

# Optimizing Binary Decision Diagrams with MaxSAT for classification

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## Abstract

The growing interest in explainable artificial intelligence (XAI) for critical decision making motivates the need for interpretable machine learning (ML) models. In fact, due to their structure (especially with small sizes), these models are inherently understandable by humans. Recently, several exact methods for computing such models are proposed to overcome weaknesses of traditional heuristic methods by providing more compact models or better prediction quality.

Despite their compressed representation of Boolean functions, Binary decision diagrams (BDDs) did not gain enough interest as other interpretable ML models. In this paper, we first propose SAT-based models for learning optimal BDDs (in terms of the number of features) that classify all input examples. Then, we lift the encoding to a MaxSAT model to learn optimal BDDs in limited depths, that maximize the number of examples correctly classified. Finally, we tackle the fragmentation problem by introducing a method to merge compatible subtrees for the BDDs found via the MaxSAT model. Our empirical study shows clear benefits of the proposed approach in terms of prediction quality and interpretability (i.e., lighter size) compared to the state-of-the-art approaches.

## 1 Introduction

Due to the increasing concerns in understanding the reasoning behind AI decisions for critical applications, interpretable Machine Learning (ML) models gained a lot of attention. Examples of such ML applications include job recruitment, bank credit applications, and justice (Voigt and Bussche 2017). Most of traditional approaches for building interpretable models are greedy, for example, decision trees (Breiman et al. 1984; Quinlan 1986, 1993), rule lists (Cohen 1995; Clark and Boswell 1991), and decision sets (Lakkaraju, Bach, and Leskovec 2016). Compared to traditional approaches, exact methods offer guarantee of optimality, such as model size and accuracy. In this context, combinatorial optimisation methods, such as Constraint Programming (Bonfietti, Lombardi, and Milano 2015; Verhaeghe et al. 2020), Mixed Integer Programming (Angelino et al. 2018; Verwer and Zhang 2019; Aglin, Nijssen, and Schaus 2020), or Boolean Satisfiability (SAT) (Bessiere,

Hebrard, and O’Sullivan 2009; Narodytska et al. 2018; Avelaneda 2020; Hu et al. 2020; Janota and Morgado 2020; Yu et al. 2020) have been successfully used to learn interpretable models. These declarative approaches are particularly interesting since they offer certain flexibility to handle additional requirements when learning a model.

By providing compact representations for Boolean functions, Binary Decision Diagrams (BDDs) (Akers 1978; Moret 1982; Bryant 1986; Knuth 2009) are widely studied for hardware design, model checking, and knowledge representation. In the context of ML, BDD could be viewed as an interpretable model for binary classification. In addition, they were extended for multi-classification, known as *decision graphs* and heuristic methods were proposed in (Oliver 1993; Kohavi 1994; Kohavi and Li 1995; Mues et al. 2004). Moreover, (Ignatov and Ignatov 2017) proposed *decision stream*, a similar topology to BDD based on merging *similar* subtrees in each split made in decision trees to improve the generalization. (Oliver 1993; Kohavi 1994) showed that *decision graphs* could avoid the *replication* problem and *fragmentation* problem of decision trees effectively, which BDDs also could avoid in binary classification. This fact indicates that generally in the practice of ML, a BDD have a smaller size than the corresponding decision tree.

In this paper, we introduce a SAT-based model for learning optimal BDDs with the smallest number of features classifying all examples correctly, and a lifted MaxSAT-based model to learn optimal BDDs minimizing the classification error. We assume that all BDDs are *ordered* and *reduced*<sup>1</sup>, the limitation on the depth for a BDD, corresponds to the number of features to be selected by our model. To the best of our knowledge, (Cabodi et al. 2021) is the only exact method of learning optimal BDDs in the context of ML. The authors proposed a SAT model to learn optimal BDDs with the smallest sizes that correctly classify all examples. In their approach, the depth of the BDD is not restrained. Therefore, it is possible that the BDD is small in size but high in depth. As the BDD is *ordered*, this approach could not limit the number of features used, making it not quite comparable with our proposition. Another related work is in (Hu et al. 2020) where the authors consider a MaxSAT model to learn optimal decision trees minimizing the classification error within

<sup>1</sup>The two notions are defined in the background

a limited depth. The usage of the same solving methodology with the same objective function and the depth limit, makes these two MaxSAT models comparable. Finally, in order to increase the scalability of our approach, we propose a heuristic extension based on a simple pre-processing step.

The rest of the paper is organized as follows. First, we give the related technical background in Section 2. Then, in Section 3, we show the proposed SAT and MaxSAT models for learning BDDs in binary classification. Finally in Section 4, we present our large experimental studies to show the competitive prediction quality of the proposed approach.

## 2 Technical Background

### Classification

Consider a dataset  $\mathcal{E} = \{e_q, \dots, e_M\}$  with  $M$  examples. Each example  $e_q \in \mathcal{E}$  is characterized by a list of binary features  $\mathcal{L}_q = [f_1, \dots, f_K]$  and a binary target  $cl_q$ , representing the class of the example ( $cl_q \in \{0, 1\}$ ). The data set is partitioned into  $\mathcal{E}^+$  and  $\mathcal{E}^-$ , where  $\mathcal{E}^+$  (respectfully  $\mathcal{E}^-$ ) is the set of positive (respectfully negative) examples. That is,  $cl_q = 1$  iff  $e_q \in \mathcal{E}^+$  and  $cl_q = 0$  iff  $e_q \in \mathcal{E}^-$ . We assume that,  $\forall 1 \leq q, q' \leq M, \mathcal{L}_q = \mathcal{L}_{q'}$  implies  $cl_q = cl_{q'}$ .

Let  $\phi$  be the function defined by  $\phi(\mathcal{L}_q) = cl_q, \forall q \in [1, M]$ . The classification problem is to compute a function  $\gamma$  (called a *classifier*) that matches as accurately as possible the function  $\phi$  on examples  $e_q$  of the training data and generalizes well on unseen test data.

### Binary Decision Diagrams

Binary Decision Diagrams (BDDs) are used to provide compact representation of Boolean functions. Let  $[x_1, \dots, x_n]$  be a sequence of  $n$  Boolean variables. A BDD is a rooted, directed, acyclic graph  $\mathcal{G}$ . The vertex set  $\mathcal{V}$  of  $\mathcal{G}$  contains two types of vertices. A *terminal* vertex  $v$  is associated to a binary value:  $value(v) \in \{0, 1\}$ . A *nonterminal* vertex  $v$ , is associated to a Boolean variable  $x_i$  and has two children  $left(v), right(v) \in \mathcal{V}$ . In this case,  $index(v) = i \in \{1, \dots, n\}$  is the index of the Boolean variable associated to  $v$ .

We assume that all BDDs are *ordered* and *reduced*. These two restrictions are widely considered in the literature as they guarantee a *unique* BDD for a given Boolean function. The restriction *ordered* indicates that for any *nonterminal* vertex  $v$ ,  $index(v) < index(left(v))$  and  $index(v) < index(right(v))$ . The restriction *reduced* indicates that the graph contains no *nonterminal* vertex  $v$  with  $left(v) = right(v)$ , nor does it contain distinct *nonterminal* vertices  $v$  and  $v'$  having isomorphic rooted sub-graphs. Therefore, given an *ordered reduced* BDD  $\mathcal{G}$  with root  $v$ , the associated Boolean function can be recursively obtained with the Shannon expansion process (Shannon 1938).

Let  $g$  be a Boolean function defined over a sequence  $\mathcal{X} = [x_1, \dots, x_n]$  of  $n$  Boolean variables. The function  $g$  can be represented by a *truth table* that lists the  $2^n$  values of all assignments of the  $n$  variables. The value of the truth table is therefore associated to a string of  $2^n$  binary values. A truth table  $\beta$  of length  $2^n$  is said to be of order  $n$ . A truth table  $\beta$  of order  $n > 0$  has the form  $\beta_0\beta_1$ , where  $\beta_0$  and  $\beta_1$  are truth tables of order  $n - 1$ , and  $\beta_0$  and  $\beta_1$  are called *subtables*

of  $\beta$ . The *subtables* of *subtables* are also considered to be *subtables*, and a table is considered as a *subtable* of itself. A *bead* of order  $n$  is a truth table  $T$  of order  $n$  that does not have the form  $\alpha\alpha$  where  $\alpha$  is a subtable of  $T$ . The *beads* of  $g$  are the *subtables* of its truth table that happen to be *beads*. Proposition 1 from (Knuth 2009) relates truth table and binary decision diagram for the same Boolean function.

**Proposition 1.** *All vertices in  $\mathcal{V}$  of a binary decision diagram  $\mathcal{G}$ , are in one-to-one correspondence with the beads of the Boolean function  $g$  it represents.*

Based on Proposition 1, we can produce the ordered and reduced binary decision diagram of a Boolean function by finding its *beads* and combine its *beads* with its sequence of variables.

**Example 1.** *Consider the Boolean function from (Knuth 2009):  $g_1(x_1, x_2, x_3) = (x_1 \vee x_2) \wedge (x_2 \vee x_3) \wedge (x_1 \vee x_3)$ . The binary string associated to its truth table  $\beta$  is 00010111. The beads of  $\beta$  are  $\{00010111, 0001, 0111, 01, 0, 1\}$ .*

From Proposition 1, we can draw the BDD with the beads found, shown as the left part of Figure 1. The dashed (solid) line of each vertex indicates the left (right) child. Then, we can replace the beads by vertices associated with the sequence of Boolean variables. The final binary decision diagram for  $g_1$  is shown as the right part of Figure 1.

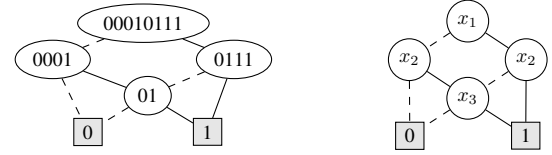


Figure 1: The Binary decision diagram for  $g_1(x_1, x_2, x_3)$

### Oblivious Read-Once Decision Graphs

Oblivious Read-Once Decision Graphs (OODGs) are proposed in (Kohavi 1994) to overcome some limitations of decision trees for multi-classification, like *replication* and *fragmentation* problem. We refer the readers to (Kohavi and Li 1995; Kohavi 1994) for details on OODGs. An OODG is a rooted, directed, acyclic graph, which contains terminal *category nodes* labelled with classes to make decisions, and non-terminal *branching nodes* labelled with features to make splits. The property “*read-once*” indicates that each feature occurs at most once along any path from the root to a category node. The property “*levelled*” indicates that the nodes are partitioned into a sequence of pairwise disjoint sets, representing the levels, such that outgoing edges from each level terminate at the next level. The property “*oblivious*” extends the idea of “*levelled*” by guaranteeing that all nodes at a given level are labelled by the same feature.

For the classification process, top-down and bottom-up heuristic methods for building OODGs are proposed in (Kohavi and Li 1995; Kohavi 1994). Here, we introduce briefly the top-down heuristic method, which is similar to the heuristic methods C4.5 and CART for computing decision trees. The top-down heuristic induction for OODG with given

depth contains three critical phases: (1) selecting a sequence of features with the help of *mutual information* (the difference of *conditional entropy* (Cover and Thomas 2006)); (2) growing an oblivious decision tree (ODT) by splitting the dataset with features in the sequence selected; and (3) merging *isomorphic* and *compatible* subtrees from top to down to build the OODG. When building the ODT, the algorithm marks nodes that capture no example of the dataset as “*unknown*”. For the merging phase, two subtrees are *compatible* if at least one root is labelled as “*unknown*”, or if the two root nodes are labelled with same feature and their corresponding children are the roots of compatible subtrees. The ODT grown could make classifications directly by assigning “*unknown*” nodes with the majority class of their parents.

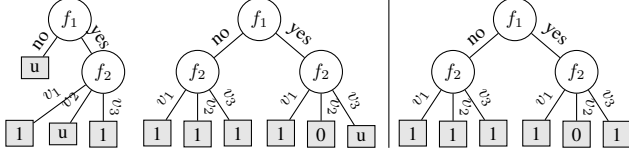


Figure 2: An example of two compatible subtrees (the left two) and the merged tree (the right one) from (Kohavi and Li 1995)

Figure 2 shows an example of two compatible subtrees and the merged tree, where “*unknown*” nodes are labelled as “*u*”. Merging compatible subtrees changes the bias by assuming that a “*unknown*” node is likely to behave the same as another child if they belong to compatible subtrees.

In binary classification for binary datasets, OODGs could be considered *equivalent* to BDDs, as the properties “*oblivious*” and “*read-once*” for OODGs are same as property “*ordered*” for BDDs. In addition, the use of merging compatible subtrees could also be applied for BDDs.

### SAT & MaxSAT

We use standard terminology for Boolean Satisfiability (Biere et al. 2009). A *literal* is a Boolean variable or its negation, and a *clause* is a disjunction of literals. An assignment of variables satisfies a clause if one of its literals is true. Given a set of Boolean variables and a set of clauses defined over these variables, the SAT problem can be defined as finding an assignment of the variables such that all the clauses are satisfied. Maximum Satisfiability (MaxSAT) is an optimization version of the SAT problem, where the clauses are partitioned into *hard* and *soft* clauses. Here we consider the Partial MaxSAT problem, that is to find an assignment of the Boolean variables that satisfies all the hard clauses and maximizes the number of satisfied soft clauses.

## 3 (Max)SAT-based model for Binary Decision Diagrams

In this section, we present our approach for learning BDDs for binary classification using SAT and MaxSAT.

### Problem Definition

We firstly consider the following decision problem for classification with BDD in a given depth.

- $P_{bdd}(\mathcal{E}, H)$  : Given a set of examples  $\mathcal{E}$ , is there a BDD of depth  $H$  that classifies correctly all examples in  $\mathcal{E}$ ?

Notice that the algorithm for  $P_{bdd}(\mathcal{E}, H)$  can be used to the alternative problem of optimizing a BDD that classifies all examples in the dataset correctly with a minimum depth. For that purpose, one can use a linear search that takes an initial depth  $H_0$  as input and progressively increases or decreases this value depending on the result of solving  $P_{bdd}(\mathcal{E}, H)$ .

Next, we consider another optimization problem for the classification with BDD in a limited depth.

- $P_{bdd}^*(\mathcal{E}, H)$  : Given a set of examples  $\mathcal{E}$ , find a BDD of depth  $H$  that maximises the number of examples in  $\mathcal{E}$  that are correctly classified.

We propose an initial SAT model for the decision problem  $P_{bdd}(\mathcal{E}, H)$ . Then, we propose an improved version in tighter formula size. Finally, we show how the improved SAT model for  $P_{bdd}(\mathcal{E}, H)$  can be used effectively to solve the optimization problem  $P_{bdd}^*(\mathcal{E}, H)$  with MaxSAT.

### SAT Model for $P_{bdd}(\mathcal{E}, H)$

As shown in Section 2, a BDD of depth  $H$  could be generated from the combination of a sequence of Boolean variables of size  $H$ :  $[x_1, \dots, x_H]$ , and a truth table of order  $H$  associated to a Boolean function. To solve the classification problem  $P_{bdd}(\mathcal{E}, H)$ , we then have to find a sequence of binary features of size  $H$  that maps one-to-one the sequence of Boolean variables, and a truth table associated to a Boolean function that well-classified all examples. We denote the sequence of binary features found as *feature ordering*. Therefore, the SAT encoding consists of two parts:

- **Part 1:** Constraints for selecting features of the dataset into the feature ordering of size  $H$ .
- **Part 2:** Constraints for generating a truth table that classifies all examples of  $\mathcal{E}$  correctly with the selected feature ordering.

To realize the SAT encoding, we introduce two sets of Boolean variables as follow:

- $a_r^i$ : the variable  $a_r^i$  is 1 iff feature  $f_r$  is selected as  $i$ -th feature in the feature ordering, where  $i = 1, \dots, H$ ,  $r = 1, \dots, K$ .
- $c_j$ : the variable  $c_j$  is 1 iff the  $j$ -th value of the truth table is 1, where  $j = 1, \dots, 2^H$ .

The set of variables  $a_r^i$  guarantees the *ordered* restriction. Then, we introduce two constraints (1) and (2) for the feature ordering. Constraint 1 ensures that any feature  $f_r$  can be selected at most once.

$$\sum_{i=1}^H a_r^i \leq 1, \quad r = 1, \dots, K \quad (1)$$

Then, there is exactly one feature selected for each index of the feature ordering.

$$\sum_{r=1}^K a_r^i = 1, \quad i = 1, \dots, H \quad (2)$$

We use the classical sequential counter encoding proposed in (Sinz 2005) to model constraints (1) and (2) as a Boolean formula.

The truth table we are looking for is the binary string of the values of variables  $c_1 c_2 \dots c_{2^H}$ . To avoid the first feature selected makes useless split, we need to make sure that the truth table is a *bead*.

$$\bigvee_{j=1}^{2^{H-1}} (c_j \oplus c_{j+2^{H-1}}) \quad (3)$$

There is a relationship between the values of a truth table and the assignments of the given sequence of Boolean variables. For example, the first value of a truth table corresponds to the assignment that  $x_1 = 0$  and  $x_2 = 0$ . Therefore, we define the following function to obtain the value of the  $i$ -th feature in the feature ordering of size  $H$  given the  $j$ -th value in the truth table.

$$rel(i, j) = \lfloor \frac{j-1}{2^{H-i}} \rfloor \bmod 2, \quad i \in [1, H], j \in [1, 2^H] \quad (4)$$

For an example  $e_q \in \mathcal{E}$ , we denote the value of the feature  $f_r$  as  $\sigma(r, q)$ . If  $rel(i, j) = \sigma(r, q)$ , it indicates that for example  $e_q$ , the feature  $f_r$  can be at the  $i$ -th position in the feature ordering to produce the  $j$ -th value in the truth table. To classify all examples correctly, we ensure that no example follows an assignment in the truth table leading to its opposite class. Thus, we propose the following constraints for classification. Let  $e_q \in \mathcal{E}^+$ , for all  $j = 1, \dots, 2^H$ :

$$\neg c_j \rightarrow \bigvee_{i=1}^H \bigvee_{r=1}^K (a_r^i \wedge rel(i, j) \oplus \sigma(r, q)) \quad (5)$$

That is, for every positive example  $e_q$ , any variable  $c_j$  assigned to 0 must be associated to an assignment of features that contains at least one feature-value that is not coherent with  $e_q$ . For negative examples, we use a similar idea. Let  $e_q \in \mathcal{E}^-$ , for all  $j = 1, \dots, 2^H$ :

$$c_j \rightarrow \bigvee_{i=1}^H \bigvee_{r=1}^K (a_r^i \wedge rel(i, j) \oplus \sigma(r, q)) \quad (6)$$

$\mathcal{E}_0$	$f_1$	$f_2$	$f_3$	$f_4$	label
$e_1$	1	0	1	0	0
$e_2$	1	0	0	1	0
$e_3$	0	0	1	0	1
$e_4$	1	1	0	0	0
$e_5$	0	0	0	1	1
$e_6$	1	1	1	1	0
$e_7$	0	1	1	0	0
$e_8$	0	0	1	1	1

Table 1: A dataset for binary classification

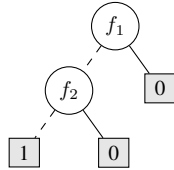


Figure 3: Decision Tree found

**Example 2.** Let  $\mathcal{E}_0$  be the given set of examples shown in Table 1. Figure 3 shows the corresponding decision tree classifying all examples correctly. We consider to encode a BDD with depth  $H = 2$  classifying all examples of  $\mathcal{E}_0$  correctly.

The two sets of variables are:  $\{a_1^1, a_1^2, a_2^1, a_2^2, a_3^1, a_3^2, a_4^1, a_4^2\}$ , and  $\{c_1, c_2, c_3, c_4\}$ . The constraints 1, 2, and 3 are:

$$\begin{aligned} a_1^1 + a_2^2 &\leq 1, & a_1^1 + a_2^2 &\leq 1, & a_3^1 + a_3^2 &\leq 1, & a_4^1 + a_4^2 &\leq 1 \\ a_1^1 + a_2^1 + a_3^1 + a_4^1 &= 1, & a_1^2 + a_2^2 + a_3^2 + a_4^2 &= 1 \\ && (c_1 \oplus c_3) \vee (c_2 \oplus c_4) && \end{aligned}$$

For classification constraints (i.e., 5 and 6), we show the encoding of  $e_1 \in \mathcal{E}^-$  with for value  $c_1$ . The encoding for other examples and other values is similar.

$$\begin{aligned} c_1 \rightarrow & (a_1^1 \wedge 0 \oplus 1) \vee (a_2^1 \wedge 0 \oplus 0) \vee (a_3^1 \wedge 0 \oplus 1) \\ & \vee (a_4^1 \wedge 0 \oplus 0) \vee (a_1^2 \wedge 0 \oplus 1) \vee (a_2^2 \wedge 0 \oplus 0) \\ & \vee (a_3^2 \wedge 0 \oplus 1) \vee (a_4^2 \wedge 0 \oplus 0) \end{aligned}$$

This could be simplified as follow:

$$\neg c_1 \vee a_1^1 \vee a_3^1 \vee a_1^2 \vee a_3^2$$

$x_1 = f_1$	$x_2 = f_2$	
0	0	$c_1 = 1$
0	1	$c_2 = 0$
1	0	$c_3 = 0$
1	1	$c_4 = 0$

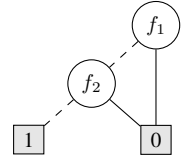


Table 2: Truth table solution for BDD

of depth 2 classifying all example of  $\mathcal{E}_0$  Figure 4: The BDD found

The values of truth table found by the SAT model are shown in Table 2, the feature ordering is  $[f_1, f_2]$ . Moreover, Table 2 illustrates the relationship between the values of truth table and the assignments of the given sequence Boolean variable of size 2. Figure 4 shows the corresponding BDD. This BDD classifies all examples of the dataset  $\mathcal{E}_0$  correctly, also provides more compact representation than the decision tree shown in Figure 3.

We refer to this first SAT encoding for  $P_{bdd}(\mathcal{E}, H)$  as BDD1. The size of BDD1 is given in Proposition 2.

**Proposition 2.** For a  $P_{bdd}(\mathcal{E}, H)$  problem with  $K$  binary features and  $M$  examples, the encoding size (in terms of the number of literals used in the different clauses) of BDD1 is  $O(M \times H \times K \times 2^H)$ .

*Proof.* Notice first that  $j$  ranges from 1 to  $2^H$ ,  $i$  ranges from 1 to  $H$ , and  $r$  ranges from 1 to  $K$ . The term  $M \times 2^H$  results from constraint (5) and (6), each contains  $O(H \times K)$  literals. For the remaining constraints, it is  $O(H \times K)$  for constraints (1) and (2),  $O(2^H)$  for constraint (3).  $\square$

The size of BDD1 is quite huge due to the size of clauses generated by constraints (5) and (6) for classification. This makes BDD1 impractical in practice.

### An improved SAT Model for $P_{bdd}(\mathcal{E}, H)$

In order to reduce the size of BDD1, we propose new classification constraints to replace constraints (5) and (6). The idea is that every positive (respectively negative) example follows an assignment leading to a positive (respectively negative) value of the truth table. We introduce a new set of Boolean variables:

- $d_i^q$ : The variable  $d_i^q$  is 1 iff for example  $e_q$  the value of the  $i$ -th feature selected in feature ordering is 1, where  $i = 1, \dots, H$ ,  $q = 1, \dots, M$ .

Then, We describe constraints that relate the values of features for each example  $e_q \in \mathcal{E}$ , for  $i = 1, \dots, H$ ,  $r = 1, \dots, K$ :

$$\begin{aligned} a_r^i &\rightarrow d_i^q & \text{if } \sigma(q, r) = 1 \\ a_r^i &\rightarrow \neg d_i^q & \text{if } \sigma(q, r) = 0 \end{aligned} \quad (7)$$

Let  $e_q \in \mathcal{E}^+$ , we have  $2^H$  constraints for classifying examples correctly:

$$\begin{aligned} \neg d_1^q \wedge \neg d_2^q \wedge \dots \wedge \neg d_{H-1}^q \wedge \neg d_H^q &\rightarrow c_1 \\ \neg d_1^q \wedge \neg d_2^q \wedge \dots \wedge \neg d_{H-1}^q \wedge d_H^q &\rightarrow c_2 \\ &\dots \\ d_1^q \wedge d_2^q \wedge \dots \wedge d_{H-1}^q \wedge d_H^q &\rightarrow c_{2^H} \end{aligned} \quad (8)$$

That is, any positive example follows an assignment of the feature ordering that leads to a positive value in the truth table.

Similarly, for any  $e_q \in \mathcal{E}^-$ , we also have  $2^H$  constraints:

$$\begin{aligned} \neg d_1^q \wedge \neg d_2^q \wedge \dots \wedge \neg d_{H-1}^q \wedge \neg d_H^q &\rightarrow \neg c_1 \\ \neg d_1^q \wedge \neg d_2^q \wedge \dots \wedge \neg d_{H-1}^q \wedge d_H^q &\rightarrow \neg c_2 \\ &\dots \\ d_1^q \wedge d_2^q \wedge \dots \wedge d_{H-1}^q \wedge d_H^q &\rightarrow \neg c_{2^H} \end{aligned} \quad (9)$$

We refer to this new SAT encoding for  $P_{bdd}(\mathcal{E}, H)$  as BDD2. The encoding size of BDD2 is given in Proposition 3.

**Proposition 3.** For a  $P_{dd}(\mathcal{E}, H)$  problem with  $K$  binary features and  $M$  examples, the encoding size of the SAT encoding (BDD2) is  $O(M \times H \times (2^H + K))$ .

*Proof.* The term  $M \times H \times K$  results from constraint (7). For constraints (8) and (9), for each example, there are  $2^H$  clauses containing  $H + 1$  literals. The term  $M \times H \times 2^H$  results from that.  $\square$

Propositions 2 and 3 show a clear theoretical advantage of BDD2 compared to BDD1 in terms of the encoding size, thus scalability.

### MaxSAT Model for $P_{bdd}^*(\mathcal{E}, H)$ :

We now present a MaxSAT encoding for the optimization problem  $P_{bdd}^*(\mathcal{E}, H)$ . That is, given a set of examples  $\mathcal{E}$ , find a binary decision diagram of depth  $H$  that maximises the number of examples correctly classified.

We transform the SAT encoding of BDDs into a MaxSAT encoding following a simple technique. The idea is to keep structural constraints as hard clauses and classification constraints as soft clauses. We consider BDD2 as it has a reduced size. Constraints (1), (2), (3) and (7) are kept as hard clauses. To classify the examples, we declare all clauses of constraints (8) and (9) as soft clauses. For any example  $e_q$ , the number of satisfied soft clauses associated to  $e_q$  is either  $2^H$  (indicating  $e_q$  is classified correctly), or  $2^H - 1$  (indicating  $e_q$  is classified wrongly). Therefore, the objective of maximising the number of satisfied soft clauses is equivalent to maximise the number of examples that are correctly classified.

## Merging Compatible Subtrees

Consider a BDD  $\mathcal{G}$  found by a MaxSAT solver and its associated truth table  $\beta$ . Based on the feature ordering of  $\mathcal{G}$ , it is possible that some values in  $\beta$  capture no (training) example (Equivalent to “unknown” nodes for OODG). Such values are decided by the MaxSAT solver in an arbitrary way, which gives a certain bias in generalisation. We propose to merge compatible subtrees in  $\mathcal{G}$  in order to handle this bias. This will result in changing some values in the truth table  $\beta$  (i.e. the arbitrary ones decided by MaxSAT).

We propose a post-processing procedure to merge compatible subtrees using the following three phase: (1) update the truth table  $\beta$  by replacing the values of  $\beta$  that capture no examples with a special value “u”; (2) for each level, check the *beads*, where “u” can be used to match 1 or 0, and create a node for each *bead*; (3) for each level, after creating the nodes, check the matches between all subtables of the next level. For matched subtables, update the corresponding *beads* of current level to eliminate the “u” values. This process is illustrated in Example 3.

**Example 3.** Assume that a MaxSAT model finds the truth table  $\beta$  00010111 with the feature ordering  $[f_1, f_2, f_3]$ , and assume that the updated truth table  $\beta'$  is u0u1011u after phase (1). For level 1, we create a root node for  $\beta'$  as it is a *bead*. Then, we check the subtables of  $\beta'$  (u0u1 and 011u). Since they do not match, we move to the next level. For level 2, we create a node for u0u1 and a node for 011u as they are *beads*. Then, we check all subtables of the next level, which are u0, u1, 01 and 1u. We observe that u0 matches 1u, and u1 matches 01, therefore, the *beads* u0u1 and 011u are updated as 1001 and 0110. Therefore, the updated *beads* of  $\beta'$  are {u0u1011u, 1001(u0u1), 0110(011u), 10, 01, 0, 1}.

Figure 5 shows the *beads* updated (in the left), the BDD before the merging process (in the right) and the final BDD found (in the middle).

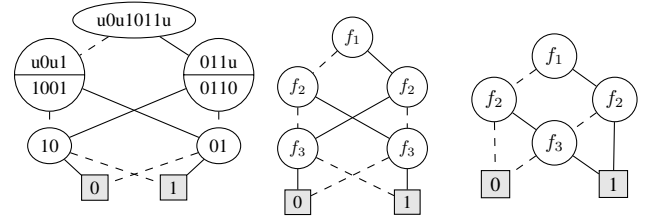


Figure 5: The BDD after merging compatible subtrees (the middle one) and the BDD before merging (the right one).

## 4 Experimental Results

We present our large experimental studies to evaluate empirically our propositions on different levels<sup>2</sup>. At first, we evaluate the prediction performance between the proposed MaxSAT-BDD model and the heuristic method, ODT and OODG. Next, we compare our model with an exact method

<sup>2</sup>The source code and datasets are available online at <https://gitlab.laas.fr/hhu/bddencoding>

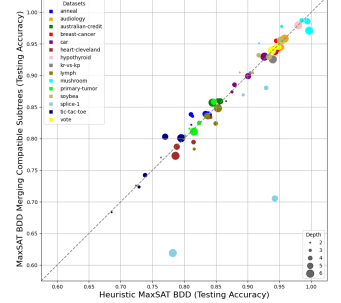
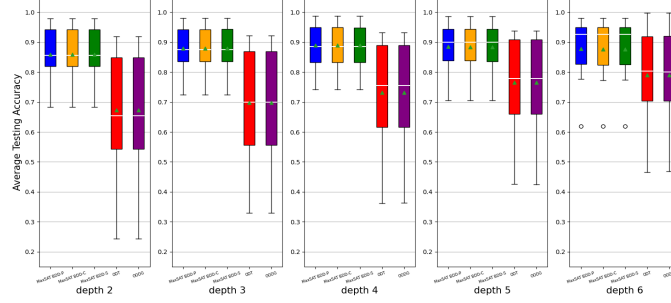
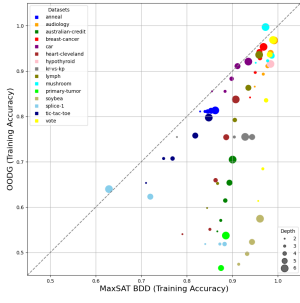


Figure 6: The left scatter shows the average training accuracy of OODG and MaxSAT model. The right Figure 7: Average testing accuracy of MaxSAT model of BDD and its heuristic approach.

for building decision trees using MaxSAT (Hu et al. 2020) in terms of prediction quality, model size, and encoding size. Finally, we propose and evaluate a scalable heuristic version of our encoding. We consider datasets from CP4IM<sup>3</sup>. These datasets are binarized with the one-hot encoding. Preliminary experiments confirm the great improvements in encoding size of BDD2 compared to BDD1, as the proposition 2 and 3 shown. Meantime, they show scalability limits of SAT encoding for just small part of dataset. Therefore, we just present results of MaxSAT-BDD. For each dataset, we use random 5-fold cross-validation with 5 different seeds. All experiments were run on a cluster using Xeon E5-2695 v3@2.30GHz CPU and running xUbuntu 16.04.6 LTS. The MaxSAT solver we used is Loandra (Berg, Demirović, and Stuckey 2019), an efficient incomplete MaxSAT solver that return the best solution found within a limited computation time or report optimality. For each experiment, the time limit for generating formulas and the time limit for solver are set to 15 minutes.

### Comparison with Existing Heuristic Approaches

We consider the  $P_{bdd}^*(\mathcal{E}, H)$  problem (Section 3) with 5 different depths  $H \in \{2, 3, 4, 5, 6\}$ . We compare our MaxSAT-BDD model with the approach proposed in (Kohavi and Li 1995) to learn ODT and OODG. For the heuristic methods, as described in the background section, after merging *isomorphic* and *compatible* subtrees of ODT, the corresponding OODG changes the bias for those “unknown” nodes. In fact, different bias affects the prediction for unseen examples, but *not* for learned examples. Therefore, the training accuracy of ODT and OODG are equals, but the testing accuracy could be different. This fact also suits to the MaxSAT-BDD with different biases for the “unknown” nodes. In this experiment, we consider three different biases: assigning for each unknown node the majority class of its branch (denoted as **MaxSAT BDD-P**), merging compatible subtrees (**MaxSAT BDD-C**), and the class decided by the MaxSAT solver (**MaxSAT BDD-S**).

The left scatter plot in Figure 6 presents the comparison of the average training accuracy between OODG and MaxSAT-BDD model. In this figure, different datasets are marked with

different colors, and different depths are labelled with points of different sizes. From the scatter plot, we observe that the average training accuracy of both approaches increase with the increase of depth. Overall, the MaxSAT-BDD model performs better than the heuristic OODG in training accuracy.

The right boxplots of Figure 6 show the average testing accuracy of MaxSAT-BDD with different biases, ODT, and OODG using different depths averaged over all datasets. The white line and green triangle of each box indicate the median and the average value, respectively. Several observations from the boxplots are presented as follows. At first, for each bias, increasing the depth could improve the prediction performance. However, compared to ODT and OODG, all biases chosen for MaxSAT-BDD get less improvements with increasing depths. Next, there are slight differences for different biases of MaxSAT-BDD, indicating that it is quite robust. Then, generally, MaxSAT-BDD gets better prediction performance than ODT and OODG, in particular when depths are small. We noticed also that when the depth is 2, all datasets (except one), MaxSAT-BDD reports optimality.

### Comparison with an Exact Decision Tree Approach

The purpose of this experiment is to compare our proposition with the exact method for learning decision trees using the same solving approach (MaxSAT). For MaxSAT-BDD, we consider only the bias of merging compatible subtrees (**MaxSAT BDD-C**) since no substantial difference was observed. We consider different values for depth:  $H \in \{2, 3, 4, 5, 6\}$ . For MaxSAT-BDD, the depth also corresponds to the number of selected features, whereas for MaxSAT-DT the depth chosen here indicate *maximum depth* of the BDD.

Table 3 presents the results of evaluation. In the column “Dataset”, the dataset size (left) and the number of binary feature (right) are shown under the name. The column “Size” and “E.Size” indicate the number of nodes of model and the encoding size (number of literals in 10 thousands). The column “F\_d” indicates the average number of different features used in the decision tree found. The columns in same colors are comparable and the best values are marked in blue.

The results in Table 3 show that the MaxSAT-BDD is competitive to MaxSAT-DT in terms of prediction quality. In most cases, the training and testing accuracy of these two approaches are close. However, the size of the models are

<sup>3</sup><https://dtai.cs.kuleuven.be/CP4IM/datasets/>



Datasets	H	MaxSAT BDD-C				MaxSAT-DT				
		Train	Test	Size	E.Size	Train	Test	Size	E.Size	F.d
anneal (812/89)	2	82.92	82.19	5	24.09	83.18	82.14	6.84	52.72	2.88
	3	84	83.55	7	37.21	85.07	84.66	12.68	126.18	5.76
	4	84.58	83.84	9.4	52.06	86.05	84.78	18.68	315.45	8.64
	5	85.33	83.92	11.72	71.08	86.44	84.88	23.88	865.26	11.08
	6	86.26	83.70	14.68	99.47	87.6	85.76	39.16	2666.67	17.32
audiology (216/146)	2	94.91	94.92	4	10.59	95.49	94.92	7	31.35	3
	3	96.78	95.84	5.04	16.41	97.82	95.56	11.56	88.75	5.28
	4	97.73	95.56	6.96	22.56	99.51	94.54	19.08	272.15	8.68
	5	98.40	94.44	9.88	29.82	99.95	93.98	27	915.29	11.72
	6	99.17	95.84	14.28	39.59	99.86	94.08	24.12	3323.61	10.88
australian (653/124)	2	86.70	85.94	4.72	26.79	86.93	85.33	6.68	59.65	2.84
	3	87.45	84.81	5.32	41.15	88.09	84.87	13.08	146.15	5.68
	4	88.45	86.03	7.4	56.85	88.74	85.18	17.48	377.62	7.92
	5	89.36	85.91	10.44	75.9	89.28	84.75	22.52	1076.35	10.08
	6	90.05	85.7	17.32	102.49	89.49	84.84	27.08	3433.64	12.20
cancer (683/89)	2	93.88	93.59	4	20.29	94.91	94.2	7	45.56	3
	3	95.02	93.91	5.84	31.37	96.6	94.73	15	110.85	6.96
	4	96.06	95.49	7.96	43.89	97.34	94.17	21	283.77	9.44
	5	95.94	93.74	10.68	59.91	97.99	94.35	29.32	800.89	13.20
	6	96.84	94.35	14.8	83.83	98.87	93.41	45.72	2536.91	19.88
car (1728/21)	2	85.53	85.53	4	13.32	85.53	85.53	6.84	32.01	2.92
	3	88.40	87.41	5.08	21.95	89.25	87.45	12.68	71.83	5.64
	4	89.84	88.54	6.84	34.44	91.62	89.68	20.36	162.46	7.68
	5	91.13	89.91	9.6	55.79	93.78	92.77	29.56	389.68	10.24
	6	93.51	92.99	13.36	97.06	95.8	95.06	31.96	1044.54	10.88
cleveland (296/95)	2	79.04	72.57	4	9.48	80.76	72.84	7	25.57	3
	3	85.07	83.37	6	14.73	85.68	76.55	12.84	68.93	5.72
	4	86.32	79.46	7.84	20.55	86.77	76.75	17.80	200.76	8.04
	5	88.65	78.72	13.08	27.89	87.26	74.45	23.96	646.75	10.84
	6	90.74	77.29	21.04	38.66	88.58	75.81	28.84	2284.76	13.08
hypothyroid (3247/86)	2	97.84	97.84	4	92.65	97.84	97.84	5.96	182.20	2.48
	3	98.09	98.04	5.12	142.78	98.14	97.82	9.72	402.98	4.32
	4	98.27	98.13	6.72	200.09	98.38	98.01	15.40	885.51	7.12
	5	98.30	98.05	9.28	274.03	98.45	98	20.04	2016.31	8.92
	6	98.37	97.95	13.68	385.4	98.46	97.91	33.16	4957.57	14.04
kr-vs-kp (3196/73)	2	77.83	77.01	4	77.88	86.92	86.92	7	155.09	3
	3	90.43	90.43	5.28	120.54	93.81	93.79	12.44	342.99	5.08
	4	94.09	94.09	7.56	170.28	94.32	94.14	17.24	753.78	7.12
	5	94.34	94.18	9.52	236.39	94.85	94.69	25.40	1717.14	10.20
	6	92.80	92.55	11.52	339.35	93.91	93.69	29.32	4227.67	12.20
lymph (148/68)	2	84.46	83.23	4	3.5	86.01	79.27	7	12.33	3
	3	86.76	78.35	5.92	5.55	91.93	80.54	14.68	36.65	6.64
	4	90.54	82.4	8.72	7.86	94.56	78.46	20.20	117.94	8.88
	5	93.51	83.6	13.52	10.94	97.09	82.46	27.08	413.09	11.88
	6	95.88	84.82	17.64	15.74	99.59	80.92	46.60	1550.34	18.96
mushroom (8124/112)	2	95.13	95.13	4	299.19	96.9	96.9	7	565.27	3
	3	97.74	97.77	6.8	458.1	99.9	99.9	13.72	1227.18	6.24
	4	98.78	98.74	9	635.09	100	100	19.80	2603.94	9.08
	5	98.63	98.57	11.32	853.68	100	100	23.40	5571.14	10.64
	6	97.28	97.10	14.6	1165.88	100	100	27.56	12376.90	12
tumor (336/31)	2	82.80	81.6	4	3.72	82.92	81.01	6.76	10.46	2.88
	3	83.84	80.43	5.3	6.02	86.16	82.97	13.88	27.24	6.08
	4	85.52	82.49	8.64	9.04	87.89	82.85	20.92	76.40	9.16
	5	87.51	85.83	13.32	13.79	90.1	79.34	47.80	239.09	16.84
	6	88.57	81.12	19.84	22.44	90.34	81.31	37.32	838.63	15.04
soybean (630/50)	2	90.48	90.48	4	10.79	91.27	91.27	7	25.55	3
	3	91.39	90.41	6.52	16.99	95.45	94.7	15	62.30	7
	4	93.24	93.21	9.04	24.54	97.25	95.9	22.20	160.18	9.88
	5	94.31	92.95	11.92	35.34	97.96	95.3	40.60	455.33	15.72
	6	96.07	95.52	14.88	53.41	98.27	96.03	33.40	1459.87	14.40
splice-1 (3190/287)	2	84.04	84.04	4	296.61	84.22	83.17	6.92	555.22	2.96
	3	87.25	86.94	5.44	449.04	87.79	87.37	11.32	1231.59	4.64
	4	88.3	88.04	7.24	608.3	86.52	85.64	16.60	2717.90	7.12
	5	71.99	70.53	10.28	783.9	77.37	76.32	21.88	6226.75	9.48
	6	62.92	61.89	16.28	996.27	60.36	58.95	29.40	15406.05	12.28
tic-tac-toe (958/27)	2	71.05	68.35	4	9.25	71.1	67.49	5.96	22.31	2.48
	3	74.91	72.36	6.16	15.01	77.15	73.55	11.48	51.98	5.20
	4	76.87	74.22	8.84	22.88	82.47	78.68	20.60	125.10	8.44
	5	81.86	80.31	13.88	35.67	83.08	79.50	28.44	328.33	11.16
	6	84.82	80.08	24.16	59.52	84.25	80.86	38.12	979.46	13.24
vote (435/48)	2	95.68	95.22	3.76	7.2	96.21	95.03	7	18.33	3
	3	96.69	94.57	5.56	11.38	97.39	93.79	13.96	46.55	6.04
	4	97.40	94.39	8.16	16.49	98.62	94.57	21.16	126.45	9.32
	5	98.21	94.57	12.4	23.83	99.47	93.84	30.52	381.95	12.96
	6	98.93	93.98	18.44	36.2	99.62	94.76	35.40	1292.44	14.88

Table 3: Comparison between MaxSAT-BDD and MaxSAT-DT.

always smaller with MaxSAT-BDD. The difference grows bigger when the depth increases. The reduction in model size provides better interpretability. Moreover, sometimes, compared to the optimal BDDs found via MaxSAT-BDD, the optimal decision trees found via MaxSAT-DT make useless splits improving no prediction performance, as we can see in the case of the datasets “car” and “hypothyroid” with depth 2. We observe also that MaxSAT-BDD has always a (far) lighter encoding size than MaxSAT-DT which makes it easier to handle and to report optimality in limited time.

## Evaluation of a Heuristic MaxSAT-BDD method

To increase the scalability of our model, we propose a heuristic version of MaxSAT-BDD using CART (Breiman et al. 1984), an efficient and scalable heuristic for learning decision trees. The idea is to run CART as a pre-processing step in order to choose a subset of (important) features. Then apply the MaxSAT-BDD approach using only the selected subset of features.

We first evaluate the prediction quality of this heuristic method with the original MaxSAT-BDD. The size of the encoding is in favor of the heuristic approach as expected, making large problems treatable. The results of average testing accuracy are shown in Figure 7. This heuristic approach is clearly very competitive to the original MaxSAT-BDD in generalization performance. Especially, for those datasets with more features, the heuristic approach obtains better prediction performance than the original within same limited time. As a consequence, compared to OODG, our heuristic approach performs much better in terms of prediction quality. We also observed no significant prediction quality difference with CART.

## 5 Conclusion

We propose exact and heuristic methods for optimizing binary decision diagrams (BDDs) based on the (Maximum) Boolean Satisfiability framework. As an interpretable ML model, in practice, BDD provides more compact topology than other interpretable ML model, like decision trees. Our large experimental studies show clear benefits of the proposed approach in terms of prediction quality and interpretability compared to the existing heuristic approaches. Compared to the existing state-of-the-art approaches, the proposed approach obtains competitive prediction performance but far lighter encoding size.

In the future, it would be interesting to extend the proposed approach for multi-valued classification. Moreover, a deeper investigation of BDDs with other interpretable models (such as decision rules and decision sets) will have significant benefits for explainable AI.

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