SAT-Based Learning of Compact Binary Decision Diagrams for Classification

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Motivation

- **Decision trees** as **interpretable classifiers**
  - However, number of splits **exponential** in depth

- **Binary Decision Diagrams** as more **compact** alternatives
  - Same split across each level

Our Contribution

- Propose **SAT-based encoding** for learning max-accuracy BDDs
- Model the **size** of the BDD as a **secondary objective**
- Introduce and model **Multi-Dimensional BDDs** as more expressive alternatives
- Demonstrate **improved compactness** with **maintained accuracy** in experiments

Background

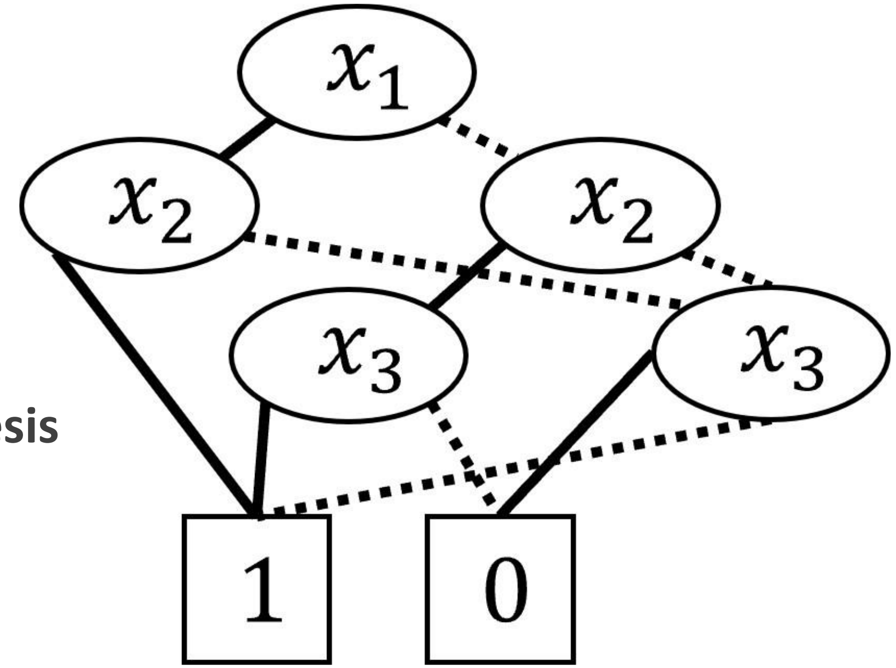
Encodings

Experiments

- Binary Decision Diagrams
- MaxSAT

Binary Decision Diagrams (BDD)

- **Rooted, directed, acyclic** graph
- Representation of a **Boolean** function
- Historically utilized towards **hardware synthesis**
- Recent focus on **BDD classifiers**



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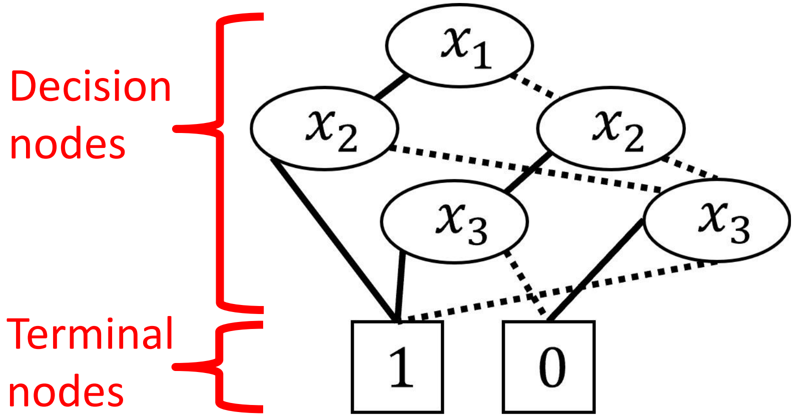

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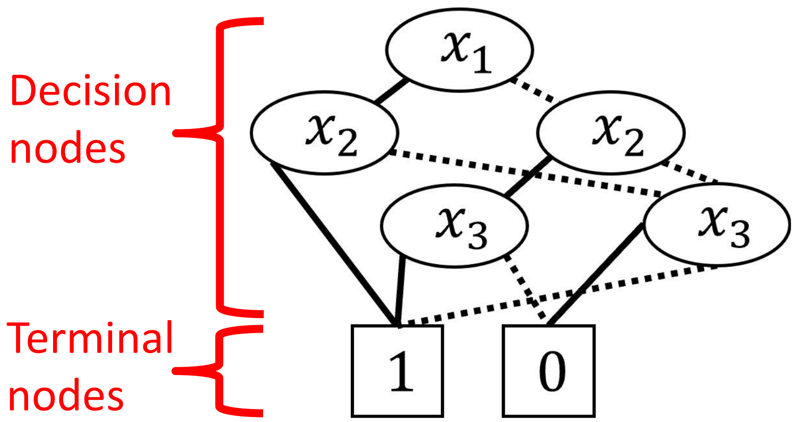

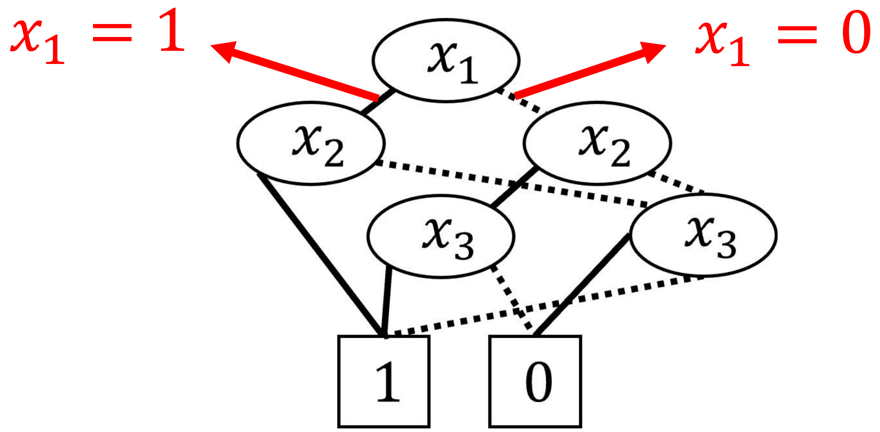

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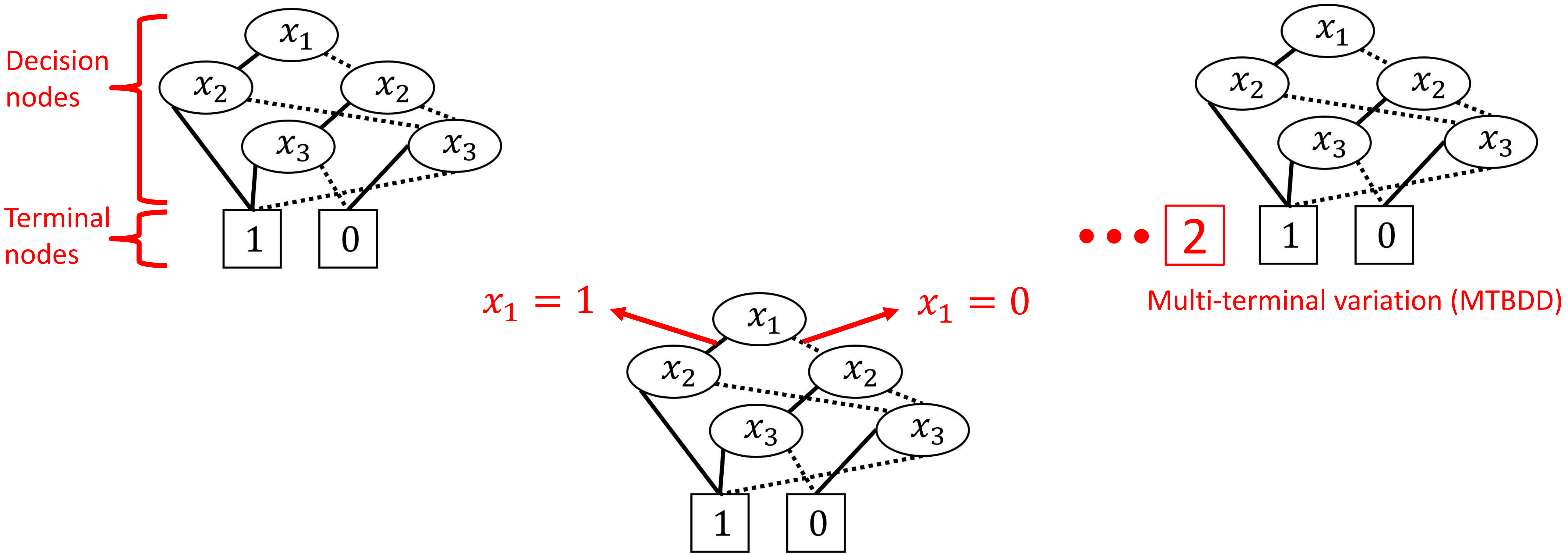

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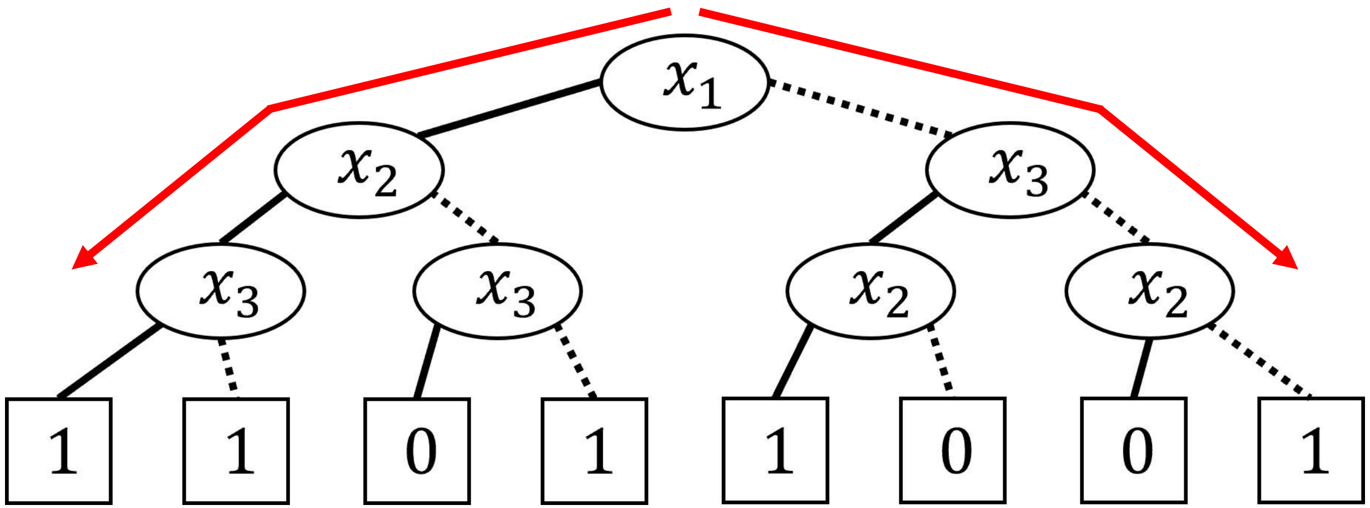
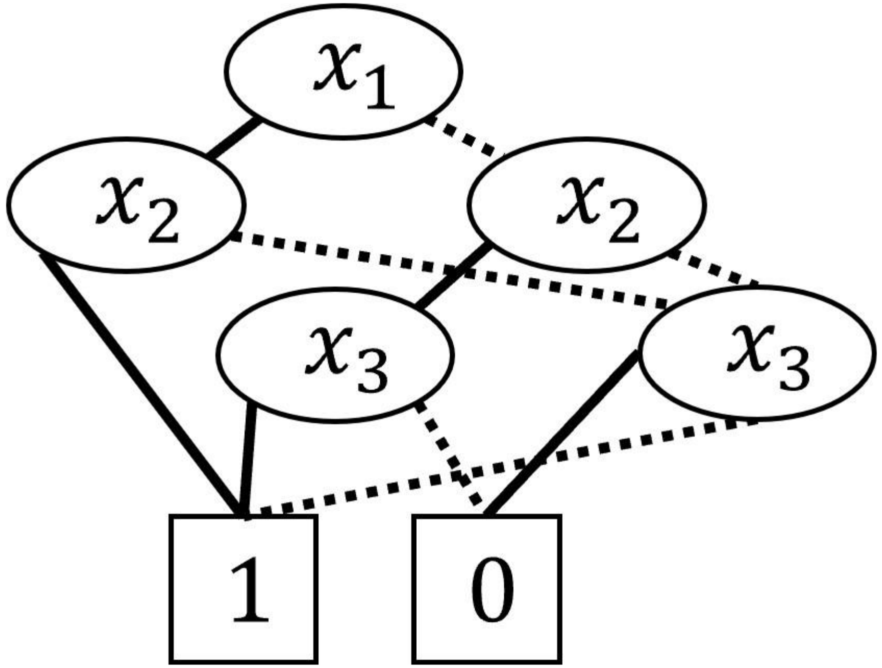


Unreduced and unordered



Reduced and ordered

MaxSAT

- Set of binary variables $\mathcal{X} = \{x_0, x_1, \ldots, x_n\}$
- Set of clauses
  - Each clause C_i is a subset of literals $\mathcal{X} \cup \neg\mathcal{X}$

- Find an assignment $\mathcal{M}: \mathcal{X} \rightarrow \{false, true\}$

- Satisfy all **hard** clauses $\mathcal{C}_h$
- Maximize the number of satisfied **soft** clauses $\mathcal{C}_s$

Background

Encodings

Experiments

- BDD Encoding
- Size Optimization
- Multi-dimensional BDDs
- Expressiveness relations

BDD Encoding

- **Direct encoding** of numerical features
  - Based on [Shati, Cohen, McIlraith, CP2021]

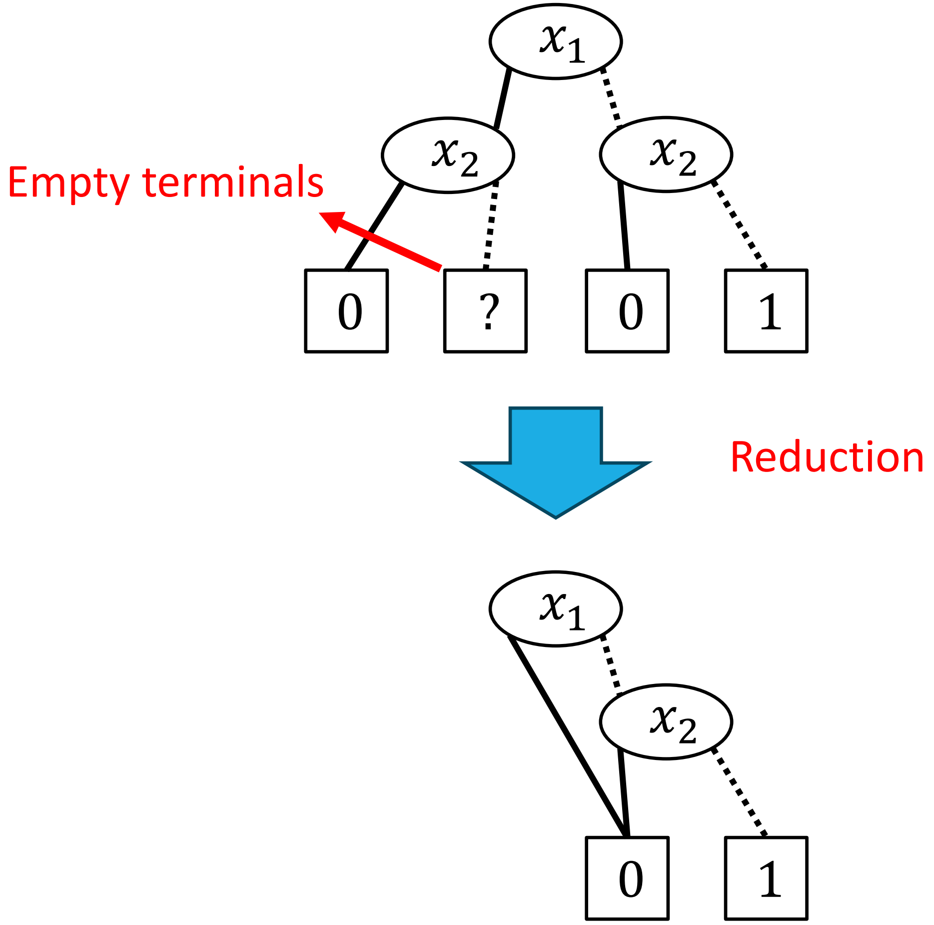
- Employ **splits** at each node
  - (feature, threshold)

- The alternative: **binarize features in advance**
  - **excessive** number of features

BDD Encoding

- **Direct encoding** of numerical features
  - Based on [Shati, Cohen, McIlraith, CP2021]

- Learn ordered but **unreduced** BDDs
  - Reduction in a **second stage**



BDD Encoding

- **Hard clauses:**

$$(a_{s,j}, \neg a_{s,j+1}) \qquad s < s_{max}, j \in F$$

$$(a_{s,0}) \qquad s < s_{max}$$

$$(\neg a_{s,j}, a_{s,j+1}, d_{s,i_1}, \neg d_{s,i_2}) \quad s < s_{max}, j \in F, (i_1, i_2) \in O_j(X)$$

$$(\neg a_{s,j}, a_{s,j+1}, \neg d_{s,i_1}, d_{s,i_2}) \quad s < s_{max}, j \in F, (i_1, i_2) \in O_j^{=}(X)$$

$$(\neg a_{s,j}, a_{s,j+1}, d_{s,\#_j^1}) \qquad s < s_{max}, j \in F$$

$$(\neg c_{t,l_1}, \neg c_{t,l_2}) \qquad t \in \mathcal{N}_T, l_1, l_2 \in K$$

$$(\bigvee_{l \in L} c_{t,l}) \qquad t \in \mathcal{N}_T$$

$$(\bigvee_{s \in A_L(t)} \neg d_{s,i}, \bigvee_{s \in A_R(t)} d_{s,i}, c_{t,y_i}, \neg o_i) \qquad t \in \mathcal{N}_T, x_i \in X$$

- **Soft clauses:**

$$(o_i) \qquad x_i \in X$$

- **Variables:**
  - $a_{s,j}$: The feature chosen at split s is or comes before j.
  - $d_{s,i}$: Point x_i is directed to the left child at split s.
  - $c_{t,l}$: Output label l is assigned to terminal node t.
  - o_i: Point x_i is classified correctly.

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- Exactly one feature is selected at each split.
- Selected feature enforces order of values.
- Exactly one label is selected at each leaf.

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- Exactly one feature is selected at each split.
- Selected feature enforces order of values.
- Exactly one label is selected at each leaf.
- The leaf and point labels match for a correctly classified point.

BDD Encoding

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- Exactly one feature is selected at each split.
- Selected feature enforces order of values.
- Exactly one label is selected at each leaf.
- The leaf and point labels match for a correctly classified point.
- Number of correctly classified points are maximized.

Size Optimization

- Model the size of BDD’s **reduced version**

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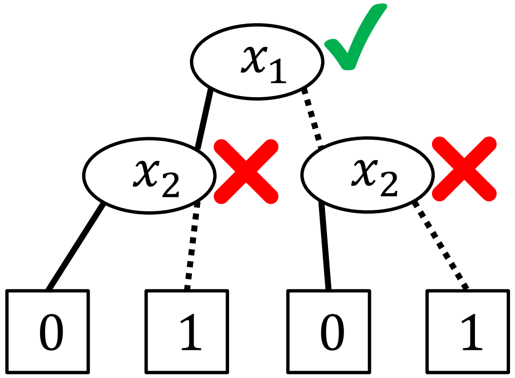
- For each decision node:
  - Can it be **replaced** by one of its **children**?



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- Model the size of BDD's **reduced version**

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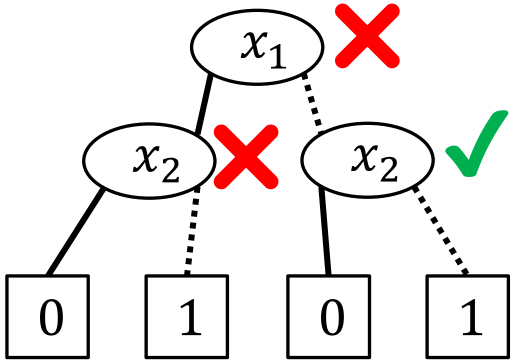

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- Two approaches:
  - **1-stage:** add as a **secondary objective** to accuracy
  - **2-stage:** use as a **post-processing step** to choose **empty** node labels

Size Optimization

- **Hard clauses:**

$(\neg c_{t_1,l}, \neg c_{t_2,l}, \neg \sigma_{t_1,t_2}) \quad (t_1, t_2, \Delta) \in G(s_{max}), l \in K$

$(\neg c_{t_1,l}, c_{t_2,l}, \sigma_{t_1,t_2}) \quad (t_1, t_2, \Delta) \in G(s_{max}), l \in K$

$(c_{t_1,l}, \neg c_{t_2,l}, \sigma_{t_1,t_2}) \quad (t_1, t_2, \Delta) \in G(s_{max}), l \in K$

$(b_{\Delta \lfloor t_1/\Delta \rfloor, \Delta}, \neg \sigma_{t_1,t_2}) \quad (t_1, t_2, \Delta) \in G(s_{max})$

$(\neg r_{t_1\Delta, t_2\Delta, \Delta}, \neg c_{t_1\Delta+\delta, l}, c_{t_2\Delta+\delta, l}) \quad \Delta \in P(s_{max}), t_1 < t_2 < 2^{s_{max}}/\Delta, \delta < \Delta, l \in K$

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- **Soft clauses:**

$(\bigvee_{0 \le t_2 < t} r_{t_2\Delta, t\Delta, \Delta}, \neg b_{t\Delta, \Delta}) \quad \Delta \in P(s_{max}), t < 2^{s_{max}}/\Delta$

- **Definitions:**

$$
\begin{aligned}
G(1) &= \{(0, 1, 2)\} \\
G(p) &= G(p-1) \cup \{(t_1 + 2^{p-1}, t_2 + 2^{p-1}, \Delta) | (t_1, t_2, \Delta) \in G(p-1)\} \\
&\quad \cup \{(t, t + 2^{p-1}, 2^p) | 0 \le t < 2^{p-1}\}
\end{aligned}
$$

- **Variables:**
  - α_{t_1,t_2}: Terminals t_1 and t_2 have been assigned different output labels.
  - $b_{t,\Delta}$: The sequence of Δ labels starting from terminal node t (inclusive) cannot be divided into two equal sub-sequences.
  - $r_{t_1,t_2,\Delta}$: The sequence of Δ labels starting from terminal node t_1 is equal to the sequence of Δ labels starting from terminal node t_2 (both inclusive).

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- The differences in labels are correctly represented.
- A node cannot be replaced by one of its children if their descendants are labelled differently.
- A node cannot be merged with one of the previous ones if their descendants are labelled differently.
- The number of nodes that can be replaced or merged are maximized.

Multi-dimensional BDD

- **Multi-dimensional** splits:
  - Specified by **directional inner BDDs (DIBDD)** rather feature threshold pairs

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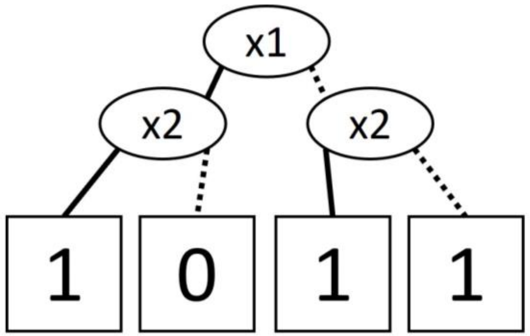
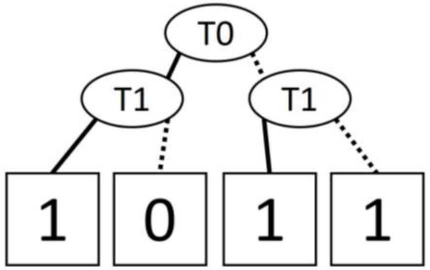
- **DIBDD** with dimension D:
  - Operates on D **ordinary splits**
  - Has two terminals, representing **left (1) and right (0)** directions



Multi-dimensional BDD

- **Multi-dimensional BDDs** (MDBDD):
  - Operates on multi-dimensional splits rather than ordinary ones



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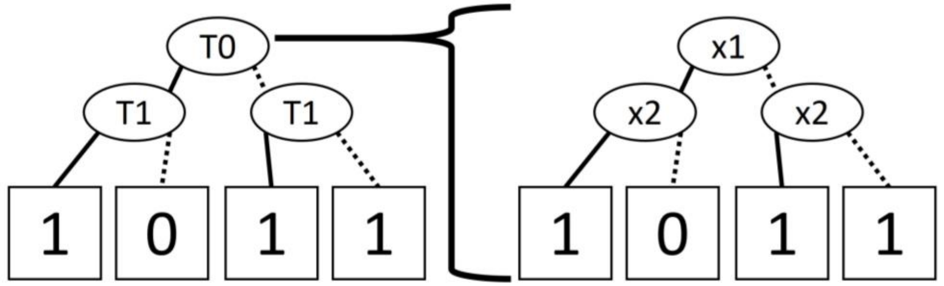

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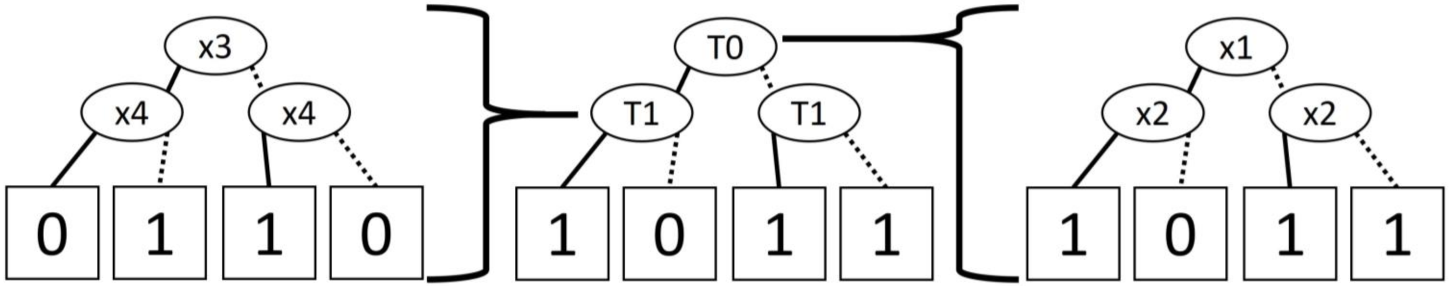
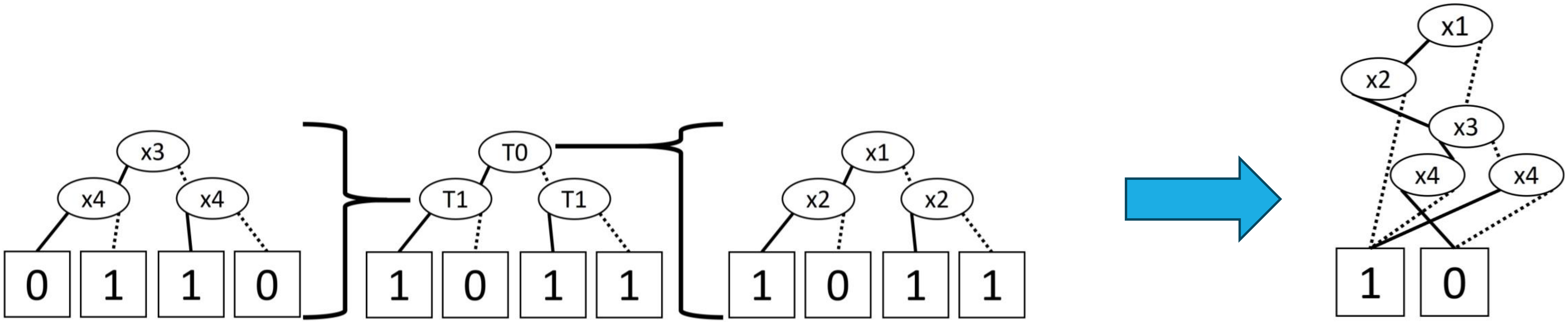


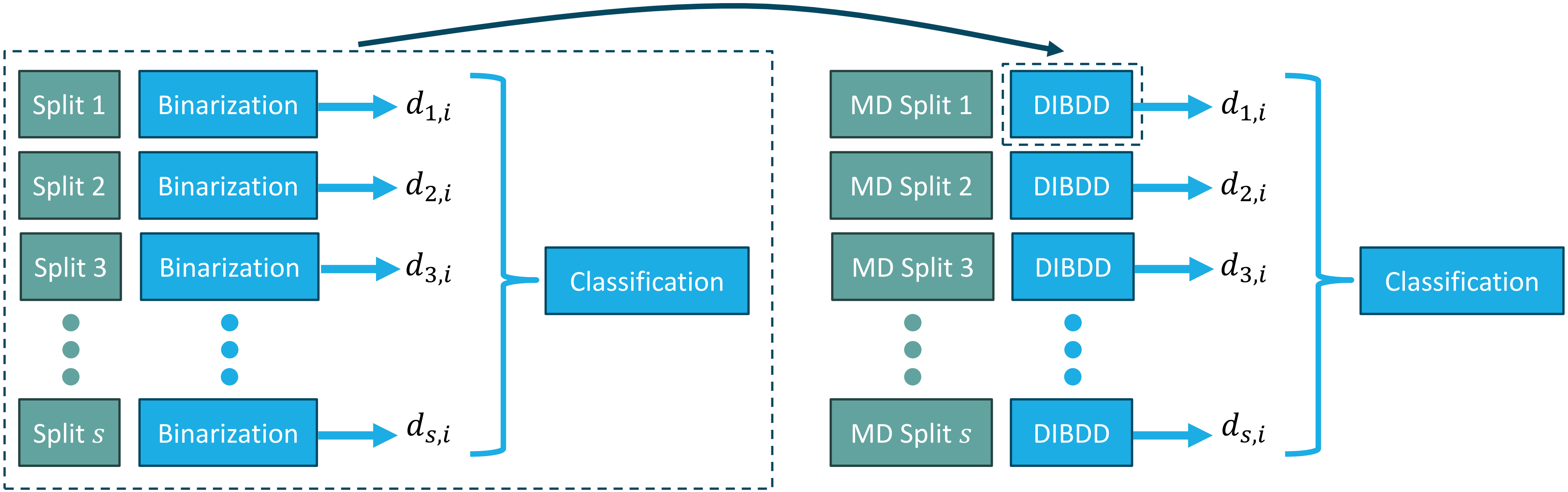
Multi-dimensional BDD

- **Multi-dimensional BDDs** (MDBDD):
  - Operates on multi-dimensional splits rather than ordinary ones
  - Can be **transformed** into ordinary BDDs



Multi-dimensional BDD

- BDD encoding:
- MDBDD encoding:



Multi-dimensional BDD

- Kept **hard clauses:** enforce labels and correct classification
- Kept **soft clauses:** maximize correct classification
- New **hard clauses:**

$$(\hat{a}_{(s,h),j}, \neg\hat{a}_{(s,h),j+1}) \qquad (s,h) \in S_H, j \in F$$

$$(\hat{a}_{(s,h),0}) \qquad (s,h) \in S_H$$

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$$(\hat{c}_{s,0}) \qquad s \in S$$

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  - $\hat{a}_{(s,h),j}$: The feature chosen at split h of directional inner BDD s is or comes before j.
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- Kept **soft clauses:** maximize correct classification
- New **hard clauses:**

$$(\hat{a}_{(s,h),j}, \neg\hat{a}_{(s,h),j+1}) \qquad (s,h) \in S_H, j \in F$$

$$(\hat{a}_{(s,h),0}) \qquad (s,h) \in S_H$$

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$$(\hat{c}_{s,0}) \qquad s \in S$$

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- The value of a multi-dimensional split matches the label of the containing leaf in the DIBDD.

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$(\neg\hat{a}_{(s,h),j}, \hat{a}_{(s,h),j+1}, \hat{d}_{(s,h),\#_j^1})$	$(s,h) \in S_H, j \in F$
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- Selected feature enforces order of values.
- The value of a multi-dimensional split matches the label of the containing leaf in the DIBDD.
- First leaf of each DIBDD is labelled 1 for breaking symmetry.

Expressiveness relations

- Given: $D_{total} = D_1 + D_2 + \cdots + D_s$

Multi-dimension BDD on s splits $\leq$ BDDs on D_{total} splits

Expressiveness relations

- Given: $D_{total} = D_1 + D_2 + \cdots + D_s$

BDDs on s splits $\leq$ Multi-dimension BDD on s splits $\leq$ BDDs on D_{total} splits

Background

Encodings

Experiments

- Objectives
- Setup
- Performance
- Size optimization
- Multi-dimensional BDD

Objectives

- Does our encoding outperform the state of the art in **runtime** and **training accuracy**?
- Do the 1-stage and 2-stage approaches **improve compactness** and how do they **affect testing accuracy**?
- Do multi-dimensional BDDs enable us to employ a **higher number of features** in our solutions?

Setup

- Baseline: **Hu et al.** [2022]
  - Learns **max-accuracy** BDDs with **binary classification** and **binary features**

- Datasets: **11** datasets from the **UCI** repository

- Solver: **Loandra** with 15 minutes time limit

Performance

- **Higher** training accuracies
- **Shorter** runtimes

	Training Accuracy			Runtime / Timeout		
Splits	Ours	Hu et al.	Tie	Ours	Hu et al.	Tie
4	2	0	6	5	0	3
5	3	1	4	3	0	5
6	3	0	5	3	0	5

Number of improvements compared to Hu et al.

Performance

- **Higher** training accuracies
- **Shorter** runtimes
- Improvements seen in both numerical and binary datasets

	Training Accuracy			Runtime / Timeout		
Splits	Ours	Hu et al.	Tie	Ours	Hu et al.	Tie
4	2	0	6	5	0	3
5	3	1	4	3	0	5
6	3	0	5	3	0	5

Number of improvements compared to Hu et al.

Dataset			Splits	Accuracy (%)		Time (s)	
				Ours	Hu et al. [16]	Ours	Hu et al. [16]
Ionosphere			4	94.9	90.6	TO	TO
$\lvert X \rvert$	$\lvert F \rvert$	$\lvert K \rvert$	5	95.2	85.8	TO	TO
351	34	2	6	96.6	90.6	TO	TO
Monk2			4	74.6	74.6	85.49	473.43
$\lvert X \rvert$	$\lvert F \rvert$	$\lvert K \rvert$	5	84.6	84.6	185.3	416.37
169	6	2	6	100	100	0.35	1.09

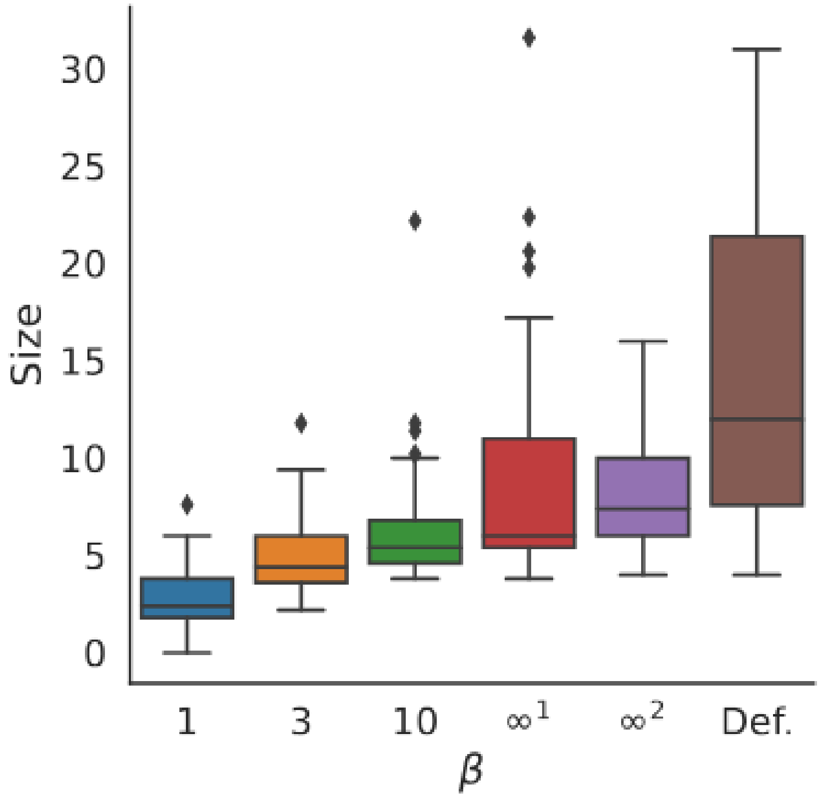
Size Optimization

- Use **5-fold cross validation** and study testing accuracy, training accuracy, and size

- Parameter $\boldsymbol{\beta}$: the weight of accuracy against size in objective
  - $\boldsymbol{\beta} \in \mathbb{R}$: Accuracy weighted (1-stage)
  - $\boldsymbol{\beta} = \infty^{\mathbf{1}}$: Accuracy prioritized (1-stage)
  - $\boldsymbol{\beta} = \infty^{\mathbf{2}}$: 2-stage approach
  - $\boldsymbol{\beta} = \boldsymbol{def}$: No size optimization

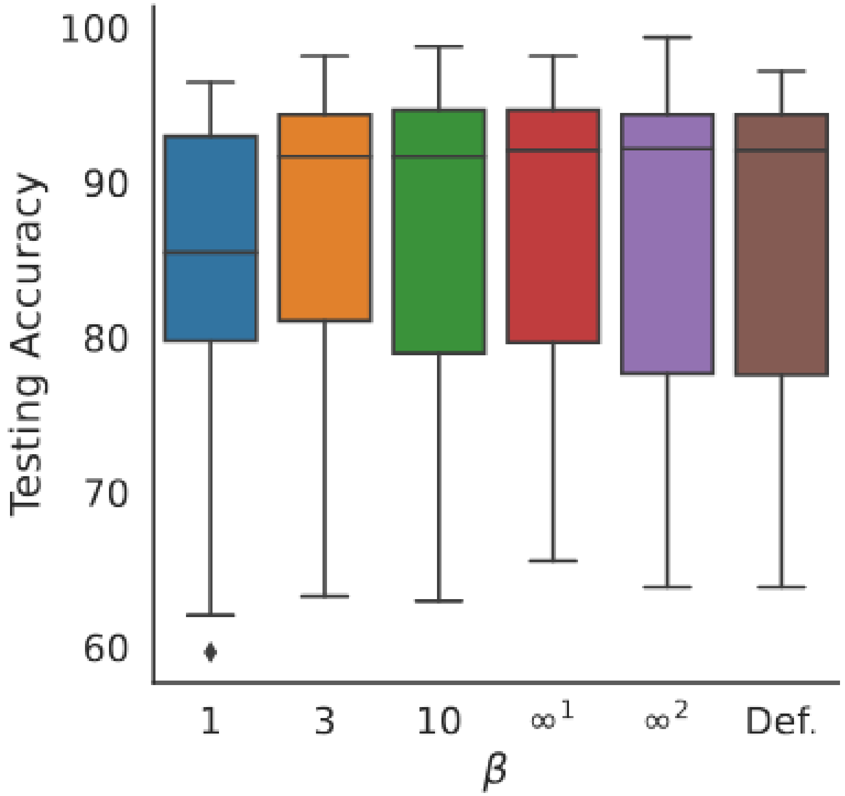
Size Optimization

- **1-stage** and **2-stage** approaches significantly improve compactness



Size Optimization

- **Compactness** helps with **testing accuracy** and **generalization**



Multi-dimensional BDD

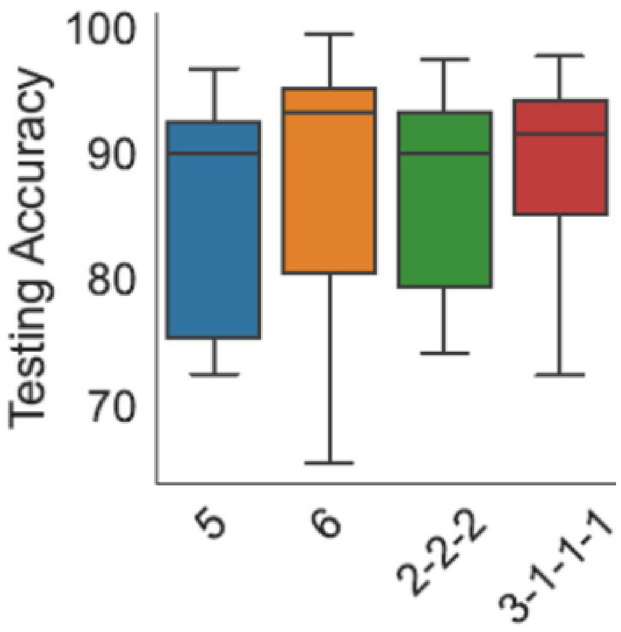
- **5-fold cross validation**

- **Sequence of dimensions** as parameter

- Utilize **2-stage** size optimization

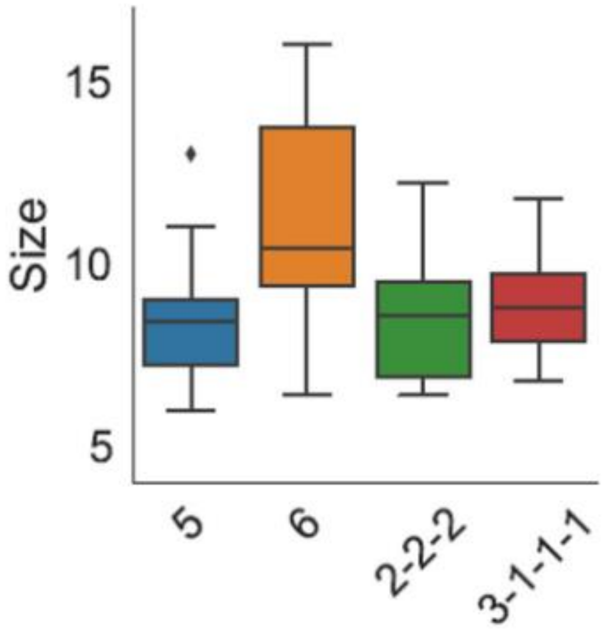
Multi-dimensional BDD

- Testing accuracy is close to **upper bound** of **expressiveness**



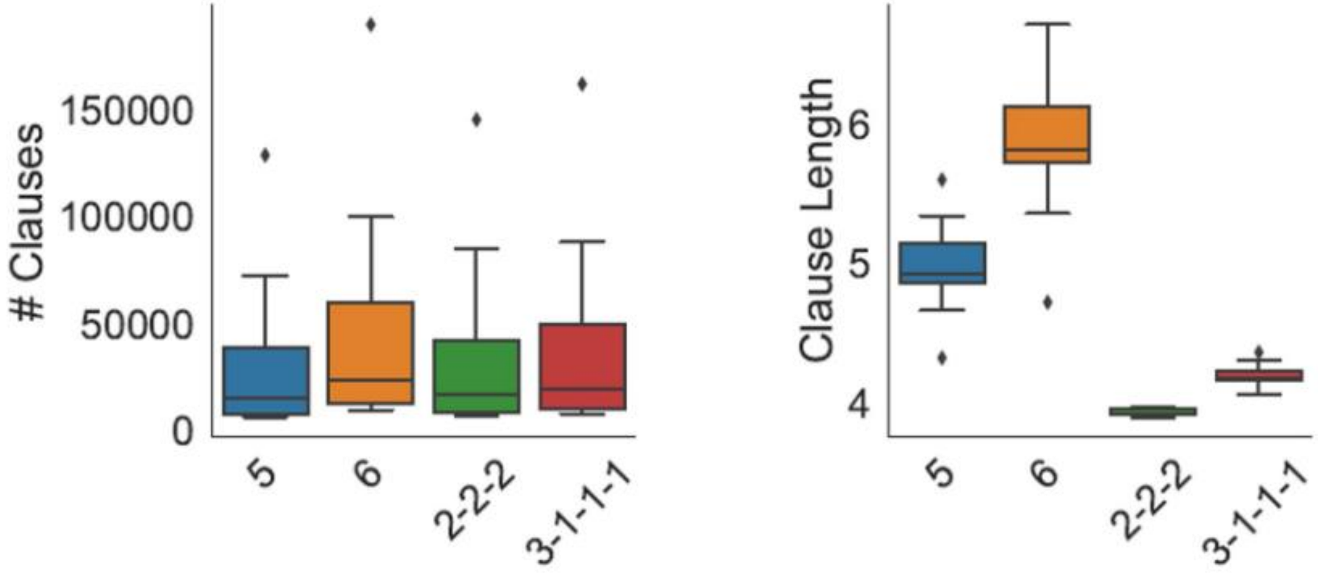
Multi-dimensional BDD

◦ Solutions are more compact than **upper bound** of **expressiveness**



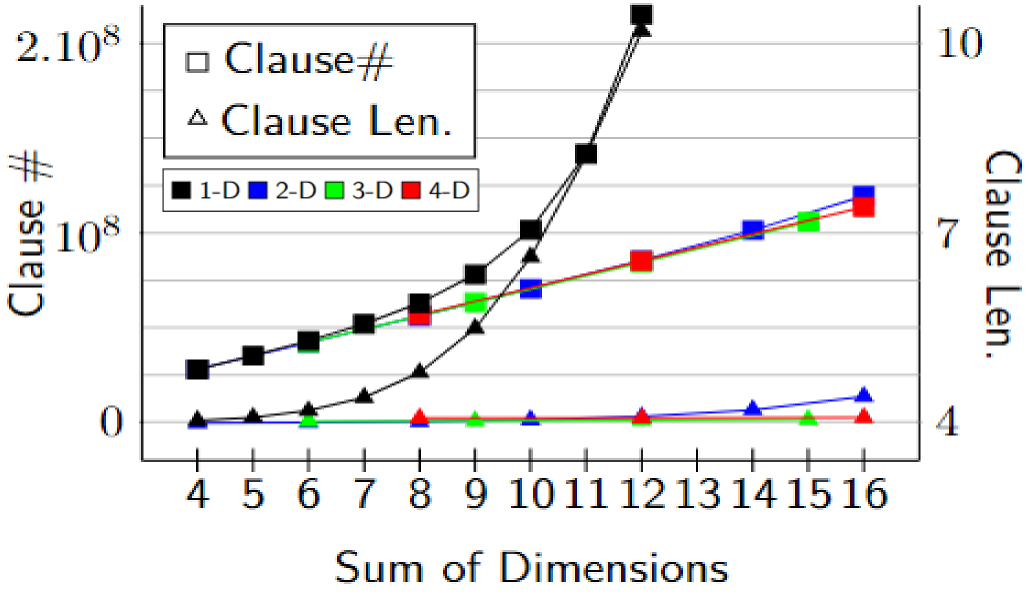
Multi-dimensional BDD

- **Clauses** are significantly **shorter**



Multi-dimensional BDD

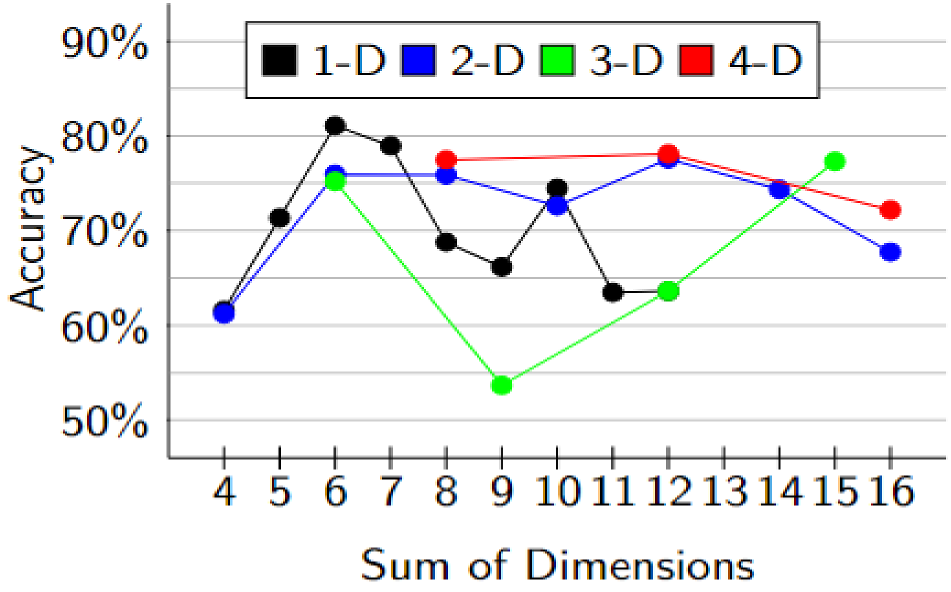
- Performance on **Adult dataset**
  - 32K points and 105 features
  - 60m timeout
- Number and length of clauses **scale significantly better**



Multi-dimensional BDD

- Performance on **Adult dataset**
  - 32K points and 105 features
  - 60m timeout

- Solutions are produced for **higher number of total dimensions**



Summary

- **SAT-based** encoding for learning **BDD classifiers**
  - Numerical feature encoding
  - Multi-label

- BDD **size optimization**
  - **1-stage** (as a secondary objective)
  - **2-stage** (as a post-processing step)

- **Multi-dimensional** BDDs
  - Directional inner BDDs and multi-dimensional splits
  - **Expressiveness** bounds

- Experiments:
  - **Better performance** than the state of the art
  - **Significant compactness** with little cost to accuracy
  - Better **generalization** through size reduction
  - **Multi-dimensional BDDs** to enable high number of total splits

Future Work

- Allow more control to **2-stage size optimization**

- Encode **nested** directional BDDs

- Investigate strategies to **balance the two objectives**

- Analyze the effects of the **dimension sequence parameter**

Thank you for your time!

Q & A

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CP-23
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