Sufficient reasons for classifier decisions in the presence of constraints

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Abstract
Recent work has unveiled a theory for reasoning about the decisions made by binary classifiers: a classifier describes a Boolean function, and the reasons behind an instance being classified as positive are the prime-implicants of the function that are satisfied by the instance. One drawback of these works is that they do not explicitly treat scenarios where the underlying data is known to be constrained, e.g., certain combinations of features may not exist, may not be observable, or may be required to be disregarded. We propose a more general theory, also based on prime-implicants, tailored to taking constraints into account. The main idea is to view classifiers in the presence of constraints as describing partial Boolean functions, i.e., that are undefined on instances that do not satisfy the constraints. We prove that this simple idea results in reasons that are no less (and sometimes more) succinct. That is, not taking constraints into account (e.g., ignored, or taken as negative instances) results in reasons that are subsumed by reasons that do take constraints into account. We illustrate this improved parsimony on synthetic classifiers and classifiers learned from real data.

1 Introduction
Machine learning models are currently used to assist decision makers. In case the domains involve high-stakes decisions (e.g., criminal justice and healthcare), model understanding can be used to help with debugging, detect bias in predictions, and vet models [Lakkaraju et al., 2020]. One form of model-understanding is to explain decisions of pre-built models in a post-hoc manner. Models that may not lend themselves easily to interpretability (e.g., some neural networks, random forests or Bayesian network classifiers) or in cases there is an accuracy-interpretability tradeoff, can be passed as inputs to algorithms to produce explanations [Lakkaraju et al., 2020].

In this paper we follow a recent line of logic-based approaches for supplying explanations behind individual classifier decisions [Shih et al., 2018; Darwiche and Hirth, 2020] (rather than explaining the whole model). These works treat the input-output behaviour of a learned binary classifier as a total Boolean function, independently of how the classifier was learned or is implemented. In order to extract specific reasons, these works encode and manipulate the functions symbolically, e.g., as BDDs.

The problem we address in this work is how to incorporate background knowledge, specifically input/domain constraints, into supplying reasons behind individual decisions of classifiers.1 Such constraints may arise from the structure and inter-dependencies between features present in data [Darwiche, 2020]. For example, in a medical setting, some combinations of drugs may never be prescribed together (and thus will not appear in any dataset or clinical setting): if we know that drug A and drug B are never prescribed together (this is the constraint), then a reason of the form “drug A was prescribed and drug B was not prescribed” is overly redundant; it is more parsimonious to supply the reason “drug A was prescribed”.

Our contributions are as follows:

1. We provide a crisp formalisation that takes constraints into account, resulting in reasons that are as least (and sometimes more) parsimonious, i.e., more general and more succinct, than not taking constraints into account. The idea is to present a classifier as a partial function that is not defined on those input instances that do not satisfy the constraint, and then to use the classic definition of prime-implicant on partial functions [Coudert, 1994] as the instantiation of the word “reason”. This immediately and naturally generalises the work of [Shih et al., 2018; Darwiche and Hirth, 2020] from the unconstrained setting to the constrained setting.

2. The main computational problem is to find all reasons of a classifier-decision (for a given instance) in the presence of constraints. We provide a simple reduction of this problem to the unconstrained setting, allowing one to re-use existing algorithms and tools. The idea is that if the constraint is given by the Boolean formula $\kappa$, and the decision function by $\varphi$, then reasons of $\varphi$-decisions that take $\kappa$ into account are exactly the reasons of $(\kappa \rightarrow \varphi)$-

1We do not deal with constraints on the possible outputs of a classifier [Xu et al., 2018].
decision. Interestingly, all other variations, (including the seemingly natural \((\kappa \land \varphi)\)), provide no more, and sometimes less, parsimonious reasons.

3. We show, both theoretically and empirically on synthetic classifiers and classifiers learned from data, that approaches that ignore constraints may supply reasons that are unnecessarily long since they redundantly encode knowledge already described in the constraints.

2 Preliminaries

We begin by recalling just enough logical background to be able to explain our theory.

Boolean logic, partial Boolean functions, and prime-implicants. Let \(X = \{X_1, X_2, \ldots, X_n\}\) be a set of \(n\) Boolean variables (aka feature variables). The set of Boolean formulas is generated from \(X\), the constants \(\top\) (verum/true) and \(\perp\) (falsum/false), and the logical operations \(\land, \lor, \lnot, \rightarrow\) and \(\leftrightarrow\). Variables \(X\) and their negations \(\lnot X\) are called literals.

A term \(t\) is a conjunction of literals; the empty-conjunction is also denoted \(\top\).

An instance (over \(X\)) is an element of \(\{0, 1\}^n\), and is denoted \(x\) (intuitively, it is an instantiation of the variables \(X\)). An instance \(x\) satisfies a formula \(\varphi\) if \(\varphi\) evaluates to true when the variables in \(\varphi\) are assigned truth-values according to \(x\). The set of instances that satisfy the formula \(\varphi\) is denoted \(\{x\}^\varphi\).

Thus we can represent sets of instances by formulas, i.e., the logical equivalence of \(s\) and \(t\) is represented by \(s \leftrightarrow t\).

A term \(t\) is an implicant of \(s\) if \([t] \subseteq [s]\), i.e., if every instance that satisfies \(t\) also satisfies \(s\). If \([t] \subseteq [s]\) then we say that \(s\) properly subsumes \(t\).

Definition 1. A partial Boolean function \(f\) (over \(X\)) is a function \(\{0, 1\}^n \rightarrow \{0, 1, \ast\}\).

For \(i \in \{0, 1, \ast\}\) define \(f^i := f^{-1}(i)\). Call \(f^1\) the function’s onset, \(f^0\) its offset, and \(f^\ast\) its don’t-care set. The care set of \(f\) is the set \(f^0 \cup f^1\). If the don’t-care set is empty, then \(f\) is a total Boolean function. The instances in the onset are called positive instances of \(f\). We can represent a total Boolean function by a formula \(\varphi\) such that \([\varphi] = f^1\).

The following definition generalises the notion of implicant and prime-implicant from total Boolean functions (cf. [Quine, 1952; Shih et al., 2018; Darwiche and Hirth, 2020]) to partial Boolean functions \(f\) (cf. [McCluskey, 1956; Coudert, 1994]).

Definition 2. A term \(t\) is an implicant of a \(f\) if \([t] \subseteq f^1 \cup f^\ast\); it is prime if no other implicant of \(f\) subsumes \(t\).

Intuitively, \(t\) is prime if removing any literal from \(t\) results in a term that is no longer an implicant.

Decision functions Total Boolean functions naturally arise as the decision-functions of threshold-based binary classifiers ([Choi et al., 2019; Shih et al., 2018]): the decision function \(f\) of a threshold-based classifier is the function that maps an instance \(x\) to 1 if \(Pr(d = 1|x) \geq T\), and to 0 otherwise; here \(d\) is a binary class variable, and \(Pr\) is the distribution specified by the classifier, and \(T\) is a user-defined classification threshold. Note that decision functions thus defined are total Boolean functions. Let \(x\) be a positive instance of \(f\).

In [Darwiche and Hirth, 2020], the sufficient reasons behind the decision \(f(x) = 1\) are defined to be the terms \(t\) such that (i) \(t\) is a prime-implicant of \(f\), and (ii) \(t\) is satisfied by \(x\).

Example 1. Consider the total Boolean function \(f\) over \(X = \{X_1, X_2\}\) represented by the formula \((X_1 \leftrightarrow X_2)\) (see the third column of Table 1). The prime-implicants of \(f\) are \((X_1 \land X_2)\) and \((\lnot X_1 \land \lnot X_2)\).

The only sufficient reason of \(f(0, 0) = 1\) is the term \((\lnot X_1 \land \lnot X_2)\), and the only sufficient reason of \(f(1, 1) = 1\) is the term \((X_1 \land X_2)\).

3 Problem Setting

The problem we address is how to define reasons behind decision-functions in the presence of domain constraints.

Definition 3. A constraint is a set \(C\) of instances over \(X\). We can represent a constraint by a formula \(\varphi\) such that \([\varphi] = C\).

The following are just a few examples that show that constraints are ubiquitous. In a medical setting, constraints of the form \((X_1 \rightarrow X_2)\) may reflect that people with condition \(X_1\) also have condition \(X_2\), e.g., \(X_1\) may mean “is pregnant” and \(X_2\) may mean “is a woman”. In a university degree structure, constraints of the form \((X_1 \rightarrow (X_2 \lor X_3))\) may reflect that \(X_2\) and \(X_3\) are prerequisites to \(X_1\); constraints of the form \((X_1 \rightarrow \lnot(X_2 \lor X_3))\) may reflect prohibitions; and constraints of the form \((X_1 \land X_2)\) may reflect compulsory courses. In configuration problems, e.g., that arise when users purchase products, the user may be required to configure their product subject to certain constraints, and constraints of the form \((X_1 \lor X_2) \land \lnot(X_1 \land X_2)\) may reflect that the user needs to choose between two basic models. These constraints also result from one-hot encodings of a categorical variables, e.g., if \(M\) is a 12-valued variable representing months, and \(X_i\) for \(i = 1, \ldots, 12\) is Boolean variable, then the induced constraint is \((\bigvee_i X_i) \land \left(\bigwedge_{i \neq j} \lnot(X_i \land X_j)\right)\). Finally, combinatorial objects have natural constraints, e.g., rankings are ordered sets, trees are acyclic graphs, and games have rules, see Section 6.

Just as a binary classifier describes a total Boolean function, a binary classifier in the presence of a constraint \(C\) describes a partial Boolean function \(f\) whose care-set is \(C\). Indeed, the assumption in this paper is that constraints are hard, i.e., instances that are not in \(C\) are not possible and can be ignored (e.g., they will not appear in training or testing data).

However, many techniques in Machine Learning, such as threshold-based classifiers, produce representations of total Boolean functions. This suggests the following terminology:

Definition 4. A constrained decision-function is a pair \((f, C)\) consisting of a total Boolean function \(f\) and a constraint \(C\).

We thus ask:

How should one define reasons behind decisions of constrained decision-functions?
We posit that a reasonable notion of "reason" that takes constraints into account should have the following properties:

1. it does not depend on the representation of \((f, C)\), i.e., it is a semantic notion;
2. it does not depend on the values \(f(x)\) for \(x \notin C\), i.e., if \(f, g\) agree on \(C\) (and perhaps disagree on the complement of \(C\)), then reasons for \((f, C)\) should be the same as reasons for \((g, C)\);
3. it is not less succinct (and is sometimes more succinct) than not taking constraints into account;
4. in case there are no constraints, i.e., \(C = \{0, 1\}^n\), we recover the notion of reasons from [Darwiche and Hirth, 2020; Shih et al., 2018].

Our formalisation in the next section satisfies these properties.

4 Formalisation of Reasons in the Presence of Constraints

The main objective of this work is to provide a principled definition for reasons behind decisions made by constrained decision-functions \((f, C)\). Let \(f_C\) be the partial Boolean function that maps \(x\) to \(f(x)\) if \(x \in C\), and to * otherwise. Item 2 above says that we want our definition to only depend on the partial Boolean function \(f_C\); so, we define reasons for partial Boolean functions \(g\).

Definition 5 (Sufficient reasons of partial Boolean function). Let \(g\) be a partial Boolean function and let \(x\) be a positive instance of \(g\). A sufficient reason of \(g(x) = 1\) is a term \(t\) such that (i) \(t\) is a prime-implicant of \(g\), and (ii) \(t\) is satisfied by \(x\).

Then: define the sufficient reasons of a constrained decision-function \((f, C)\) to be those of the induced partial Boolean function \(f_C\), i.e., if \(x \in C\) is a positive instance of \(f\), then a sufficient reason of \(x\) wrt \((f, C)\) is a term \(t\) such that (i) \(t\) is a prime-implicant of \(f_C\), and (ii) \(t\) is satisfied by \(x\).

Example 2. Continuing the Example, suppose a constraint is specified by the formula \((X_1 \rightarrow X_2)\), thus \(C = \{(0, 0), (0, 1), (1, 1)\}\). Table 1 provides both \(f\) and the partial Boolean function \(f_C\). The prime-implicants of \(f_C\) are \(\neg X_2\) and \(X_1\). The only sufficient reason for \(f_C(0, 0) = 1\) is \(\neg X_2\), and the only sufficient reason for \(f_C(1, 1) = 1\) is \(X_1\).

Remark 1. Sufficient reasons of a negative instances can be handled by sufficient reasons of positive instances of the dual function \(g\) defined as follows: \(g(x) = 0\) if \(f(x) = 1\); \(g(x) = 1\) if \(f(x) = 0\); and \(g(x) = *\) otherwise.

We now justify Definition 5 (Sufficient Reasons).

1. Our definition is a generalisation of sufficient reason from [Darwiche and Hirth, 2020], called PI-explanation in [Shih et al., 2018]. Indeed, those works only handle decision-functions without constraints (i.e., in our terminology, those works have \(f^* = \emptyset\)). This explains why we use the same terminology, i.e., sufficient reasons.

2. Using prime implicants to explain Boolean functions as well as individual instances has a long history in Science (see Section 7 for a full discussion). This is generally motivated by the principle of parsimony, also known as Occam’s razor in scientific domains, i.e., a reason should not be any more complicated than it needs to be.

3. Subtle changes in the definition result in radically different types of reasons. This is discussed at the end of Section 4.1.

Assuming the constraints are known, the second justification means that reasons should not contain redundancies that are captured by the constraint. We illustrate this point by showing that, given a constrained decision function \((f, C)\), simply considering reasons of the total Boolean function \(f\) (and ignoring the constraint \(C\)), may supply less parsimonious reasons.

Example 3. Continuing the Example, note that the only sufficient reason for \(f(0, 0) = 1\) is \((\neg X_1 \land \neg X_2)\) which is subsumed by \(\neg X_2\), a sufficient reason of \(f_C(0, 0) = 1\); similarly, the only sufficient reason for \(f(1, 1) = 1\) is \((X_1 \land X_2)^\perp\) which is subsumed by \(X_1\), a sufficient reason of \(f_C(1, 1) = 1\).

Example 3 accords with the intuition that, in light of the constraint \((X_1 \rightarrow X_2)\), reason \(X_1\) is preferred to reason \((X_1 \land X_2)^\perp\). This is no accident: reasons using \(f_C\) are as least as parsimonious as reasons using \(f\), as we know prove.

Lemma 1. If \(f, g\) are partial functions such that \(f^1 \cup f^* \subseteq g^1 \cup g^*\), then every sufficient reason for \(f(x) = 1\) is subsumed by some sufficient reason of \(g(x) = 1\).

Proof. Note that a sufficient reason of \(f(x) = 1\), being an implicant of \(f\), is also an implicant of \(g\) (since \(f^1 \cup f^* \subseteq g^1 \cup g^*\)), and that every implicant of a function is subsumed by some prime-implicant of that function.

The following proposition establishes that \(f_C\) supplies reasons that are as least as parsimonious as reasons using \(f\):

Proposition 1. Let \((f, C)\) be a constrained decision-function, and suppose \(x \in C\) is a positive instance of \(f\). Then every sufficient reason of \(f(x) = 1\) is subsumed by some sufficient reason of \(f_C(x) = 1\).

Proof. Lemma 1 applies since \(f^1 \cup f^* = f^1 \subseteq (f_C)^1 \cup (f_C)^*\). Indeed, the equality holds since \(f\) is assumed total, and the containment holds by definition of \(f_C\).

It is not hard to find examples where the subsumption in Proposition 1 is always strict, see Example 3. In particular, if \(t\) properly subsumes \(s\) then, \(t\) is smaller than \(s\) (i.e., contains less literals). And indeed, it is not hard to find examples where every sufficient reason of \(f(x) = 1\) is much larger than
every sufficient reason of \( f_C(x) = 1 \). To do this, consider the constraint \( X_1 \rightarrow (X_2 \land X_3 \cdots \land X_n) \); then every reason of the form \( X_1 \land X_2 \land \cdots \land X_n \) is subsumed by the reason \( X_1 \).

4.1 Reducing the Constrained Case to the Unconstrained Case

It turns out that that there is a particular total function whose reasons are exactly the same as those of a given partial Boolean function. This will allow us to reuse algorithms and tools that are already developed for reasoning about total Boolean functions, e.g., [Shih et al., 2018; Darwiche and Hirth, 2020].

Definition 6. For a partial Boolean function \( f \), define the total Boolean function \( \bar{f} \) as follows: the value of \( \bar{f} \) on \( x \) is equal to 1 if \( f(x) = 1 \) or \( f(x) = * \), and equal to 0 otherwise.

Sufficient reasons using \( f \) and \( \bar{f} \) are the same:

Proposition 2. Let \( f \) be a partial Boolean function and \( x \) a positive instance of \( f \). A term is a sufficient reason of \( f(x) = 1 \) iff it is a sufficient reason of \( \bar{f}(x) = 1 \).

Proof. Follows from the definitions, i.e., the implicants of \( f \) and \( \bar{f} \) are the same (since \( f^1 \cup f^* = \bar{f}^1 \)), and thus the prime implicants of \( f \) and \( \bar{f} \) are the same, and a positive instance of \( f \) is also a positive instance of \( \bar{f} \).

Thus, for a constrained decision-function \((f,C)\) with \( f \) represented by the formula \( \varphi \), and \( C \) by the formula \( \kappa \), the total function \( \bar{f} \) is represented by \( \kappa \Rightarrow \varphi \). We are now in a position to illustrate the third point in the justification of Definition 5, i.e., that subtle changes in the definition result in radically different types of reasons. First, we have seen in the Examples that ignoring the constraints does not provide the most parsimonious reasons. Second, consider the variation in which one uses the total function represented by the formula \( \kappa \land \varphi \). Although seemingly natural (indeed, why not assign a negative value to instances that do not satisfy the constraint), it is not hard to see, using Lemma 1, that this results in the least parsimonious reasons for \( f \). On the other hand, using the formula \( \kappa \Rightarrow \varphi \) (or equivalently \( f_C \) or equivalently \( \bar{f} \)), results in the most parsimonious reasons. We find it striking that this change of perspective (implication vs conjunction) has such drastic changes on the parsimony of the produced reasons.

4.2 Equivalent reasons

We now explain that syntactically different reasons may be semantically equivalent, and thus we only need to consider one representative from each equivalence-class.

Suppose \( s, t \) are syntactically different terms, but logically equivalent, i.e., \([t] = [s]\). Then there is no semantic difference between the terms, and so we do not distinguish between them. E.g., \( t = X_1 \land X_2 \) and \( s = X_2 \land X_1 \) are logically equivalent, and thus we generally do not distinguish between \( s, t \). However, even if \( s, t \) are not logically equivalent, they may be logically equivalent modulo \( C \), i.e., \( C \cap [s] = C \cap [t] \). In this case, we say that \( s, t \) are or simply constraint-equivalent. For instance, if \( C \) is represented by \( (X_1 \lor X_2) \land \neg(X_1 \land X_2) \) then \( t = \neg X_1 \) is \( C \)-equivalent to \( s = X_2 \). Thus, we do not distinguish between \( s \) and \( t \). Practically speaking, we will only consider reasons up to constraint-equivalence, i.e., we will pick an arbitrary representative from each constraint-equivalence class.

More generally, say that \( s \) is constraint-subsumed by \( t \) if \([s] \cap C \subseteq [t] \cap C \). Just as in the unconstrained case sufficient reasons are maximal in the subsumption order, it may be reasonable in the constrained case to require that reasons are maximal in the constraint-subsumption order. We do not require this in our notion of sufficient reason since, doing it may eliminate more succinct reasons, which might be undesirable. These tensions are illustrated in the Case Studies in Section 6, and further discussed in Section 7.

5 Illustration

In this section we illustrate sufficient reasons on a complete synthetic example of a learned classifier, inspired by an example in [Kisa et al., 2014].

Consider a tech-company that is trying to decide whether or not to shortlist a recent graduate from a particular school of computer science for a job interview. The company considers students who took any of Probability (P), Logic (L), Artificial Intelligence (A) or Knowledge Representation (K). Suppose that the company uses data on students who were hired in the past to learn a threshold-based classifier, and let \( f \) be the associated total decision function over \( X = \{L, K, P, A\} \) with onset \( f^1 = \{(0011), (0110), (0111), (1100), (1101), (1110), (1111)\} \).

The details of how such an \( f \) can be learned is not the focus of this paper, see, e.g., [Shih et al., 2018] for the case of Bayesian networks, [Choi et al., 2019] for the case of Neural Networks or to [Audemard et al., 2020] for Random Forests.

Consider an instance \( x = (0011) \) corresponding to students that did not take L or K, but did take P and A. Note that \( f(x) = 1 \), i.e., the classifier decides to grant such students interviews. What is the reason behind this decision? Table 2 gives the reasons, and we see that the only reason behind the decision of \( f \) for \( x = (0011) \) is \((\neg L \land P \land A)\), i.e., that the student did not take L, but did take P and A.

| L | K | P | A | Reasons for \( f(x) = 1 \) |
|---|---|---|---|---|
| 0 | 0 | 1 | 1 | \((\neg L \land P \land A)\) |
| 0 | 1 | 1 | 1 | \((\neg L \land P \land A), (K \land P)\) |
| 1 | 1 | 0 | 0 | \((L \land K)\) |
| 1 | 1 | 1 | 0 | \((L \land K), (K \land P)\) |
| 1 | 1 | 1 | 1 | \((L \land K), (K \land P)\) |

Table 2: Positive instances that satisfy the constraints, and reasons.

Suppose, that a student’s enrolments must satisfy the following constraints \( C \): a student must take P or L. \((P \lor L)\); the prerequisite for A is P. \((A \rightarrow P)\); the prerequisite for K is A or L, \((K \rightarrow (A \lor L))\). Reasons of the constrained decision-function \( f_C \) are given in Table 2. Note \((\neg L \land A)\) and \( K \) are not constraint-equivalent, and indeed are incomparable in the constraint-subsumption order.
Consider the reason behind the decision \( f(x) = 1 \) where \( x = (0011) \), i.e., \( \neg L \land A \). This reason strictly subsumes the reason \( \neg L \land P \land A \) used by the original (unconstrained) classifier \( f \). This phenomenon, that for every positive instance \( x \) in \( C \), every sufficient reason of \( f(x) = 1 \) is subsumed by some sufficient reason of \( f_C(x) = 1 \), can be seen in all other rows of Table 2. This illustrates that our notion of sufficient reason (Definition 5) systematically eliminates such redundancies, a fact we formalised in Proposition 1.

6 Case Studies and Validation

In this section we validate our theory on constrained decision-functions learned from data.\(^3\) Figure 1 illustrates the workflow. The case-studies showcase two major types of constraints that can arise in AI: (i) constraints due to pre-processing of data (e.g. one-hot, or other categorical, encodings); (ii) inherent semantic-constraints in input space.

We focus on interpretable classifiers, namely decision trees (learned using the Recursive Partitioning RPART algorithm in R [Therneau et al., 1997]). This allows us to compare sufficient reasons (both with and without constraints) of decisions with the reasons specified by the corresponding branch of the decision tree [Breiman et al., 1984]

**Algorithms** We consider the following computational problem: given a partial Boolean function \( f \), and a positive instance \( x \), find all sufficient reasons of \( f(x) = 1 \). By Proposition 2, one can reuse algorithms developed for total Boolean functions: simply replace \( f \) by the total Boolean function \( \tilde{f} \).

For instance, the computational problem is solved in [Shih et al., 2018] for total Boolean functions by computing prime-implicants using the Shannon-expansion recursive procedure [Coudert, 1994] and limiting the recursive calls at every step to those that satisfy a given instance \( x \).

Moreover, [Shih et al., 2018] use circuit-representations of functions and sets of prime-implicants. This is the approach we use in our experiments.

In particular, for a given variable order \( v \), we build a few OBDDs [Darwiche and Marquis, 2002] with variable order \( v \). First, an OBDD\(_C\) representing \( C \) which we complement, and then disjoint that complement with an OBDD\(_L\) representing the decision-function \( f \), in order to get the OBDD\(_C\) representing the function \( f_C \).

\(^3\)For the experiments, we restrict our attention to binary data. Continuous data can be discretised, and discrete/categorical data can be binarised as shown in [Breiman et al., 1984].

**Case Study 1.** We used the dataset of Corticosteroid Randomization after Significant Head Injury (CRASH) trial [Collaborators and others, 2008] and based our study on 11 clinically relevant variables described in [Zador et al., 2016]. Input variables include demographics, injury characteristics and image findings, six of which are categorical, and the rest are Boolean.\(^4\)

Outcome variable \( gos \) (0) indicates favourable (un-favourable) outcomes (e.g., death or severe disability).

Categorical variables are encoded using a one-hot encoding, which induces the constraint \( C \) as follows. For a categorical variable \( X \), let \( D \) denote a set of Boolean variables corresponding to the set of categories of \( X \). The corresponding constraint says that exactly one of the variables in \( D \) must be true. For example, variable \( Eye \) (shortened to \( E \)) has 4 categories, which we encode by the Boolean variables in \( D_E = \{E_1, E_2, E_3, E_4\} \). The corresponding constraint is \( \lor_i E_i \land \lor_{i \neq j} \lnot (E_i \land E_j) \), where \( i, j \) vary over \( \{1, 2, 3, 4\} \). The constraint \( C \) is the conjunction of all such constraints, one for each categorical variable.

Following [Steyerberg et al., 2008] we base our example on 6945 cases with no missing values. RPART (seed: 25, train: 0.75, cp: 0.005) correctly classifies 75.69% of instances in the test set (ROC 0.77).

Figure 2 illustrates the model.

**Discussion of Case-Study 1.** The standard explanation from the learned decision tree is \( E_1 \lor P_1 \lor \lnot A_7 \lor M_5 \lor \lnot A_6 \). It is strictly subsumed by (and thus longer than) the sufficient reason using \( \tilde{f} \). This shows that decision-rules may not be the best explanations. Further, as we see, taking the constraints into account may result in more succinctness. Note that, as guaranteed by Proposition 1, the reason using \( f \) is subsumed by some reason using \( f_C \), in fact it appears as the second reason.

\(^4\)Categorical variables are: \( Age(7) \), \( Eye(4) \) \( Motor(6) \), \( Verbal(5) \), \( Pupils(3) \). The Boolean are: \( EC, PH, OB, SA, MD, HM \).
We remark that reasons 1) and 2) are not constraint-equivalent (and thus should be considered different reasons). Which reason should one prefer? On the one hand, Reason 1) is more succinct. On the other hand, Reason 2) strictly constraint-subsumes Reason 1), i.e., it applies to more instances. Without additional preferences regarding succinctness versus generality, there is no reason to prefer one over the other, and thus we return both of them.

Finally, we remark that if one had used the function \( \tilde{f}_C \) instead, one would get one sufficient reason for this decision that is highly redundant in light of the one-hot constraint, i.e., \((A_1 \land E_1 \land M_5 \land V_2 \land F_1 \land \land X_{E,V} ¬X)\) where \( V \) consists of all the remaining variables \( A_2, A_3, \ldots, E_2, E_3, \ldots \).

**Case Study 2.** We used the Tic-Tac-Toe Endgame dataset from the UCI machine learning repository as binarised in [Verwer and Zhang, 2019]: for each of the 9 board positions (labelled as in Table 3a.), introduce variables \( F_{i,X} \) (resp. \( F_{i,O} \)) capturing whether or not \( X \) (resp. \( O \)) was placed in that position. This induces constraints \( C \) that are different to Case Study 1. We let \( C \) be the constraint that expresses that no position contains both an \( X \) and an \( O \) (although it may have neither), i.e., \( C \) is represented by \( \bigwedge_{i\leq 5} \neg(F_{i,X} \land F_{i,O}) \).

Outcome variable \( \text{won} \) 1 (0) is a win (loss) for player \( X \).

Consider the following constraint \( C' \) that captures that \( X \) moves first and players alternate moves: \( \sqrt{S,T}(ψ_S \land ψ_T) \) where \( S, T \) vary over all subsets \( S, T \) of \( \{0, 1, 2, \ldots, 8\} \) such that \( S \cap T = \emptyset \), and \( 0 \leq |S| - |T| \leq 1 \), and

\[
ψ_S = \bigwedge_{i\notin S} F_{N,X} \land \bigwedge_{i\in S \cup T} ¬F_{N,X} \land ψ_T = \bigwedge_{i\notin T} F_{N,O} \land \bigwedge_{i\in S \cup T} ¬F_{N,O}.
\]

The formula expresses that the set \( S \) of positions where \( X \) has played is disjoint from the set \( T \) where \( O \) has played, and that either there are the same number of moves, or \( X \) has played one more. In this case there are 46 sufficient reasons for the instance above, none of which are constraint-\( C' \) equivalent, including the following which are not subsumed by any of the reasons using just the binarisation constraint \( C \).

|       |       |       |
|-------|-------|-------|
| 0-0-0- | 0-0-0- | 0-0-0- |
| 1-0-0- | 1-0-0- | 1-0-0- |
| 2-0-0- | 2-0-0- | 2-0-0- |
| 3-0-0- | 3-0-0- | 3-0-0- |
| 4-0-0- | 4-0-0- | 4-0-0- |

For instance, Reason ii says that, *given that we know the board is the result of a valid play, if positions 4, 5, 7 are blank and position 8 has an \( O \), then player \( O \) must have won.* This is indeed correct: player \( O \) could not have won (since with 5 moves in the game player \( O \) can only move twice), and there could not be a draw (because not all positions were filled yet).

**7 Related Work and Discussion**

Our theory generalises [Shih et al., 2018; Darwiche and Hirth, 2020] to handle domain constraints. We also show how to reduce the constrained-case to the unconstrained case, thus allowing one to reuse existing symbolic algorithms and tools [Shih et al., 2018]. There are other approaches to handle the unconstrained case: purely heuristic (which do not provide guarantees on the quality of explanations) [Ribeiro et al., 2016; Lakkaraju et al., 2019; Iyer et al., 2018] and a combination of heuristic and abductive reasoning [Ignatiev et al., 2019a].

**Prime-implicants as Explanations.** Prime implicants have been used for reasoning and providing explanations in a number of different settings: in Electrical Engineering for circuit minimisation [Brayton and Somenzi, 1989; McGeer et al., 1993]; in model-based diagnosis in AI, as a set of diagnoses sufficient to explain every state of a system in which faulty behaviour is observed [De Kleer et al., 1992; Reiter, 1987]; in system reliability analysis, as smallest combinations of events that could lead a system to failure [Coud-
Prime implicants of partial Boolean functions [Coudert, 1994] are based on the early works of [Nelson, 1955; McCluskey, 1956] and were used to further minimize a Boolean function when the output of the function for some instance was considered to be inconsequential/undefined. Those instances are often assigned to an arbitrary output if doing so results in obtaining prime implicants with fewest numbers of literals [McCluskey, 1956]. Inspired by these earlier works, our definition of sufficient reasons for constrained decision functions, treats constraints in a systematic manner to produce more parsimonious explanations.

**Explanations in ML literature.** The ML literature has techniques for producing (post-hoc local) rule-based explanations which are similar in spirit to the logic-based method of this paper. Notably, the anchors of [Ribeiro et al., 2018] are analogous to implicants. That work: 1) is probabilistic, e.g., it works directly on a probabilistic model while our method works on Boolean functions representing a possibly probabilistic model; 2) aims to optimize the coverage of anchors (i.e., the probability that the anchor applies to a random instance), which is not an analogue of prime-implicant, and thus potentially misses out valid explanations (indeed, that work has no analogue of subsumption); 3) does not explicitly handle constraints, while this is the main focus of our work.

**Discussion** The crux of our paper shows how to handle constraints, and that ignoring constraints could result in unnecessarily long/complex reasons, as well as some reasons that may be missed altogether.

A general critique of the prime-implicant based approach to reasoning is that reasons may become too large to comprehend when the number of variables is large. Notice that our method is a step towards improving this problem in the presence of constraints. If the shortest reason in presence of constraints is still too large to comprehend, not taking constraints into account may result in reasons that are even larger and even harder to comprehend.

To validate the claim that using constraints results in no longer, and sometimes shorter reasons, in the two case studies, we compared (with equivalence, subsumption, constraint-equivalence and constraint-subsumption tests), every single reason obtained from decision function \( f \) with that of \( \bar{f} \) and observed that while adding constraints may decrease or increase the number of reasons, it never increases the size of the shortest reasons (guaranteed by Proposition 1).

In the illustrative example of Section 5, adding constraints reduced the number, as well as the size of reasons for some instances, while in both of the case studies of Section 6, adding constraints increased the number of reasons, but reduced the size of some reasons. Furthermore, in Case Study 2 we demonstrated that when constraints are not taken into account, some reasons may be missed altogether, and provided some examples of such reasons.

In cases of multiple (constraint-inequivalent) reasons for a decision (even amongst the shortest ones), we do not supply a way to pick one reason over another, a challenging problem [Lakkaraju et al., 2019]. Indeed, preferring one reason over another would require additional assumptions about preferred reasons, e.g., favouring succinctness over generality [Miller, 2019].

Another noteworthy point is that in both of the case studies, we used decision trees. In effect, what matters in our investigation, is not the type of a classifier, nor the method of obtaining its decision-function.

What matters is how constraints are handled at the level of the decision function (not its representation), i.e., what values the instances ruled out by the constraints are mapped to.

Since small decision trees are often considered interpretable, we chose them for our experiments, as they also allow one to “read-off” reasons from their branches in order to compare with our most-parsimonious reasons. In fact, using decision trees yielded the following observations. In Case Study 1, we showed that while being indeed interpretable, the decision rules derived from decision trees may not be the most parsimonious explanations, and demonstrated this point with an example in the discussion of Case Study 1. This left us with a question: are decision rules derived from an optimal decision tree, sufficient reasons? A question we leave for future investigations.

Another avenue for future work is to experiment with models that are considered to be less interpretable, such as Bayesian Networks, Random Forests or Neural Networks. In these cases one might compare our most-parsimonious reasons with local reasons produced by the machine-learning community, such as “anchors” [Ribeiro et al., 2018], which would amount to finding approximate reasons [Ignatiev et al., 2019b], clearly out of the scope of this paper.

Finally, our work opens up applications that are currently only available in the unconstrained setting, e.g., computing complete reasons, decision counterfactuals, and classifier bias [Darwiche and Hinth, 2020].

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