Learning Optimal Decision Trees Using MaxSAT

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Abstract

We present a Combinatorial Optimization approach based on Maximum Satisfiability technology to compute Minimum Pure Decision Trees (MPDTs) for the sake of interpretability. We show that our approach outperforms clearly in terms of runtime previous approaches to compute MPDTs. We additionally show that these MPDTs can outperform on average the DT classifiers generated with sklearn in terms of accuracy. Therefore, our approach tackles favourably the challenge of balancing interpretability and accuracy.

Keywords  Decision trees, MaxSAT, XAI

1 Introduction

Recently, there has been a growing interest in creating synergies between Combinatorial Optimization (CO) and Machine Learning (ML), and vice-versa. This is a natural connection since ML algorithms can be seen in essence as optimization algorithms that try to minimize prediction error. In this paper, we focus on how CO techniques can be applied to improve decision tree classifiers in ML.

A decision tree classifier is a supervised ML technique that builds a tree-structured classifier, where internal nodes represent the features of a dataset, branches represent the decision rules and each leaf node represents the outcome. In essence, every path from the root to a leaf is a classification rule that determines to which class belongs the input query.

ML research has been traditionally concerned with developing accurate classifiers, i.e., classifiers whose prediction error is as low as possible. However, lately, the research community is looking at the trade-off between accuracy and interpretability, where the latter refers to the human ability to understand how the classifier works. Interpretability is fundamental in many senses: to explain ML models and understand their value and accuracy, to debug machine learning algorithms, to make more informed decisions, etc.

Among supervised learning techniques, decision tree classifiers are interpretable in itself, as long as they are small, i.e., as few rules as possible, and as short as possible. As stated in Bessiere et al. [2009], informally, this follows from the principle of Occam’s Razor that states that one should prefer simpler hypotheses. However, notice that this is just one of the diverse aspects that may have to do with interpretability at least from a human perspective.

CO approaches have been applied to compute small trees in the sense of building Decision Trees (DTs) of minimum size (number of nodes) or minimum depth. Minimizing the size corresponds indirectly to minimizing the number of rules associated with the DT and minimizing the depth corresponds to minimizing the length of the rules. Among these approaches we find several contributions coming from Operation Research (OR) [Agin et al. [2020], Verwer and Zhang [2019] and from Constraint Programming (CP) [Hu et al. [2019], Verhaeghe et al. [2019].

Another question is whether these DTs are pure (i.e., classify correctly the training dataset). To avoid overfitting on the training set, and therefore get lower accuracy on the test set, there is a rule of thumb that makes us prefer some impurity to get more generalization power. However, it is difficult to anticipate how much we should allow.
In this paper, we first address specifically the question of how to efficiently compute minimum pure DTs and discuss later how accurate they are with respect to DTs with similar size computed using other approaches. We focus on CP techniques where SATisfiability (SAT) based approaches have been shown to be very effective. Particularly, we will work on the Maximum Satisfiability (MaxSAT) problem.

In particular, we revisit the SAT approach in Narodytska et al. [2018] which encodes into SAT the decision query of whether there is a pure DT of exactly $n$ nodes. Then, by performing a sequence of such SAT queries the optimum can be located. We extend this SAT approach to the MaxSAT case, i.e., we encode into MaxSAT the query representing which is the minimum $n$ for which such a pure DT exists.

Equipped with a MaxSAT encoding we can now leverage the power of MaxSAT solvers. Our experimental results show that our approach in practice is able to obtain faster minimal pure DTs on a wide variety of benchmarks.

Secondly, we show that by extracting multiple optimal solutions from the MaxSAT solver we can build more efficient classifiers. We show that this approach is able to return comparable or better accuracies on average than the DT classifiers generated with sklearn. This is an interesting result since all the optimal solutions are minimum pure DTs for the training set.

2 Preliminaries

Definition 1 An example $e$ is a set of pairs $(f_r, v)$ plus the class label $c$, where $f_r$ is a feature and $v$ is the value assigned to the feature.

Definition 2 A Decision Tree (DT) is a set of rules (namely paths) that are constructed by traversing a tree-like structure composed of questions (decision nodes) and answers until a terminal node with a label (leaf) is found. Each decision node has as many direct successors as possible answers to the question assigned to it [Breiman et al. 1984].

Definition 3 The depth of a node in a DT is the length of the path (i.e., count of nodes traversed) from the root to this node. The depth of the DT is the length of the largest path from the root to any leaf.

Definition 4 A Complete Decision Tree (CDT) is a tree where all the leaves are located at the same depth.

Definition 5 A Pure Decision Tree (PDT) for a set of examples $\varepsilon$, $PDT(\varepsilon)$, is a DT that classifies correctly all the examples [Hautaniemi et al. 2005]. By definition, its accuracy on this set is 100%.

Definition 6 A Minimum Pure Decision Tree (MPDT) for a set of examples $\varepsilon$, $MPDT(\varepsilon)$, is a DT that is proven to be the smallest PDT for $\varepsilon$ in terms of size (i.e., the number of nodes in the DT). We denote the minimum size as $|MPDT(\varepsilon)|$.

Definition 7 A literal is a propositional variable $x$ or a negated propositional variable $\neg x$. A clause is a disjunction of literals. A Conjunctive Normal Form (CNF) is a conjunction of clauses.

Definition 8 A weighted clause is a pair $(c, w)$, where $c$ is a clause and $w$, its weight, is a natural number or infinity. A clause is hard if its weight is infinity (or no weight is given); otherwise, it is soft. A Weighted Partial MaxSAT instance is a multiset of weighted clauses.

Definition 9 A truth assignment for an instance $\phi$ is a mapping that assigns to each propositional variable in $\phi$ either 0 (False) or 1 (True). A truth assignment is partial if the mapping is not defined for all the propositional variables in $\phi$.

Definition 10 A truth assignment $I$ satisfies a literal $x$ ($\neg x$) if it maps $x$ to 1 (0); otherwise, it is falsified. A truth assignment $I$ satisfies a clause if $I$ satisfies at least one of its literals; otherwise, it is violated or falsified. The cost of a clause $(c, w)$ under $I$ is 0 if $I$ satisfies the clause; otherwise, it is $w$. Given a partial truth assignment $I$, a literal or a clause is undefined if it is neither satisfied nor falsified. A clause $c$ is a unit clause under $I$ if $c$ is not satisfied by $I$ and contains exactly one undefined literal.

Definition 11 The cost of a formula $\phi$ under a truth assignment $I$, denoted by $\text{cost}(I, \phi)$, is the aggregated cost of all its clauses under $I$.

Definition 12 The Weighted Partial MaxSAT problem for an instance $\phi$ is to find an assignment in which the sum of weights of the falsified soft clauses is minimal, denoted by $\text{cost}(\phi)$, and all the hard clauses are satisfied. The Partial
MaxSAT problem is the Weighted Partial MaxSAT problem where all weights of soft clauses are equal. The SAT problem is the Partial MaxSAT problem when there are no soft clauses. An instance of Weighted Partial MaxSAT, or any of its variants, is unsatisfiable if its optimal cost is \( \infty \). A SAT instance \( \phi \) is satisfiable if there is a truth assignment \( I \), called model, such that cost\((I, \phi) = 0\).

**Definition 13** A pseudo-Boolean constraint (PB) is a Boolean function of the form \( \sum_{i=1}^{n} q_i l_i \circ k \), where \( k \) and the \( q_i \) are integer constants, \( l_i \) are literals, and \( \circ \in \{<,\leq,=,\geq,>\} \) is a comparison operator.

**Definition 14** An At Least K (AtLeastK) constraint is a PB of the form \( \sum_{i=1}^{n} l_i \geq k \). An At Most K (AtMostK) constraint is a PB of the form \( \sum_{i=1}^{n} l_i \leq k \).

**Definition 15** An At Least One (AtLeastOne) constraint is a PB of the form \( \sum_{i=1}^{n} l_i \geq 1 \). An At Most One (AtMostOne) constraint is a PB of the form \( \sum_{i=1}^{n} l_i \leq 1 \).

### 3 Related Work

Table 1 summarizes the main SAT-based approaches to compute small trees. In a pioneering work, Bessiere et al. [2009], the first SAT approach to compute MPDTs was presented. They encode into SAT the decision query of whether there exists a PDT of size \( n \). They use as upper bound the solution from a CP model. Then, they perform a sequence of queries to a SAT solver (in the SAT4J package Le Berre and Parrain [2010]) where \( n \) is iteratively bounded by adding an AtLeastK constraint on the number of useless nodes that must be in the solution.

Recently, in Narodytska et al. [2018] a more efficient SAT encoding was provided to encode the decision query of whether there exists a PDT of size \( n \). The authors also solve the problem through a sequence of SAT queries. In this case, the upper bound is computed with the algorithm ITI Ugolli [1989]. Then, at every iteration, they reencode the problem with the next possible value of \( n \). We refer to this approach as MinDT.

In Avenelona [2020] the authors propose two SAT-based methods. The Infer-depth approach iteratively decreases the depth of the tree represented by the SAT encoding, till it locates the minimum depth to build a complete PDT. The Infer-size approach computes the MPDT with the depth found with Infer-depth. While both approaches compute small PDTs, none of them guarantee to find MPDTs.

In Janota and Morgado [2020] dtfinder, the authors fix heuristically an initial layout of the DT for the first levels and then extend it to a PDT with the minimum possible number of nodes having that layout. This approach also does not guarantee to compute MPDTs since the initial layout is not guaranteed to belong to an MPDT.

In Hu et al. [2020] DT(max), the authors’ approach answers which is the best tree in terms of accuracy in the training set that can be obtained given an upper bound on the depth. Note that if the upper bound is smaller than the minimal depth of MPDT, their approach reports a tree with less than 100% of accuracy on the training set (i.e. impure tree). However, as discussed in the introduction in terms of expected maximum accuracy for the test set this has not to be a limitation.

In Table 1 we summarize the main properties of the SAT-based approaches for computing DTs as described above. We present the algorithm, the objective function that they optimize, whether they guarantee to find a minimum PDT in size or not, and if they return a PDT for the input dataset. The only algorithms that are complete in the sense of certifying the minimum size of the PDTs are Bessiere et al. [2009] and MinDT Narodytska et al. [2018]. While Bessiere et al. [2009] is the first SAT approach presented, it was clearly outperformed by MinDT. Therefore, we will focus on comparing our approach MPDT (see section 4) with MinDT in terms of computing efficiently MPDTs. In terms of computing rather small trees with good accuracy, we will compare with DT(max) Hu et al. [2020] which in contrast to the other approaches focuses also on maximizing the accuracy.

### 4 Computing MPDTs with MaxSAT

In this section, we show how to extend the SAT encoding described in Narodytska et al. [2018], here referred to as MinDT SAT encoding, which asks whether there is a PDT of size \( n \) (number of nodes) for a binary classification problem. In particular, we describe a Partial and Weighted Partial MaxSAT encoding that represents the query of asking which is the minimum PDT that can be built given an upper bound \( n \) on the number of nodes. We refer the reader to the appendix for the complete description of the variables, symbols, and constraints used in the encoding.
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| Algorithm     | Objective       | Min size | PDT |
|---------------|-----------------|----------|-----|
| Bessiere et al. | min. size       | yes      | yes |
| MinDT         | min. size       | yes      | yes |
| Infer-depth   | min. depth      | no       | yes |
| Infer-size    | min. depth, size| no       | yes |
| dtfinder      | min. depth, size| no       | yes |
| DT(max)       | max. accuracy   | no       | no  |
| MPDT          | min. size       | yes      | yes |

Table 1: State-of-the-art: SAT-based approaches for computing DTs

The MinDT SAT encoding assumes that: (1) the problem to solve with a DT is a binary classification problem; (2) the DT is binary; (3) the root node is labeled as node 1 (the rest of them are labeled into breadth-first or level order traversal); and (4) positive (negative) answers at decision nodes are assigned to the right (left) child node.

We summarize the relevant symbols and functions used in the encoding in table 2.

| Sym/func | Definition |
|----------|------------|
| $\varepsilon$ | The set of observations used to train the tree |
| $N$ | Range of nodes, starting at 1 |
| $N^e$ | Range of even-indexed nodes |
| $N^o$ | Range of odd-indexed nodes |
| $K$ | Range of features for each observation |
| $lr(i)$ | Set of potential left child nodes for node $i$ |

Table 2: Symbols and functions for MinDT SAT encoding [Narodytska et al. 2018]

We have added a new variable $\eta_i$, to the ones used in MinDT SAT encoding, which represents if a node $i$ is used or not in the DT.

The MaxSAT encoding works on an upper-bounded number of nodes to be in the DT (see experimental results on how we compute the upper bound). Therefore, if the upper bound is not the optimal solution, some nodes will not be used.

We apply a further refinement, based on the following observation: since nodes are numbered in breadth-first order, two consecutive nodes with the same parent will be both in the solution or not. Therefore, we define function $\eta(i)$ as:

$$\eta(i) = \begin{cases} 
\eta_{i+1} & \text{if } i \in N^e \\
\eta_i & \text{if } i \in N^o 
\end{cases}$$

We first introduce the soft constraints in the Partial MaxSAT encoding that describe the objective function of the Minimum PureDT optimization problem:

$$\bigwedge_{i \in N^o} (\neg \eta_i, 1) \quad (\text{SoftN})$$

We also introduce the Weighted variant, as follows:

$$\bigwedge_{i \in N^o} (\neg \eta_i, i) \quad (\text{WSoftN})$$

The weighted variant is useful for SAT-based solvers (in particular, for core-guided approaches [Ansótegui et al. 2013], [Morgado et al. 2013]) that iteratively refine the lower bound. If we want these solvers to force the upper bound we can achieve with the combination of the Weighted encoding and the activation of the stratified approach [Ansótegui et al. 2012]. This approach partitions the soft clauses according to their weight. Then, each subset is added in decreasing order (according to their weight) and the subproblem is solved to optimality. The approach ends when the current subproblem involves all the soft clauses.

Now, we describe the constraints with the modifications needed to connect the soft clauses (objective function) from the original SAT encoding in [Narodytska et al. 2018]. To encode the PB Exactly-One constraints on a set of literals $L$...
we use a custom Python framework [Ansótegui et al. [2021]]. In particular we use the Encoder.at_most_one with option best to encode a PB AtMostOne constraint of \( L \) and we simply write a clause containing the disjunction of literals in \( L \) to write a PB AtLeastOne constraint.

### 4.1 Node usage hard clauses:

- If an odd node is not used, then both himself and the previous one are not leaves (note that we do not have to set the root as it is never a leaf in this encoding).

  \[
  \bigwedge_{i \in N^o \mid i > 1} \neg \eta_i \rightarrow \neg v_i \land \neg v_{i-1}
  \]  
  (1)

- If a node is used, then all the nodes with a smaller index must be used:

  \[
  \bigwedge_{i \in N^o \mid i > 1} \eta_i \rightarrow \eta_{i-2}
  \]  
  (2)

- Enforce the lower bound \( lb \). By setting \( \eta(lb) \) to True, and combined with constraint 2, we ensure that at least \( lb \) nodes are used. We set the lower bound to 3 nodes, as any smaller tree would have a single node:

  \[
  \eta(lb)
  \]  
  (3)

### 4.2 Tree layout hard clauses:

- (i) Leaves do not have a left child, and (ii) if node \( i \) is used in the DT, and has no left child candidates, then it is a leaf.

  \[
  \bigwedge_{i \in N} \left\{ \bigwedge_{j \in lr(i)} (v_i \rightarrow \neg l_{i,j}) \right\} \text{ if } |lr(i)| \neq 0
  \]  
  (4)

- If node \( i \) is not a leaf and is used in the DT, then it has exactly one left child.

  \[
  \bigwedge_{i \in N} \left( \neg v_i \land \eta(i) \right) \rightarrow \left( \sum_{j \in lr(i)} l_{i,j} = 1 \right)
  \]  
  (5)

- If node \( j \) is used in the DT (and it is not the root) it will have exactly one parent.

  \[
  \bigwedge_{j \in N \mid j > 1} \left( \eta(j) \rightarrow \sum_{i = \left\lfloor \frac{j}{2} \right\rfloor}^{j-1} p_{j,i} = 1 \right)
  \]  
  (6)

### 4.3 Feature assignment hard clauses:

- If node \( j \) is not a leaf and it is in the DT, then it has exactly one feature assigned to.

  \[
  \bigwedge_{j \in N} \left( \neg v_j \land \eta(j) \right) \rightarrow \sum_{r \in K} a_{r,j} = 1
  \]  
  (7)

### 4.4 Additional Pruning hard clauses:

Depending on which nodes are decided to be leaves or not, the possible list of children for a given node may change. These constraints enforce this simplification. We refer to the original description [Narodytska et al. [2018]]. We incorporate as in previous constraints the \( \eta(i) \) variable to take into account in counters \( \tau_{t,i} \) and \( \lambda_{t,i} \) only the nodes that are
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used in the solution.

\[ \bigwedge_{i \in N} \lambda_{0,i} \land \tau_{0,i} \quad (8) \]

\[ \bigwedge_{i \in N, t \in [1, \lfloor \frac{i}{2} \rfloor]} (\lambda_{t,i} \leftrightarrow (\lambda_{t-1,i} \lor v_i \land \eta(i))) \quad (9) \]

\[ \bigwedge_{i \in N, t \in [1, i]} (\tau_{t,i} \leftrightarrow (\tau_{t-1,i} \lor \neg v_i \land \eta(i))) \quad (10) \]

\[ \bigwedge_{i \in N, t \in [1, \lfloor \frac{i}{2} \rfloor]} \lambda_{t,i} \rightarrow \neg l_i,2(i-t+1) \land \neg r_i,2(i-t+1) + 1 \quad (11) \]

\[ \bigwedge_{i \in N, t \in [\lceil \frac{i}{2} \rceil, i]} \tau_{t,i} \rightarrow \neg l_i,2(t-1) \land \neg r_i,2t-1 \quad (12) \]

4.5 Multilabel encoding

When dealing with multilabel datasets (with a label domain \( Cls \)) we do not use the \( c_j \) variable, but the \( c_{k,j} \) variable to represent that the leaf \( j \) has the class \( k \) assigned. We modify the constraints 17 and 18 (see supplementary material) as follows:

\[ \bigwedge_{k \in Cls, j \in N, q \in \varepsilon_k, i} (v_j \land c_{k,j}) \rightarrow \bigvee_{r \in K} d_{r,j}^{(r,q)} \quad (13) \]

We add the following additional clauses:

• A decision node has no class assigned:

\[ \bigwedge_{j \in N, k \in Cls} (\neg v_j \rightarrow \neg c_{k,j}) \quad (14) \]

• A leaf has only one label:

\[ \bigwedge_{j \in N} (v_j \rightarrow \sum_{k \in Cls} = 1) \quad (15) \]

4.6 MaxSAT encodings:

See the appendix A for the full description of equations.

Proposition 1 Let \( PMSat_{\epsilon,n}^{e,n=ub,lh} \) be SoftN \( \land (\text{eq. (19)}) \land \ldots \land (\text{eq. (33)}) \). The optimal cost of the Partial MaxSAT instance \( PMSat_{\epsilon,n}^{e,n=ub,lh} \) is \( \lceil \frac{\text{MPDT}(e)}{2} \rceil \).

Proposition 2 Let \( W PMSat_{\epsilon,n}^{e,n=ub,lh} \) be WSoftN \( \land (\text{eq. (19)}) \land \ldots \land (\text{eq. (33)}) \). The optimal cost of the Weighted Partial MaxSAT instance \( PMSat_{\epsilon,n=ub,lh} \) is \( \lceil \frac{\sum_{\text{MPDT}(e)} \rceil}{2} \).

5 The Linear MaxSAT algorithm

In this section, we present an slightly variation of the Linear SAT-based MaxSAT algorithm Eén and Sörensson [2006], Berre and Parrain [2010], that we will use to compute MPDTs as we describe in section 6. In particular, we will apply the Linear algorithm on the Partial MaxSAT instance \( PMSat_{\epsilon,n=ub,lh} \) to compute MPDTs.

Essentially, this algorithm solves a (Weighted) Partial MaxSAT optimization problem through a sequence of SAT decision queries. The pseudocode is shown in Algorithm 1. It receives as input parameter a (Weighted) Partial MaxSAT formula \( \phi \) (which consists on a set of soft \( \phi_s \) and hard \( \phi_h \) clauses) and an optional timeout \( t \). First, we create an incremental SAT solver \( s \) (line 1). Then, we add all the hard clauses \( \phi_h \) and a copy of the clauses in \( \phi_s \) where each soft clause is extended with a new blocking variable \( b_i \) (line 2). Then, the upper bound \( ub \) of \( \phi \) is computed as the sum of the weights \( w_i \) in \( \phi_s \) plus one (line 3). An incremental PB encoder (i.e., a PB encoder whose \( k \) can be updated) is initialized in line 4. This PB encoder initially restricts the sum of the \( b_i \) variables and their associated weights \( w_i \) to
be \( \leq ub \). In line 5, we use the PB encoder to translate into CNF the initial PB constraint. While this PB constraint in combination with the hard constraints is satisfiable, we extract the model, update the \( ub \) to the cost of this model and refine the PB constraint (lines 7-12). Finally, we return the upper bound \( ub \), the model \( m \) and a reference to the incremental SAT solver \( s \).

Algorithm 1 Linear MaxSAT algorithm (LMS)

**Input:** (Weighted) Partial MaxSAT formula \( \phi \equiv \phi_h \cup \phi_t \), Timeout \( t \) (defaults to \( \infty \))

**Output:** Best upper bound \( ub \), Best model \( m \), SAT solver \( s \)

1. \( s \leftarrow SAT\_Solver() \)
2. \( s.add\_clauses(\phi_h \cup \{ c_i \lor b_i \mid (c_i, w_i) \in \phi_t \}) \)
3. \( ub \leftarrow \sum_{(c_i, w_i) \in \phi_t} w_i + 1 \)
4. \( pb \leftarrow \sum_{(c_i, w_i) \in \phi_t} w_i \cdot b_i \leq ub \)
5. \( s.add\_clauses(pb.to\_cnf()) \)
6. \( is\_sat, m \leftarrow True, \emptyset \)
7. **while** \( is\_sat = True \) and \( ub > 0 \) **and** within timeout \( t \) **do**
8. \( s.add\_clauses(pb.update(ub - 1)) \)
9. \( is\_sat \leftarrow s.solve() \)
10. **if** \( is\_sat = True \) **then**
11. \( m \leftarrow s.model() \)
12. \( ub \leftarrow cost(m) \)
13. **end if**
14. **end while**
15. **return** \( ub, m, s \)

### 6 Extracting Multiple Diverse Solutions

We can obtain multiple solutions of a given optimal cost \( c \) by generating the SAT instance representing the query of whether there is a solution of cost \( c \). Then, we execute a SAT solver in incremental mode on the SAT instance, and whenever we get a solution, we add its negation to the SAT solver and ask the solver to solve the augmented instance.

In our approach, we take advantage of the fact that the SAT instance representing the optimal solutions is already created during the execution of the Linear MaxSAT algorithm which may be also augmented by useful learned clauses added in previous calls to the SAT solver. In particular, it is the last satisfiable SAT instance seen by Linear MaxSAT.

To be able to access to the clauses of this last satisfiable instance we modify the Linear MaxSAT algorithms as follows. We move statement of line 8 \((s.add\_clauses(pb.update(ub - 1)))\) inside the conditional \( (is\_sat = True) \) of line 10 and add as an assumption to the solver in line 8 the auxiliary variables that reify the clauses in \( pb.update(ub - 1) \). At this point, the formula containing all the possible optimal solutions corresponds to \( s\_clauses() \).

However, these solutions may be too similar. In our case, we expect that diverse solutions (diverse MPDTs) may help to get a more robust approach in terms of accuracy.

To enforce a bit this diversity we will solve another MaxSAT problem. Algorithm MSOL (alg. 2) shows the pseudocode to extract multiple diverse solutions. As input we have the SAT formula that compiles the solutions, the number of solutions we want to extract the vars on which we will enforce our diversity criterion.

The set of hard clauses of the MaxSAT formula we iteratively solve contains the clauses of the input SAT instance and the clauses discarding the solutions extracted so far (line 8) restricted to the target vars.

The soft clauses contain, as unit clauses of cost 1, the negation of the literals (restricted to the target vars) appearing in the solutions retrieved so far (line 10). This way we prefer solutions where the polarity of the target vars appear less in the previous retrieved solutions. Notice that eventually, this approach can return all the optimal solutions.

Finally, algorithm MPDT (alg. 3) describes how we compute MPDTs for a given dataset. We split randomly the input dataset into training and selection datasets, where \( p \) is the percentage for examples to add to the training set (line 1).

Then, we create the MaxSAT encoding for computing MPDTs described in section 4 (line 3), on the training set \( \varepsilon_{tr} \) and the lower and upper bounds computed with additional applications (line 3 see section 8).

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1. If \( pb.update(ub - 1) \) is a unit clause, we just add its literal as an assumption
Algorithm 2 Multiple Solutions (MSOL)

**Input**: SAT instance $\varphi$, Num solutions $k$, target vars $vars$

**Output**: Set of solutions $sols$

1. $\phi_h, \phi_s, sols \leftarrow \varphi, \emptyset, \emptyset$
2. while $|sols| < k$ do
3.   $ub, m, _ \leftarrow LMS(\phi_h \cup \phi_s)$
4.   if $ub = \sum (c_i, w_i) \in \phi_s w_i + 1$ then
5.     return $sols$
6.   end if
7.   $sols \leftarrow sols \cup \{m\}$
8.   $lits \leftarrow \{l | l \in m(vars)\}$
9.   $\phi_h \leftarrow \phi_h \cup \{(\lor_{l \in lits} \neg l, \infty)\}$
10.  $\phi_s \leftarrow \phi_s \cup \{(-l, 1) | l \in lits\}$
11. end while
12. return $sols$

Then, in line 5 we call the MaxSAT solver. We assume that as in the Linear MaxSAT pseudocode the MaxSAT solver returns a container for the SAT clauses compiling all the optimal solutions.

Then, in line 6 we call MSOL (alg 2) that extracts $k$ multiple diverse MPDTs. We add as target vars the $a_{r,j}$ vars which represent that feature $r$ is assigned to node $j$.

From lines 8 to 10 we add to $best_dts$ the MPDTs such that their accuracy, evaluated on the selection set $\varepsilon_{sel}$ is greater than or equal the best accuracy in $best_dts$ minus a deviation percentage $\delta$ (line 10). Finally, we return the set $best_dts$.

In this paper, we just take randomly one of the MPDTs from $best_dts$ but other solutions combining more than one MPDT can be applied as other well-known approaches in machine learning (e.g. random forests).

Algorithm 3 Minimum Pure Decision Tree (MPDT)

**Input**: Dataset $\varepsilon$, MaxSAT solver $msat$, Split pctg $p$,
Num solutions $k$, Accuracy deviation $\delta$

**Output**: Best sample-based MPDTs $best_dts$

1. $\varepsilon_{tr}, \varepsilon_{sel} \leftarrow$ split $\varepsilon$ randomly according to $p$
2. $best_dts \leftarrow \emptyset$ (Pairs of decision trees and accuracies)
3. $ub, lb \leftarrow get\_bounds(\varepsilon_{tr})$
4. $\phi \leftarrow encode(\varepsilon_{tr}, ub, lb)$
5. $\_\_\_, s \leftarrow msat(\phi)$
6. $sols \leftarrow MSOL(s.clauses, k, \{a_{r,j} | a_{r,j} \in vars(\phi)\})$
7. for $sol \in sols$ do
8.   $dt \leftarrow decode(sol)$
9.   $acc_{dt} \leftarrow evaluate(dt, \varepsilon_{sel})$
10.  $best_dts \leftarrow update(best_dts, dt, acc_{dt}, \delta)$
11. end for
12. return $best_dts$

7 Preprocessing Datasets

The MaxSAT-based solving approach deals with datasets with binary features. Therefore, we first convert non-binary features (i.e. categorical, discrete, and continuous) into binary features. We use a direct conversion from a discrete or a categorical feature into multiple binary features. We use the `KBinsDiscretizer` transformer from sklearn to convert the continuous variables into discrete values using 8 bins (intervals of values) with the uniform strategy (same amount of values for each range). Then, we convert all the features that are non-binary to binary using either a one-hot encoding (OHE) from sklearn or our custom binary encoding.

The OHE encoding creates a new feature for each possible value in the original feature domain, assigning True to the new feature that corresponds to the value in the original one, while all the other new features are set to False.
The binary encoding applies a mapping from the original domain to a numeric domain. If the feature is ordinal, the order is kept. Then, those numeric values are represented in binary, and a new feature is created for each bit required to encode the entire domain for the original feature. Thus, for a feature with a domain \( D \) we replace it with \( \log_2(|D|) \) new features.

As described in Narodytska et al. [2018], the size of the encoding grows in \( O(kn^2 + mnk) \), with \( k \) being the number of features. Note that the binary encoding should have a natural advantage in the encoding size compared to OHE for non-binary datasets.

Finally, for each dataset benchmark, we split (following the stratification strategy) the dataset into a 64% training set, 16% selection set, and 20% test set.

8 Experimental Results

As benchmarks we use datasets (binary and non-binary) from the CP4IM repository [De Raedt et al. 2008], the UCI repository [Dua and Graff 2017], and the PennML repository [Romano et al. 2021, Olson et al. 2017]. Our execution environment consists of a computer cluster with nodes equipped with two AMD 7403 processors (24 cores at 2.8 GHz) and 21 GB of RAM per core.

8.1 On MPDT computation efficiency

The first question we address is whether the MPDT MaxSAT encoding described in section 4 in combination with a MaxSAT solver allows us to compute faster MPDTs than the MinDT approach described in Narodytska et al. [2018].

For this experiment, we used a time limit of 1h and a memory limit of 20GB and used 20 datasets for the OHE encoding and 14 for Binary encoding. To evaluate the two approaches on hard benchmarks, we focused on large datasets (rows/features) and took 20 samples at each percentage \( S_{\text{ptgs}} = \{10\%, 20\%, 30\%, 40\%\} \). This is a relevant experiment since if one wants to scale to large datasets as in Sch磷ler and Sz磷der [2021] using a kind of Large Neighborhood Search approach, it needs to efficiently solve samples of the original dataset with a SAT-based approach.

On each sample \( \varepsilon_{\text{ptgs}} \), we evaluate the Linear MaxSAT algorithm (algorithm[1]), which has been implemented using a custom Python library [Ans╝tegui et al. 2021], on the Partial \( PMSat^{\varepsilon_{\text{ptgs}},n=ub,lb}_{\text{PDT}} \) encoding for MPDTs, and the RC2 core-guided algorithm [Ignatiev 2020] on the Weighted \( WPMSat^{\varepsilon_{\text{ptgs}},n=ub,lb}_{\text{PDT}} \) variant. The \( \text{ub} \) is computed using the same approach as Narodytska et al. [2018], i.e. the upper bound is the size of the computed \( PDT(\varepsilon_{\text{ptgs}}) \) using ITI algorithm [Utgoff 1989]. The \( \text{lb} \) is trivially set to 3. The Linear MaxSAT algorithm and the MinDT approach use both the Cadical [Biere 2019] SAT solver. We exclude multilabel datasets since the MinDT approach cannot manage them.

|          | Avg. PAR10 | #Solved |
|----------|------------|---------|
|          | MPDT | MinDT | MPDT | MinDT |
| Binary   |       |       |       |       |
| 10%      | 238   | 2747  | 260   | 256   |
| 20%      | 472   | 828   | 223   | 221   |
| 30%      | 758   | 2554  | 190   | 184   |
| 40%      | 974   | 3738  | 138   | 130   |
| OHE      |       |       |       |       |
| 10%      | 277   | 12082 | 363   | 262   |
| 20%      | 621   | 10709 | 267   | 214   |
| 30%      | 840   | 8026  | 169   | 146   |
| 40%      | 4515  | 15204 | 99    | 77    |

Table 3: MinDT vs MPDT comparison for the Binary and OHE encodings

Table 3 shows the experimental results for our first experiment. We show for each competitive approach the average PAR10 on the union of all the samples from the datasets, and the number of solved samples.

As we can see, the MPDT approach (Linear MaxSAT algorithm on the Partial \( PMSat^{\varepsilon_{\text{ptgs}},n=ub,lb}_{\text{PDT}} \) encoding) becomes more efficient as we increase the size of the sample. There may be a horizon effect due to the time and memory limits

\(^2\text{RC2 was not competitive enough perhaps because it uses SAT solver Glucose 3.0.}\)
This result can be explained by the fact the Linear MaxSAT algorithm may perform fewer SAT queries and can share learnt clauses. Also, it confirms it is useful to solve optimization problems as MaxSAT instances rather with agnostic incremental approach provided memory requirements hold.

8.2 On MPDT accuracy

The second question we want to address is how accurate can be the MPDT algorithm described in section 6. We compare with the DecisionTreeClassifier model from sklearn [Scikit-learn developers, 2020]. For these experiments, we set a time limit of 1 day and 200GB of memory.

We recall that datasets are split into 64% training set, 16% selection set and 20% test set. For each approach we generate several DTs, choose the best one according to its accuracy on the selection set and report its accuracy on the test set. We try exactly 50 different random splits of the selection and test sets, select the best DT for each split and report the average accuracy on the test set.

For MPDT we retrieve at most 20 MPDTs from one execution as described in section 6. For sklearn, we evaluate three variations. In pure sklearn (psk) we run sklearn till it achieves 100% accuracy on the training set with as many seeds as DTs returned by MDPT. In limited sklearn (lsk) we restrict the DT size to the one reported by MPDT and execute it also with the same number of seeds. Finally, in All sklearn (ask) we try 20 different seeds for each possible DT size from 3 to the maximum size reached by the psk version. Notice that in ask we evaluate many more DTs than for the previous approaches. Notice that lsk and ask may not compute Pure DTs in contrast to MPDT and psk.

Table 4 shows the average accuracy and tree size for the Binary encoding. We provide the same table for OHE in the appendix C. DTs are selected taking into account the methodology described above.

MPDT obtains an average improvement on accuracy of 1.9%, 3.52% and 1.71% respect to psk, lsk and ask (see row DIFF). It is remarkable that MPDT using much less DTs than ask, and using Pure DTs, it is yet able to get a better average result.

For OHE, MPDT solves to optimality 4 instances less, and reports similar improvements on accuracy (0.44%, 4.70% and 2.41%) respect with to sklearn variations.

We also studied, whether any approach was able to see a DT with better accuracy on the test set but was not chosen with the selection set. For both OHE and Binary encodings we found that MPDT can report better DTs than sklearn. In particular, for the Binary encoding, MPDT obtains an average improvement on accuracy of 2.35%, 4.32% and 0.32% respect to psk, lsk and ask. For OHE the average improvements on accuracy are 0.39% (psk) and 4.69% (lsk). However, we found that in this case ask obtains an improvement of 0.74% respect to MPDT. Notice though that ask generated many more DTs and we could instruct MPDT to extract more solutions.

From these results, we conclude that there is room for improvement in the selection strategy, but MPDT focusing on the optimal size (without any ML heuristic) is able to see on average more accurate trees than sklearn. Moreover, it seems that exploring DTs around the optimal size is promising.

We also compare with DT(max) [Hu et al., 2020] which uses the incomplete MaxSAT solver Loandra [Berg et al., 2020]. Although Loandra is superior to the Linear MaxSAT solver we use, according to the results of the MaxSAT evaluation Bacchus et al. [2020], our approach still reports better results than DT(max) with depths of 2, 3 and 4 as in the original paper (see section 3). In particular, for the Binary encoding, we find improvements of 8.54%, 4.17%, and 2.34% respect to DT(max) limited on depths 2, 3, and 4 respectively. Similarly, for OHE the average accuracy improvements are 9.97%, 5.47%, and 4.11% respect to DT(max).

9 Conclusions and Future Work

We have presented a new efficient approach for computing MPDTs based on MaxSAT technology aiming to improve DT-based classifiers’ interpretability. Additionally, we have shown that by focusing on computing MPDTs for the training set, we can get in practice accurate DTs on the test set without applying any DT heuristic approach from ML literature. This is a curious result since technically we overfit on the training set. As future work, we will explore further the relation of the size of the tree and its pureness in terms of prediction accuracy. We will also explore how to produce better multiple optimal solutions from our MaxSAT approach and combine them effectively to construct other predictors.

We will extend results for the authors answer period if needed.
Learning Optimal Decision Trees Using MaxSAT

### A Appendix: Computing MPDTs with MaxSAT

In this appendix we present the entire encoding used for the problem of finding a minimum (in size) pure decision tree (MPDT), extending the explanation in section 4. This encoding is the optimization problem version of the original encoding [Narodytska et al. 2018].

The encoding assumes that:

- The problem to solve with a DT is a binary classification problem
- The DT is binary
- The root node is labeled as node 1
- The rest of the nodes are labeled into breadth-first or level order traversal
- Positive (negative) answers at decision nodes are assigned to the right (left) child node

Table 4 shows the symbols and functions used, and table 5 shows the propositional variables of the encoding.

We apply a further refinement, based on the following observation: since nodes are numbered in breadth first order, two consecutive nodes (with same parent) will be both in the solution or not. Therefore, we define function $\eta(i)$ as:

$$
\eta(i) = \begin{cases} 
\eta_{i+1} & \text{if } i \in N^c \\
\eta_i & \text{if } i \in N^o 
\end{cases}
$$

### A.1 Objective function

When a node is used to construct the tree, it has cost 1.

$$
\bigwedge_{i \in N^o} (\neg \eta_i, 1) \quad (SoftN)
$$
Learning Optimal Decision Trees Using MaxSAT

| Symbol/function | Definition |
|-----------------|------------|
| \( \varepsilon \) | The set of observations used to train the tree |
| \( \varepsilon^+(-) \) | The set of positive (negative) observations |
| \( n \) | The upper bound on the number of nodes |
| \( N \) | Range of nodes from 1 to \( n \) |
| \( N_e \) | Range of even-indexed nodes, from 1 to \( n \) |
| \( N_o \) | Range of odd-indexed nodes, from 1 to \( n \) |
| \( k \) | Number of features for each observation |
| \( K \) | Range of features for each observation |
| \( lr(i) = \{ j \in [i, \min(2i, n)] \mid j \in N_e \} \) | Set of potential left child nodes for node \( i \) |
| \( rr(i) = \{ j \in [i, \min(2i, n)] \mid j \in N_o \} \) | Set of potential right child nodes for node \( i \) |
| \( \sigma(r, q) = e_{q,f_r} \mid e_q \in \varepsilon \) | The value of the feature \( f_r \) at observation \( e_q \) |
| \( \eta(i) \) | Variable \( \eta_i \) relevant for the node \( i \) |

\( \eta_i \) (18)

A.2 PDT constraints

The following constraints define the layout of the decision tree and the restriction that a given assignment of features for each used decision node and classes for each used leaf results in a pure decision tree.

### A.2.1 Node usage clauses:

Those constraints force the nodes to be used in breadth-first order.

- If an odd node is not used, then both himself and the previous one are not leaves (note that we do not have to set the root as it is never a leaf by eq. [19].

\[ \bigwedge_{i \in N^o \mid i > 1} \neg \eta_i \rightarrow \neg \psi_i \land \neg \psi_{i-1} \] (16)

- If a node is used, then all the nodes with a smaller index must be used:

\[ \bigwedge_{i \in N^o \mid i > 1} \eta_i \rightarrow \eta_{i-2} \] (17)

- Enforce the lower bound \( lb \). By setting \( \eta(lb) \) to True, and combined with constraint(19) we ensure that at least \( lb \) nodes are used.

\[ \eta(lb) \] (18)
A.2.2 Tree layout hard clauses:

Those constraints ensure the solution is a valid DT.

• Root node is not a leaf.
  \[ \neg v_1 \] (19)

• (i) Leaves do not have a left child, and (ii) if node \( i \) is used in the DT, and has no left child candidates, then it is a leaf.
  \[ \bigwedge_{i \in N} \left\{ \left( \bigwedge_{j \in lr(i)} (v_i \rightarrow \neg l_{i,j}) \right) \text{ if } |lr(i)| \neq 0 \right. \]
  \[ \left. \quad \bigwedge_{j \in lr(i)} (\eta(i) \rightarrow v_i) \text{ if } |lr(i)| = 0 \right\} \] (20)

• Node \( j \) is the left child of node \( i \) iff node \( j + 1 \) is the right child of node \( i \).
  \[ \bigwedge_{i \in N} \bigwedge_{j \in lr(i)} (l_{i,j} \leftrightarrow r_{i,j+1}) \] (21)

• If node \( i \) is not a leaf and is used in the DT, then it has exactly one left child.
  \[ \bigwedge_{i \in N} \left( (\neg v_i \land \eta(i)) \rightarrow \left( \sum_{j \in lr(i)} l_{i,j} = 1 \right) \right) \] (22)

• The symmetry equations on \( p_{j,i}, l_{i,j} \) and \( r_{i,j} \).
  \[ \bigwedge_{i \in N} \bigwedge_{j \in lr(i)} (p_{j,i} \leftrightarrow l_{i,j}) \bigwedge_{i \in N} \bigwedge_{j \in rr(i)} (p_{j,i} \leftrightarrow r_{i,j}) \] (23)

Given a pair of \( i,j \) nodes, we have that \( j \in lr(i) \cup rr(i) \), and \( lr(i) \cap rr(i) = \emptyset \). This, combined with constraint 23, sets an equivalence between the variable \( p_{j,i} \) and one of \( l_{i,j} \) or \( r_{i,j} \) depending on the \( j \) node. Thus, in practice, we can perform a direct substitution of the variable \( p_{j,i} \) with the corresponding one of those two variables in the encoding, and remove the \( p_{j,i} \) variable and the constraint 23 altogether. In this description, for clarity purposes, we kept the \( p_{j,i} \) variable in the encoding.

• If node \( j \) is used in the DT (and it is not the root) it will have exactly one parent.
  \[ \bigwedge_{j \in N \mid j > 1} (\eta(j) \rightarrow \sum_{i=\lfloor \frac{j}{2} \rfloor}^{j-1} p_{j,i} = 1) \] (24)

A.2.3 Feature assignment hard clauses:

Those constraints enforce the assignment of features and classes result in a PDT.

• Feature \( f_r \) with value 0 (1) is already discriminated by node \( j \) iff the feature \( f_r \) is attached to the parent of \( j \) and node \( j \) is the right (left) child or the feature \( f_r \) with value 0 (1) is already discriminated by the parent of \( j \).
  \[ \bigwedge_{j \in N, r \in K} \left( d^{0}_{r,j} \leftrightarrow \bigvee_{i=\lfloor \frac{j}{2} \rfloor}^{j-1} (a_{r,i} \land r_{i,j}) \lor (p_{j,i} \land d^{0}_{r,i}) \right) \] (25)
  \[ \bigwedge_{j \in N, r \in K} \left( d^{1}_{r,j} \leftrightarrow \bigvee_{i=\lfloor \frac{j}{2} \rfloor}^{j-1} (a_{r,i} \land l_{i,j}) \lor (p_{j,i} \land d^{1}_{r,i}) \right) \] (26)

• No feature is discriminated at root node.
  \[ \bigwedge_{r \in K} (\neg d^{0}_{r,1} \land \neg d^{1}_{r,1}) \] (27)
• If some feature \( f_r \) is already discriminated by node \( i \), then the feature can not be assigned to any of its children.

\[
\bigwedge_{j \in N, r \in K} \bigwedge_{i=\left\lfloor \frac{j}{2} \right\rfloor}^{j-1} (u_{r,i} \land p_{j,i}) \rightarrow \neg a_{r,j} \tag{28}
\]

• Feature \( f_r \) is discriminated at node \( j \) iff \( f_r \) has been assigned to node \( j \) or it is already discriminated at the parent of \( j \).

\[
\bigwedge_{j \in N, r \in K} \left( u_{r,j} \leftrightarrow \left( a_{r,j} \lor \bigvee_{i=\left\lfloor \frac{j}{2} \right\rfloor}^{j-1} (u_{r,i} \land p_{j,i}) \right) \right) \tag{29}
\]

• If node \( j \) is not a leaf and it is in the DT, then it has exactly one feature assigned to.

\[
\bigwedge_{j \in N} \left( \neg v_j \land \eta(j) \rightarrow \sum_{r \in K} a_{r,j} = 1 \right) \tag{30}
\]

• If node \( j \) is a leaf, then it has no feature assigned to.

\[
\bigwedge_{j \in N} \left( v_j \rightarrow \sum_{r \in K} a_{r,i} = 0 \right) \tag{31}
\]

• For every positive (negative) example, if node \( j \) is a leaf and it is assigned to class 0 (1), then at least one feature is discriminated with the value in the example at node \( j \).

\[
\bigwedge_{j \in N, e_q \in \varepsilon^+} \left( v_j \land \neg c_j \rightarrow \bigvee_{r \in K} d_r^{e(r,q)} \right) \tag{32}
\]

\[
\bigwedge_{j \in N, e_q \in \varepsilon^-} \left( v_j \land c_j \rightarrow \bigvee_{r \in K} d_r^{e(r,q)} \right) \tag{33}
\]

### A.3 Additional Pruning hard clauses

Depending on which nodes are decided to be leaves or not, the possible list of children for a given node may change. These constraints enforce this simplification. We refer to the original description [Narodytska et al. 2018]. We incorporate as in previous constraints the \( \eta(i) \) variable to take into account in counters \( \tau_{t,i} \) and \( \lambda_{t,i} \) only the nodes that are used in the solution.

\[
\bigwedge_{i \in N} \lambda_{0,i} \land \tau_{0,i} \tag{34}
\]

\[
\bigwedge_{i \in N, t \in [1,\frac{i}{2}]} \left( \lambda_{t,i} \leftrightarrow \left( \lambda_{t-1,i-1} \lor v_i \land \eta(i) \right) \right) \tag{35}
\]

\[
\bigwedge_{i \in N, t \in [1,\frac{i}{2}]} \left( \tau_{t,i} \leftrightarrow \left( \tau_{t-1,i-1} \land \neg v_i \land \eta(i) \right) \right) \tag{36}
\]

\[
\bigwedge_{i \in N, t \in [1,\frac{i}{2}]} \lambda_{t,i} \rightarrow \neg l_{i,2(t-1)+1} \land \neg r_{i,2(t+1)+1} \tag{37}
\]

\[
\bigwedge_{i \in N, t \in [\frac{i}{2},i]} \tau_{t,i} \rightarrow \neg l_{i,2(t-1)} \land \neg r_{i,2t-1} \tag{38}
\]

### A.4 Multilabel encoding

When dealing with multilabel datasets (with a label domain \( C(l) \)) we do not use the \( c_j \) variable, but the \( c_{k,j} \) variable to represent that the leaf \( j \) has the class \( k \) assigned. We modify the constraints 17 and 18 as follows:

\[
\bigwedge_{k \in C(l), j \in N, e_q \in \varepsilon} \left( v_j \land c_{k,j} \rightarrow \bigvee_{r \in K} d_r^{e(r,q)} \right) \tag{39}
\]
We add the following additional clauses:

• A decision node has no class assigned:
  \[ \bigwedge_{j \in N, k \in \text{Cls}} (\neg v_j \rightarrow \neg c_{k,j}) \]  
  (40)

• A leaf has only one label:
  \[ \bigwedge_{j \in N} (v_j \rightarrow \sum_{k \in \text{Cls}} = 1) \]  
  (41)

A.5 MaxSAT encodings:

**Proposition 3** Let \( P_{\text{MSat}}^{\varepsilon,n=ub,lb} \) be \( \text{SoftN} \land (\text{eq. 19}) \land \ldots \land (\text{eq. 33}) \). The optimal cost of the Partial MaxSAT instance \( P_{\text{MSat}}^{\varepsilon,n=ub,lb} \) is \( \lceil \frac{|MP_{DT}(\varepsilon)|}{2} \rceil \).

**Proposition 4** Let \( W_{\text{MSat}}^{\varepsilon,n=ub,lb} \) be \( W_{\text{SoftN}} \land (\text{eq. 19}) \land \ldots \land (\text{eq. 33}) \). The optimal cost of the Weighted Partial MaxSAT instance \( P_{\text{MSat}}^{\varepsilon,n=ub,lb} \) is \( \lceil \frac{\sum_{i=1}^{\text{MP}_{DT}(\varepsilon)}}{2} \rceil \).

B Appendix: Datasets

Table 7 show the datasets used during the experimental results.

|       | #Columns | #Labels | #Rows |
|-------|----------|---------|-------|
|       | binary   | ohe     | total | train | sel  | test  |
| append| 22       | 56      | 2     | 105   | 67   | 17    | 21    |
| audio | 146      | 146     | 2     | 216   | 137  | 35    | 44    |
| back  | 50       | 89      | 2     | 180   | 115  | 29    | 36    |
| corral| 7        | 7       | 2     | 160   | 102  | 26    | 32    |
| habar | 11       | 28      | 2     | 266   | 169  | 43    | 54    |
| hayes-r| 9       | 16      | 3     | 120   | 76   | 20    | 24    |
| hepa  | 58       | 321     | 2     | 155   | 99   | 25    | 31    |
| h-votes| 17      | 17      | 2     | 435   | 278  | 70    | 87    |
| iris  | 13       | 32      | 3     | 150   | 96   | 24    | 30    |
| irish | 16       | 53      | 2     | 500   | 320  | 80    | 100   |
| lympho| 30       | 51      | 4     | 148   | 94   | 24    | 30    |
| monks-1| 11      | 16      | 2     | 556   | 355  | 89    | 112   |
| monks-3| 11      | 16      | 2     | 548   | 350  | 88    | 110   |
| mushr | 112      | 112     | 2     | 8124  | 5199 | 1300  | 1625  |
| mux6  | 7        | 7       | 2     | 128   | 81   | 21    | 26    |
| new-thy| 16      | 39      | 3     | 212   | 135  | 34    | 43    |
| promo | 115      | 229     | 2     | 106   | 67   | 17    | 22    |
| spect | 23       | 23      | 2     | 251   | 160  | 40    | 51    |
| wine  | 47       | 263     | 3     | 178   | 113  | 29    | 36    |
| zoo   | 26       | 122     | 7     | 101   | 64   | 16    | 21    |

Table 7: Statistics from the datasets used in the experimental results. In order: the number of features for both the binary encoding and the OHE, the number of labels (2 for binary, more for multilabel), the total number of rows in the dataset, and the number of rows used as train, selection, and test.

C Appendix: Experimental results

Tables 9 and 8 show the extended experimental results for the comparison in accuracy with DT(max) and Sklearn respectively.
|     | MPDT acc | MPDT sz | psk acc | psk sz | lsk acc | lsk sz | ask acc | ask sz |
|-----|----------|---------|---------|--------|---------|--------|---------|--------|
| append | 71.9 17 | 75.2 17 | 75.2 17 | 75.1 11 |
| audio | 92.2 17 | 91.1 17 | 93.8 17 | 93.6 9  |
| corral | 100 13 | 100 27 | 87.4 13 | 98.8 26 |
| haber | 79.7 35 | 84.0 47 | 79.8 35 | 72.1 7  |
| hayes-r | 81.6 23 | 84.4 27 | 86.3 23 | 86.2 19 |
| h-votes | 93.7 33 | 93.3 39 | 93.5 33 | 94.2 11 |
| iris | 92.5 19 | 92.5 26 | 88.9 19 | 89.9 22 |
| irish | 100 7 | 100 7 | 100 7 | 99.3 6  |
| lympho | 76.3 23 | 77.2 33 | 72.9 23 | 73.1 16 |
| monks-1 | 100 13 | 100 31 | 85.3 13 | 100 31 |
| mushr | 100 15 | 100 23 | 99.9 15 | 100 23 |
| mux6 | 100 15 | 90.9 37 | 59.6 15 | 90.7 37 |
| new-thy | 90.9 21 | 86.9 32 | 85.3 21 | 82.8 16 |
| promo | 78.7 13 | 81.2 17 | 80.1 13 | 79.8 14 |
| spect | 87.5 35 | 77.2 56 | 77.9 35 | 71.0 9  |
| zoo | 91.7 15 | 95.9 15 | 95.9 15 | 91.7 13 |

DIFF -0.44 -4.70 -2.41

Table 8: Average accuracy scores and DT sizes for OHE. Table shows the algorithms MPDT, psk (pure Sklearn), lsk (limited Sklearn), and ask (All Sklearn).
|        | MPDT | d2  | d3  | d4  |
|--------|------|-----|-----|-----|
| **OHE** |      |     |     |     |
| append | 71.9 | 70.7| 70.7| 70.7|
| audio  | 92.2 | 98.1| 91.5| 92.5|
| corral | 100  | 73.1| 90.4| 93.3|
| haber  | 79.7 | 75.1| 76.9| 78.0|
| h-votes| 93.7 | 95.9| 93.6| 90.6|
| irish  | 100  | 97.8| 100 | 100 |
| monks-1| 100  | 72.8| 85.3| 100 |
| mushr  | 100  | 97.0| 100 | 100 |
| mux6   | 100  | 64.1| 100 | 100 |
| promo  | 78.7 | 72.5| 61.5| 60.0|
| spect  | 87.5 | 77.1| 73.6| 73.4|
| **DIFF** | -9.97| -5.47| -4.11|     |
|        |      |     |     |     |
| **Binary** |      |     |     |     |
| append | 70.3 | 75.2| 75.8| 73.7|
| audio  | 92.2 | 98.1| 91.5| 92.5|
| back   | 74.1 | 73.6| 69.3| 76.5|
| corral | 100  | 73.1| 90.4| 93.3|
| haber  | 79.0 | 82.6| 78.7| 78.2|
| hepa   | 68.4 | 65.4| 64.1| 64.2|
| h-votes| 93.7 | 95.9| 93.6| 90.6|
| irish  | 100  | 95.3| 100 | 100 |
| monks-1| 100  | 65.3| 74.5| 95.6|
| monks-3| 98.6 | 94.9| 97.5| 95.3|
| mush   | 100  | 97.0| 100 | 100 |
| mux6   | 100  | 64.1| 100 | 100 |
| promo  | 73.7 | 60.4| 70.2| 71.4|
| spect  | 87.5 | 77.1| 73.6| 73.4|
| **DIFF** | -8.54| -4.17| -2.34|     |

Table 9: Average accuracy scores for MPDT and DT(max) [Hu et al. 2020] for OHE and Binary encoding. d2, d3, and d4 show the accuracy for DT(max) using a limit on depth of 2, 3, and 4 respectively.

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