

Learning Optimal Decision Trees using Constraint Programming

CP2025 - Constraints Journal Prominent Paper Award

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13 August 2025

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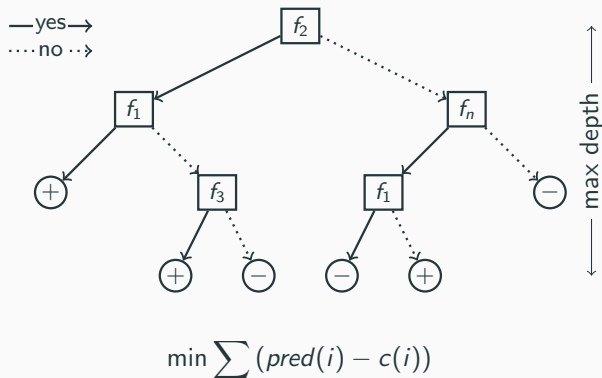
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³Université Laval, Québec, Canada, *claudc — guy.quimper@ift.ulaval.ca*



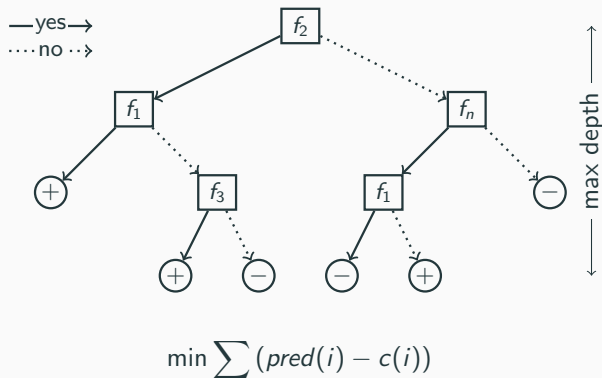
Database					
f_1	f_2	f_3	$\dots$	f_n	c
1	0	1	$\dots$	1	+
0	1	0	$\dots$	1	-
1	1	0	$\dots$	0	+
0	0	0	$\dots$	0	+
1	0	0	$\dots$	0	+
0	1	1	$\dots$	1	-
1	1	1	$\dots$	0	-
$\vdots$	$\vdots$	$\vdots$	$\ddots$	$\vdots$	$\vdots$
1	1	1	$\dots$	1	+

Database					
f_1	f_2	f_3	$\dots$	f_n	c
1	0	1	$\dots$	1	+
0	1	0	$\dots$	1	-
1	1	0	$\dots$	0	+
0	0	0	$\dots$	0	+
1	0	0	$\dots$	0	+
0	1	1	$\dots$	1	-
1	1	1	$\dots$	0	-
$\vdots$	$\vdots$	$\vdots$	$\ddots$	$\vdots$	$\vdots$
1	1	1	$\dots$	1	+



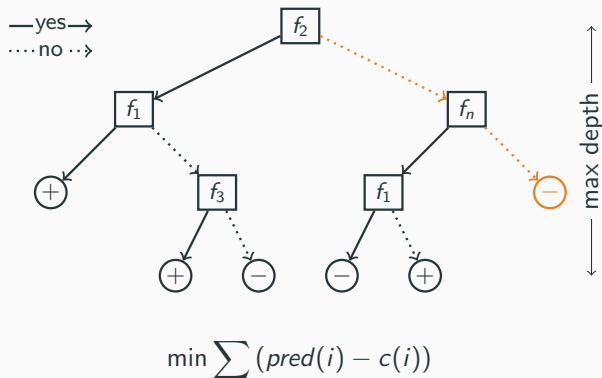
Database					
f_1	f_2	f_3	...	f_n	c
1	0	1	...	1	+
0	1	0	...	1	-
1	1	0	...	0	+
0	0	0	...	0	+
1	0	0	...	0	+
0	1	1	...	1	-
1	1	1	...	0	-
$\vdots$	$\vdots$	$\vdots$	$\ddots$	$\vdots$	$\vdots$
1	1	1	...	1	+

New sample					
0	0	1	...	0	?



Database					
f_1	f_2	f_3	...	f_n	c
1	0	1	...	1	+
0	1	0	...	1	-
1	1	0	...	0	+
0	0	0	...	0	+
1	0	0	...	0	+
0	1	1	...	1	-
1	1	1	...	0	-
$\vdots$	$\vdots$	$\vdots$	$\ddots$	$\vdots$	$\vdots$
1	1	1	...	1	+

New sample					
0	0	1	...	0	-

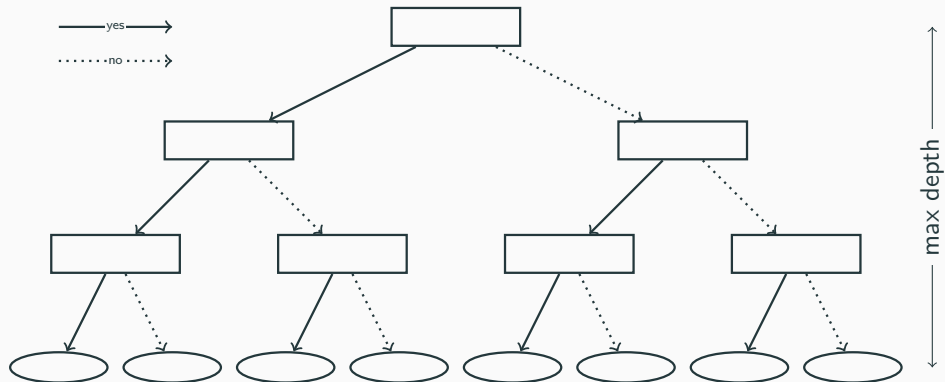


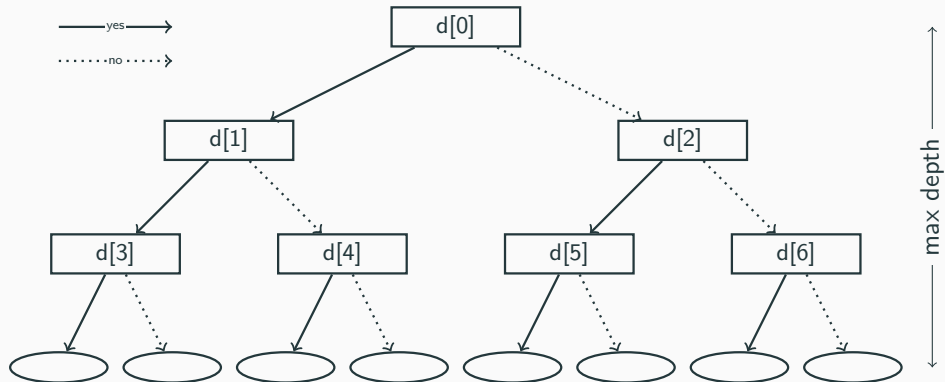
Greedy methods:

- ✓ easy construction
- ✗ hard to impose additional constraints
- ✗ potentially unnecessarily complex tree

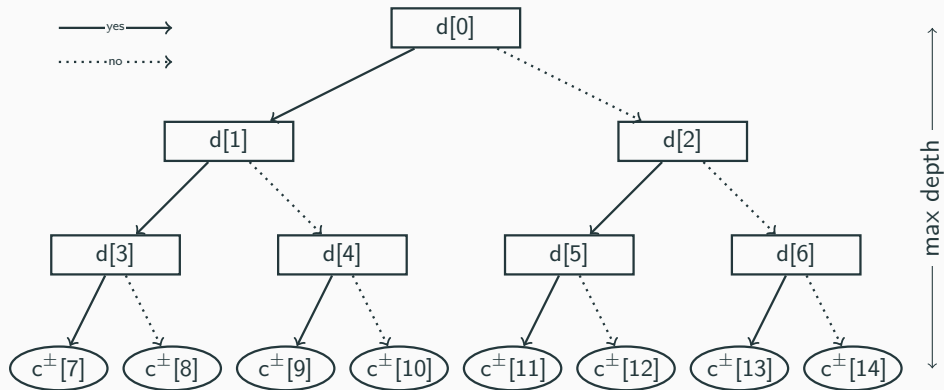
- Mining optimal decision trees from itemset lattices, Nijssen, S., Fromont, E., 2007
- Minimising decision tree size as combinatorial optimisation, Bessiere, C., Hebrard, E., O'Sullivan, B., 2009
- Optimal constraint-based decision tree induction from itemset lattices, Nijssen, S., Fromont, É., 2010
- **Optimal classification trees**, Bertsimas, D., Dunn, J., 2017
- Learning optimal decision trees with sat, Narodytska, N., Ignatiev, A., Pereira, F., Marques-Silva, J., RAS, I., 2018
- Learning optimal and fair decision trees for non-discriminative decision-making, Aghaei, S., Azizi, M.J., Vayanos, P., 2019
- Learning optimal classification trees using a binary linear program formulation, Verwer, S., Zhang, Y., 2019

CP Model



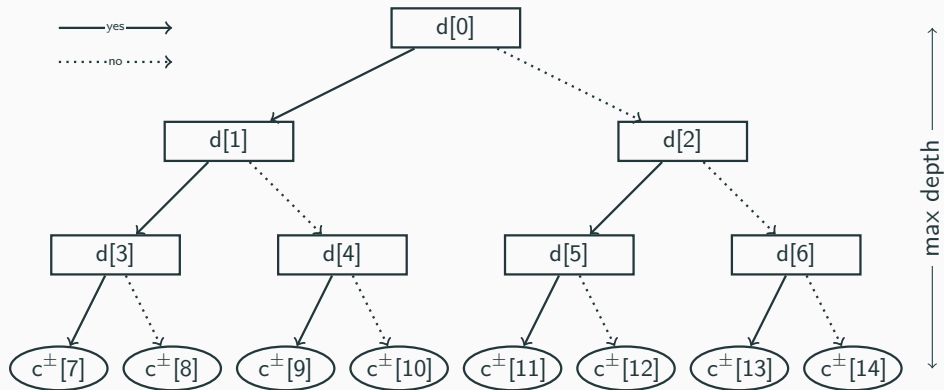


$$\text{dom}(d[i]) = \{1, \dots, n\}$$



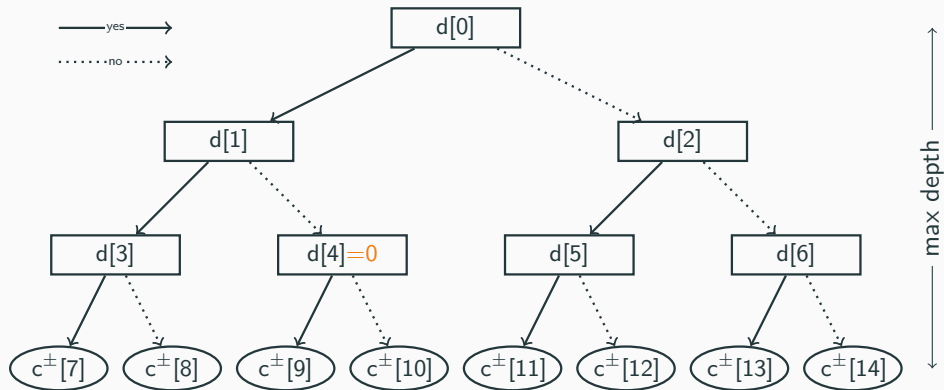
$$\text{dom}(d[i]) = \{1, \dots, n\}$$

$$\text{dom}(c[i]) = \{0, \dots, N\}$$



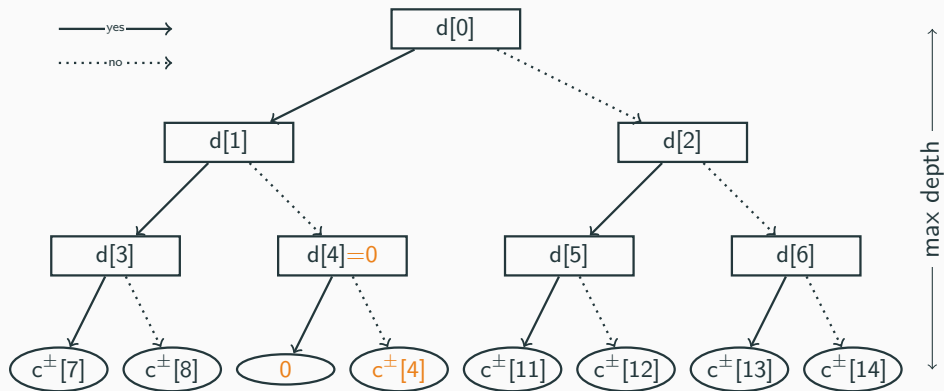
$$\text{dom}(d[i]) = \{0, 1, \dots, n\}$$

$$\text{dom}(c[i]) = \{0, \dots, N\}$$



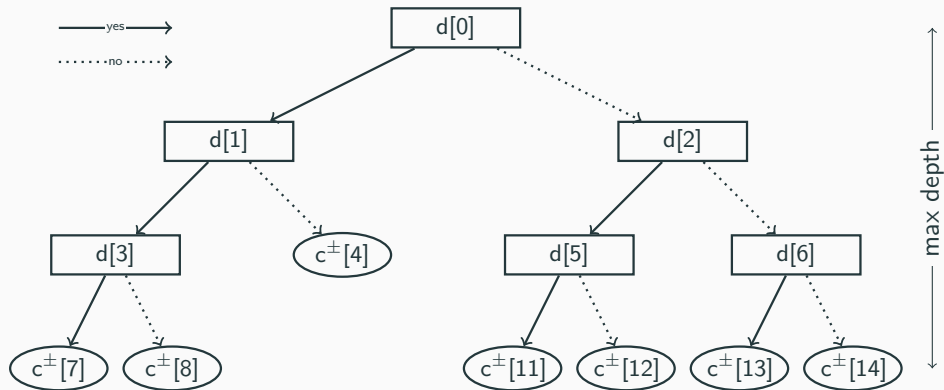
$$\text{dom}(d[i]) = \{0, 1, \dots, n\}$$

$$\text{dom}(c[i]) = \{0, \dots, N\}$$



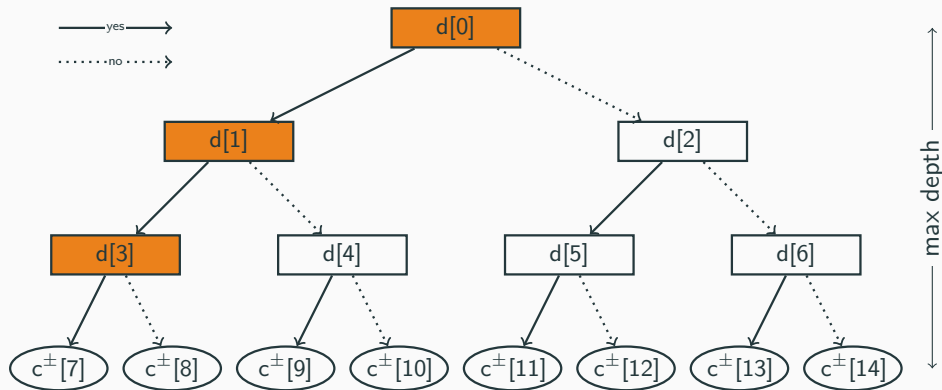
$$\text{dom}(d[i]) = \{0, 1, \dots, n\}$$

$$\text{dom}(c[i]) = \{0, \dots, N\}$$



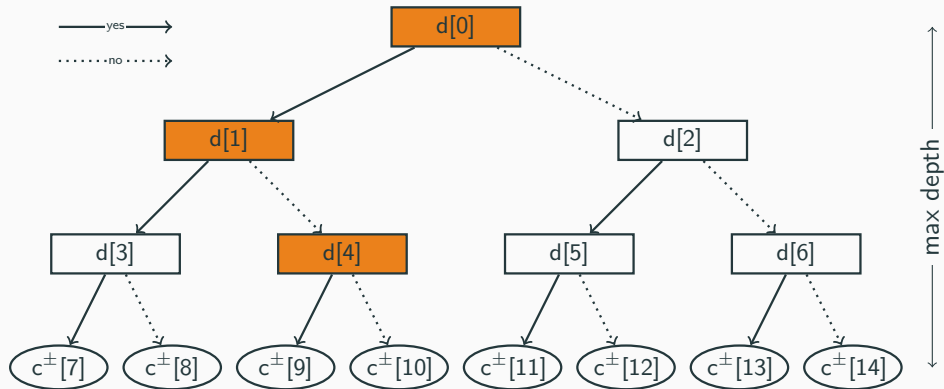
$$\text{dom}(d[i]) = \{0, 1, \dots, n\}$$

$$\text{dom}(c[i]) = \{0, \dots, N\}$$



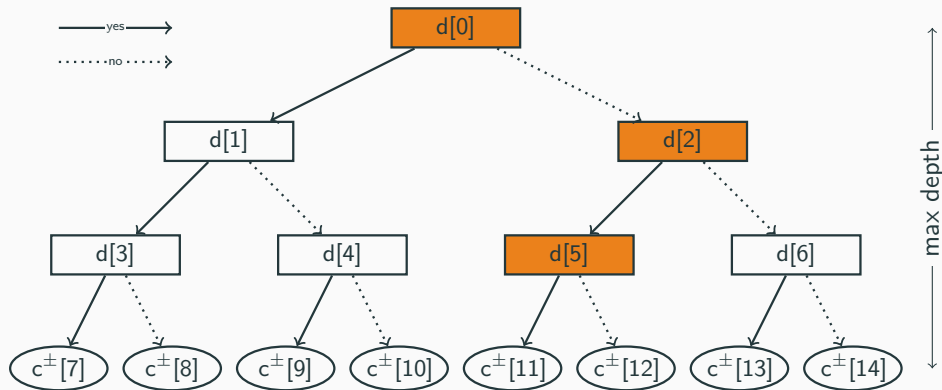
$$\text{dom}(d[i]) = \{0, 1, \dots, n\}$$

$$\text{dom}(c[i]) = \{0, \dots, N\}$$



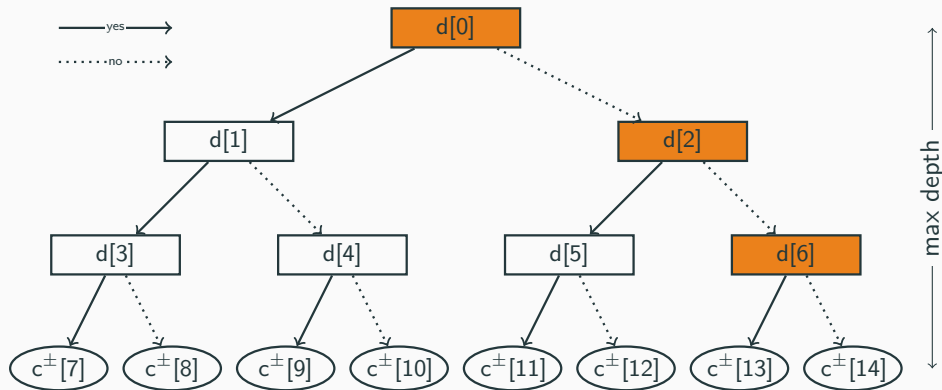
$$\text{dom}(d[i]) = \{0, 1, \dots, n\}$$

$$\text{dom}(c[i]) = \{0, \dots, N\}$$



$$\text{dom}(d[i]) = \{0, 1, \dots, n\}$$

$$\text{dom}(c[i]) = \{0, \dots, N\}$$



$$\text{dom}(d[i]) = \{0, 1, \dots, n\}$$

$$\text{dom}(c[i]) = \{0, \dots, N\}$$

f_1	f_2	f_3	f_4
1	0	1	1
0	1	0	1
1	1	0	0
0	0	0	0
1	0	0	0
0	1	1	1
1	1	1	0
1	1	1	1

Features (Dense)				Counter
x_1	x_2	x_3	x_4	

f_1	f_2	f_3	f_4
1	0	1	1
0	1	0	1
1	1	0	0
0	0	0	0
1	0	0	0
0	1	1	1
1	1	1	0
1	1	1	1

Features (Dense)				Counter
x_1	x_2	x_3	x_4	
0	1	0	1	

f_1	f_2	f_3	f_4
1	0	1	1
0	1	0	1
1	1	0	0
0	0	0	0
1	0	0	0
0	1	1	1
1	1	1	0
1	1	1	1

Features (Dense)				Counter
x_1	x_2	x_3	x_4	
0	1	0	1	3

f_1	f_2	f_3	f_4
1	0	1	1
0	1	0	1
1	1	0	0
0	0	0	0
1	0	0	0
0	1	1	1
1	1	1	0
1	1	1	1

Features (Dense)				Counter
x_1	x_2	x_3	x_4	
0	1	0	1	3

- Dense representation
- No feature rejection

f_1	f_2	f_3	f_4
1	0	1	1
0	1	0	1
1	1	0	0
0	0	0	0
1	0	0	0
0	1	1	1
1	1	1	0
1	1	1	1

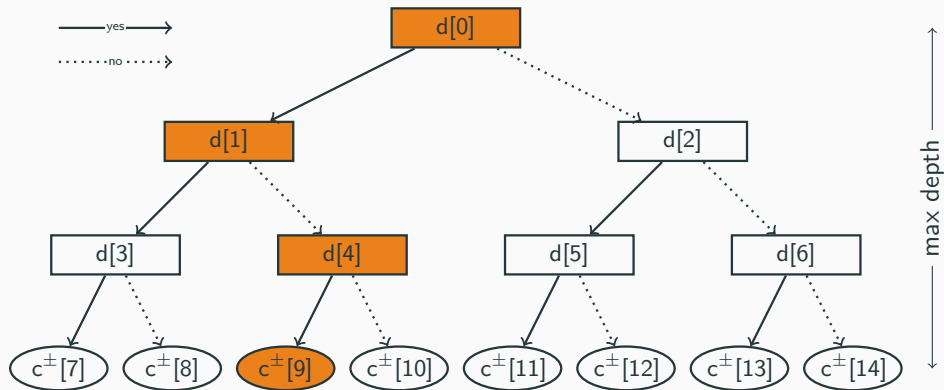
Features (Sparse)		Counter
y_1	y_2	
2	4	3

- Dense representation
- No feature rejection

f_1	f_2	f_3	f_4
1	0	1	1
0	1	0	1
1	1	0	0
0	0	0	0
1	0	0	0
0	1	1	1
1	1	1	0
1	1	1	1

✓Features (Sparse)		✗Features (Sparse)	Counter
y_1	y_2	z_1	
2	4	3	1

- ~~Dense representation~~
- ~~No feature rejection~~



$$\text{Coversize}(\{d[0], d[4]\}, \{d[1]\}, c^+[9])$$

$$\text{Coversize}(\{d[0], d[4]\}, \{d[1]\}, c^-[9])$$

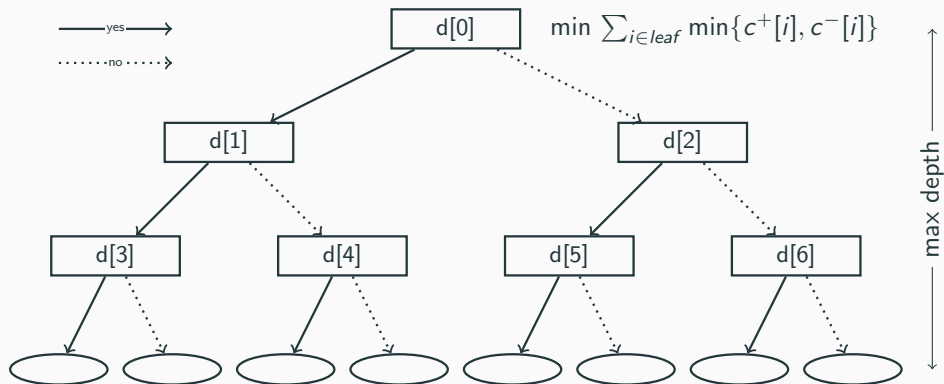
- constraints imposing minimum at leaf

$$c^+[i] + c^-[i] \geq N_{min}$$

- constraints avoiding useless decisions

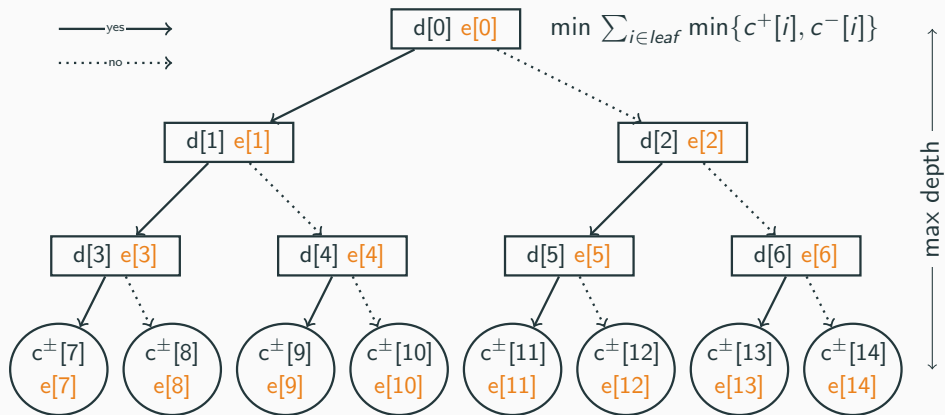


- redundant constraints improving speed



$$\text{dom}(d[i]) = \{0, 1, \dots, n\}$$

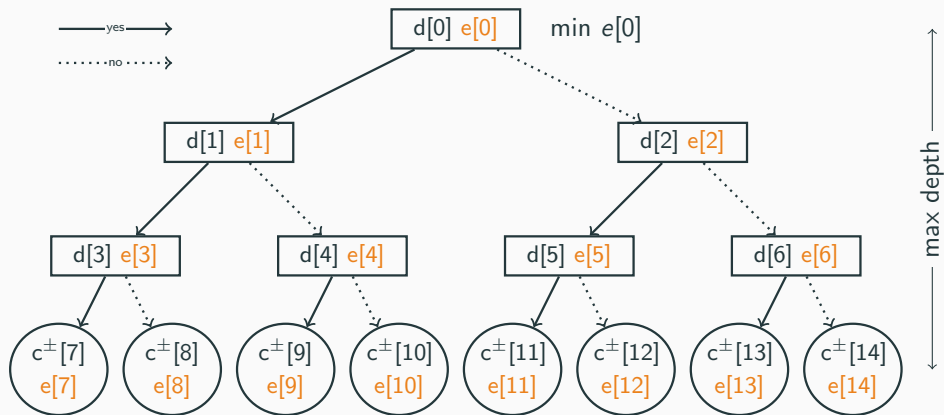
$$\text{dom}(c[i]) = \{0, \dots, N\}$$



$$\text{dom}(d[i]) = \{0, 1, \dots, n\}$$

$$\text{dom}(c[i]) = \{0, \dots, N\}$$

$$\text{dom}(e[i]) = \{0, \dots, N\}$$



$$\text{dom}(d[i]) = \{0, 1, \dots, n\}$$

$$\text{dom}(c[i]) = \{0, \dots, N\}$$

$$\text{dom}(e[i]) = \{0, \dots, N\}$$

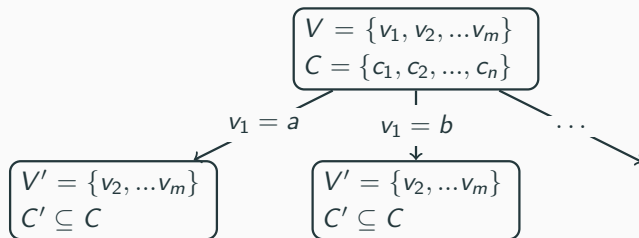
Search

$$V = \{v_1, v_2, \dots, v_m\}$$

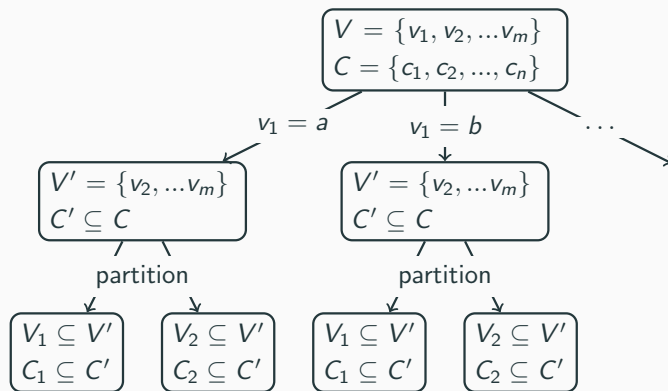
$$C = \{c_1, c_2, \dots, c_n\}$$

OR nodes

$SOL = SOL_1 \text{ or } SOL_2 \text{ or } \dots$

**OR nodes**

$SOL = SOL_1 \text{ or } SOL_2 \text{ or } \dots$

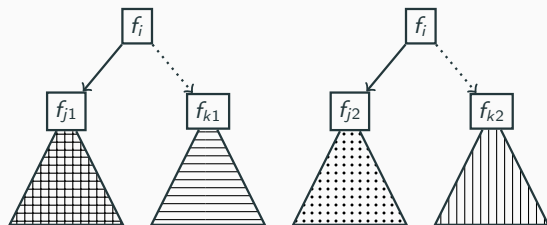


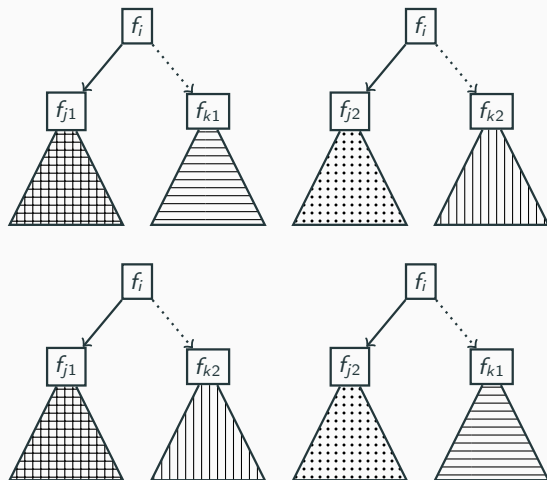
OR nodes

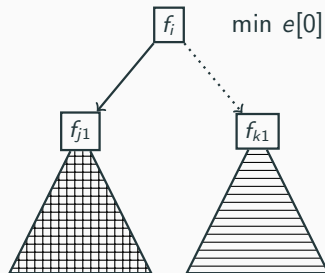
$SOL = SOL_1$ or SOL_2 or $\dots$

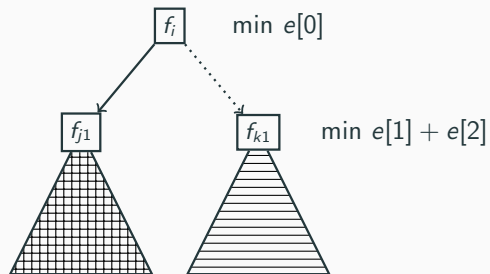
AND nodes

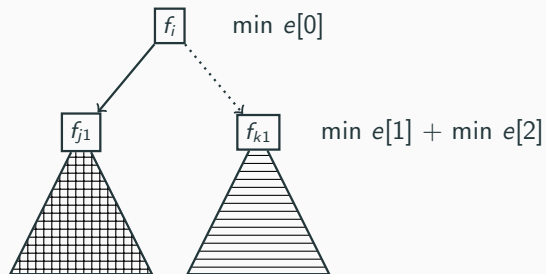
$SOL = SOL_1$ and SOL_2 and $\dots$

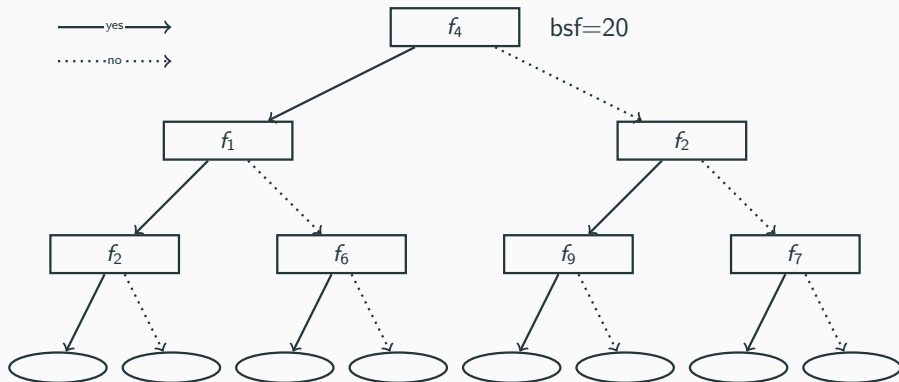


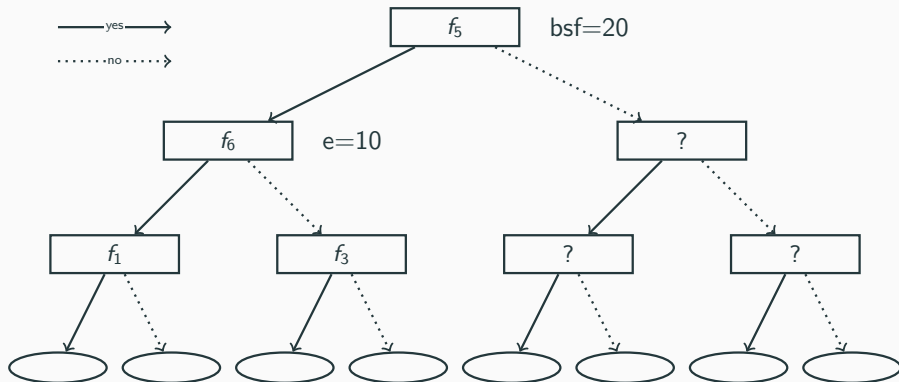


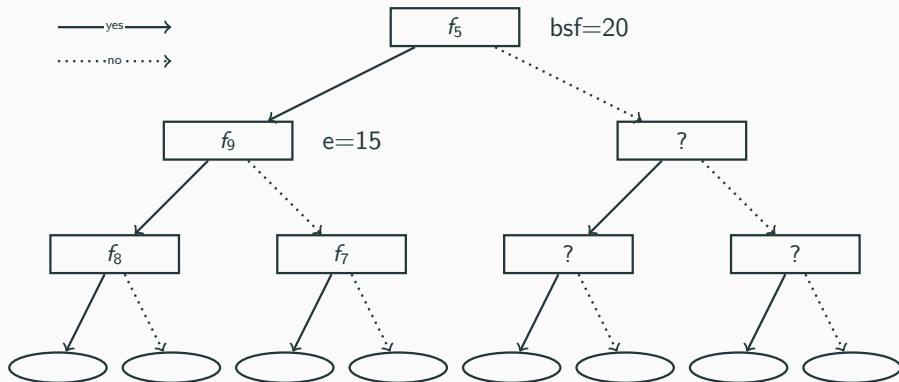




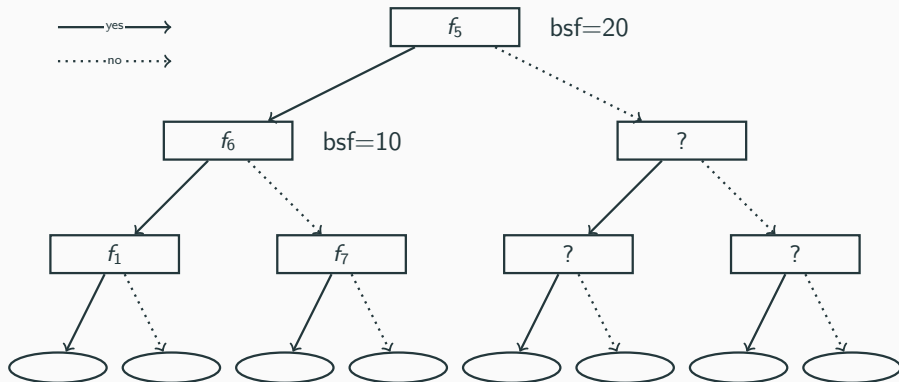


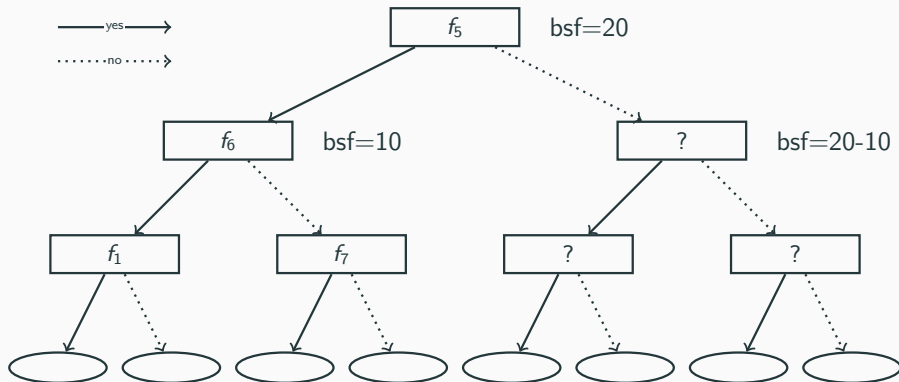




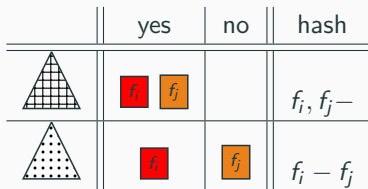












Results

	$N_{\min} = 1$			$N_{\min} = 5$			
	DL8	BinOCT	CP	DL8	CP	CP-c	CP-m
Proven optimality	49(61%)	13(16%)	68 (85%)	54(67%)	65 (81%)	63(79%)	59(74%)
Best solution found	49(61%)	21(26%)	80 (100%)	54(67%)	79 (99%)	77(96%)	72(90%)
Fastest	17(21%)	1(1%)	63 (79%)	26(32%)	52 (65%)	36(45%)	27(34%)
Time out	31(39%)	67(84%)	12 (15%)	25(31%)	15 (19%)	17(21%)	21(26%)

23 instances, depths from 2 to 5, 10 min TO

DL8: Dynamic programming approach using frequent itemsets mining

BinOCT: MIP-based approach running on CPLEX

To summarize

- efficient method
- cp based
- exploits the structure of the problem
- anytime best solution

To go further

- multi-class decision trees
- continuous features through binarization
- other sum-based cost functions
- ...

And since...

Nombre total de
citations

Cité 135 fois



The Thirty-Fourth AAAI Conference on Artificial Intelligence (AAAI-20)

Learning Optimal Decision Trees Using Caching Branch-and-Bound Search

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Louvain-la-Neuve, Belgium

Abstract

Several recent publications have studied the use of Mixed Integer Programming (MIP) for finding an optimal decision tree, that is, the best decision tree under formal requirements on accuracy, fairness or interpretability of the predictive model. These publications used MIP to deal with the hard computational challenge of finding such trees. In this paper, we introduce a new efficient algorithm, DL8.5, for finding optimal decision trees, based on the use of itemset mining techniques. We show that this new approach outperforms

- the trees found are accurate while satisfying additional constraints such as on the *fairness* of the trees: in their predictions, the trees may favor one group of individuals over another.

With the increasing interest in explainable and fair models in machine learning, recent years have witnessed a renewed interest in alternative algorithms for learning decision trees that can provide such optimality guarantees.

Most attention has been given in recent years and in

Proceedings of the Twenty-Ninth International Joint Conference on Artificial Intelligence (IJCAI-20)

Learning Optimal Decision Trees with MaxSAT and its Integration in AdaBoost

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{hhu, siala, hebrard, huguet}@laas.fr

Abstract

Recently, several exact methods to compute decision trees have been introduced. On the one hand, these approaches can find optimal trees for vari-

methods might exist [Bennett, 1994]. Moreover, simpler (e.g. smaller) trees, are often more accurate on unknown data.

Recently, several exact methods have been introduced to find optimal decision trees for some combinations of criteria involving, their size (i.e., nodes), depth, and their empirical

Journal of Machine Learning Research 23 (2022) 1-47

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MurTree: Optimal Decision Trees via Dynamic Programming and Search

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SAT-based Decision Tree Learning for Large Data Sets

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Abstract

Decision trees of low depth are beneficial for understanding and interpreting the data they represent. Unfortunately, finding a decision tree of lowest complexity (depth or size) that correctly represents given data is NP-hard. Hence known algorithms either (i) utilize heuristics that do not minimize the depth or (ii) are exact but scale only to small or medium-sized instances. We propose a new hybrid approach to decision tree learning, combining heuristic and exact methods in a novel way. More specifically, we employ SAT encodings repeatedly to local parts of a decision tree provided by a standard heuristic.

Decision trees: from efficient prediction to responsible AI

H. Blockeel, L. Deous, B. Falcourt, G. Naeffels, ... - Frontiers in artificial ... - 2023 - frontiersin.org

This article provides a birds-eye view on the role of decision trees in machine learning and data science over roughly four decades. It sketches the evolution of decision tree research ...

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Machine learning in agriculture: A comprehensive updated review

I. Benros, A.C. Tzavaras, G. Dotsis, R. Barrio, D. Kateris, ... - Sensors, 2021 - mdpi.com

The digital transformation of agriculture has evolved various aspects of management into artificial intelligent systems for the sake of making value from the ever-increasing data ...

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Mathematical optimization in classification and regression trees

E. Carrizosa, G. Mulet-Silla, D. Romero Morales, ... - Top, 2021 - Springer

Classification and regression trees, as well as their variants, are off-the-shelf methods in Machine Learning. In this paper, we review recent contributions within the Continuous ...

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On tackling explanation redundancy in decision trees

Y. Jizba, A. Ignatiev, J. Marques-Silva, ... - Journal of Artificial Intelligence ..., 2022 - jair.org

Decision trees (DTs) epitomize the ideal of interpretability of machine learning (ML) models. The interpretability of decision trees motivates explainability approaches by so-called ...

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Logic-based explainability in machine learning

J. Marques-Silva, ... - Knowledge, 18th International Summer School 2022 ..., 2023 - Springer

The last decade witnessed an ever-increasing stream of successes in Machine Learning (ML). These successes offer clear evidence that ML is bound to become pervasive in a wide ...

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Learning optimal decision trees using caching branch-and-bound search

G. Aspin, S. Nilsson, P. Schaus, ... - Proceedings of the AAAI conference on ..., 2020 - ojs.aaai.org

Several recent publications have studied the use of Mixed Integer Programming (MIP) for finding an optimal decision tree, that is, the best decision tree under formal requirements on ...

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On explaining decision trees

Y. Jizba, A. Ignatiev, J. Marques-Silva, ... - arXiv preprint arXiv:2010.11034, 2020 - arxiv.org

Decision trees (DTs) epitomize what have become to be known as interpretable machine learning (ML) models. This is informally motivated by paths in DTs being often much smaller ...

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Murtree: Optimal decision trees via dynamic programming and search

E. Demirozic, A. Lukina, E. Hebrard, J. Chan, ... - Journal of Machine ..., 2022 - jmlr.org

Decision tree learning is a widely used approach in machine learning, favoured in applications that require concise and interpretable models. Heuristic methods are ...

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SAT-based decision tree learning for large data sets

A. Scheder, S. Seidenberg, ... - Journal of Artificial Intelligence Research, 2024 - jair.org

Decision trees of low depth are beneficial for understanding and interpreting the data they represent. Unfortunately, finding a decision tree of lowest complexity (depth or size) that ...

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Constraint enforcement on decision trees: A survey

G. Naeffels, P. Terno, B. Falcourt, ... - ACM Computing Surveys (CSUR), 2022 - dl.acm.org

Decision trees have the particularity of being machine learning models that are visually easy to interpret and understand. Therefore, they are primarily suited for sensitive domains like ...

Strong optimal classification trees

☆ [A Gómez, P Werners](#) - arXiv preprint arXiv:2103.11986, 2021 - [arxiv.org](#)

Decision trees are among the most popular machine learning models and are used routinely in applications ranging from machine learning and medicine to bioinformatics. In this ...

☆ [Engraeher](#) ☆ [Citer](#) [Cite](#) 74 times [Autres articles](#) [Les 5 versions](#) [30](#)

Necessary and sufficient conditions for optimal decision trees using dynamic programming

☆ [van der Linden, M de Weert](#) - ... - [Advances in Neural ...](#), 2023 - [proceedings.neurips.cc](#)

Global optimization of decision trees has shown to be promising in terms of accuracy, but, consequently, has been limited in terms of the number of models that can be used. In this ...

☆ [Engraeher](#) ☆ [Citer](#) [Cite](#) 24 fois [Autres articles](#) [Les 5 versions](#) [30](#)

Optimal survival trees

☆ [Bertalmio, J Datto, E Gibson, A O'Donovan](#) - [Machine Learning](#), 2022 - [Springer](#)

Tree-based models are increasingly popular due to their ability to identify complex relationships that are beyond the scope of parametric models. Survival tree methods adapt ...

☆ [Engraeher](#) ☆ [Citer](#) [Cite](#) 64 fois [Autres articles](#) [Les 5 versions](#) [30](#)

pmu] Solid waste management techniques powered by bio-silico approaches with a special focus on municipal solid waste management: Research trends and ...

☆ [S Vyas, K Dhakar, S Varjari, RP Singhania](#) - [Science of the Total Environment](#), 2023 - [Elsevier](#)

Many technical, chemical, environmental, biological, financial, educational, and regulatory factors are typically involved in solid waste management (SWM). Artificial Intelligence (AI) ...

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Recent progress in recent
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Interpretable Machine
J. A. S. S. S. S. S. S. S. S.
The research requires multi-
discrete event simulation mod
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Interpretable and Com
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The research requires multi-
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Interpretable and Com
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Revisiting column-gene
J. A. S. S. S. S. S. S. S. S.
Decision trees are highly in
learning (ML) models. This
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Thank you for listening!

Any questions?

<https://hverhaeghe.bitbucket.io/>