Leveraging Association Rules for Better Predictions and Better Explanations

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Abstract. We present a new approach to classification that combines data and knowledge. In this approach, data mining is used to derive association rules (possibly with negations) from data. Those rules are leveraged to increase the predictive performance of tree-based models (decision trees and random forests) used for a classification task. They are also used to improve the corresponding explanation task through the generation of abductive explanations that are more general than those derivable without taking such rules into account. Experiments show that for the two tree-based models under consideration, benefits can be offered by the approach in terms of predictive performance and in terms of explanation sizes.

1 Introduction

Hybrid AI is concerned with the design of more efficient AI systems based on both data and knowledge. Hybridizing data-driven techniques and knowledge-driven techniques can be achieved in many distinct ways and for a large number of purposes. Thus, beyond augmenting the predictive performance of the ML-based AI system one starts with, the use of symbolic information can be beneficial for better explaining the predictions that are made. Such an interpretability issue (see e.g., [27,2]) is relevant to an XAI perspective that is crucial when dealing with critical applications [15].

In this paper, we present a new approach to classification where data and knowledge are combined. Our objective is *to determine to which extent the performance of a tree-based model (a decision tree or a random forest) used for a classification task can be enhanced as to inference and explanation by taking advantage of symbolic information under the form of association rules mined from the available data*. To achieve this goal, our approach exploits recent results concerning the correction of tree-based models [9,10] and the efficient computation of abductive explanations for such models [4].

Our approach basically consists of the following steps. Given a random forest F (possibly reduced to a single decision tree) that has been learned from a dataset D, one first translates the instances from D into instances over the Boolean conditions X encountered in F, giving rise to a binarized dataset D_b^F. In general, the elements of X do not represent independent conditions because they come from the same numerical or

categorical attributes used to describe the instances considered at start (those of D). As a consequence, a domain theory Th, represented as a Boolean formula on X, must be considered as well so as to make precise how the Boolean conditions in X are logically connected (the pair (F, Th) is a *constrained decision-function* in the sense of [14]). Then, a data mining algorithm is used to derive a (conjunctively-interpreted) set A of association rules (possibly with negations) from D_b^F. Only rules with 100% confidence and a non-null support are targeted. Among those rules, classification rules (alias class association rules - *CAR*, i.e., those rules from A concluding about the membership to a class) forming a subset A_c of A are used to modify F in such a way that the updated forest complies with the rules. Accordingly, primacy is given to the predictions that can be obtained using the classification rules over those coming from the random forest. The rectification operation from [9,10] is used to update the forest. Algorithm 1 gives a pseudo-code of the operations that are achieved.

Algorithm 1 Computing a tree-based model rectified by a set of classification rules and a domain theory extended by association rules that are mined as well.

Require: a tabular dataset D.
Ensure: a tree-based model F^{A_c} complying with the classification rules from A_c and an extended domain theory Th_e.

$(F, Th) \leftarrow learn(D)$
$D_b^F \leftarrow binarize(D, F)$
$A \leftarrow mine(D_b^F)$
$A_c \leftarrow select - CAR(A)$
$F^{A_c} \leftarrow rectify(F, A_c)$
$Th_e \leftarrow Th \wedge (A \setminus A_c))$
return $((F^{A_c}, Th_e))$

One is also interested in deriving (local) abductive explanations for the predictions made. Thus, given an instance $\boldsymbol{x}$ and the corresponding classification $F(\boldsymbol{x})$ to be explained, one looks for a subset t of the characteristics over X used to represent $\boldsymbol{x}$ such that every instance $\boldsymbol{x}'$ that is covered by t (i.e., such that t is a subset of the characteristics of $\boldsymbol{x}'$) and that satisfies $Th_e = Th \wedge (A \setminus A_c)$ is classified by the rectified forest in the same way as $\boldsymbol{x}$. By considering instances that satisfies the *extended domain theory Th_e* (and not only Th), it is known that, in theory, more general explanations can be obtained [14,31]. Since the explanations that are considered are based on Boolean conditions on X, minimum-size abductive explanations for an instance are among its most general explanations. Thus, the explanations computed using the extended domain theory are in general shorter than those obtained when the initial domain theory is considered, and as a consequence, the extension of Th achieved by considering in addition the rules from $A \setminus A_c$ leads to abductive explanations that are typically easier to understand.

The contributions of the paper are as follows. We first show that it is possible to take advantage of the change operation for tree-based models, called *rectification* [9,10], in

order to incorporate the classification rules from A_c into F. The rectification operation ensures that F, once rectified, classifies every instance on X classified by a classification rule R of A_c in the way the rule R asks for, while every other instance on X is classified as required by F before the rectification takes place. Especially, we show that the rectification of F by A_c an be achieved in an iterative way (i.e., on a rule-per-rule basis) provided that A_c is non-conflicting (meaning that one cannot find in A_c two classification rules with compatible premises but contradictory conclusions). In our approach, the conflict-freeness of A_c is ensured by the process used for generating it.

In order to derive valuable abductive explanations suited to tree-based models, a complexity challenge must be dealt with. Indeed, the generation of non-trivial abductive explanations for random forests is known to be computationally hard in general, even in the case when no domain theory is considered [21]. It is also known as hard for random forests with a single decision tree when a domain theory is taken into account [8]. To tackle this issue, we show how to generalize the concept of *majoritary reasons* introduced in [4] to decision trees and random forests based on Boolean conditions X that are not independent but are connected through a domain theory on X; to ensure that the tractability of the computation of such abductive explanations, the inference relation used to reason from the domain theory is not full logical entailment but unit propagation.

A last contribution of the paper consists of an empirical evaluation of the approach in order to assess the benefits it offers. Interestingly, the experiments made show that the objectives of improving the predictive performance of the classifiers and of diminishing the size of the explanations can be met. In a nutshell, for 12 out of 13 datasets used in the experiments, rectifying the random forest used by the classification rules that have been mined leads to slightly increase its predictive performance. The increase is small in general but it can exceed 10%. As to the size of the abductive explanations that have been generated, the reduction achieved can be huge (more than 96%) and effective for a large proportion of instances (up to 100%), depending on the number of association rules that have been extracted. Depending on the dataset, the improvement observed is higher when the classifier used is a random forest or when it is a decision tree.

Additional empirical results and the code used in our experiments are available online at [7].

2 Formal Preliminaries

2.1 Decision tree, random forests, and classifiers

We consider a dataset D consisting of classified instances from a binary classification problem and represented as tabular data. A finite set $\mathcal{A}$ of p *attributes* (aka *features*) (where each attribute $A_i \in \mathcal{A}$ takes a value (called a *characteristic*) in a domain Dom_i). Each attribute A_i is numerical, categorical, or Boolean. An instance over $\mathcal{A}$ is a tuple from $Dom_1 \times \ldots \times Dom_p$. The class of an instance in D is made precise by the Boolean value of a specific column y of D (the instance is positive when y takes value 1 and negative when it takes value 0). Thus, a classified instance is a tuple from $Dom_1 \times \ldots \times Dom_p \times \{0, 1\}$.

When dealing with a binary classification problem, a *decision tree* over $\mathcal{A}$ is a binary tree T, each of whose internal nodes (aka decision nodes) is labeled with a Boolean condition over $A_i \in \mathcal{A}$, and each leaf is labeled by a Boolean value denoting a class (positive or negative). The value $T(\boldsymbol{x})$ of T on an input instance $\boldsymbol{x}$ is given by the label of the leaf reached from the root, which is either a 1-leaf (i.e., a leaf labelled by 1) or a 0-leaf (i.e., a leaf labelled by 0). The unique root-to-leaf path p characterizing the leaf that is met is defined as follows: at each decision node go to the left (resp. right) child if the Boolean condition labelling the node is evaluated to 0 (resp. 1) for $\boldsymbol{x}$. $leaf(p)$ denotes the leaf of p.

A *random forest* over $\mathcal{A}$ is an ensemble $F = \{T_1, \cdots, T_m\}$, where each T_i ($i \in [m]$) is a decision tree over $\mathcal{A}$. The value $F(\boldsymbol{x})$ of F on an input instance $\boldsymbol{x}$ is given by

$$F(\boldsymbol{x}) = \begin{cases} 1 & \text{if } \frac{1}{m} \sum_{i=1}^{m} T_i(\boldsymbol{x}) > \frac{1}{2} \\ 0 & \text{otherwise.} \end{cases}$$

The *size* of F is given by $|F| = \sum_{i=1}^{m} |T_i|$, where $|T_i|$ is the number of nodes occurring in T_i. Clearly enough, any decision tree T over $\mathcal{A}$ is equivalent to the random forest $F = \{T\}$ in the sense that $T(\boldsymbol{x}) = F(\boldsymbol{x})$ for every instance $\boldsymbol{x}$ over $\mathcal{A}$. Therefore, in the rest of the paper, decision trees will also be viewed (wlog) as random forests with a single tree.

$X = \{x_1, \ldots, x_n\}$ denotes the set of Boolean conditions labelling decision nodes in F. A term (resp. a clause) on X is a conjunction (resp. disjunction) of literals on X, i.e., of elements from X, possibly negated. A *positive literal* is an element $x \in X$, and a *negative literal* is the negation $\overline{x}$ of an element $x \in X$. When ℓ is a literal on X, its *complementary literal*, noted $\sim \ell$, is given by $\overline{x}$ when $\ell = x$ is a positive literal, and x when $\ell = \overline{x}$ is a negative literal. A formula in *disjunctive (resp. conjunctive) normal form* is a disjunction of terms (resp. a conjunction of clauses).

Every root-to-leaf path p of a decision tree T_i is associated with a term (noted p as well to avoid heavy notations). For each decision node in p labelled by $x \in X$, x is a literal of p when the condition x is evaluated to 1 and $\overline{x}$ is a literal of p otherwise. It is well-known (see e.g., [4]) that any decision tree T_i on X can be turned in linear time into an equivalent disjunction of consistent terms over X, noted $\text{DNF}(T_i)$ and into an equivalent conjunction of non-valid clauses over X, noted $\text{CNF}(T_i)$. Each term in $\text{DNF}(T_i)$ corresponds to a 1-path of T_i and each clause in $\text{CNF}(T_i)$ is the negation of a term describing a 0-path of T_i.

Finally, Th denotes a domain theory, i.e., a Boolean formula on X that indicates how the Boolean conditions in X are logically connected. Every instance $\boldsymbol{x}$ over $\mathcal{A}$ can be rewritten into a (usually more general) instance over X [6] that is classified by F in the same way as $\boldsymbol{x}$ so that each T_i in F can be viewed as a decision tree over X, and F can be viewed as a random forest over X. Each T_i and F itself can thus be considered as Boolean formulas on X. In the following, $\boldsymbol{X}$ denotes the set of all instances over X.

Example 1. As a matter of illustration, consider the following loan allocation problem. The goal is to determine whether a loan of $\$100k$ must be granted to an applicant, described using three attributes from $\mathcal{A} = \{A, I, S\}$: his/her age A (a numerical attribute), his/her annual income I (in $\$k$, a numerical attribute), and his/her professional status S (a categorical attribute). In the available dataset D, three values for S
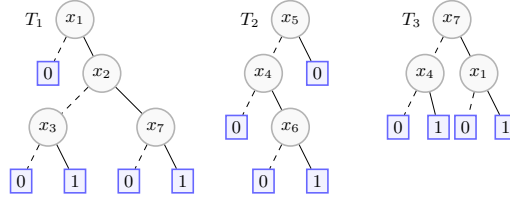
Fig. 1. A random forest for a loan allocation problem. The left (resp. right) child of any decision node labelled by x_i corresponds to the assignment of x_i to 0 (resp. 1).

are encountered ("unemployed (U)", "temporary position (TP)", or "permanent position"). The random forest $F = \{T_1, T_2, T_3\}$ given at Figure 1 has been learned from D. F is based on 7 Boolean conditions: $X = \{x_1, \ldots, x_7\}$, where $x_1 = (A > 25)$, $x_2 = (A > 60)$, $x_3 = (I > 30)$, $x_4 = (I > 50)$, $x_5 = (S = U)$, $x_6 = (S = TP)$, and $x_7 = (S = PP)$. Those conditions are logically connected as given by the domain theory $Th = (x_2 \Rightarrow x_1) \wedge (x_4 \Rightarrow x_3) \wedge (x_5 \Rightarrow \overline{x_6}) \wedge (x_5 \Rightarrow \overline{x_7}) \wedge (x_6 \Rightarrow \overline{x_7})$. The implications $x_2 \Rightarrow x_1$ and $x_4 \Rightarrow x_3$ simply reflect that $60 > 25$ and $50 > 30$ (respectively). The remaining implications state that S cannot take two distinct values in its domain at the same time. Here, the domain of the categorical attribute S is considered open (i.e., we do not not assume that the only possible values for S are U, TP, and PP).

The instance $(33, 52, PP)$ over $\mathcal{A}$ representing an applicant aged 32, having \$$52k$ annual income, and a permanent position, corresponds to the instance $\boldsymbol{x} = (1, 0, 1, 1, 0, 0, 1)$ of $\boldsymbol{X}$. $\boldsymbol{x} = (1, 0, 1, 1, 0, 0, 1)$ is more general than the instance $(33, 52, PP)$ one started with, in the sense that other instances over $\mathcal{A}$ (e.g., $(48, 60, PP)$) also corresponds to $\boldsymbol{x}$. We can easily check that the instance $\boldsymbol{x}$ is such that $F(\boldsymbol{x}) = 1$ (indeed, we have $T_1(\boldsymbol{x}) = 1$, $T_2(\boldsymbol{x}) = 0$, and $T_3(\boldsymbol{x}) = 1$).

Each instance $\boldsymbol{x}$ of $\boldsymbol{X}$ can be considered as an interpretation on X that satisfies Th. This interpretation can be represented by a (canonical) term $t_{\boldsymbol{x}}$ on X, formed by the set (interpreted as a conjunction) of the positive literals x_i ($i \in [n]$), such that $\boldsymbol{x}_i = 1$ and by the negative literals $\overline{x_i}$ ($i \in [n]$) such that $\boldsymbol{x}_i = 0$. $\top$ is the Boolean constant always true that evaluates to the Boolean value 1 and $\bot$ is the Boolean constant always false that evaluates to the Boolean value 0. In the following, $\models$ denotes logical entailment and $\equiv$ logical equivalence.

Definition 1. *A binary classifier* on X *is a mapping C from $\boldsymbol{X}$ to the set of Boolean values $\{0, 1\}$. $\boldsymbol{x} \in \boldsymbol{X}$ is a positive instance if $C(\boldsymbol{x}) = 1$ and a negative one if $C(\boldsymbol{x}) = 0$.*

Every ML model that is based on Boolean conditions (such as a decision tree or a random forest) and targets two classes only can be represented by a Boolean formula of the form $\Sigma_X \Leftrightarrow y$ where Σ_X is a formula on X and $y \notin X$ is a propositional variable that denotes the class of positive instances. Indeed, it is sufficient to consider any Σ_X such that $\boldsymbol{x}$ is a model of Σ_X if and only if $\forall \boldsymbol{x} \in \boldsymbol{X}$, $C(\boldsymbol{x}) = 1$.

Accordingly, any binary classifier can be represented by a classification circuit in the sense of [9]:

Definition 2. *A* classification circuit Σ *on* $X \cup \{y\}$ *is a circuit equivalent to a formula of the form* $\Sigma_X \Leftrightarrow y$ *where* Σ_X *is a Boolean formula on* X.

In the following, when Φ is a Boolean circuit or a formula on $X \cup \{y\}$ and z is any variable from $X \cup \{y\}$, $\Phi(z)$ (resp. $\Phi(\overline{z})$) denotes the *conditioning* of Φ by z (resp. by $\overline{z}$). $\Phi(z)$ (resp. $\Phi(\overline{z})$) is the circuit (or the formula) obtained by replacing in Φ any occurrence of z by the Boolean constant $\top$ (resp. $\bot$). When $\Sigma = \Sigma_X \Leftrightarrow y$ is a classification circuit on $X \cup \{y\}$, the set of models of $\Sigma(y)$ consists precisely of the models of Σ_X and the set of models of $\Sigma(\overline{y})$ consists precisely of the counter-models of Σ_X. Finally, when $x \in X$ is an instance, $\Phi(x)$ denotes the iterative conditioning of Φ by each literal of t_x. Thus, $x \in X$ is classified positively (resp. negatively) by Σ when $\Sigma(x)$ is equivalent to y (resp. $\overline{y}$).

2.2 Implicants and abductive explanations

Given two formulas Φ and Th on X, a term t on X is an *implicant* of Φ modulo Th iff Φ is a logical consequence of $t \wedge Th$. A term t is an *implicant* of Φ iff Φ is a logical consequence of t. Thus, a term t is an implicant of a formula Φ iff t is an implicant of Φ modulo a valid formula Φ.

Based on these notion of implicants, we can now make precise the notion of abductive explanation for an instance given a constrained decision-function based on a random forest [14]:

Definition 3. *Let* (F, Th) *be a constrained decision-function where* F *is a random forest on* X *and* Th *a Boolean formula on* X. *Let* x *be an instance from* X *that satisfies* Th *and is s.t.* $F(x) = 1$ *(resp.* $F(x) = 0$).

- *An* abductive explanation *for* x *given* (F, Th) *is a (conjunctively-interpreted) set* $t \subseteq t_x$ *such that* t *is an implicant of* F *modulo* Th *(resp.* t *is an implicant of* $\overline{F}$ *modulo* Th).
- *A* subset-minimal abductive explanation *for* x *given* (F, Th) *is an abductive explanation* t *for* x *given* (F, Th) *such that no proper subset of* t *is an abductive explanation for* x *given* (F, Th).

Abductive explanations t provide subsets of characteristics of the instance x (thus, literals over X) that explain why x is classified by F in the way it has been classified (possibly, taking Th into account).[3] Subset-minimal abductive explanations are also called sufficient reasons [12] and prime-implicant explanations [30].

Example 2 (Example 1, cont'ed). A subset-minimal abductive explanation for $x = (1, 0, 1, 1, 0, 0, 1)$ given (F, Th) is given by $t = x_1 \wedge \overline{x_2} \wedge x_4$. This means that any applicant with age between 26 and 60 and annual income greater than \$50k will be classified by F in the same way as x (i.e., as a positive instance), but if one of the three conditions (being older than 25, at least 60 years old, and having more than \$50k income) is relaxed, the same conclusion about the loan granted cannot be guaranteed.

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[3] As in [19] and unlike [18], in this paper, abductive explanations are not required to be minimal w.r.t. set inclusion. The notion of abductive explanations considered here corresponds to so-called weak abductive explanations in [16].

2.3   Association rules

In the following, we also need the notion of association rule:

Definition 4. *An association rule $R = b \Rightarrow h$ is a clause over $X \cup \{y\}$, where $y \notin X$ denotes the class of positive instances. The body (aka premises) b of such a rule always is a conjunction of literals over X and the head (aka conclusion) h of R is a literal over $X \cup \{y\}$. When h is a literal over y, the association rule $R = b \Rightarrow h$ is a classification rule (aka a class association rule - CAR).*

Example 3 (Example 1, cont'ed). $(x_4 \wedge x_7) \Rightarrow y$ and $\overline{x_2} \Rightarrow \overline{x_7}$ are two association rules. $(x_4 \wedge x_7) \Rightarrow y$ is a classification rule.

The rules we consider may contain negations in their bodies and in their heads. Obviously, any (conjunctively-interpreted) set A of association rules can also be viewed as a Boolean formula (in conjunctive normal form) on $X \cup \{y\}$.

Clearly enough, when it holds, a classification rule $R = b \Rightarrow y$ (resp. $R = b \Rightarrow \overline{y}$) indicates that each instance $\boldsymbol{x} \in \boldsymbol{X}$ satisfying b has to be positively (resp. negatively) classified. Indeed, $R(\boldsymbol{x}) \equiv y$ (resp. $R(\boldsymbol{x}) \equiv \overline{y}$) is true.

Association rules can be generated using data mining techniques, including the seminal Apriori algorithm [1]. To do so, the classified instances over $\mathcal{A}$ from D are first rewritten into classified instances over X (the Boolean conditions used in F), giving rise to the binarized dataset D_b^F. In this dataset, each Boolean condition $x \in X$ is used to give rise to two columns, one related to x, the other one to $\overline{x}$. This is useful to extract a set A of association rules with negations from D_b^F using standard data mining algorithms. Two key scores are typically used to assess the quality of an association rule. The *support* of an association rule $R = b \Rightarrow h$ given a dataset D_b^F is the number of instances ("transactions") in D_b^F satisfying $b \wedge h$ divided by the number of instances in D_b^F. The *confidence* of a rule $R = b \Rightarrow h$ given a dataset D_b^F is the number of instances in D_b^F satisfying $b \wedge h$ divided by the number of instances satisfying b.

In general, the subset A_c of A consisting of classification rules derived from D_b^F using a data mining algorithm corresponds to an *incomplete* classifier since instances may exist that are not covered by the body of any rule from A_c. Furthermore, in the general case, A_c can be *conflicting* given the domain theory Th on X. This means that one can find in A_c two rules $R_1 = b_1 \Rightarrow h_1$ and $R_2 = b_2 \Rightarrow h_2$ such that $b_1 \wedge b_2 \wedge Th$ is consistent and $h_1 \equiv \overline{h_2}$. When A_c contains conflicting rules $R_1 = b_1 \Rightarrow h_1$ and $R_2 = b_2 \Rightarrow h_2$, one does not know how to classify instances $\boldsymbol{x}$ satisfying $b_1 \wedge b_2 \wedge Th$ since the two rules give contradictory conclusions about the class of $\boldsymbol{x}$.

3   Rectifying Decision Trees and Random Forests

To take advantage of the classification rules of A_c (or, at least, those the user is sufficiently confident to them) to improve the predictive performance of F, the *rectification operation* [9,10] can be used. To this purpose, class labels (reduced to y or $\overline{y}$ here) are required to be explicit. Notably, rectification is not specific to tree-based models but it

applies to *classification circuits* Σ on $X \cup \{y\}$. This is not an issue since when viewing a random forest F as a Boolean formula over X, the formula $F \Leftrightarrow y$ is such a classification circuit Σ.

Rectifying $F \Leftrightarrow y$ by A_c then amounts to generate a classification circuit noted $(F \Leftrightarrow y) \star A_c$ such that for every instance $\boldsymbol{x} \in \boldsymbol{X}$, if A_c classifies $\boldsymbol{x}$, then $(F \Leftrightarrow y) \star A_c$ classifies $\boldsymbol{x}$ in the same way as A_c, else $(F \Leftrightarrow y) \star A_c$ classifies $\boldsymbol{x}$ in the same way as F. The rectified circuit $(F \Leftrightarrow y) \star A_c$ of $F \Leftrightarrow y$ by A_c [10] is characterized (up to logical equivalence) by $(F \Leftrightarrow y) \star A_c \equiv F^{A_c} \Leftrightarrow y$ where

$$F^{A_c} \equiv (F \wedge \neg(A_c(\overline{y}) \wedge \neg A_c(y))) \vee (A_c(y) \wedge \neg A_c(\overline{y})).$$

As explained in [10], the rationale of this characterization is as follows. For an instance $\boldsymbol{x}$ to be classified as positive by the rectified classification circuit, it must be the case that either A_c consistently asks for it (this corresponds to the disjunct $A_c(y) \wedge \neg A_c(\overline{y})$), or that the classification circuit considered at start classifies $\boldsymbol{x}$ as positive, provided that T does not consistently ask $\boldsymbol{x}$ to be classified as negative (this corresponds to the disjunct $F \wedge \neg(A_c(\overline{y}) \wedge \neg A_c(y))$). When A_c is conflict-free, every instance that can be classified using rules from A_c is consistently classified by A_c.

In our approach, the rules in A that are generated by the data mining algorithm $mine$ used in Algorithm 1 can be filtered by the user if needed (only those rules in which the user has sufficient trust must be used). A 100% confidence score and a non-null support score is considered so that each rule put forward by the data mining algorithm meets these conditions (the goal is generate only rules that are not contradicted by any piece of available evidence in D_b^F since we want to use them as if they were true pieces of knowledge). The set A of association rules is expected to be conflict-free but considering rules with a 100% confidence score and a non-null support score is not enough to ensure it. In our approach, the lack of conflicts is ensured by the way the procedure $mine$ works: rules are generated one by one, by decreasing support, and a generated rule R is put into A whenever it does not conflict with any of the rule R' that precedes R in the enumeration (provided that R' has been kept so far and put into A). The absence of conflicts makes it possible to rectify F by A_c in an iterative way, rule by rule (the order with which the classification rules of A_c are taken into account does not matter when A_c is conflict-free).

Furthermore, in order to use XAI techniques developed so far for decision trees and random forests (especially, the computation of abductive explanations as presented in Section 4), we would like the resulting classification circuit $(F \Leftrightarrow y) \star A_c$ to be represented as a decision tree when F is a decision tree and as a random forest when F is a random forest. It is possible to ensure this property without requiring additional heavy computational costs. Indeed, in order to rectify a random forest F by a classification rule R, it is enough to rectify every tree $T_i \in F$ by R. Furthermore, rectifying a decision tree T_i by a classification rule $R = b \Rightarrow h$ amounts to rectify every branch of T_i by R, leading to a tree. Thus, all the branches of the trees in F can be rectified by R in parallel.

More precisely, rectifying T_i by $R = b \Rightarrow h$ amounts to update only those root-to-leaf paths p of T_i such that $p \wedge b \wedge Th$ is consistent and the leaf of p conflicts with the conclusion h of the rule (i.e., when $h = y$ and the leaf of p is a 0-leaf and when $h = \overline{y}$
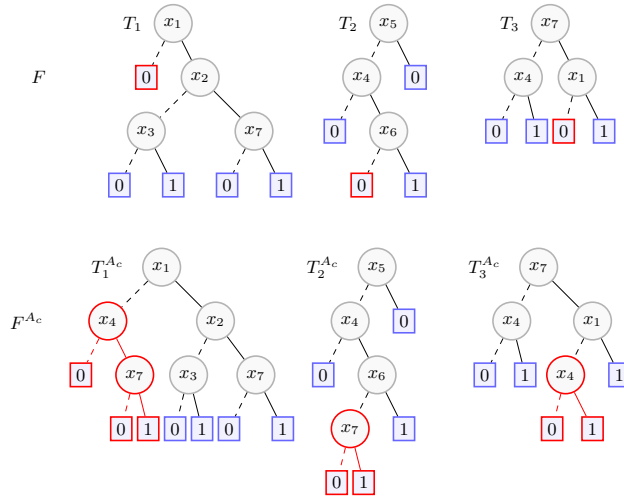
Fig. 2. The random forest F^{A_c} obtained by rectifying F by $A_c = \{(x_4 \wedge x_7) \Rightarrow y\}$. The modifications achieved w.r.t. F are printed in red.

and the leaf of p is a 1-leaf). Let $patch(p, R)$ the *comb-shaped tree* with its main branch labelled by conditions from $b \setminus p$ leading to a 0-leaf if $h = \overline{y}$ and to a 1-leaf if $h = y$, while every other branch of the comb-shaped tree is labelled by $leaf(p)$. A rectification of p by R can be obtained by replacing the leaf node of p by $patch(p, R)$.

Example 4 (Example 1, cont'ed). Suppose that the data mining algorithm has produced a unique classification rule with confidence 100% and a non-null support, namely $R = (x_4 \wedge x_7) \Rightarrow y$. This rule is not a logical consequence of the classification circuit $F \Leftrightarrow y$. Indeed, the instance $\boldsymbol{x} = (0, 0, 1, 1, 0, 0, 1)$ is such that $F(\boldsymbol{x}) = 0$ while $\boldsymbol{x}$ is classified as a positive instance by R. If R is considered reliable enough by the user, $F \Leftrightarrow y$ can be rectified by $A_c = \{R\}$. The resulting random forest F^{A_c} is given at Figure 2. In detail, with $b = x_4 \wedge x_7$ and $h = y$:

- The unique branch of T_1 that needs to be rectified is the one corresponding to $\overline{x_1}$ since it ends with a 0-leaf while $h = y$. The two other branches of T_1 ending with a 0-leaf are associated with terms p (namely, $x_1 \wedge \overline{x_2} \wedge \overline{x_3}$ and $x_1 \wedge \overline{x_2} \wedge \overline{x_7}$) such that $p \wedge b \wedge Th$ is inconsistent (keep in mind that $x_4 \Rightarrow x_3$ is part of Th). Thus, the 0-leaf node corresponding to the path $\overline{x_1}$ in T_1 is replaced by the comb-shaped tree $patch(\overline{x_1}, R)$ in $T_1^{A_c}$. This comb-shaped tree simply ensures that a 1-leaf is reached when $x_4 \wedge x_7$ holds, while a 0-leaf (i.e., $leaf(\overline{x_1})$) is reached otherwise.
- The unique branch of T_2 that needs to be rectified is the one corresponding to $\overline{x_5} \wedge x_4 \wedge \overline{x_6}$ since it ends with a 0-leaf while $h = y$. The two other branches of T_2 ending with a 0-leaf are associated with terms p (namely, $\overline{x_5} \wedge \overline{x_4}$ and x_5) such that $p \wedge b \wedge Th$ is inconsistent (keep in mind that $x_5 \Rightarrow \overline{x_7}$ is part of Th). Thus, the 0-leaf node corresponding to the path $\overline{x_5} \wedge x_4 \wedge \overline{x_6}$ in T_2 is replaced by the comb-shaped tree $patch(\overline{x_5} \wedge x_4 \wedge \overline{x_6}, R)$ in $T_2^{A_c}$. This comb-shaped tree simply ensures

that a 1-leaf is reached when $x_4 \wedge x_7$ holds, while a 0-leaf (i.e., $leaf(\overline{x_5} \wedge x_4 \wedge \overline{x_6})$) is reached otherwise. In the comb-shaped tree $patch(\overline{x_5} \wedge x_4 \wedge \overline{x_6}, R)$, there is no need to repeat the condition x_4 since it belongs to the path $\overline{x_5} \wedge x_4 \wedge \overline{x_6}$.

– Finally, the unique branch of T_3 that needs to be rectified is the one corresponding to $x_7 \wedge \overline{x_1}$ since it ends with a 0-leaf while $h = y$. The other branch of T_3 ending with a 0-leaf is associated with the term $p = \overline{x_7} \wedge \overline{x_4}$ such that $p \wedge b \wedge Th$ is inconsistent. Thus, the 0-leaf node corresponding to the path $x_7 \wedge \overline{x_1}$ in T_3 is replaced by the comb-shaped tree $patch(x_7 \wedge \overline{x_1}, R)$ in $T_3^{A_c}$. This comb-shaped tree simply ensures that a 1-leaf is reached when $x_4 \wedge x_7$ holds, while a 0-leaf (i.e., $leaf(x_7 \wedge \overline{x_1})$) is reached otherwise. In the comb-shaped tree $patch(x_7 \wedge \overline{x_1}, R)$, there is no need to repeat the condition x_7 since it belongs to the path $x_7 \wedge \overline{x_1}$.

The rectification of F by R can be achieved in time $\mathcal{O}(|F| \cdot |R|)$, leading to a model F^{A_c} of size upper bounded by $\mathcal{O}(|F| \cdot |R|)$. Notably, the branches of each resulting tree $T_i^{A_c}$ in F^{A_c} can be *simplified* using Th: from bottom to top, starting from the leaf of a branch p up to the root of the tree T_i, an arc of p can be removed when the literal ℓ labelling it is a logical consequence of $(p \setminus \{\ell\}) \wedge Th$. In addition, any internal node of $T_i^{A_c}$ having a left subtree identical to its right subtree can be replaced by one of its two subtrees. Though such a simplification process would let unchanged the rectified model F^{A_c} considered in the running example, in the general case it may have a significant effect on the size of the resulting model, leading sometimes to a model that is smaller than the one F we started with. To illustrate this point, consider the running example again: it is easy to verify that rectifying T_3 by $(\overline{x_7} \wedge \overline{x_4}) \Rightarrow y$ and simplifying the resulting tree would lead to a tree smaller than T_3 itself (we would get a tree with 5 nodes instead of 7 nodes for T_3).

4   Deriving Abductive Explanations

Let us turn now to the second problem tackled, i.e., computing better explanations by leveraging association rules. A first important remark is that, though no consensus exists about what a "good" explanation should be [26,27], many criteria for evaluating explanations (and/or the XAI methods used to produce them) have been pointed out [28]. Some of those criteria are antagonistic, so trade-offs must be considered. Among other criteria, *correctness* indicates to which extent explanations capture the actual behaviour of the AI system (and not the one of a surrogate model). *Compactness* concerns the size of the explanations (shorter explanations are usually easier to interpret). When dealing with (local) abductive explanations based on Boolean conditions (as it is the case in this paper), the size of the explanations is also related to their *generality*, i.e., the set of instances covered by the explanation. Indeed, in this case, minimum-size abductive explanations are among the subset-minimal abductive explanations, i.e., those that are as general as possible. *Coherence* is about whether explanations comply with the domain knowledge, while *controllability* refers to the possibility for a user to influence the explanations that are provided.

Unlike other notions of explanations based on feature attribution techniques (especially Shapley values [25,17]), abductive explanations t for an instance $\boldsymbol{x}$ given (C, Th),

are formal explanations that are *correct by design*: it is ensured that for any feasible instance $\boldsymbol{x}'$ (i.e., an instance that satisfies Th), if $\boldsymbol{x}'$ is covered by t, then $C(\boldsymbol{x}') = C(\boldsymbol{x})$. Stated otherwise, t being true is enough to explain the way $\boldsymbol{x}$ has been classified by C. The coherence criterion is also met given that pieces of domain knowledge (given as a domain theory) are exploited in the computation of explanations.

Computing an abductive explanation for $\boldsymbol{x} \in \boldsymbol{X}$ given (C, Th) is an easy task when no requirement are imposed about the generality of the explanation that is generated. Indeed, $t_{\boldsymbol{x}}$ is a (trivial) abductive explanation for $\boldsymbol{x} \in \boldsymbol{X}$ given (C, Th). The direct reason for $\boldsymbol{x}$, i.e., the set of characteristics of $t_{\boldsymbol{x}}$ that can be found in the unique path of C compatible with $t_{\boldsymbol{x}}$ when C is a decision tree, and the union of all those characteristics over the trees of C when C is a random forest, is an alternative abductive explanation for $\boldsymbol{x} \in \boldsymbol{X}$ given (C, Th). However, such a direct reason (aka the path-restricted explanation for $\boldsymbol{x}$ when C is a decision tree) may contain many redundant conditions that are not present in subset-minimal abductive explanations [22].

The difficulty is to thus to find more general explanations, especially subset-minimal abductive explanations or even minimum-size abductive explanations. Going a step further in this direction requires to address *a complexity issue* because generating subset-minimal abductive explanations or minimum-size abductive explanations is computationally difficult. The presence of a domain theory makes (in general) the problem harder. Thus, while the generation of a subset-minimal abductive explanation for an instance given a decision tree can be achieved in polynomial time when no domain theory is considered, the problem becomes (in general) NP-hard when a domain theory must be taken into account [8]. On the other hand, the problem of generating a subset-minimal abductive explanation for $\boldsymbol{x}$ given a random forest is intractable (DP-hard) [21], even when no domain theory is taken into account. Of course, generating minimum-size abductive explanations is at least as hard as generating subset-minimal abductive explanations since every minimum-size abductive explanation necessarily is a subset-minimal abductive explanation.

To deal with such a complexity issue, the concept of *majoritary reason* [4] has been pointed out as a valuable trade-off in terms of tractability of the computation and generality. Majoritary reasons are abductive explanations (thus satisfying the correctness criterion above) that can be computed in polynomial time in the case of random forests and that coincides with subset-minimal abductive explanations in the case of decision trees (i.e., random forests with a single tree). Furthermore, even if majoritary reasons may contain irrelevant characteristics in general, in practice one can often derive majoritary reasons that are shorter than subset-minimal abductive explanations [4]. Formally, majoritary reasons have been defined as follows [4]:

Definition 5. *Let $F = \{T_1, \ldots, T_m\}$ be a random forest over X and $\boldsymbol{x} \in \boldsymbol{X}$. A majoritary reason for $\boldsymbol{x}$ given F is a term t covering $\boldsymbol{x}$ (i.e., t a subset of $t_{\boldsymbol{x}}$), such that t is an implicant of at least $\lfloor \frac{m}{2} \rfloor + 1$ decision trees T_i (resp. $\neg T_i$) if $F(\boldsymbol{x}) = 1$ (resp. $F(\boldsymbol{x}) = 0$), and for every $\ell \in t$, $t \setminus \{\ell\}$ does not satisfy this last condition.*

In the following, we show how the concept of majoritary reason for random forests F presented in [4] can be extended to the case when a domain theory Th_e is considered. The extended domain theory used here includes constraints that encode the logical

connections between Boolean conditions used in F, possibly completed by association rules that have been derived from D_b^F.

Definition 6. *Let $F = \{T_1, \ldots, T_m\}$ be a random forest over X, Th_e a domain theory on X, and $\boldsymbol{x} \in \boldsymbol{X}$. A* majoritary reason *for $\boldsymbol{x}$ given (F, Th_e) is a term t covering $\boldsymbol{x}$ (i.e., t a subset of $t_{\boldsymbol{x}}$), such that t is an implicant modulo Th_e of at least $\lfloor \frac{m}{2} \rfloor + 1$ decision trees T_i (resp. $\neg T_i$) if $F(\boldsymbol{x}) = 1$ (resp. $F(\boldsymbol{x}) = 0$), and for every $\ell \in t$, $t \setminus \{\ell\}$ does not satisfy this last condition.*

The problem with this definition is that it leads to a concept of reason that cannot be computed in polynomial time (unless $P = NP$). Indeed, in the general case, no constraint bears on the association rules that can be generated, so they can be any clauses. As a consequence, testing whether t is an implicant modulo Th of a tree T_i is a coNP-complete problem, which precludes the existence of polynomial-time algorithms for generating majority reasons.

To deal with this problem while taking into account within the extended domain theory Th_e the set of all the association rules produced by the data mining algorithm used, the approach we followed consists in *weakening the inference relation used to reason*. Let us remind that *unit resolution* is an inference rule allowing to derive a clause δ on X from a literal ℓ on X (called a unit clause) and a clause $\sim \ell \vee \delta$ on X. A literal ℓ is *derivable by unit propagation* from a domain theory Th_e in conjunctive normal formal (CNF), noted $Th_e \vdash_1 \ell$ iff there exists a finite sequence of clauses $\delta_1, \ldots, \delta_k$ on X such that $\delta_k = \ell$ and every clause δ_i ($i \in [k]$) in the sequence is a clause of Th_e or can be obtained by applying the unit resolution rule to two clauses δ_a, δ_b of the sequence such that $a < i$ and $b < i$. The set of all the literals on X that are derivable by unit propagation (UP) from Th_e can be computed in time linear in the size of Th_e (see e.g., [11,32]). Every literal from this set is a logical consequence of Th (in symbols, if $Th \vdash_1 \ell$ then $Th \models \ell$), but the converse does not hold in general.

Let Φ be a formula on X in CNF that does not contain any valid clause. When t is a consistent term, t is an implicant of Φ iff every clause δ of Φ contains a literal ℓ of t. Given a domain theory Th in conjunctive normal term, let us say that a term t on X is a *UP-implicant* of Φ iff for every clause δ of Φ, δ contains a literal ℓ that belongs the set of literals derivable by unit propagation from $t \wedge Th$. Clearly enough, if t is a UP-implicant of Φ given Th, then t is an implicant of Φ modulo Th, but the converse does not hold in general. For instance, $\overline{b}$ is a logical consequence of $t \wedge Th$, with $t = \top$ (the empty term) and $Th = (a \vee \overline{b}) \wedge (\overline{a} \vee \overline{b})$ but $\overline{b}$ is not derivable by unit propagation from $t \wedge Th$. Based on this notion of UP-implicant, a corresponding notion of majoritary reason can be defined as well:

Definition 7. *Let $F = \{T_1, \ldots, T_m\}$ be a random forest over X, Th_e a domain theory on X, and $\boldsymbol{x} \in \boldsymbol{X}$. A* UP-majoritary reason *for $\boldsymbol{x}$ given (F, Th_e) is a term t covering $\boldsymbol{x}$, such that t is a UP-implicant given Th_e of at least $\lfloor \frac{m}{2} \rfloor + 1$ decision trees T_i (resp. $\neg T_i$) if $F(\boldsymbol{x}) = 1$ (resp. $F(\boldsymbol{x}) = 0$), and for every $\ell \in t$, $t \setminus \{\ell\}$ does not satisfy this last condition.*

The tractability of generating UP-majoritary reasons lies in the fact that they can be computed using a simple greedy algorithm equipped with unit propagation instead of full logical entailment.

Proposition 1. *Given a random forest F over a set of Boolean conditions X, a domain theory Th over X in conjunctive normal form, and an instance $\boldsymbol{x} \in \boldsymbol{X}$, a UP-majoritary reason for $\boldsymbol{x}$ given (F, Th) can be computed in time polynomial in the size of the input.*

Considering distinct orderings over the literals of $t = t_{\boldsymbol{x}}$ within the greedy algorithm may easily lead it to generate distinct majoritary reasons. Since the greedy algorithm is efficient, several orderings can be tested and finally, for taking the compactness criterion into account, one of the shortest majoritary reasons among those that have been produced can be retained. Furthermore, the fact that the greedy algorithm is order-driven can be exploited to focus the search for majoritary reasons to explanations that preferentially contain (or not contain) some characteristics (to do so, it is enough to order the literals of $t_{\boldsymbol{x}}$ from the least preferred to the most preferred). The ordering used thus reflects some user preferences (this is a first way to meet the controllability criterion).

In our approach, association rules that are not classification rules are added to the initial domain theory Th composed of clauses that encode the logical connections between Boolean conditions used in F. This leads to an extended domain theory Th_e in conjunctive normal form. As it was the case for the classification rules considered in Section 3, only rules having a 100% confidence score and a non-null support are extracted by the data mining algorithm (again, the goal is generate only rules that are not contradicted by any piece of available evidence in D_b^F since we want to use them as if they were true pieces of knowledge). Among them, only those rules in which the user is trustful enough can be kept (this is another way to meet the controllability criterion).

Interestingly, extending Th to Th_e may lead to the generation of more general explanations. Indeed, whenever a domain Th_e is at least as strong as another domain theory Th from a logical point of view (here, because Th has been completed by association rules to get Th_e), the formula $Th_e \Rightarrow F$ is a logical consequence of the formula $Th \Rightarrow F$ (and similarly for $\overline{F}$ instead of F). As a consequence, for every implicant t of F modulo Th, there exists an implicant t' of F modulo Th_e such that t' is implied by t. Similarly, for every UP-implicant t of F given Th, since the set of literals derivable by unit propagation from Th is a subset of the set of literals derivable by unit propagation from Th_e when $Th \subseteq Th_e$, there exists an implicant t' of F given Th_e such that t' is a logical consequence of t. In both cases, t' is at least as general as t.

Example 5 (Example 1, cont'ed). Consider the rectified random forest F^{A_c} at Figure 2 and $\boldsymbol{x} = (1, 0, 1, 1, 0, 0, 1)$. We have $F^{A_c}(\boldsymbol{x}) = 1$. We can check that $t = x_1 \wedge \overline{x_2} \wedge x_4$ is a UP-majoritary reason for $\boldsymbol{x}$ given (F^{A_c}, Th), and even a subset-minimal abductive explanation for $\boldsymbol{x}$ given (F^{A_c}, Th). Suppose that a unique association rule $R = (x_1 \wedge \overline{x_2}) \Rightarrow x_4$ with a 100% confidence score and a non-null support has been extracted and that the user is confident that this rule is correct. Then R can be added to Th, to give the extended domain theory Th_e. t is not a UP-majoritary reason for $\boldsymbol{x}$ given (F^{A_c}, Th_e) but the more general term $t' = x_1 \wedge \overline{x_2}$ is such a reason.

Table 1. Description of the empirical setting.

Dataset	$\lvert D\rvert$	$\lvert\mathcal{A}\rvert$	X_{RF}	X_{DT}	R_{RF}	R_{DT}	Repository
arrowhead_0_vs_1	146	249	611.5	6.8	100.0	16.6	UCR
arrowhead_0_vs_2	146	249	341.4	5.4	100.0	6.8	UCR
arrowhead_1_vs_2	130	249	593.0	6.7	100.0	10.8	UCR
australian	690	38	1299.8	47.5	100.0	99.2	openML
balance	576	4	28.0	19.4	30.3	18.8	UCI
biodegradation	1055	41	4320.4	76.6	100.0	100.0	openML
breast-tumor	286	37	112.1	38.8	100.0	100.0	openML
cleveland	303	22	551.0	27.3	100.0	40.7	openML
cnae	1080	856	75.8	45.8	99.6	14.5	UCI
compas	6172	11	68.0	49.1	97.9	70.6	openML
contraceptive	1473	21	108.6	75.3	100.0	100.0	UCI
divorce	170	54	83.3	1.7	100.0	2.8	UCI
german	1000	58	406.5	34.4	100.0	100	UCI

5   Experiments

5.1   Empirical protocol

Table 1 shows the description of the 13 datasets D used in our experiments and indicates the repositories where they can be found: UCR,[4] UCI,[5] and openML.[6]

Categorical features have been treated as nominal variables and encoded as arbitrary numbers. As to numerical features, no explicit preprocessing was performed: these features were binarized on-the-fly by the decision tree and/or random forest algorithms used for learning (we used the latest version of the `Scikit-Learn` library [29]). All hyperparameters of the learning algorithms were set to their default values (no preset depth for the trees and 100 trees in the random forests).

For every dataset D, a repeated random sub-sampling cross validation process has been achieved. D has been split 10 times into two subsets: a training set gathering 70% of the available instances from D (chosen at random) and a test set composed of the remaining 30% of instances from D. For each partition, a decision tree (resp. a random forest) F has been learned from the corresponding training set of the partition and the performance of the classifier has been evaluated on the corresponding test set. This performance scores (as well as the sizes of the classifiers and other characteristics of them) are averaged over the 10 models F that have been learned.

Then, for each dataset D and classifier F, an associated binarized dataset D_b^F was generated using the Boolean conditions occurring in F. A set A of association rules R with negations was derived from D_b^F using the ad-hoc data mining algorithm $mine$. Only rules R having a confidence of 100%, a non-null support and that are not falsified

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[4] www.timeseriesclassification.com

[5] https://archive.ics.uci.edu/ml/index.php

[6] https://www.openml.org/

by any element $(\boldsymbol{x}, \ell)$ of D_b^F have been extracted from the training set of D_b^F. This means that whenever the body b of R is satisfied by $\boldsymbol{x}$, the head h of R agrees with the label ℓ of $\boldsymbol{x}$. Those conditions are considered to limit the risk that the association rules that are mined do not hold. No specific properties (e.g., closed itemset) were targeted for the antecedent of the classification rules. Finally, the rules R of A were generated by decreasing support[7], and, once generated, a rule was kept if and only if it does not conflict with a rule that has been generated and kept before. A timeout of 3600 seconds was considered for the generation of classification rules of A_c, with a limit of 100 rules to maintain the size of the trees in F^{A_c} "small enough". A timeout of 3600 seconds was considered as well for the generation of other association rules, i.e., those from $A \setminus A_c$, with various limits in the number of rules (100 to 100 000) in order to evaluate the impact of the logical strength of Th_e on the size of the explanations. Only association rules of size 2 and 3 have been mined by $mine$ (indeed, most general rules are the most interesting ones).

Since some of the datasets used in the experiments are unbalanced, the classification performance of each model on a dataset was measured using the average F-score, average G-mean, and average AUC score of the corresponding classifiers over the 10 test sets before any rectification, and once the classifiers have been rectified by the corresponding set A_c of classification rules.

In order to measure the impact of using the association rules from $A \setminus A_c$ on the size of explanations, 100 instances have been selected from each test set and those violating any association rule from $A \setminus A_c$ have been discarded. Then for every remaining instance $\boldsymbol{x}$, UP-majority reasons for $\boldsymbol{x}$ given (F, Th) were generated using a greedy algorithm that starts with $t_{\boldsymbol{x}}$ and exploits an (elimination) ordering over the features of $t_{\boldsymbol{x}}$. 100 orderings per $\boldsymbol{x}$ have been selected at random, leading possibly to 100 distinct reasons for $\boldsymbol{x}$. A shortest reason among those generated has been retained, and the mean size of those shortest reasons over the set of instances has been computed. The mean number of instances (out of 100) for which a size decrease has been observed has also been computed. Finally, the same task has been achieved but considering this time the extended domain theory $Th_e = Th \wedge (A \setminus A_c)$ instead of Th.

In addition to the specification of the repositories where the datasets used come from, Table 1 provides different statistics. Column $|D|$ represents the number of instances in dataset D. $|\mathcal{A}|$ represents the number of primitive features used to describe the instances of D, X_{RF} (resp. X_{DT}) represents the average number of features in the 10 binarized datasets D_b^F, obtained from D by using the Boolean conditions in the 10 random forests (resp. in the 10 decision trees) that have been generated. R_{RF} and R_{DT} represents the average number of classification rules extracted from the 10 binarized datasets D_b^F. For more details, we refer the reader to the supplementary material available from [7].

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[7] Note that generating the rules by decreasing lift would not be discriminant enough. Indeed, the lift of a rule can be computed by dividing its confidence by the unconditional probability of its head, so when dealing with rules having a confidence of 100%, all the rules with the same head have the same lift.

Table 2. The impact of rectifying a random forest by classification rules, in terms of F-score, G-mean, AUC score, size, and computation time.

Dataset	$\mathcal{IF}$	$\mathcal{FF}$	$\mathcal{IG}$	$\mathcal{FG}$	$\mathcal{IA}$	$\mathcal{FA}$	$\mathcal{IN}$	$\mathcal{FN}$	$\mathcal{ID}$	$\mathcal{FD}$	$\mathcal{TR}$	$\mathcal{NR}$
arrowhead_0_vs_1	0.88	0.90	0.85	0.87	0.85	0.87	980.2	44693.6	6.7	12.4	1.22e-01	2.2
arrowhead_0_vs_2	0.89	0.91	0.85	0.88	0.86	0.89	658.4	19252.8	5.3	13.4	2.78e-01	10.3
arrowhead_1_vs_2	0.78	0.87	0.79	0.85	0.80	0.86	1037.4	25144.4	6.7	14	3.40e-01	7.0
australian	0.73	0.74	0.76	0.78	0.77	0.78	11104.2	18725.2	16.3	18.4	5.30e+01	62.2
balance	0.93	0.95	0.93	0.95	0.93	0.95	8857	15349.6	12.1	14	4.76e+00	21.4
biodegradation	0.77	0.78	0.84	0.85	0.84	0.85	12611.8	398474.8	16.4	27.3	5.17e+02	90.0
breast-tumor	0.43	0.47	0.51	0.54	0.54	0.57	9513.8	24956.4	19.2	20.9	1.00e+01	15.4
cleveland	0.70	0.75	0.72	0.75	0.72	0.76	2518	11923.2	10.6	15.3	4.52e-01	19.5
cnae	0.86	0.94	0.88	0.96	0.88	0.96	2100	39332.2	23.7	28.8	4.46e-01	12.8
compas	0.57	0.58	0.62	0.63	0.63	0.64	77957	81260.4	19.7	20.9	2.86e+01	69.7
contraceptive	0.58	0.60	0.64	0.65	0.65	0.66	18479.8	39696.6	21.5	23.5	8.49e+00	53.0
divorce	0.95	0.96	0.95	0.96	0.95	0.96	442.6	7875.8	3.7	14.9	2.73e+00	19.3
german	0.98	0.98	0.02	0.02	0.49	0.50	5457	56676	15.1	24.9	5.15e+01	100.0

5.2 Empirical results

Tables 2 and 3 give, respectively for the random forest model and the decision tree model, the initial and final (i.e., after rectification) average F-scores, G-mean scores, and AUC scores $(\mathcal{IF}, \mathcal{FF})(\mathcal{IG},\mathcal{FG})$ $(\mathcal{IA}, \mathcal{FA})$, the initial and final average numbers of nodes $(\mathcal{IN}, \mathcal{FN})$, and the initial and final average depths $(\mathcal{ID}, \mathcal{FD})$. $\mathcal{TR}$ represents the average cumulative time (in seconds) required to perform all rectifications. $\mathcal{NR}$ denotes the percentage of rectifications that led to change F. We observe that, for the majority of the datasets used in the experiments, rectifying both random forests and decision trees with the mined classification rules leads to an increase in predictive performance, ranging from 1% to more than 10%. For the three metrics used, namely F-score, G-mean and AUC, an improvement is typically achieved. This improvement is small most of the time, but it can be very significant in some cases (see e.g., the `arrowhead_1_vs_2` and the `cnae` datasets when a random forest is used).

The average computation times required to achieved the full rectification of F by A_c were reasonable (less than 517 seconds for the random forests and less than 5 seconds for the decision trees).

The numbers of nodes and the depths increased for both classifiers, which is not a surprise given the way the rectification algorithm works. This increase can be significant and it may question the readability by humans of the rectified trees for some datasets. However, assuming that a tree-based model is "human comprehensible" when it contains at most 50 nodes, only 4 models out of the 26 models considered in our experiments were already "small enough" at start to be viewed as "human comprehensible" ($\mathcal{IN} \leq 50$ for 4 decision trees, only). And all of them of them remained "small enough" after the rectification step ($\mathcal{FN} \leq 50$ for 3 decision trees). The limit of 50 nodes was systematically exceeded by the random forests that have been learned. Fur-

Table 3. The impact of rectifying a decision tree by classification rules, in terms of F-score, G-mean, AUC score, size, and computation time.

Dataset	$\mathcal{IF}$	$\mathcal{FF}$	$\mathcal{IG}$	$\mathcal{FG}$	$\mathcal{IA}$	$\mathcal{FA}$	$\mathcal{IN}$	$\mathcal{FN}$	$\mathcal{ID}$	$\mathcal{FD}$	$\mathcal{TR}$	$\mathcal{NR}$
arrowhead_0_vs_1	0.82	0.86	0.80	0.85	0.81	0.85	20.4	39	5.4	6.3	1.06e-03	5.6
arrowhead_0_vs_2	0.83	0.86	0.80	0.84	0.81	0.84	12.8	20.2	4.2	5	1.38e-03	4.6
arrowhead_1_vs_2	0.74	0.78	0.74	0.77	0.74	0.78	19.2	33.2	5.3	6	7.24e-04	4.8
australian	0.70	0.74	0.73	0.77	0.73	0.77	141.4	5325.2	12.5	24.2	2.06e-01	28.0
balance	0.87	0.90	0.87	0.89	0.87	0.89	97	144.4	10	10.7	8.41e-03	15.9
biodegradation	0.62	0.69	0.73	0.77	0.73	0.78	189	97609.2	14.3	33.7	5.91e+00	74.3
breast-tumor	0.37	0.44	0.46	0.51	0.50	0.54	85.2	854.4	11.1	15.3	3.15e-02	12.8
cleveland	0.70	0.74	0.72	0.75	0.73	0.76	58.6	596	9	13.3	1.46e-02	12.9
cnae	0.90	0.95	0.95	0.98	0.95	0.98	54.4	3530.6	20.3	33.4	2.05e-01	34.9
compas	0.55	0.57	0.61	0.62	0.62	0.63	772.2	810	15.2	16.1	1.25e-01	49.5
contraceptive	0.57	0.60	0.62	0.64	0.62	0.65	448.8	689	17.6	17.6	9.15e-02	40.2
divorce	0.92	0.92	0.93	0.93	0.93	0.93	4	4.4	1.5	1.7	2.01e-04	2.3
german	0.96	0.98	0.27	0.29	0.54	0.56	64	1197.4	10.4	19.4	1.05e-01	48.9

thermore, preserving human interpretability was not an objective of our approach: what was expected instead (and actually achieved) was to keep the *computational intelligibility* of the model [5], i.e., the ability to support efficiently a number of XAI queries. Especially, our experiments have shown that the ability to compute in an efficient way abductive explanations from tree-based models has been preserved after the rectification step.[8]

The time required by the data mining algorithm to compute A_c depends on the dataset and varies between 0.15 and 1656.46 seconds for the random forests. For decision trees, it ranges from 0.01 to 0.46 seconds.

Tables 4 and 5 give statistics about the evolution of the size of the smallest abductive explanations that have been found for the tree-based models F considered at start, depending on the number of association rules that have been generated (up to 100, 1000, 10000, and 100000) and added to the initial domain theory Th to get the extended domain theory Th_e. Such statistics are reported both for the random forests (Table 4) and for the decision trees (Table 5). In these tables, Red represents the reduction achieved, i.e., on average over 100 instances x, the ratio between the size of the smallest UP-majoritary reason found for x using Th minus the size of the smallest UP-majoritary reason found for x using Th_e, divided by the size of the smallest UP-majoritary reason found for x using Th. Ins represents on average over 100 instances, the number of instances x for which the size of the smallest abductive explanation found has decreased when switching from Th to Th_e.

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[8] It must also be kept in mind that if decision trees with a limited depth are more "human comprehensible", they are also less robust. Indeed, changing a few characteristics (no more than the depth of the tree) in an input instance (whatever it is) is enough to change the prediction made for this instance. See Proposition 5 in [3] for details.

Table 4. The impact of taking association rules into account on the size of abductive explanations given a random forest.

Dataset	100000		10000		1000		100	
	Red	*Ins*	*Red*	*Ins*	*Red*	*Ins*	*Red*	*Ins*
arrowhead_0_vs_1	29.83	100.00	10.52	97.01	5.18	96.12	2.29	80.62
arrowhead_0_vs_2	72.84	100.00	25.62	100.00	14.23	73.98	5.31	55.56
arrowhead_1_vs_2	55.73	100.00	16.11	98.08	4.84	92.59	2.36	64.96
australian	3.68	43.90	1.70	23.57	0.66	10.62	0.11	1.92
balance	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
biodegradation	37.38	99.60	5.36	90.30	1.48	46.90	0.13	9.70
breastTumor	19.62	91.96	0.55	6.32	0.00	0.00	0.00	0.00
cleveland	0.59	19.09	0.27	8.43	0.22	4.33	0.17	2.65
cnae	96.73	100.00	41.74	98.85	21.42	95.05	16.75	92.30
compas	7.37	37.40	0.00	0.00	0.00	0.00	0.00	0.00
contraceptive	1.59	22.50	0.15	0.80	0.00	0.00	0.00	0.00
divorce	82.63	100.00	82.88	100.00	43.09	100.00	9.53	58.94
german	0.78	28.30	0.4	9.50	0.12	9.31	0.09	0.60

The results obtained show that for the two tree-based models considered in the experiments (decision trees and random forests), the reduction of the size of abductive explanations obtained by considering association rules heavily varies with the dataset and with the number of association rules that are considered. Indeed, *Red* is null or very small for some configurations and quite high for others. Of course, it increases with the number of association rules that are generated (since the logical strength of the theory cannot decrease when a rule is added to it). Similarly, the number *Ins* of instances concerned by such a reduction heavily varies with the dataset and with the number of association rules that have been generated. It is null or very small for some configurations but reaches 100% for other configurations when random forests are considered. Again, *Ins* cannot decrease when the theory used is strengthened.

The time required by the data mining algorithm to compute the association rules that are not classification rules (i.e., those rules from $A \setminus A_c$) also depends on the dataset; it varies between 0.33 and 3600 seconds for the random forests and between 0.1 and 39.54 seconds for the decision trees. When deriving abductive explanations while taking advantage of association rules as a domain theory, experiments have not shown any huge extra computational cost, i.e., UP-majoritary reasons can be derived efficiently in practice (with computation times that are usually close to those required by majoritary reasons). More in detail, the computation time required to derive one UP-majoritary reason was on average less than 1s, whatever the dataset used and even when the domain theory has been completed with 100 000 rules). This lack of extra cost can be explained by the efficiency with which unit propagation can be achieved in practice.

Tables 2 and 3 have shown that after rectification, the number of nodes in the models F can increase significantly. Thus, it was important to assess whether this increase may have a significant impact on the time needed to compute abductive explanations for instances given F. From such a perspective, Tables 6 and 7 report for the datasets con-

Table 5. The impact of taking association rules into account on the size of abductive explanations given a decision tree.

Dataset	100000		10000		1000		100	
	Red	*Ins*	*Red*	*Ins*	*Red*	*Ins*	*Red*	*Ins*
arrowhead_0_vs_1	17.62	43.18	17.62	43.18	17.62	43.18	17.06	41.67
arrowhead_0_vs_2	11.12	26.76	11.12	26.76	11.12	26.76	11.12	26.76
arrowhead_1_vs_2	13.26	28.69	13.26	28.69	13.26	28.69	13.26	28.69
australian	21.15	72.91	5.96	26.49	1.82	10.95	0.25	2.04
balance	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
biodegradation	38.68	85.51	19.93	68.52	3.20	17.72	0.55	3.70
breastTumor	17.09	65.29	11.59	54.03	3.42	19.78	0.39	1.77
cleveland	4.29	24.73	4.29	24.73	0.48	2.88	0.17	0.66
cnae	71.06	95.43	71.06	95.43	41.40	78.26	3.48	28.90
compas	3.76	19.10	0.00	0.00	0.00	0.00	0.00	0.00
contraceptive	4.90	27.70	0.3	1.30	0.00	0.00	0.00	0.00
divorce	19.54	33.33	19.54	33.33	19.54	33.33	19.54	33.33
german	5.38	20.63	5.38	20.63	2.19	7.63	0.00	0.00

sidered in our experiments average computation times (in seconds, over 100 instances) to generate one *sufficient reason* for an instance given a decision tree and one *majoritary reason* for an instance given a random forest. $\mathcal{T}_{bef}$ denotes the time needed to compute a sufficient reason before the rectification of the model F, and $\mathcal{T}_{aft}$ the average time needed to compute a sufficient reason after the rectification of the model F by A_c. The domain theory considered here is the initial one Th. From these tables, we can observe that while the time required to compute explanations increases after rectification, it remains very reasonable (in the worst case, less than 1s) whatever the model F.

6   Other Related Work

Though the issue of rule learning in a classification perspective has been considered for decades, our work departs significantly from previous approaches by the fact that it is also guided by the explanation issue. Instead, the goal pursued by most of the previous approaches was to generate rule-based classifiers using classification rule mining. Furthermore, most of the time, in such previous approaches, tree-based models were not involved in addition to rule mining.

   An exception concerns the CBA system [23] based on Apriori algorithm [1]. In the CBA system, classification rules R are generated by decreasing confidence, then decreasing support unless preset minimal values are reached (in the reported experiments, 50% for confidence $minconf$, and 1% for the support $minsup$). A default class is considered as well so as to get a complete classifier whatever the number of rules generated. The accuracy of the classifier is evaluated. The set of rules is pruned to get a minimal number of rules that cover the training data and achieve satisfying accuracy. In particular, every rule that does not enhance the accuracy of the classifier is removed. [24]

Table 6. Average computation time (in seconds, over 100 instances) for extracting a sufficient reason for an instance given a decision tree

Dataset	$\mathcal{T}_{bef}$	$\mathcal{T}_{aft}$
arrowhead_0_vs_1	0.00037 ± 0.00028	0.00042 ± 0.00024
arrowhead_0_vs_2	0.00030 ± 5.21e-05	0.00054 ± 0.00032
arrowhead_1_vs_2	0.00040 ± 0.00024	0.00045 ± 0.00028
australian	0.00056 ± 0.00015	0.00157 ± 0.00095
balance	0.00089 ± 0.00101	0.00061 ± 0.00017
biodegradation	0.00045 ± 0.00025	0.00401 ± 0.00515
breast-tumor_0	0.00060 ± 8.15e-05	0.00136 ± 0.00112
cleveland	0.00053 ± 9.90e-05	0.00112 ± 0.00107
cnae_0	0.00037 ± 0.00012	0.00139 ± 0.00098
compas	0.00051 ± 0.00027	0.00041 ± 0.00020
contraceptive_0	0.00079 ± 0.00012	0.00116 ± 0.00099
divorce	0.00028 ± 0.00014	0.00031 ± 0.00016
german	0.00043 ± 5.56e-05	0.00066 ± 0.00025

improves the previous CBA approach in two directions. First, by considering minimal values $minsup$ that depend on the targeted class (this is important to get accurate rules when dealing with imbalanced datasets). Second, by making a competition of several classifiers on different segments of the training data. Each rule R that is generated is thus used to select a subset of training instances, those covered by the body of the rule. Then several models are learned from the resulting set of instances and evaluated: R is replaced by the model that minimizes the number of classification errors (provided that this number is lower than the number of errors coming from R). As remarked in [24], considering decision trees as one of the competitors is valuable since it makes it possible to generate deep trees (i.e., with paths corresponding to rules with many conditions) which can be necessary to get an accurate classification but can hardly be achieved by the rules generated by the CBA algorithm for combinatorial reasons. Thus, decision trees are used in this approach to improve a rule-based classifier, while in some sense a converse path is followed in our work.

In contrast to such works, rule mining is leveraged in our approach to improve a tree-based classifier as to inference and explanation. Unlike the previous approaches focused solely on the inference issue, only rules with 100% confidence and non-null support are looked for. In our approach, for the inference task, primacy is given to classification rules over the tree-based classifier. A rectification algorithm is used to update the tree-based classifier with each classification rule that is generated. Finally, not only classification rules are extracted but other association rules are generated as well and exploited to improve the explanation task by strengthening the domain theory associated with the tree-based model.

As far as we know, the use of mined rules for generating more general abductive explanations has hardly been considered previously. As a notable exception, let us mention [31], which shows that taking into account mined rules is useful to diminish the size of sufficient reasons for decision lists (boosted trees and binarized neural networks are also

Table 7. Average computation time (in seconds, over 100 instances) for extracting a majoritary reason for an instance given a random forest

Dataset	$\mathcal{T}_{bef}$	$\mathcal{T}_{aft}$
arrowhead_0_vs_1	0.00108 ± 9.61e-05	0.03399 ± 0.01488
arrowhead_0_vs_2	0.00105 ± 0.00051	0.00984 ± 0.00510
arrowhead_1_vs_2	0.01427 ± 0.00317	0.02419 ± 0.02181
australian	0.06901 ± 0.02262	0.08253 ± 0.02014
balance	0.00880 ± 0.00190	0.01038 ± 0.00276
biodegradation	0.09015 ± 0.02015	1.05798 ± 1.01648
breast-tumor_0	0.01202 ± 0.00430	0.04102 ± 0.01813
cleveland	0.02420 ± 0.00565	0.06865 ± 0.02992
cnae_0	0.00273 ± 0.00033	0.01250 ± 0.00358
compas	0.00994 ± 0.00592	0.00803 ± 0.00317
contraceptive_0	0.01224 ± 0.00394	0.01418 ± 0.00612
divorce	0.00537 ± 0.00106	0.05882 ± 0.04120
german	0.02064 ± 0.00688	0.03661 ± 0.01331

mentioned). In this approach, rule induction is achieved using a specific MaxSAT-based algorithm to learn decision sets [20]. Unsurprisingly, the empirical results presented in [31] cohere with the ones pointed out in the previous section. The main differences between [31] and our own work are actually threefold. First of all, [31] also presents the impact of mined rules on the size of (subset-minimal) contrastive explanations (in theory, it is known that they can be lengthened) while only abductive explanations are considered in our work. Furthermore, in [31] the mined rules are not used for the inference purpose. Finally, the ML models considered in the two papers differ ([31] focuses on decision list, boosted trees, and binarized neural networks, while we have considered decision trees and random forests).

7   Conclusion

In this paper, we have shown how to combine association rules derived using data mining techniques with decision tree and random forest classifiers. Classification rules are exploited to tentatively enhance the predictive performance of the classifier at hand using a rectification operation. Other association rules are leveraged to produce more general abductive explanations. Computational guarantees about the tractable generation of those explanations have been provided. An important feature of our approach is that at each step the user *can keep the control* of the association rules from A he/she is ready to consider (he/she can simply select those rules in which he/she is confident enough and filters out the other ones). Experiments have been conducted showing that the proposed approach is practical enough. Computation times remain reasonable, even for large datasets (see e.g., the results for `biodegradation` and `cnae` in the tables) The empirical results have shown that the objective of improving the predictive performance of the classifiers can be reached, even if they are often modest for the inference

task. On the contrary, they have also shown that the reduction of the size of abductive explanations can be very significant.

This work calls for further research. A perspective is to compile Th_e in order to make it tractable for clausal entailment [13]. This would be an alternative to unit propagation as used in the proposed approach. Provided that the compiled forms remain small enough (which cannot be guaranteed in the general case), this could be a way to benefit from the full power of logical entailment, and as a consequence, to get even more general explanations. Experiments will be run to determine whether this is actually the case in practice.

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Appendix: Proofs

Proof of Proposition 1

Proof. Our greedy algorithm is as follows. For the case when $F(\boldsymbol{x}) = 1$, start with $t = t_{\boldsymbol{x}}$, and iterate over the literals ℓ of t by checking whether t deprived of ℓ is a UP-implicant given Th of at least $\lfloor \frac{m}{2} \rfloor + 1$ decision trees of F. If so, remove ℓ from t and proceed to the next literal. Once all literals in $t_{\boldsymbol{x}}$ have been examined, the final term t is by construction a UP-implicant given Th of a majority of decision trees in F, such that removing any literal from it would lead to a term that is no longer a UP-implicant given Th of this majority. So, t is by construction a UP-majoritary reason. The case when $F(\boldsymbol{x}) = 0$ is similar, by simply replacing each T_i by its negation (which can be obtained in linear time by replacing every 0-leaf in T_i by a 1-leaf and vice-versa). This greedy algorithm runs in time polynomial in the size of the input $t_{\boldsymbol{x}}$, F and Th since on each iteration, checking whether t is a UP-implicant given Th of T_i (for each $i \in [m]$) can be done in time polynomial in the size of t, T_i, and Th. Indeed, in order to decide whether t is a UP-implicant given Th of a decision tree T_i of F, it is enough to test that for every clause $\delta \in \mathtt{CNF}(T_i)$, δ contains a literal derivable by unit propagation from $t \wedge Th$. The fact that this set can be derived in time linear in the size of $t \wedge Th$ completes the proof.