# LEARNING OPTIMAL DECISION TREES USING CONSTRAINT PROGRAMMING

BNAIC19

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[3] Université Laval, Québec, Canada, $claude-guy.quimper@ift.ulaval.ca$

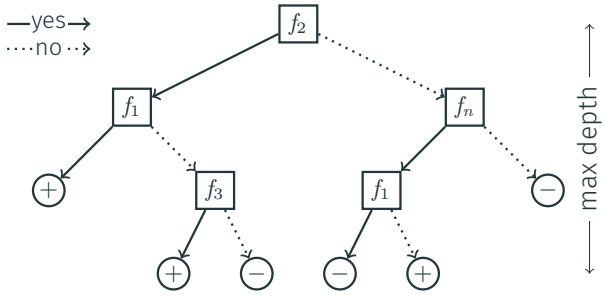
Database

| $f_1$ | $f_2$ | $f_3$ | $\dots$ | $f_n$ | $c$ |
|---|---|---|---|---|---|
| 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 | $+$ |

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 | + |




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

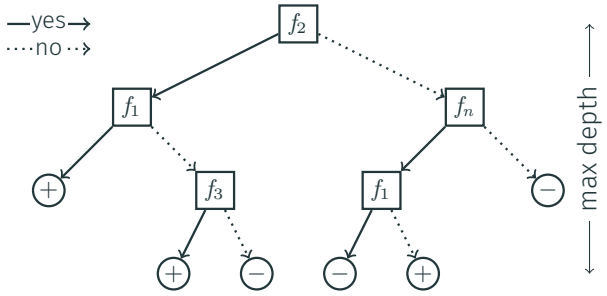
UCLouvain

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 | + |

New sample

| | | | | | |
|---|---|---|---|---|---|
| 0 | 0 | 1 | $\dots$ | 0 | ? |




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

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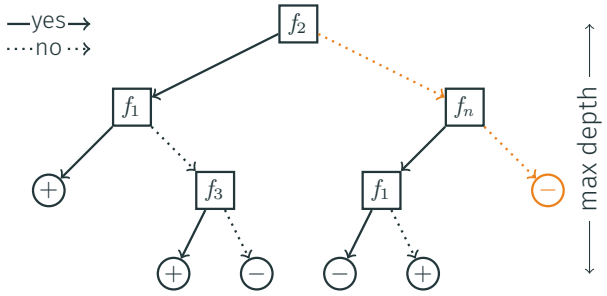
Database

| $f_1$ | $f_2$ | $f_3$ | $\dots$ | $f_n$ | $c$ |
|---|---|---|---|---|---|
| 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 | + |

New sample

| | | | | | |
|---|---|---|---|---|---|
| 0 | 0 | 1 | $\dots$ | 0 | − |



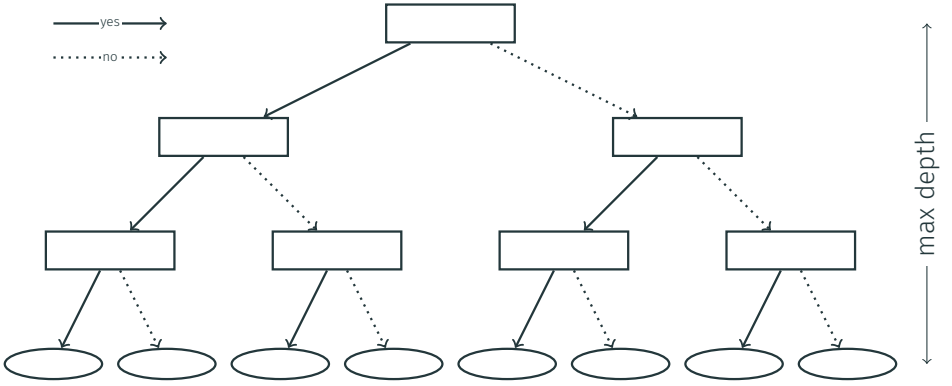

$$\min \sum (pred(i) - c(i))$$

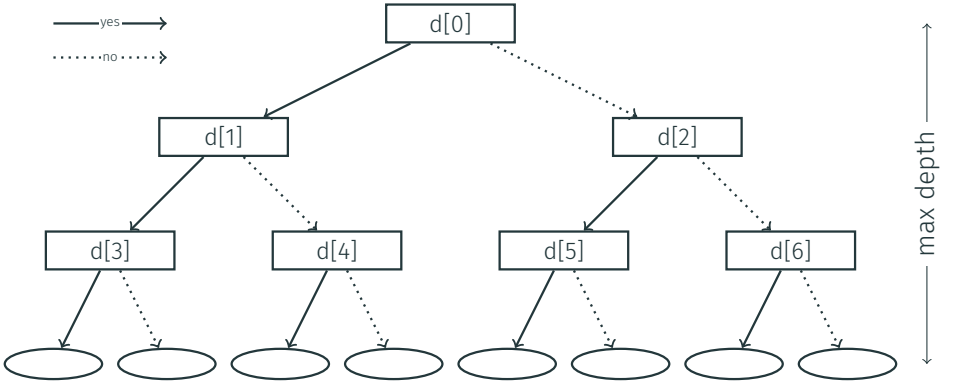
Greedy methods:

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

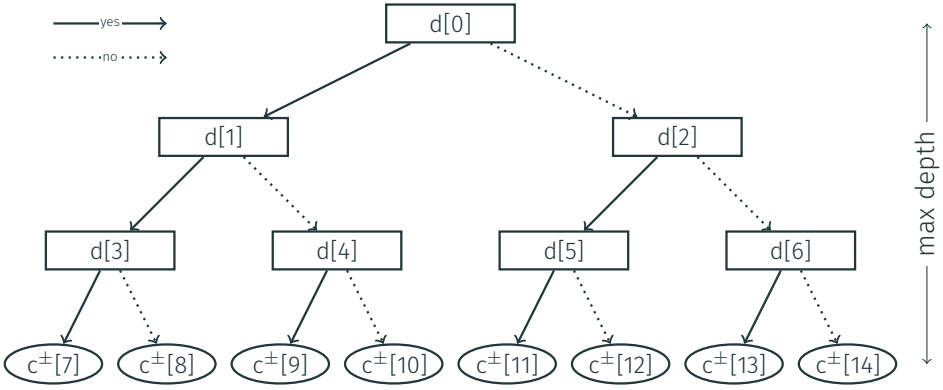
- Mining optimal decision trees from itemset lattices, Nijssen, S., Fromont, E., 2007
- Minimising decision tree size as combinatorial optimisation, Bessiere, C., Hebrard, E., O'Sullivan, B., 2009
- Optimal constraint-based decision tree induction from itemset lattices,Nijssen, S., Fromont, É., 2010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


yes
no
max depth

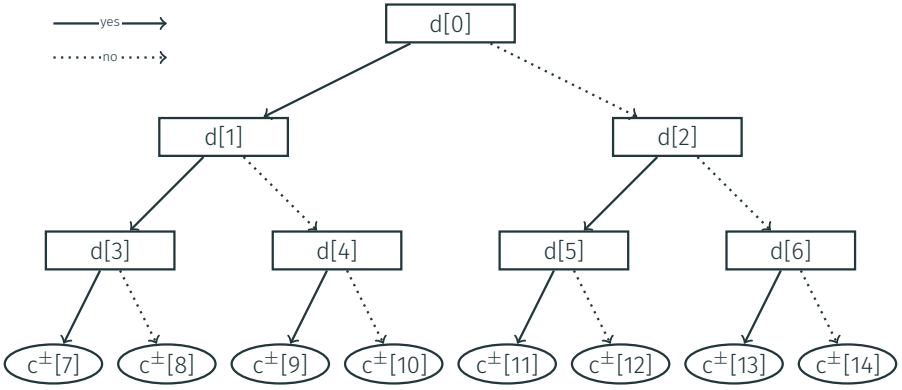



$$dom(d[i]) = \{1, ..., n\}$$



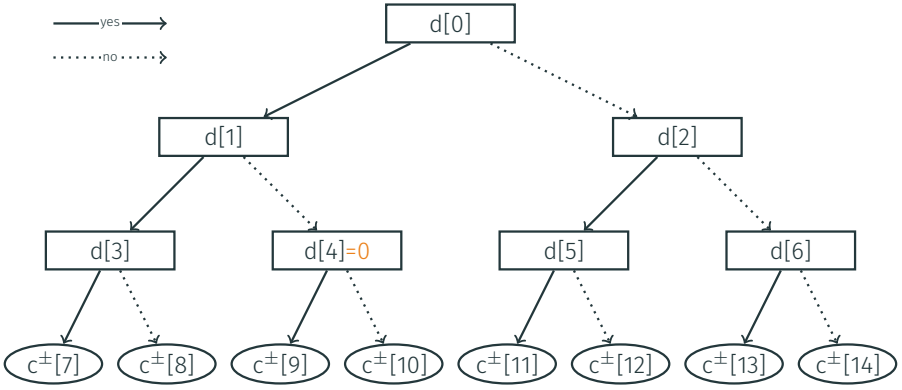

$dom(d[i]) = \{1, ..., n\}$

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



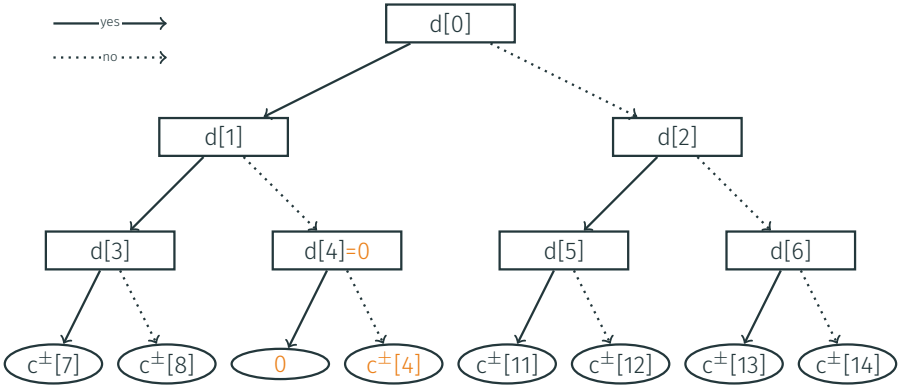

$dom(d[i]) = \{0, 1, ..., n\}$

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



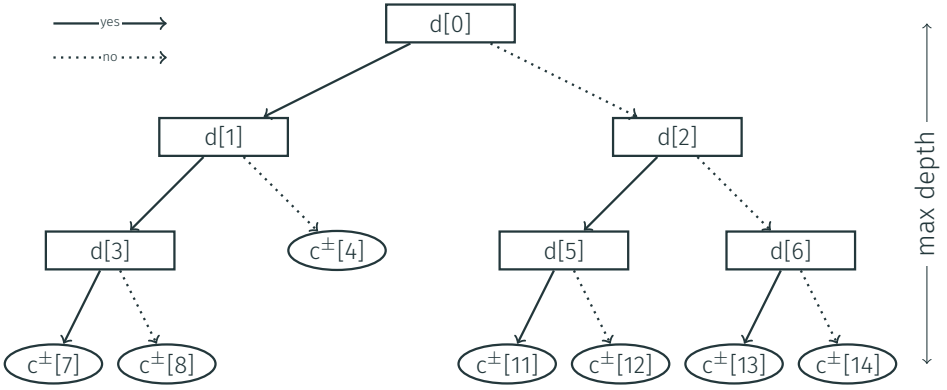

$dom(d[i]) = \{0, 1, ..., n\}$

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



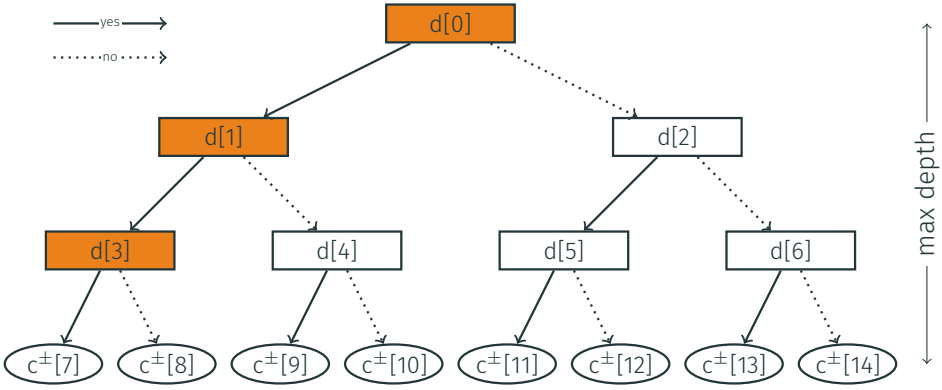

$dom(d[i]) = \{0, 1, ..., n\}$

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



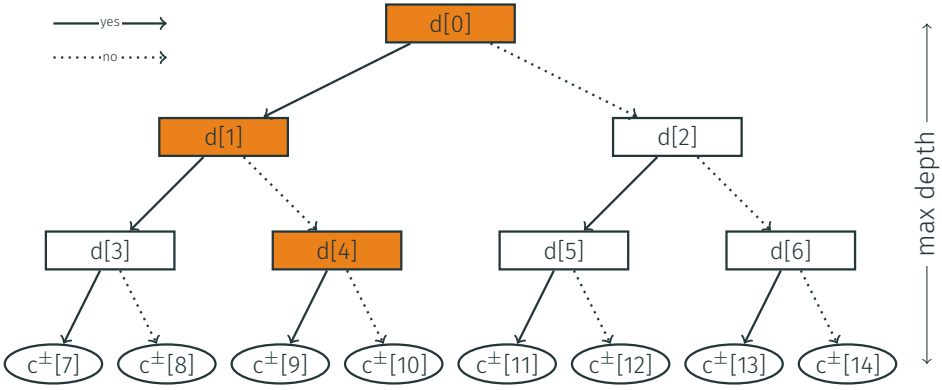

$dom(d[i]) = \{0, 1, ..., n\}$

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



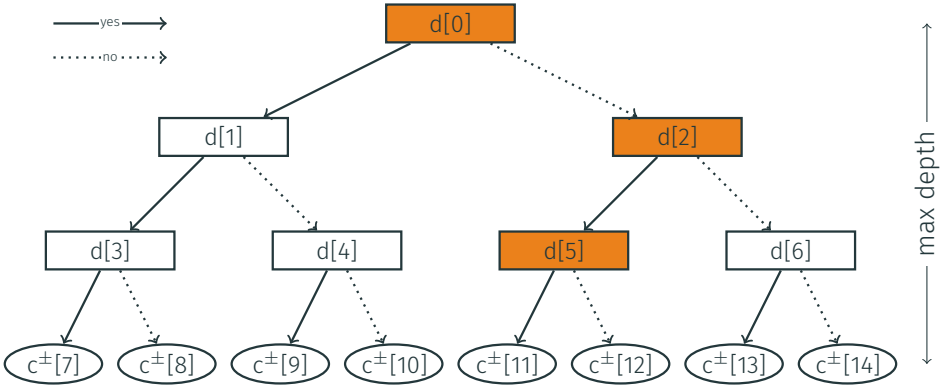

$dom(d[i]) = \{0, 1, ..., n\}$

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



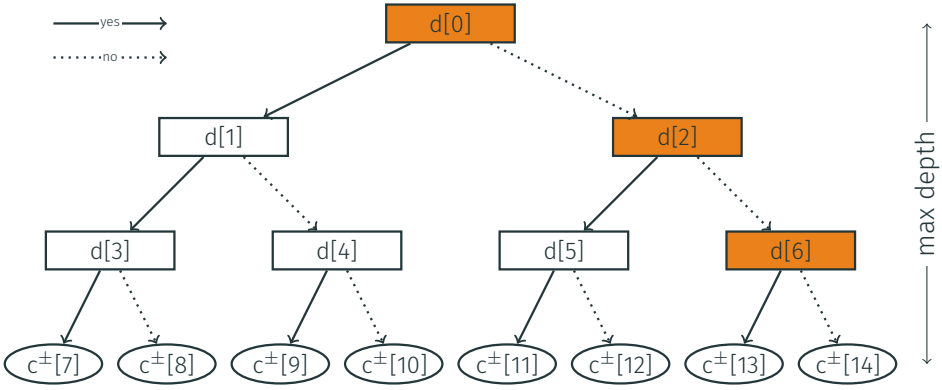

$dom(d[i]) = \{0, 1, ..., n\}$

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




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

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




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

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

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 (Dense) | | | | Counter |
|---|---|---|---|---|
| $x_1$ | $x_2$ | $x_3$ | $x_4$ | |
| | | | | |

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 (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 |

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 (Dense) | | | | Counter |
|---|---|---|---|---|
| $x_1$ | $x_2$ | $x_3$ | $x_4$ | |
| 0 | 1 | 0 | 1 | 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) | | Counter |
|---|---|---|
| $y_1$ | $y_2$ | |
| 2 | 4 | 3 |

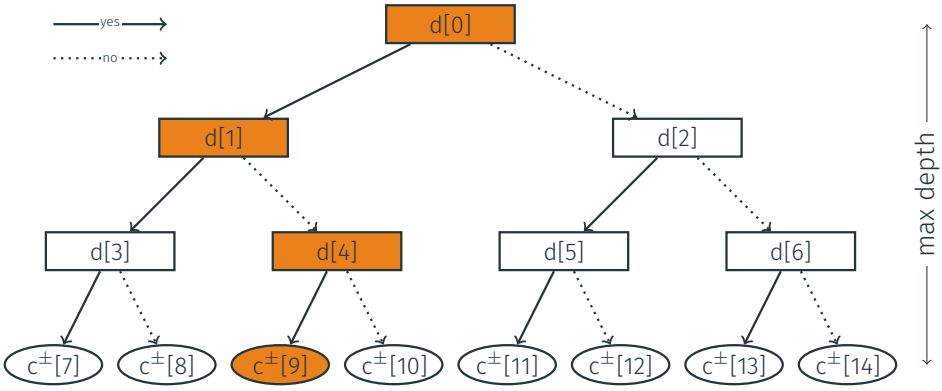
- ~~Dense representation~~
- No feature rejection

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~~




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

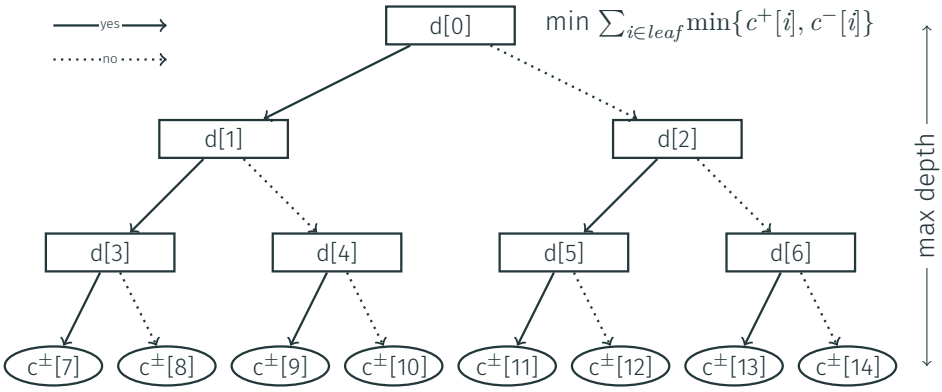
$Coversize(\{d[0], d[4]\}, \{d[1]\}, c^{-}[9])$

- constraints imposing minimum at leaf

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

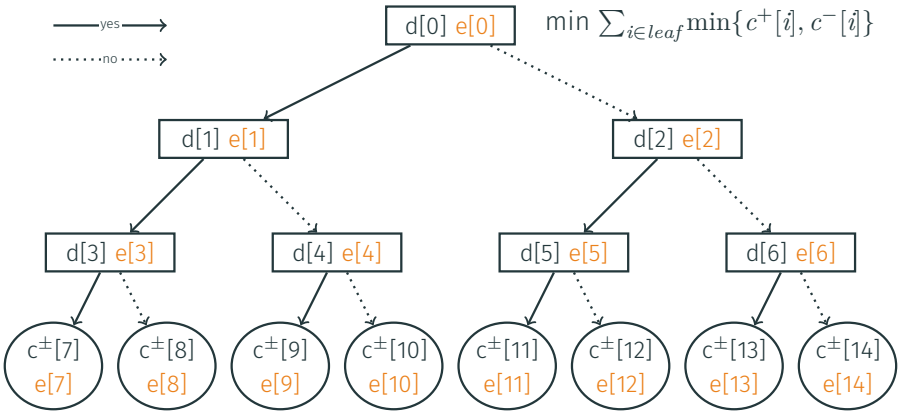
- constraints avoiding useless decisions


- redundant constraints improving speed

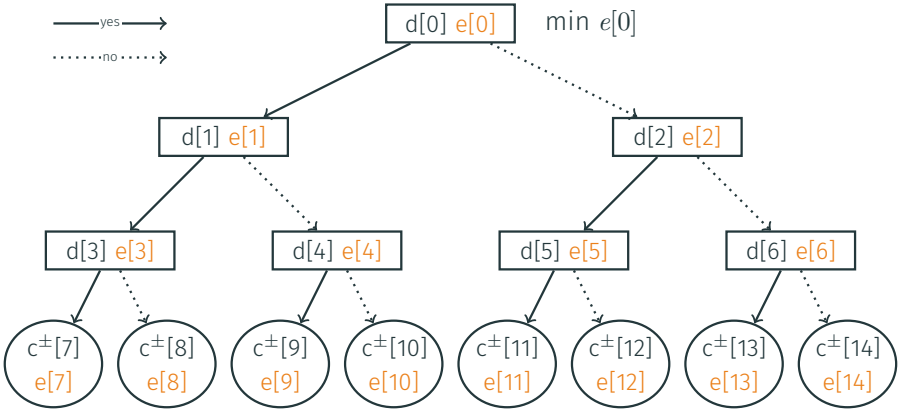



$dom(d[i]) = \{0, 1, ..., n\}$

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




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




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

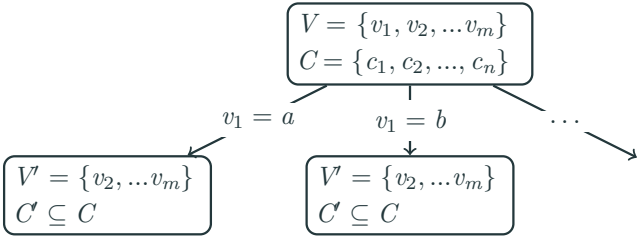
# SEARCH

UCLouvain

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

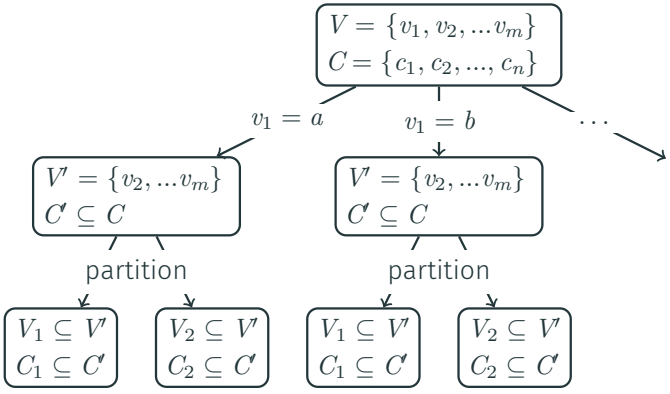
**OR nodes**

SOL = $SOL_1$ or $SOL_2$ or ...



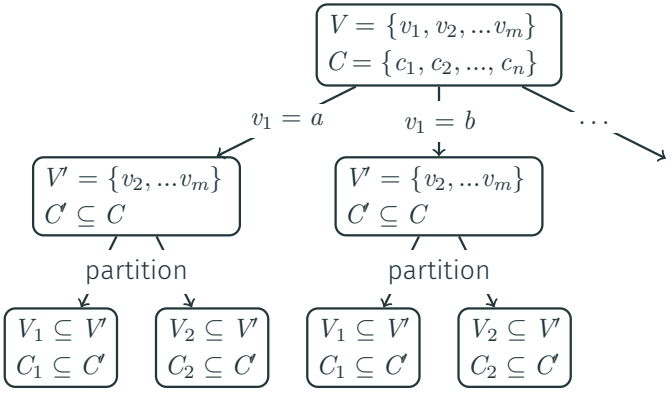

**OR nodes**

SOL = $SOL_1$ or $SOL_2$ or ...




**OR nodes**

SOL = $SOL_1$ or $SOL_2$ or ...

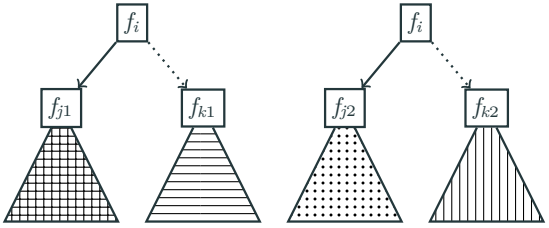


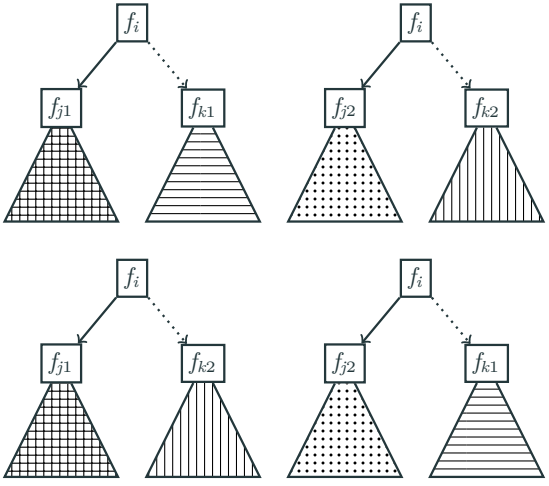

**OR nodes**

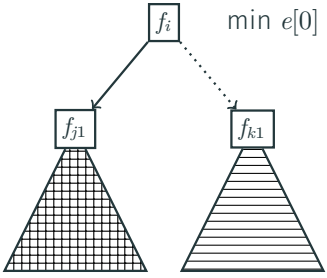
SOL = $SOL_1$ or $SOL_2$ or ...

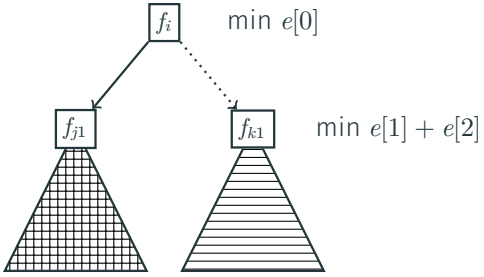
**AND nodes**

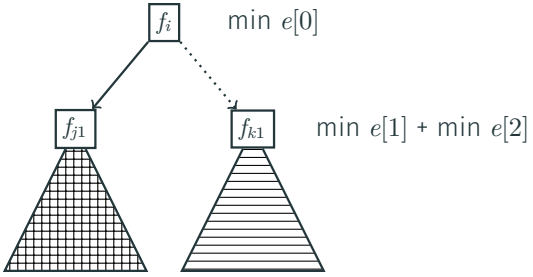
SOL = $SOL_1$ and $SOL_2$ and ...

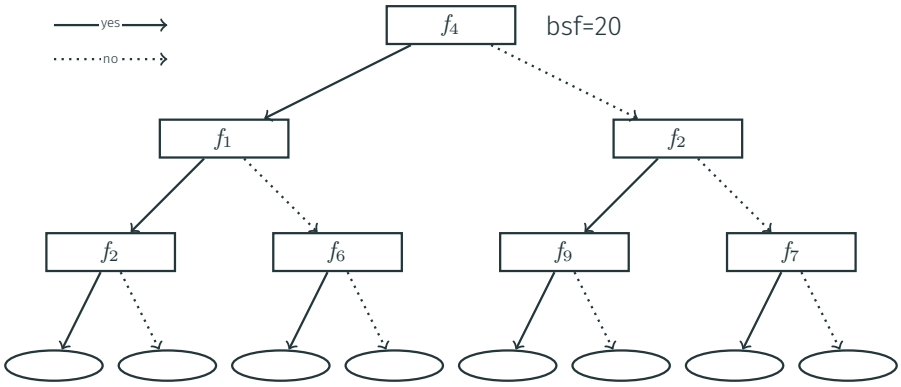

$f_i$
$f_{j1}$
$f_{k1}$
$f_i$
$f_{j2}$
$f_{k2}$


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


$f_i$
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 $e[2]$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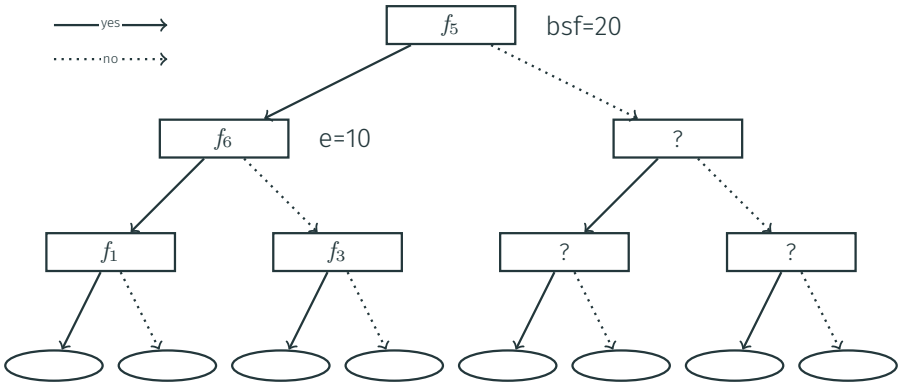
$f_7$


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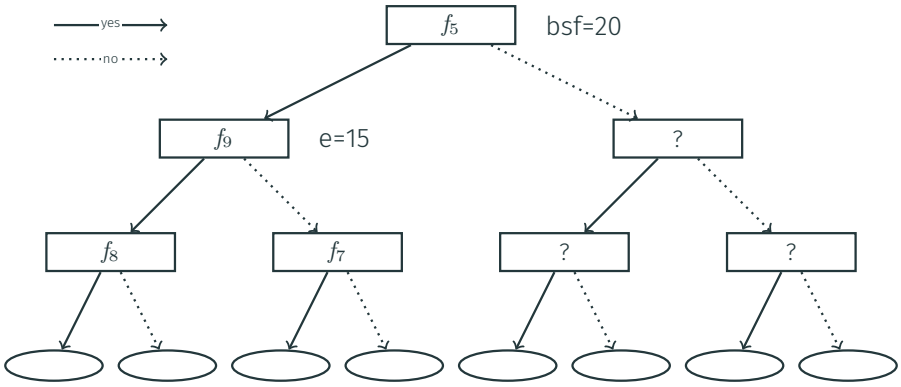
bsf=20
$f_6$
e=10
?
$f_1$
$f_3$
?
?


yes
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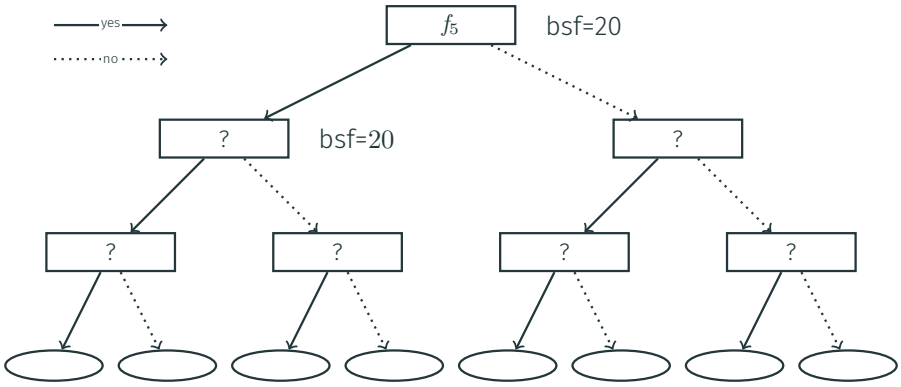
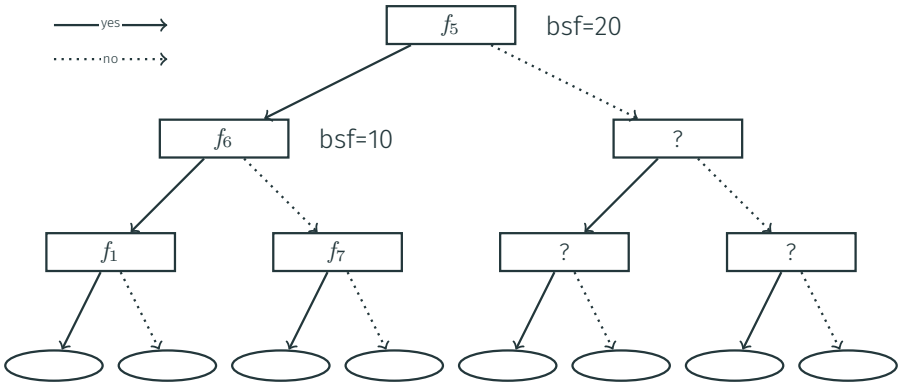
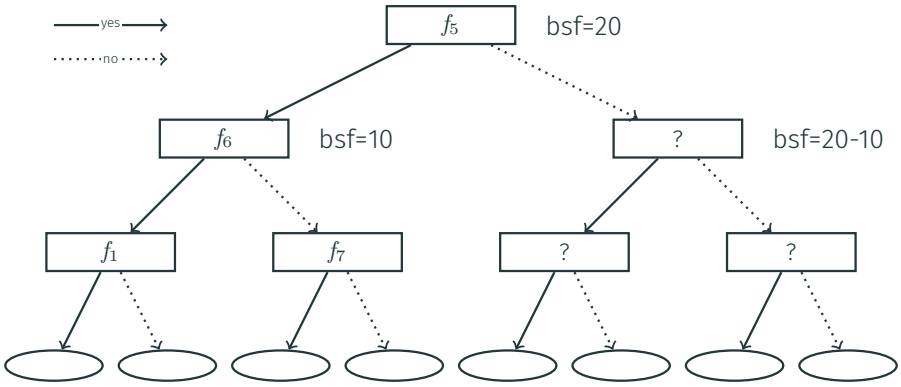
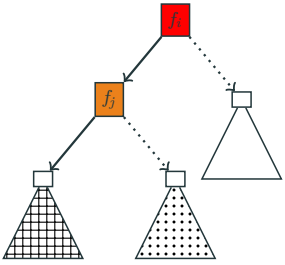
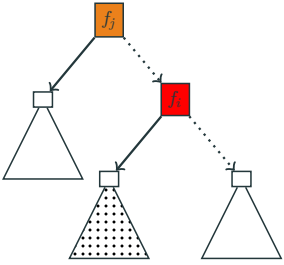
$f_5$
bsf=20
$f_9$
e=15
?
$f_8$
$f_7$
?
?

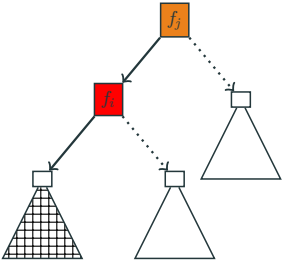

yes
no
$f_5$
bsf=20
?
bsf=20
?
?
?
?
?

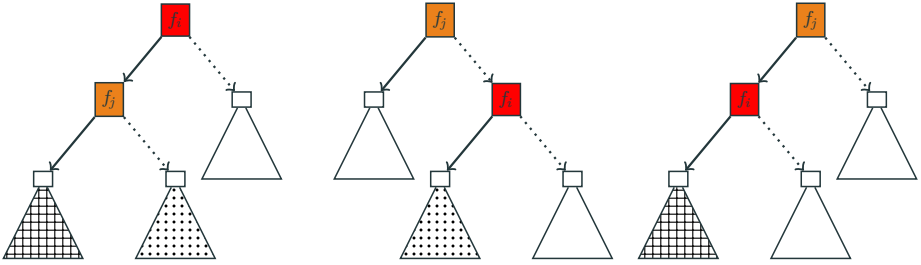

yes
no
$f_5$
bsf=20
$f_6$
bsf=10
?
$f_1$
$f_7$
?
?


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

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| | $N_{\min} = 1$ | | | $N_{\min} = 5$ | | | |
|---|---|---|---|---|---|---|---|
| | DL8 | BinOCT | CP | DL8 | CP | CP-c | CP-m |
| Proven optimality | 49(64%) | 13(17%) | **57**(75%) | 54(71%) | 56(74%) | 56(74%) | **58**(76%) |
| Best solution found | 49(64%) | 21(28%) | **76**(100%) | 54(71%) | **74**(97%) | **74**(97%) | 70(92%) |
| Fastest | 23(30%) | 11(14%) | **49**(64%) | 28(37%) | **40**(53%) | 33(43%) | 22(29%) |
| Time out | 27(36%) | 63(83%) | **19**(25%) | 22(29%) | 21(28%) | 21(28%) | **19**(25%) |

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

UCLouvain

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
- ...

Thank you for listening!

Any questions?