Learning Optimal Decision Trees using Constraint Programming

CP2025 - Constraints Journal Prominent Paper Award

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The Problem

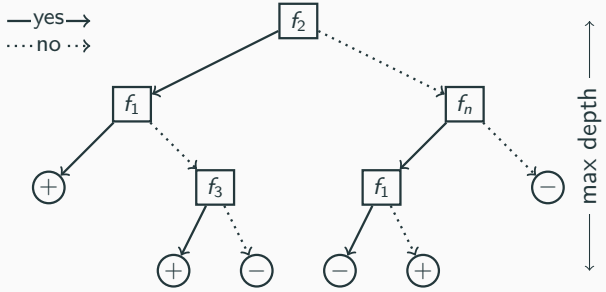
UCLouvain

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	$+$

UCLouvain

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	−
⋮	⋮	⋮	⋱	⋮	⋮
1	1	1	...	1	+



$$\min \sum (pred(i) - c(i))$$

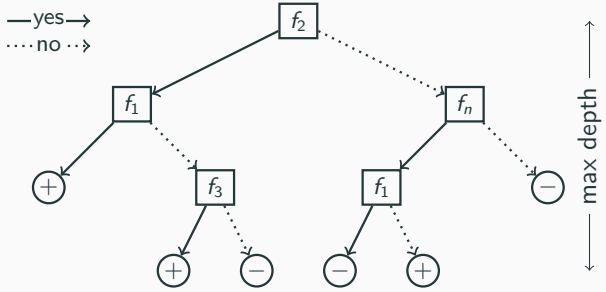
UCLouvain

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	−
⋮	⋮	⋮	⋱	⋮	⋮
1	1	1	...	1	+

New sample

0	0	1	...	0	?



$$\min \sum (pred(i) - c(i))$$

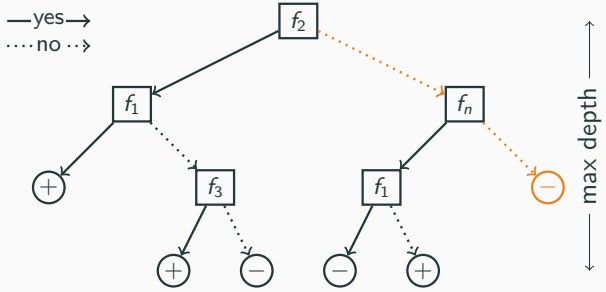
UCLouvain

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	−
⋮	⋮	⋮	⋱	⋮	⋮
1	1	1	...	1	+

New sample

0	0	1	...	0	−



$$\min \sum (pred(i) - c(i))$$

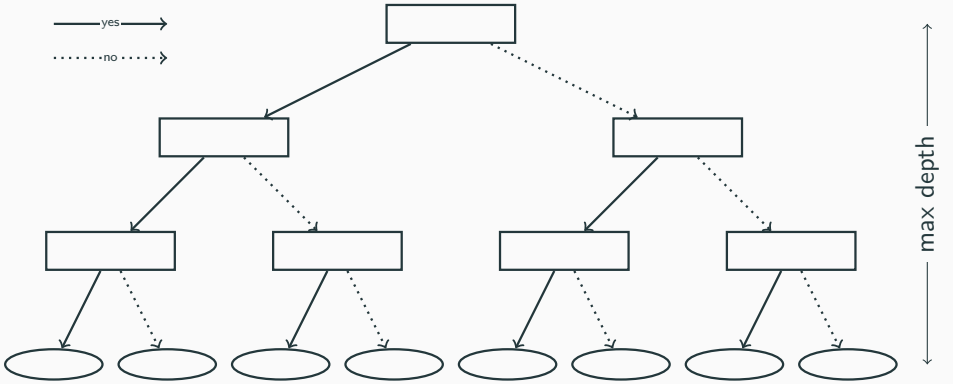
Greedy methods:

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

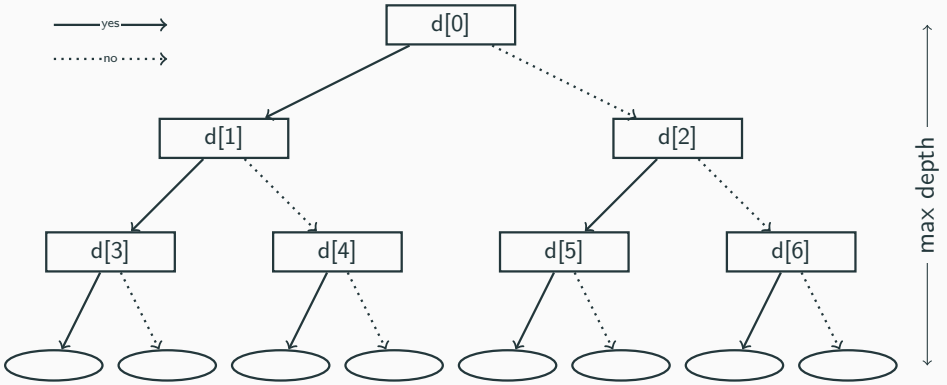
- Mining optimal decision trees from itemset lattices, Nijssen, S., Fromont, E., 2007
- Minimising decision tree size as combinatorial optimisation, Bessiere, C., Hebrard, E., O'Sullivan, B., 2009
- Optimal constraint-based decision tree induction from itemset lattices,Nijssen, S., Fromont, É., 2010
- **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

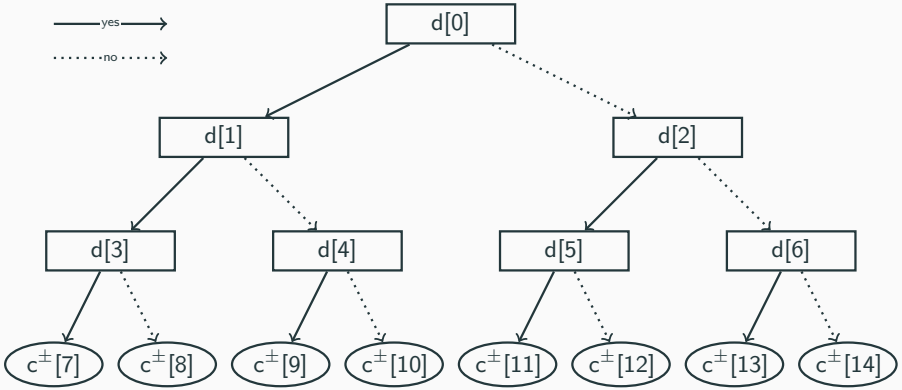
Model - Decision variables



Model - Decision variables

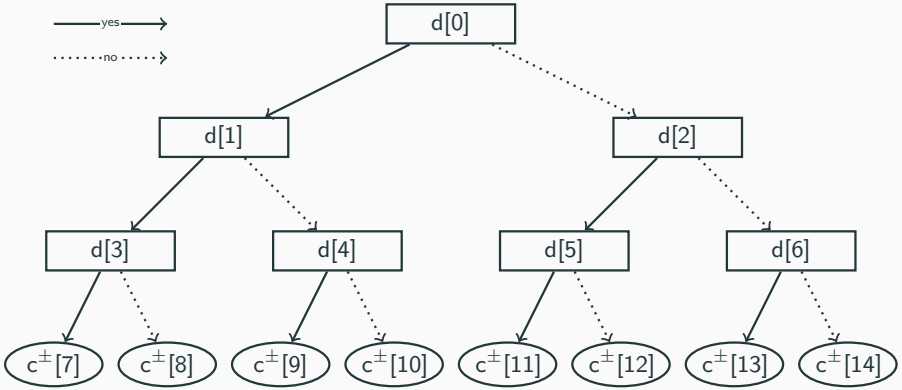


$dom(d[i]) = \{1, ..., n\}$



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

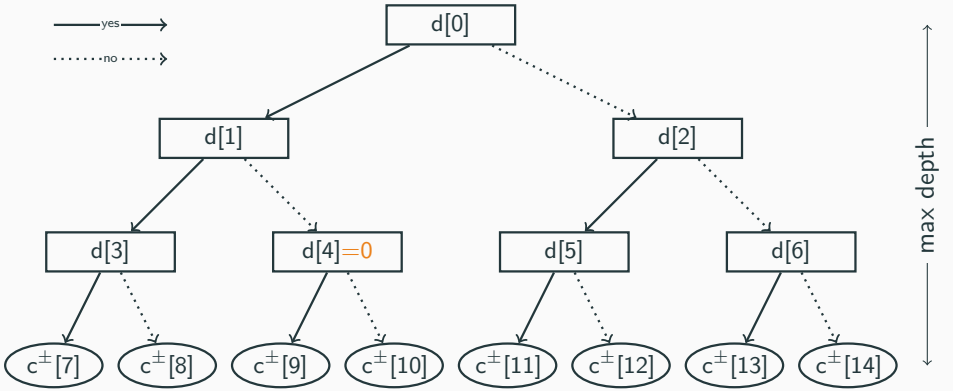
$dom(c[i]) = \{0, ..., N\}$



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

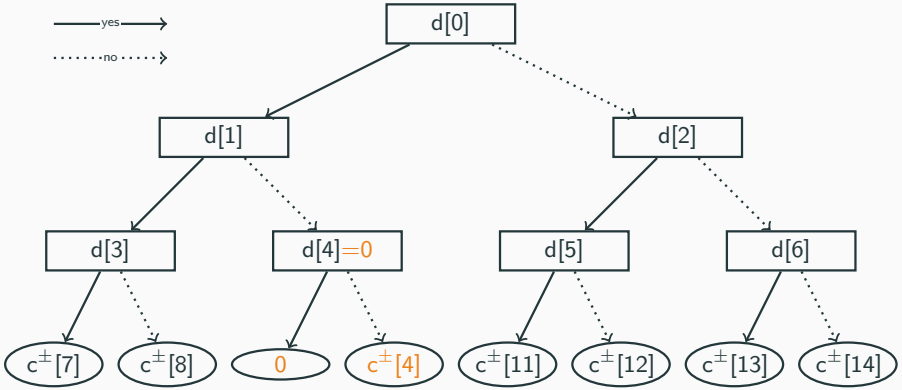
$dom(c[i]) = \{0, ..., N\}$

Model - Unbalanced Tree



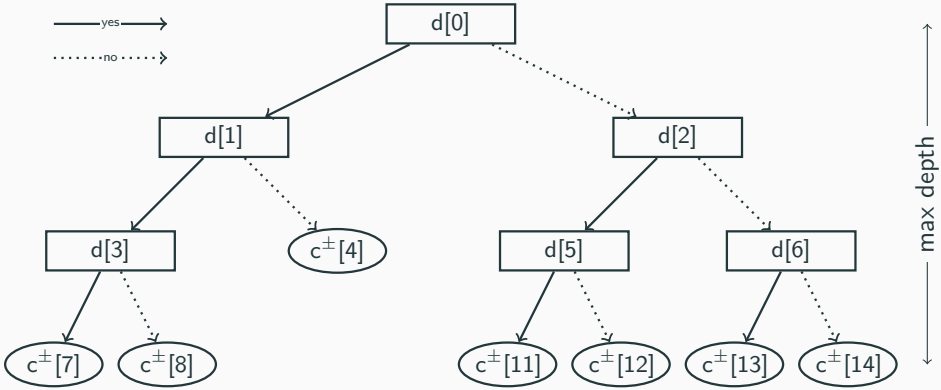
$dom(d[i]) = \{0, 1, ..., n\}$

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



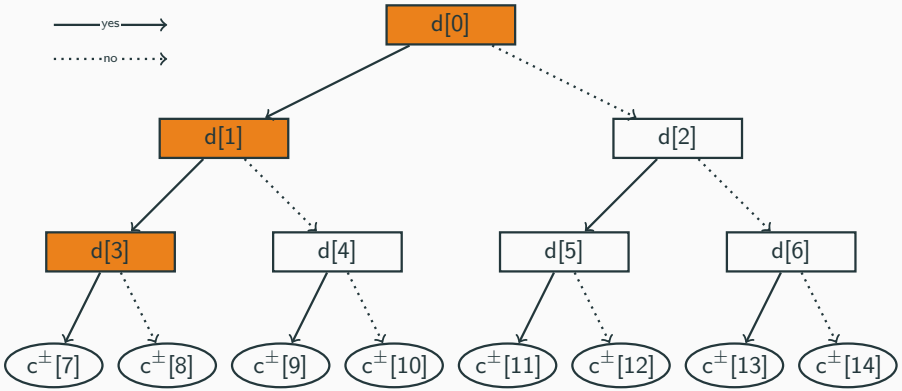
$dom(d[i]) = \{0, 1, ..., n\}$

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



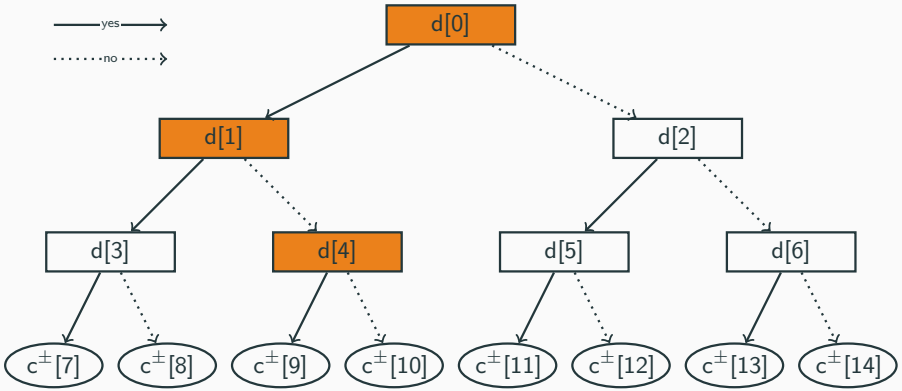
$dom(d[i]) = \{0, 1, ..., n\}$

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



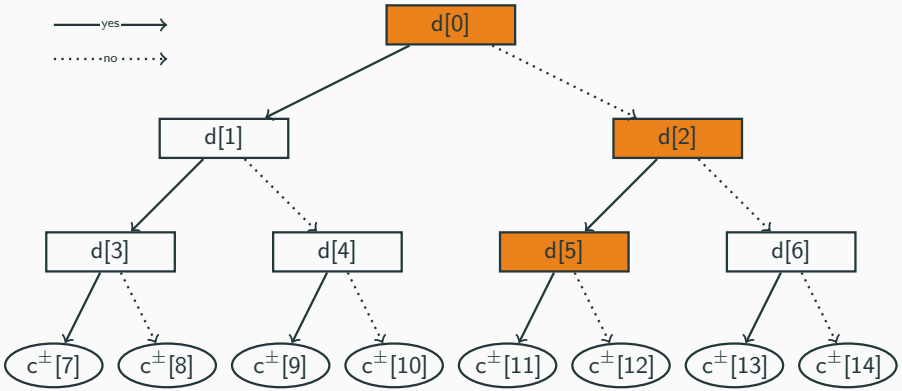
$dom(d[i]) = \{0, 1, ..., n\}$

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



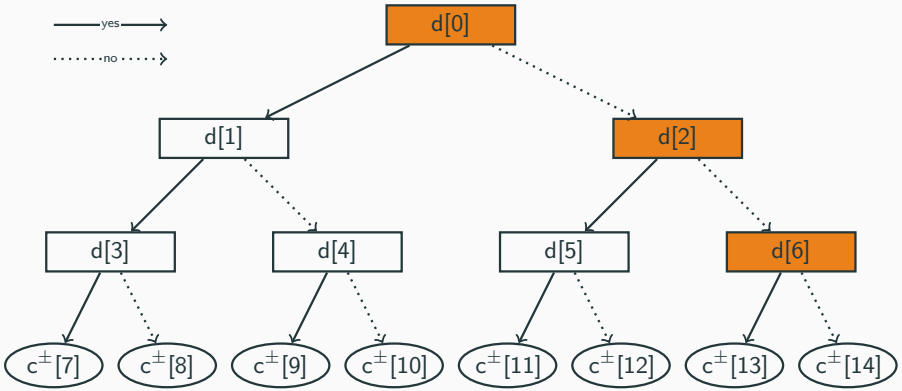
$dom(d[i]) = \{0, 1, ..., n\}$

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



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

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



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

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

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

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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

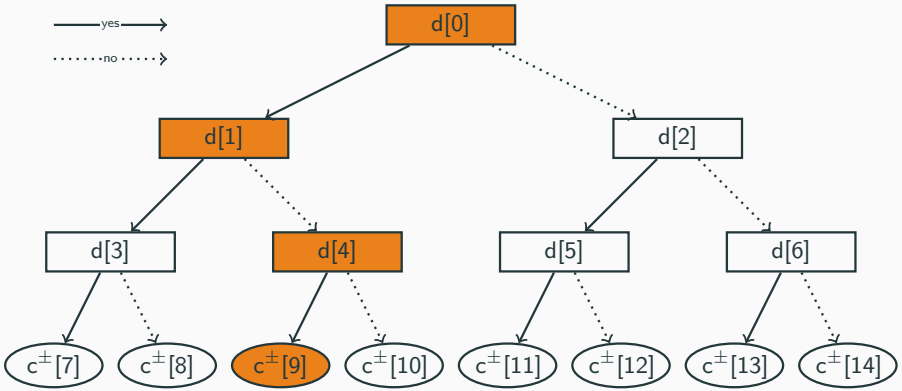
- ~~Dense representation~~
- No feature rejection

UCLouvain

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~~



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

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

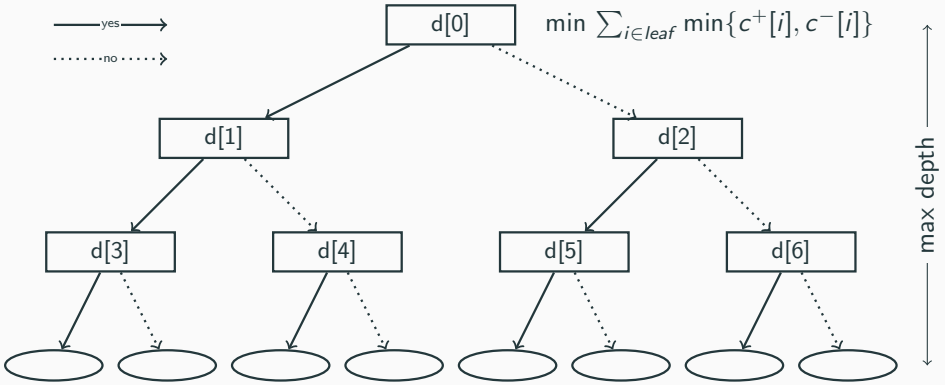
UCLouvain

- constraints imposing minimum at leaf

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

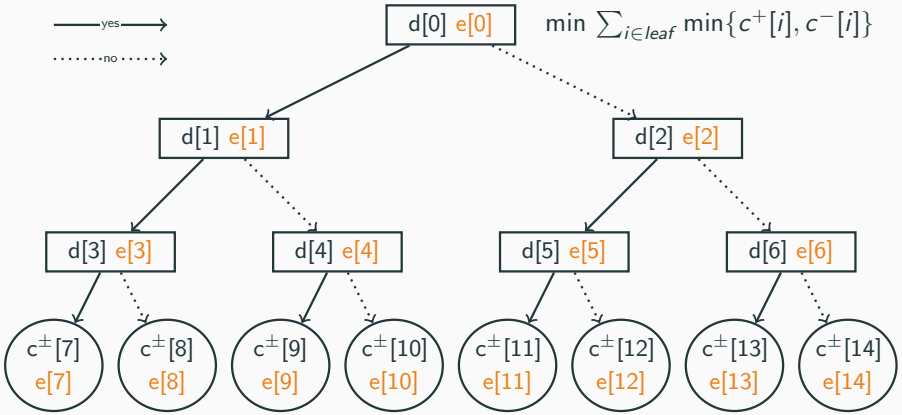
- constraints avoiding useless decisions

- redundant constraints improving speed

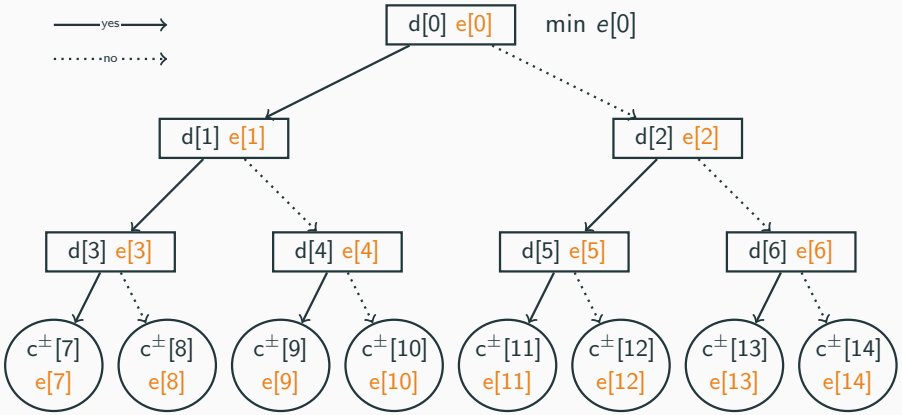


$dom(d[i]) = \{0, 1, ..., n\}$

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



$dom(d[i]) = \{0, 1, ..., n\}$ $dom(c[i]) = \{0, ..., N\}$ $dom(e[i]) = \{0, ..., N\}$



$dom(d[i]) = \{0, 1, ..., n\}$ $dom(c[i]) = \{0, ..., N\}$ $dom(e[i]) = \{0, ..., N\}$

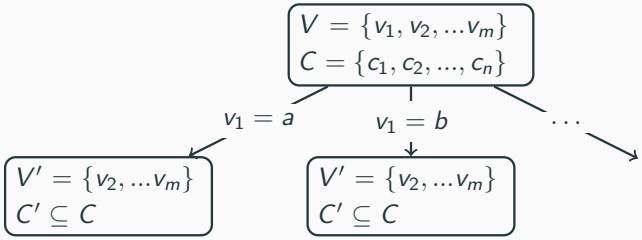
Search

UCLouvain

$V = \{v_1, v_2, ...v_m\}$
$C = \{c_1, c_2, ..., c_n\}$

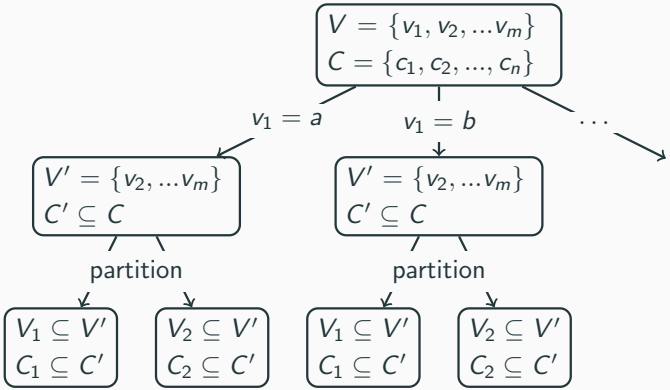
OR nodes

SOL = SOL_1 or SOL_2 or ...



OR nodes

SOL = SOL_1 or SOL_2 or ...

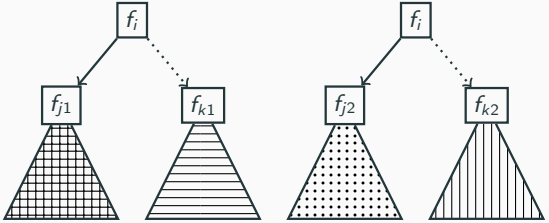


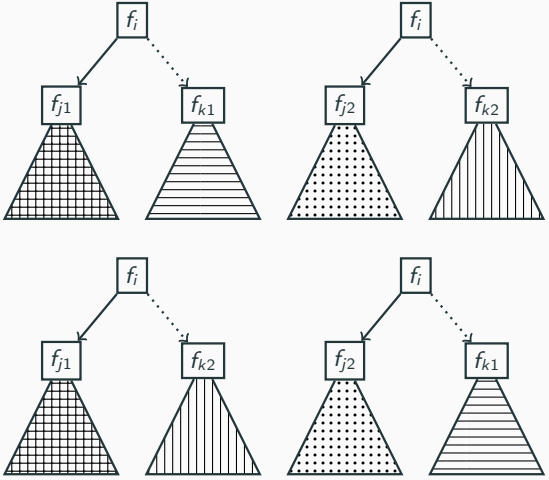
OR nodes

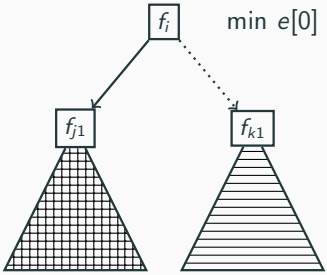
SOL = SOL_1 or SOL_2 or ...

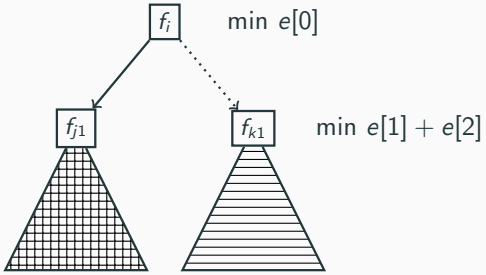
AND nodes

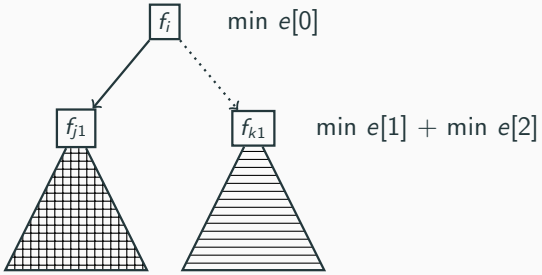
SOL = SOL_1 and SOL_2 and ...

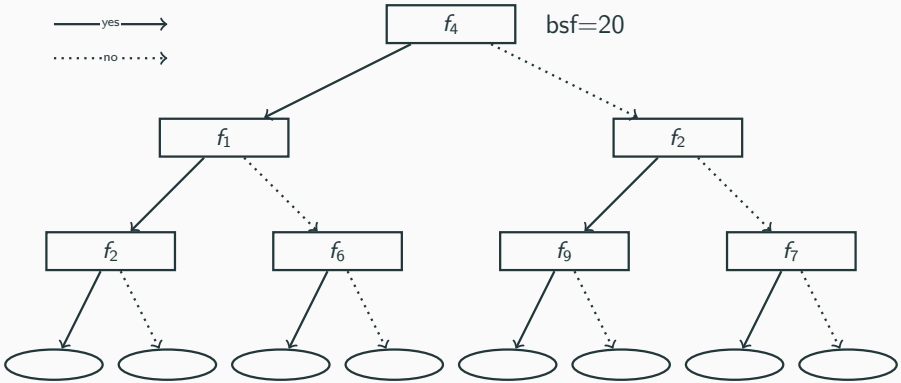

f_i
f_{j1}
f_{k1}
f_i
f_{j2}
f_{k2}

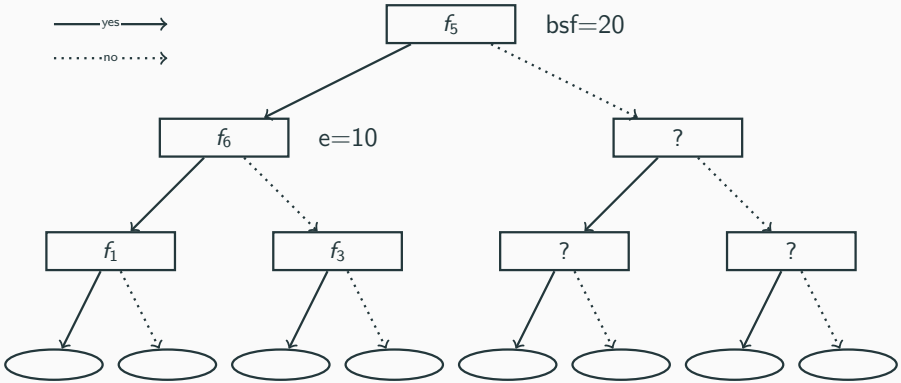

f_i
f_{j1}
f_{k1}
f_i
f_{j2}
f_{k2}
f_i
f_{j1}
f_{k2}
f_i
f_{j2}
f_{k1}

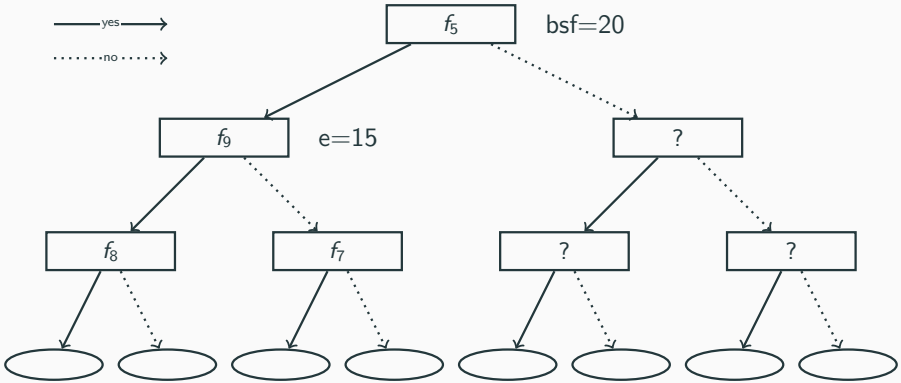

f_i
min $e[0]$
f_{j1}
f_{k1}

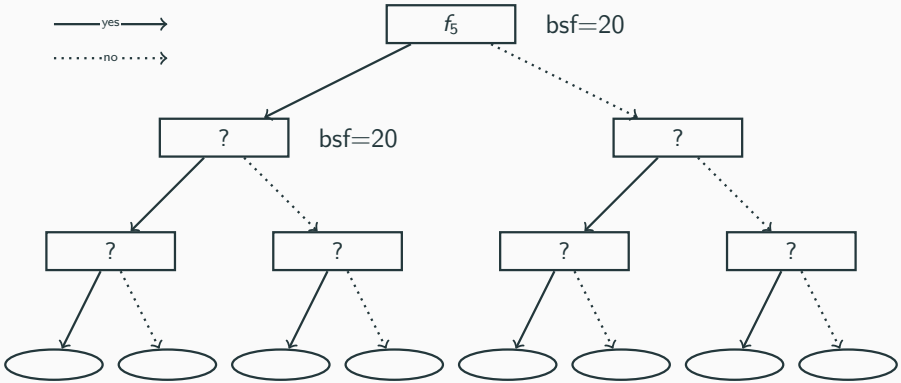

f_i
min $e[0]$
f_{j1}
f_{k1}
min $e[1] + e[2]$

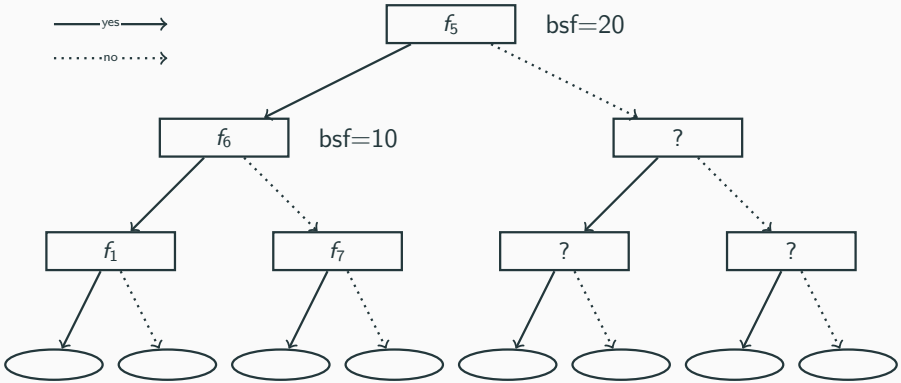

f_i
min $e[0]$
f_{j1}
f_{k1}
min $e[1]$ + min $e[2]$

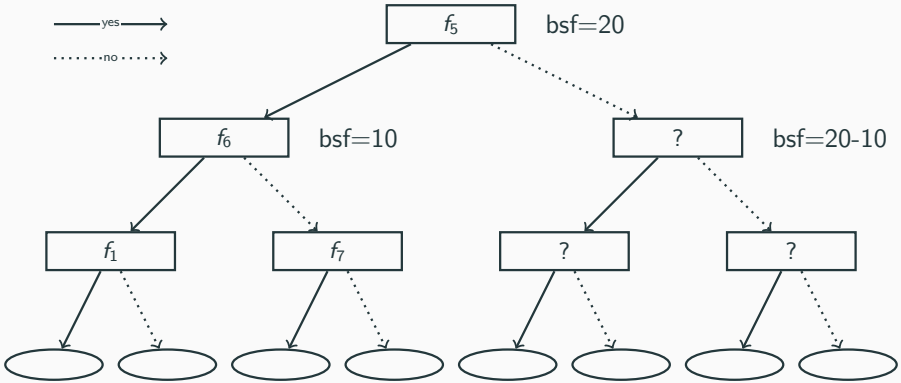

yes
no
f_4
bsf=20
f_1
f_2
f_2
f_6
f_9
f_7

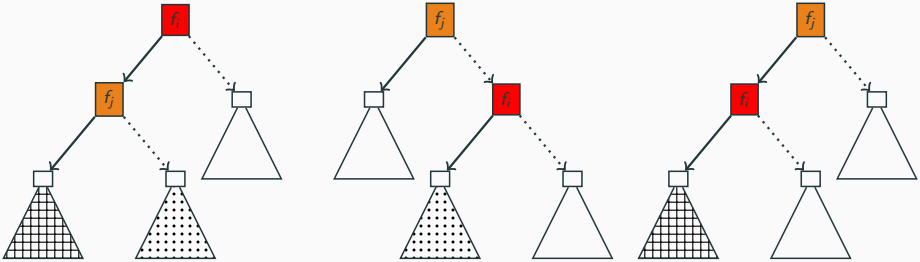

yes
no
f_5
bsf=20
f_6
e=10
?
f_1
f_3
?
?

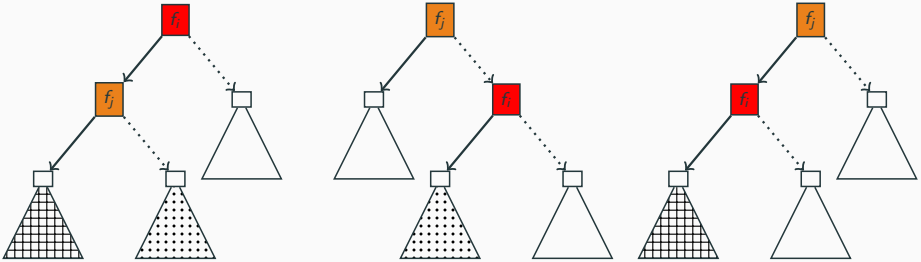

yes
no
f_5
bsf=20
f_9
e=15
?
f_8
f_7
?
?


yes
no
f_5
bsf=20
?
bsf=20
?
?
?
?
?


yes
no
f_5
bsf=20
f_6
bsf=10
?
f_1
f_7
?
?


yes
no
f_5
bsf=20
f_6
bsf=10
?
bsf=20-10
f_1
f_7
?
?


f_i
f_j
f_j
f_i
f_j
f_i



	yes	no	hash
	f_i f_j		$f_i, f_j -$
	f_i	f_j	$f_i - f_j$

Results

UCLouvain

	$N_{min} = 1$			$N_{min} = 5$			
	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

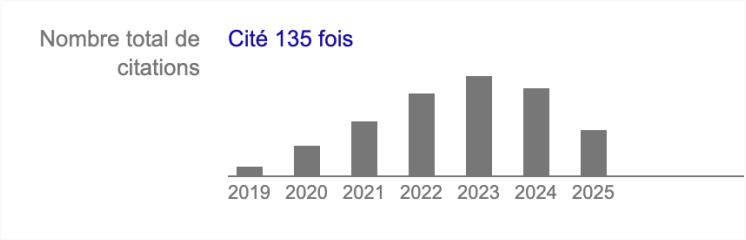
- efficient method
- cp based
- exploits the structure of the problem
- anytime best solution

To go further

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

And since...

And since...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2025

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

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

Gaël Aglin, Siegfried Nijssen, Pierre Schaus
firstname.lastname@uclouvain.be
ICTEAM, UCLouvain
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

- 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

MaxSat and integration in AdaBoost (IJCAI 2020)

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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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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 Submitted 5/20; Revised 10/21; Published 2/22

MurTree: Optimal Decision Trees via Dynamic Programming and Search

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DT-Slim with SAT and local encoding (JAIR 2024)

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Journal of Artificial Intelligence Research 80 (2024) 875-918 Submitted 01/2024; published 07/2024

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,

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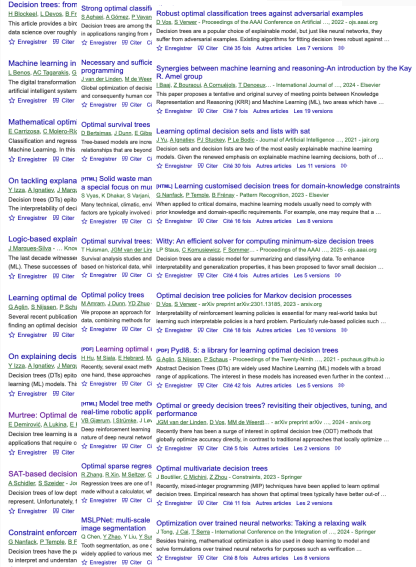

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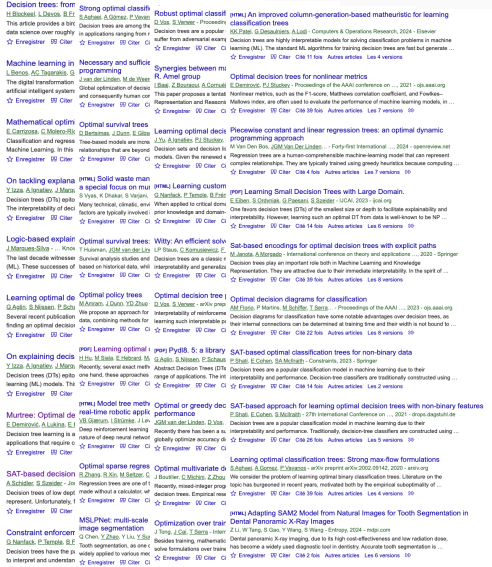

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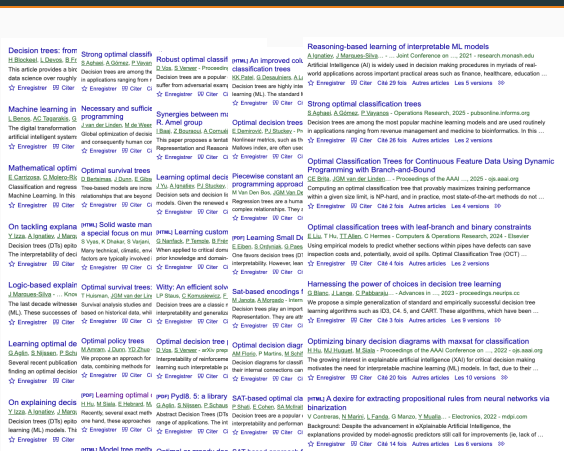

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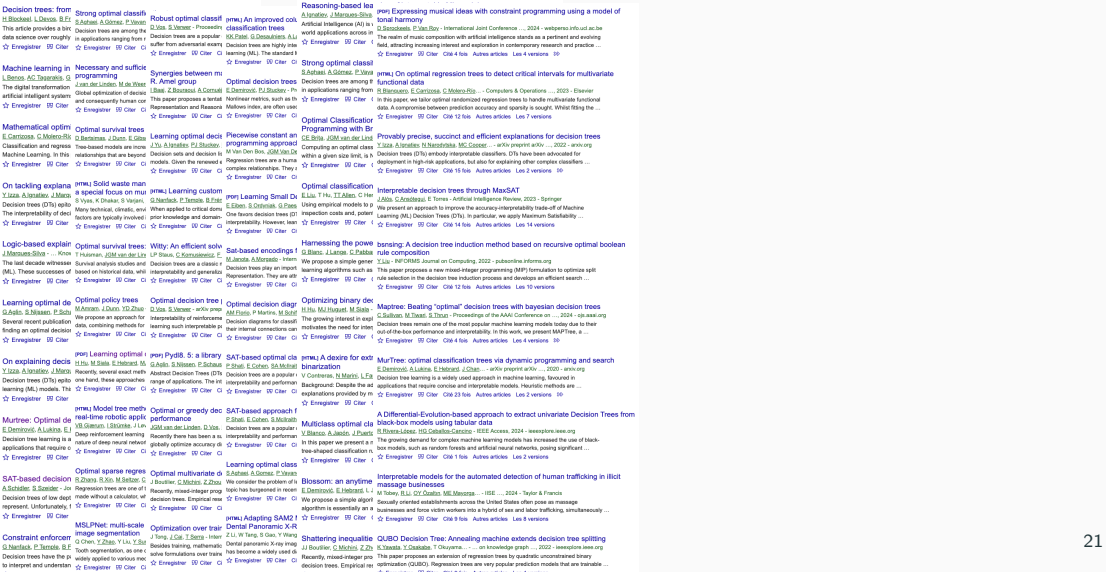

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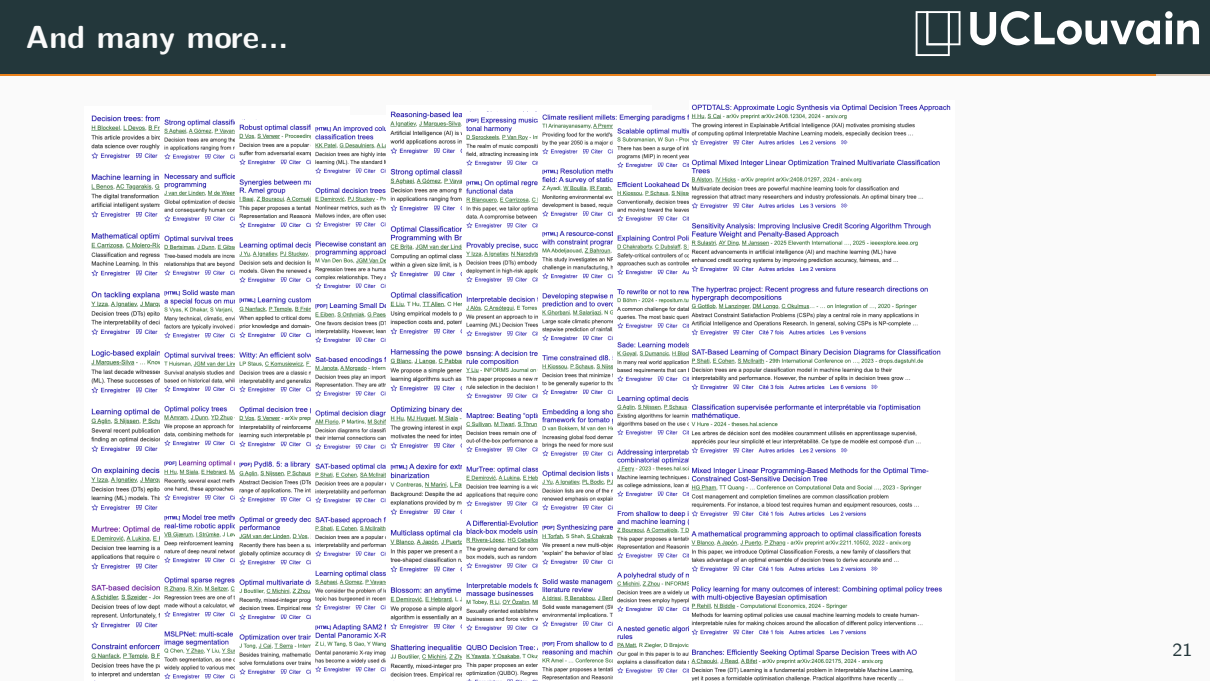

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Thank you for listening!

Any questions?

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