similar ideas are yet to be investigated in the case of other ML models.
Localized explanations. Non-formal explainability methods emphasize the local nature of their explanations. In situations where such locality is of interest, one may wonder whether formal explainability can be adapted to further emphasize locality. Given the diverse nature of features, we opt to define the Hamming distance between two points in feature space,

$$D_h(x_1, x_2) = \sum_{i=1}^{m} IT(x_{1i} = x_{2i}, 1, 0)$$

(36)

Given the definition of Hamming distance, we can now propose a definition of localized weak abductive and contrastive explanations.

$$\text{WeakLAXp}(\mathcal{X}) := \forall (x \in \mathcal{F}). \left[ D_h(x, v) \leq \epsilon \land \bigwedge_{i \in \mathcal{X}} (x_i = v_i) \rightarrow (\kappa(x) = c) \right]$$

(37)

$$\text{WeakLCXp}(\mathcal{Y}) := \exists (x \in \mathcal{F}). \left[ D_h(x, v) \leq \epsilon \land \bigwedge_{i \notin \mathcal{Y}} (x_i = v_i) \land (\kappa(x) \neq c) \right]$$

(38)

for some target $\epsilon > 0$. The definitions of subset-minimal sets remain unchanged, i.e. localized AXp’s and CXp’s can be computed using (8) and (9), by replacing WeakAXp and WeakAXp, respectively by WeakLAXp and WeakLCXp. Finally, although we opted to use Hamming distance, (37) and (38) could consider other measures of distance.

Explanations beyond ML. Although at present ML model explainability of ML models is the most studied theme in the general field of explainability, it is also the case that explainability has been studied in AI for decades [14–16, 111, 118, 119, 128, 283, 313, 317, 331, 332], with a renewed interest in recent years. For example, explanations have recently been studied in AI planning [76, 109, 110, 126, 158, 215, 327, 328, 330, 344], constraint satisfaction and problem solving [62, 114, 130, 150, 328], among other examples [329]. Furthermore, there is some agreement that regulations like EU’s General Data Protection Regulation (GDPR) [115] effectively impose the obligation of explanations for any sort of algorithmic decision making [144,208]. Despite representing fairly distinct areas of research, it is the case that most explainability approaches focus on computing explanations by computing MUSes or variants thereof. This is the case in planning [109], in constraint solving [62], besides explanations in ML as detailed in earlier sections of this paper (see Section 4).

11 Future Research & Conclusions

This section concludes the paper. As the previous sections illustrate, formal explainability has blossomed into a number of important areas of research. Thus, we start by overviewing a number of research directions. Afterwards, we summarize the paper’s contributions.
11.1 Research Directions

As the second part of the paper reveals (see Sections 6 to 10), there exist a vast number of ongoing research topics in the field of formal explainability.

Definitions of explanations. Although the existing definitions of (formal) explanations offer important theoretical advantages, e.g. duality of explanations, researchers have looked at alternative definitions, with the purpose of improving the efficiency of algorithms for computing explanations, or improving the expressiveness of explanations [26, 28].

Computation of explanations. The ability to devise more efficient tools to reason about NNs represents a critical topic of research. Significant improvements in the tools used to reason about NNs would allow explaining more complex classifiers, and so extend the rage of applicability of formal explainability. The grand challenges in the computation of explanations is to devise novel methods for efficiently computing explanations of neural networks and bayesian network classifiers. Recent progress in the analysis of NNs [202, 203, 229] suggests initial directions. A related line of research is the computation of approximate explanations with formal guarantees [40].

Explainability queries. Besides enumeration of explanations, a related question is the enumeration of explanations that are preferred or that take user suggestions into account. This is the subject of future research. Regarding the feature membership, several research problems can be envisioned. One is to efficiently decide membership in the case of arbitrary classifiers, e.g. random forests and other tree ensembles. Another direction of research is to chart the complexity of FMP for the many families of classifiers that can be used in practical settings. For example, given the result that FMP is in NP for families of classifiers for which computing one explanation is in P, then proving/disproving hardness results would allow selecting the most adequate tools to use when solving FMP in practice.

Probabilistic explanations. One key difficulty of computing probabilistic explanations is the computational complexity of the problem [355]. Although researchers have made progress in devising efficient algorithms for efficiently computing probabilistic explanations for specific families of classifiers [190, 192], but also in understanding the computational hardness of computing probabilistic explanations in such cases [22], a number of topics of research can be envisioned. Concretely, one topic is to devise a more complete chart of the computational complexity of the problem, and a second topic is to devise practically efficient algorithms for families of classifiers that have not yet been investigated, e.g. decision lists and sets and tree ensembles, among others.
Explanation certification. It is well-known that algorithms proved correct can be implemented incorrectly. In areas where the rigor of results is paramount, there have been efforts to devise mechanisms for ascertaining the correctness of either implemented algorithms or their computed results [8,9,88,89,92,113,139–141,154,155,250,359]. A natural topic of research is to apply similar solutions in the case of the computation of explanations, but also in the case of explainability queries. For example, existing algorithms for computing one explanation can be formalized in a proof assistant (e.g. [50]), from which a certified executable can then be extracted. Explanation of certification is expected to be relevant in settings that are deemed high-risk or safety-critical.

Additional topics. The accounting for input constraints can play a key role in formal explainability. As a result, the inference of good constraints from training data is a promising direction of research. The goal will be to find the best possible rules, that improve the accuracy of explanations, but that do not impact significantly the performance of formal explainers. Another line of research is to account input distributions when these are either known or can be inferred. As noted in Section 9, the use of surrogate models to compute explanations of complex models holds great promise, but it also requires further assessment. It is open such assessment is to be made. In classification problems with a large number of features, it is often important to be able to aggregate features. In formal explainability, this issue has not yet been addressed, and it is a topic of future research. The previous sections also mentioned in passing several topics of research, that could contribute to raising the impact of formal explainability.

11.2 Concluding Remarks

This paper summarizes the recent developments in the emerging field of formal explainability. The paper overviews the definition of explanations, and covers the computation of explanations, addressing specific families of classifiers, both families for which computing one explanation is computationally hard, and families for which computing one explanation is tractable. The paper also covers a wide range of ongoing topics of active research including explainability queries, probabilistic explanations, accounting for input constraints, and formal explainability using surrogate models. In most cases, the paper also highlights existing topics of research.

As shown throughout the paper, formal explainability borrows extensively from a number of areas of research in AI, including automated reasoning and model-based diagnosis. Different reasoners, including SAT, MILP, and SMT, among others, have been and continue to be exploited in devising ways of computing explanations, both exact and probabilistic, but also answering explainability queries.
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