Exact Combinatorial Optimization with Graph Convolutional Neural Networks

Maxime Gasse, Didier Chételat, Nicola Ferroni, Laurent Charlin, Andrea Lodi

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GERAD GROUPE D'ÉTUDES ET DE RECHERCHE EN ANALYSE DES DÉCISIONS
DATA SCIENCE FOR REAL-TIME DECISION-MAKING
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Overview

The Branching Problem

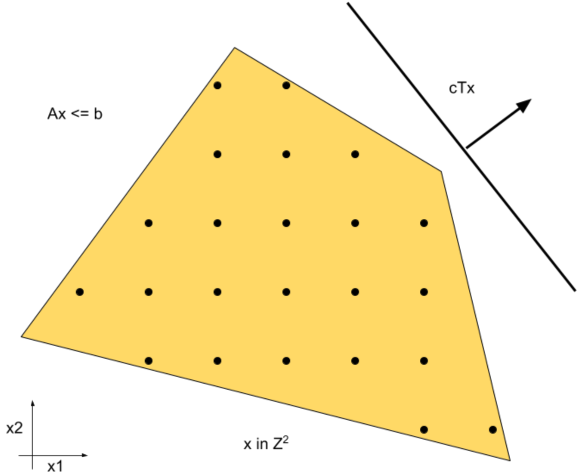
Mixed-Integer Linear Program (MILP)

$$\begin{aligned} \arg\min_{\mathbf{x}} \quad & \mathbf{c}^\top \mathbf{x} \\ \text{subject to} \quad & \mathbf{A}\mathbf{x} \leq \mathbf{b}, \\ & \mathbf{l} \leq \mathbf{x} \leq \mathbf{u}, \\ & \mathbf{x} \in \mathbb{Z}^p \times \mathbb{R}^{n-p}. \end{aligned}$$

- $\mathbf{c} \in \mathbb{R}^n$ the objective coefficients
- $\mathbf{A} \in \mathbb{R}^{m \times n}$ the constraint coefficient matrix
- $\mathbf{b} \in \mathbb{R}^m$ the constraint right-hand-sides
- $\mathbf{l}, \mathbf{u} \in \mathbb{R}^n$ the lower and upper variable bounds
- $p \leq n$ integer variables

NP-hard problem.

Mixed-Integer Linear Program (MILP)



Linear Program (LP) relaxation

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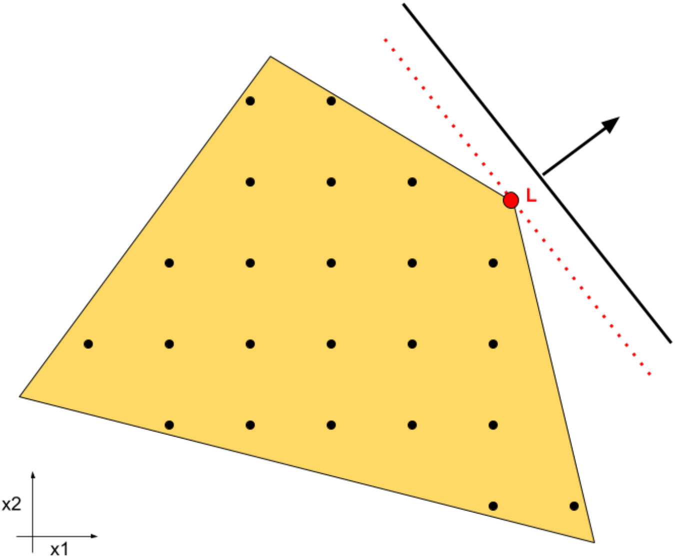
& \mathbf{x} \in \mathbb{R}^n.
\end{aligned}
$$

Convex problem, efficient algorithms (e.g., simplex).

- $\mathbf{x}^\star \in \mathbb{Z}^p \times \mathbb{R}^{n-p}$ (lucky) $\rightarrow$ solution to the original MILP
- $\mathbf{x}^\star \notin \mathbb{Z}^p \times \mathbb{R}^{n-p}$ $\rightarrow$ lower bound to the original MILP

Linear Program (LP) relaxation



Branch-and-Bound

Split the LP recursively over a non-integral variable, i.e. $\exists i \leq p \mid x_i^\star \notin \mathbb{Z}$

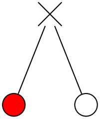
$$x_i \leq \lfloor x_i^\star \rfloor \quad \vee \quad x_i \geq \lceil x_i^\star \rceil .$$

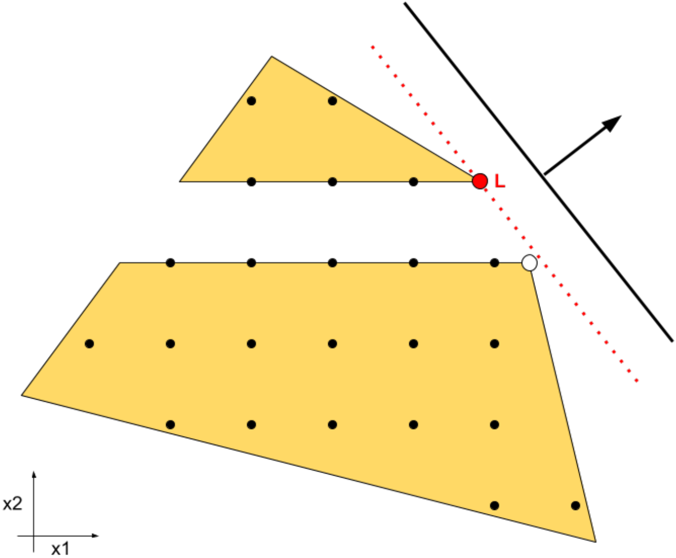
Lower bound (L): minimal among leaf nodes.
Upper bound (U): minimal among leaf nodes with integral solution.

Stopping criterion:

- L = U (optimality certificate)
- L = ∞ (infeasibility certificate)
- L - U < threshold (early stopping)

Branch-and-Bound





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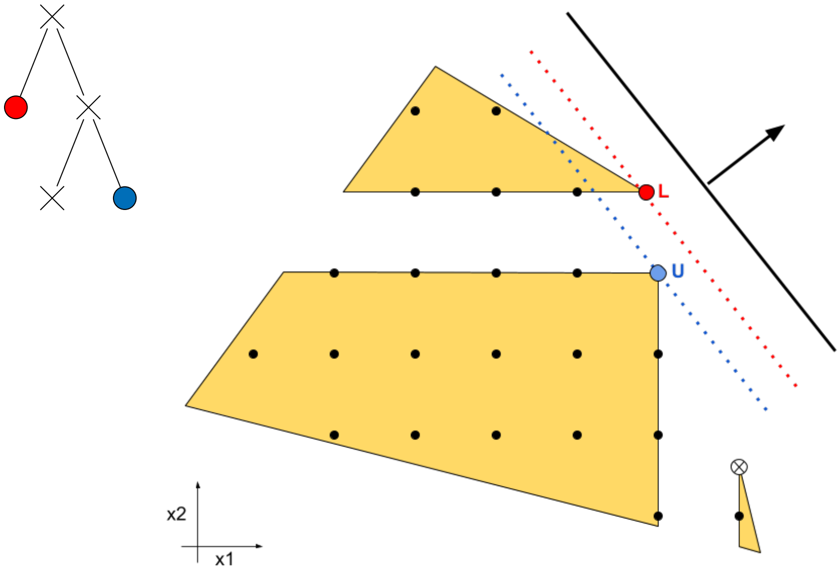

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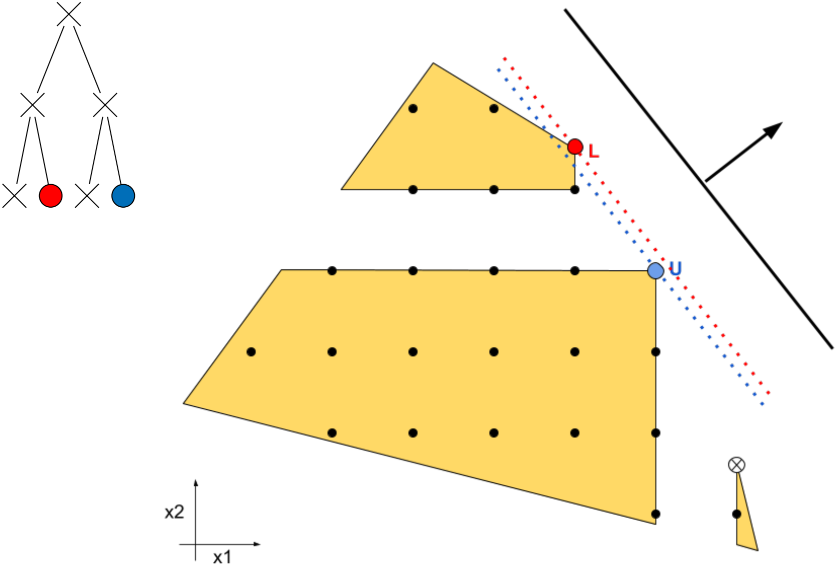

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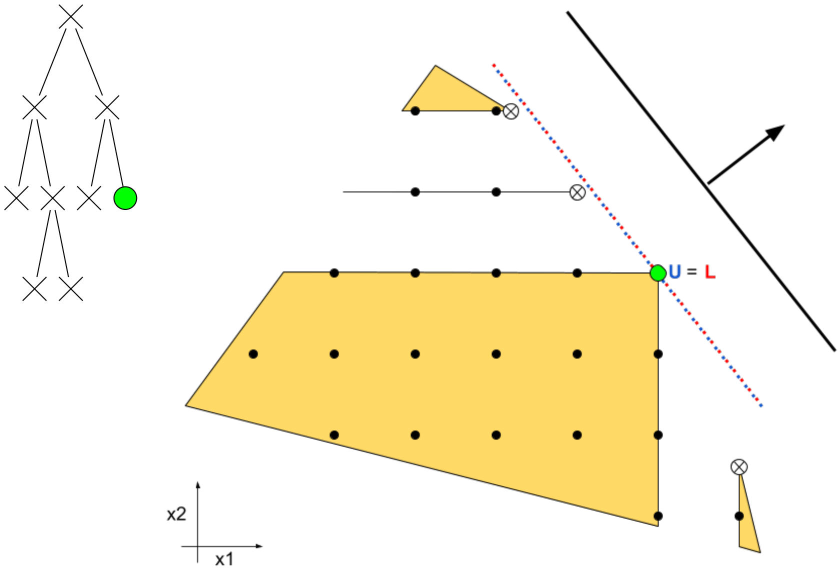
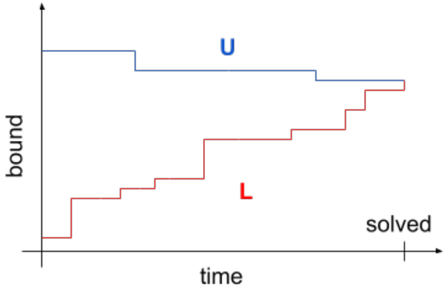


Branch-and-bound: a sequential process

Sequential decisions:

- variable selection (branching)
- node selection
- *cutting plane selection*
- *primal heuristic selection*
- *simplex initialization*
- ...



State-of-the-art in B&B solvers: expert rules

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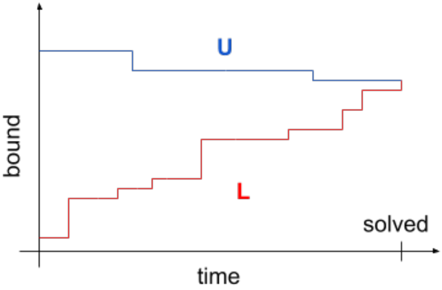

State-of-the-art in B&B solvers: expert rules

Objective: no clear consensus

- L = U fast ?
- U - L ↘ fast ?
- L ↗ fast ?
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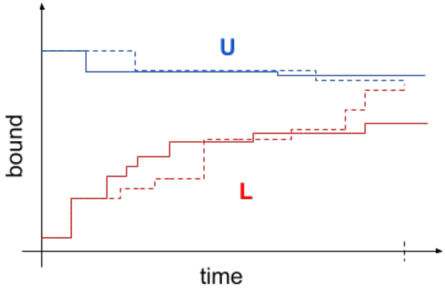

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State-of-the-art in B&B solvers: expert rules

Expert branching rules: state-of-the-art

Strong branching: one-step forward looking (greedy)

- solve both LPs for each candidate variable
- pick the variable resulting in tightest relaxation
- \+ small trees
- − computationally expensive

Pseudo-cost: backward looking

- keep track of tightenings in past branchings
- pick the most promising variable
- \+ very fast, almost no computations
- − cold start

Reliability pseudo-cost: best of both worlds

- compute SB scores at the beginning
- gradually switches to pseudo-cost (+ other heuristics)
- \+ best overall solving time trade-off (on MIPLIB)

Markov Decision Process

Objective: take actions which maximize the long-term reward

$$\sum_{t=0}^{\infty} r(\mathbf{s}_t),$$

with $r : \mathcal{S} \to \mathbb{R}$ a reward function.

Branching as a Markov Decision Process

State: the whole internal state of the solver, $\mathbf{s}$.

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$$\mathbf{s}_{t+1} \sim p_\pi(\mathbf{s}_{t+1}|\mathbf{s}_t) = \sum_{a \in \mathcal{A}} \underbrace{\pi(a|\mathbf{s}_t)}_{\text{branching policy}} \underbrace{p(\mathbf{s}_{t+1}|\mathbf{s}_t, a)}_{\text{solver internals}}.$$

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Branching problem: solve

$$\pi^\star = \arg\max_\pi \mathop{\mathbb{E}}_{\tau \sim p_\pi} [r(\tau)],$$

with $r(\tau) = \sum_{\mathbf{s} \in \tau} r(\mathbf{s})$.

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A policy $\pi^\star$ may not be optimal in two distinct configurations.

Challenges

MDP $\implies$ Reinforcement learning (RL) ?

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State representation: $\mathbf{s}$

- global level: original MILP, tree, bounds, focused node...
- node level: variable bounds, LP solution, simplex statistics...

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- – variable-size instances (cols, rows) $\implies$ Graph Neural Network

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- collect one τ = solving a MILP (with π likely not optimal)
- expensive $\Longrightarrow$ train on small instances

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Reward function: r

- no consensus
- \+ a strong expert exists $\implies$ imitation learning

Machine learning approaches

Node selection

- He et al., 2014
- Song et al., 2018

Variable selection (branching)

- Khalil, Le Bodic, et al., 2016 $\Longrightarrow$ "online" imitation learning
- Hansknecht et al., 2018 $\Longrightarrow$ offline imitation learning
- Balcan et al., 2018 $\Longrightarrow$ theoretical results

Cut selection

- Baltean-Lugojan et al., 2018
- Tang et al., 2019

Primal heuristic selection

- Khalil, Dilkina, et al., 2017
- Hendel et al., 2018

The Graph Convolution Neural Network Model

Node state encoding

Natural representation : variable / constraint bipartite graph

$$
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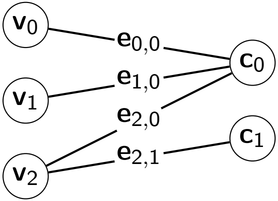
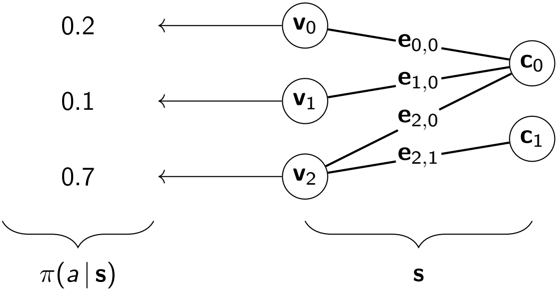


- $\mathbf{v}_i$: variable features (type, coef., bounds, LP solution...)
- $\mathbf{c}_j$: constraint features (right-hand-side, LP slack...)
- $\mathbf{e}_{i,j}$: non-zero coefficients in $\mathbf{A}$

D. Selsam et al. (2019). Learning a SAT Solver from Single-Bit Supervision.

Branching Policy as a GCNN Model

Neighbourhood-based updates: $\mathbf{v}_i \leftarrow \sum_{j \in \mathcal{N}_i} \mathbf{f}_\theta(\mathbf{v}_i, \mathbf{e}_{i,j}, \mathbf{c}_j)$



T. N. Kipf et al. (2016). Semi-Supervised Classification with Graph Convolutional Networks.

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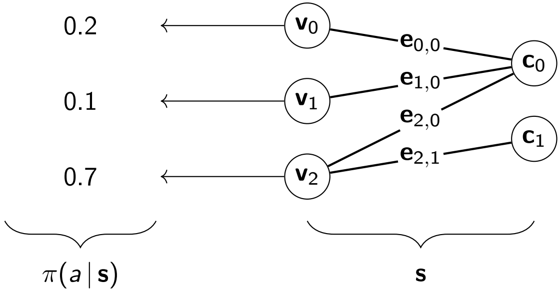

Natural model choice for graph-structured data

- permutation-invariance
- benefits from sparsity

T. N. Kipf et al. (2016). Semi-Supervised Classification with Graph Convolutional Networks.

Experiments

Imitation learning

Full Strong Branching (FSB): good branching rule, but expensive.
Can we learn a fast, good-enough approximation ?

[1] A. Gleixner et al. (July 2018). The SCIP Optimization Suite 6.

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Behavioural cloning

- collect $\mathcal{D} = \{(\mathbf{s}, a^\star), \dots\}$ from the expert agent (FSB)
- estimate $\pi^\star(a \mid \mathbf{s})$ from $\mathcal{D}$
- \+ no reward function, supervised learning, well-behaved
- − will never surpass the expert...

Implementation with the open-source solver SCIP[1]

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Implementation with the open-source solver SCIP[1]

Not a new idea

- Alvarez et al., 2017 predict SB scores, XTrees model
- Khalil, Le Bodic, et al., 2016 predict SB rankings, SVMrank model
- Hansknecht et al., 2018 do the same, λ-MART model

[1] A. Gleixner et al. (July 2018). The SCIP Optimization Suite 6.

Minimum set covering[2]

Model	Easy Time	Easy Wins	Easy Nodes	Medium Time	Medium Wins	Medium Nodes	Hard Time	Hard Wins	Hard Nodes
FSB	17.30	0 / 100	17	411.34	0 / 90	171	3600.00	0 / 0	n/a
RPB	8.98	0 / 100	**54**	60.07	0 / 100	1741	1677.02	4 / 65	47 299
XTrees	9.28	0 / 100	187	92.47	0 / 100	2187	2869.21	0 / 35	59 013
SVMrank	8.10	1 / 100	165	73.58	0 / 100	1915	2389.92	0 / 47	42 120
λ-MART	7.19	14 / 100	167	59.98	0 / 100	1925	2165.96	0 / 54	45 319
GCNN	**6.59**	**85** / 100	134	**42.48**	**100** / 100	**1450**	**1489.91**	**66** / 70	**29 981**

3 problem sizes

- 500 rows, 1000 cols (easy), training distribution
- 1000 rows, 1000 cols (medium)
- 2000 rows, 1000 cols (hard)

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Generalizes to harder problems !

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Combinatorial auction[3]

	Easy			Medium			Hard		
Model	Time	Wins	Nodes	Time	Wins	Nodes	Time	Wins	Nodes
FSB	4.11	0 / 100	6	86.90	0 / 100	72	1813.33	0 / 68	400
RPB	2.74	0 / 100	10	17.41	0 / 100	689	136.17	13 / 100	5511
XTrees	2.47	0 / 100	86	23.70	0 / 100	976	451.39	0 / 95	10 290
SVMrank	2.31	0 / 100	77	23.10	0 / 100	867	364.48	0 / 98	6329
λ-MART	**1.79**	**75** / 100	77	14.42	1 / 100	873	222.54	0 / 100	7006
GCNN	1.85	25 / 100	**70**	**10.29**	**99** / 100	**657**	**114.16**	**87** / 100	**5169**

3 problem sizes

- 100 items, 500 bids (easy), training distribution
- 200 items, 1000 bids (medium)
- 300 items, 1500 bids (hard)

[3] K. Leyton-Brown et al. (2000). Towards a Universal Test Suite for Combinatorial Auction Algorithms.

Capacitated facility location[4]

Model	Easy			Medium			Hard		
	Time	Wins	Nodes	Time	Wins	Nodes	Time	Wins	Nodes
FSB	30.36	4 / 100	14	214.25	1 / 100	76	742.91	15 / 90	55
RPB	26.55	9 / 100	**22**	156.12	8 / 100	**142**	631.50	14 / 96	**110**
XTrees	28.96	3 / 100	135	159.86	3 / 100	401	671.01	1 / 95	381
SVMrank	23.58	11 / 100	117	130.86	13 / 100	348	586.13	21 / 95	321
λ-MART	23.34	16 / 100	117	128.48	23 / 100	349	582.38	15 / 95	314
GCNN	**22.10**	**57** / 100	107	**120.94**	**52** / 100	339	**563.36**	**30** / 95	338

3 problem sizes

- 100 facilities, 100 customers (easy), training distribution
- 100 facilities, 200 customers (medium)
- 100 facilities, 400 customers (hard)

[4] G. Cornuejols et al. (1991). A comparison of heuristics and relaxations for the capacitated plant location problem.

Maximum independent set[5]

	Easy			Medium			Hard		
Model	Time	Wins	Nodes	Time	Wins	Nodes	Time	Wins	Nodes
FSB	23.58	9 / 100	7	1503.55	0 / 74	38	3600.00	0 / 0	n/a
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XTrees	10.75	1 / 100	76	1183.37	1 / 47	4664	3565.12	0 / 3	38 296
SVMrank	8.83	2 / 100	46	242.91	1 / 96	**546**	2902.94	1 / 18	6256
λ-MART	7.31	30 / 100	52	219.22	15 / 91	747	3044.94	0 / 12	8893
GCNN	**6.43**	51 / 100	43	192.91	**42** / 82	1841	**2024.37**	**25** / 29	2997

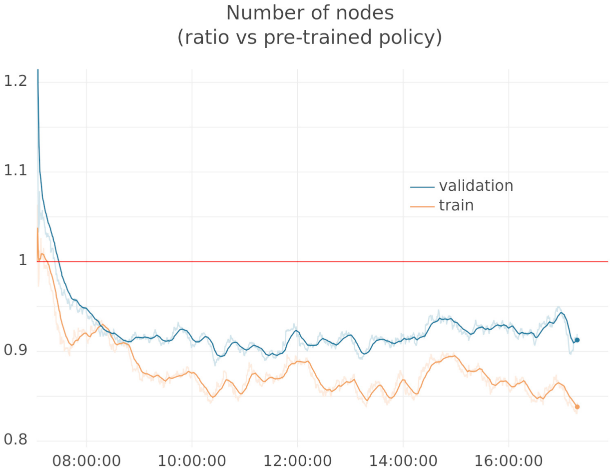
3 problem sizes, Barabási-Albert graphs (affinity=4)

- 500 nodes (easy), training distribution
- 1000 nodes (medium)
- 1500 nodes (hard)

[5] D. Chalupa et al. (2014). On the Growth of Large Independent Sets in Scale-Free Networks.

Reinforcement learning

Early results: set covering problem



Reward: negative number of nodes

Proximal Policy Optimization (PPO)

Challenging. . . but promising !

Conclusion

Heuristic vs data-driven branching:

+ tune B&B to your problem of interest automatically
– no guarantees outside of the training distribution
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What next:

- real-world problems
- other solver components: node selection, cut selection...
- reinforcement learning: still a lot of challenges
- interpretation: which variables are chosen ? Why ?
- provide an clean API + benchmarks for MILP adaptive solving (based on the open-source SCIP solver)

Paper: `https://arxiv.org/abs/1906.01629` M. Gasse et al. (2019). Exact Combinatorial Optimization with Graph Convolutional Neural Networks.

Code: `https://github.com/ds4dm/learn2branch`

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Thank you!

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DATA SCIENCE FOR REAL-TIME DECISION-MAKING

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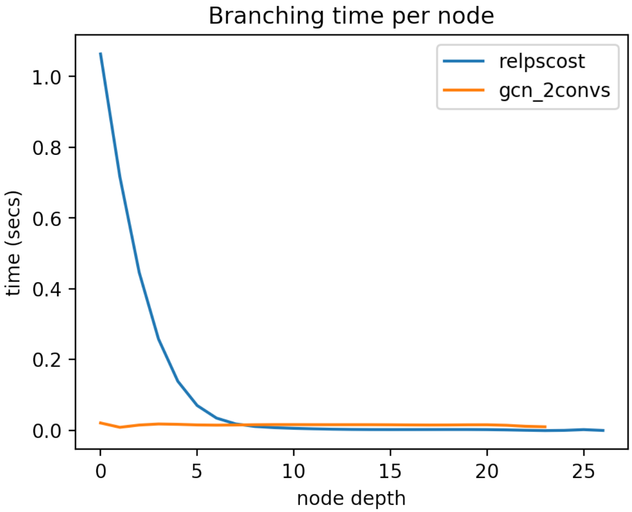
Learned Policy vs Reliability Pseudocost (SCIP default)



Time delta:
- python overhead
- data extraction (**s**)
- model evaluation

Close the gap:
- engineering ?
- efficient heuristics (reliability) ?