

Hybrid Models for Learning to Branch

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Huawei London Research Center, Nov. 26th 2021



Resources



Paper: <https://arxiv.org/abs/2006.15212>



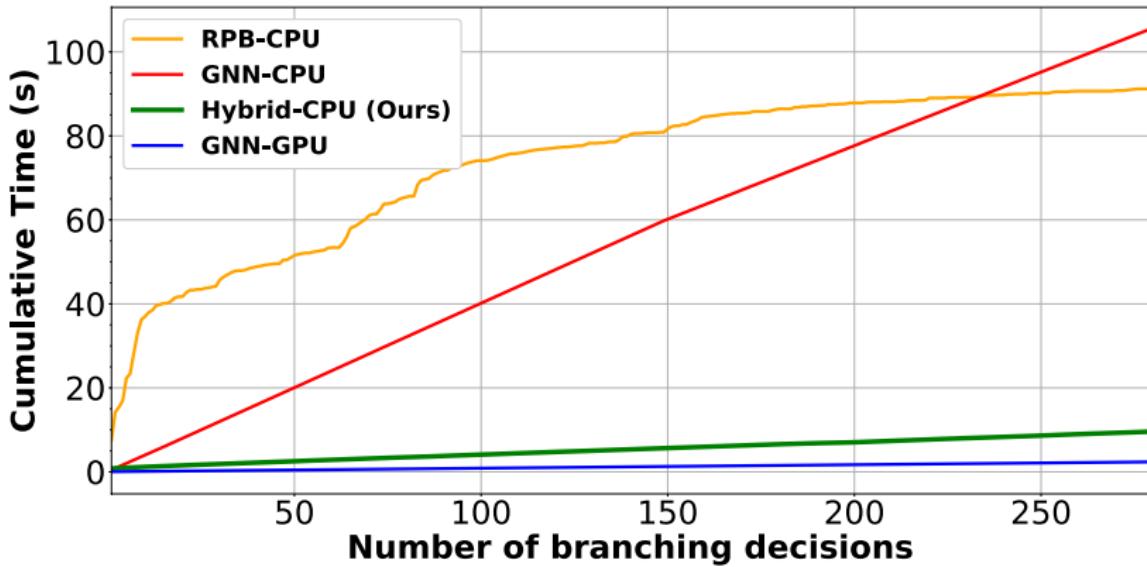
Code: <https://github.com/pg2455/Hybrid-learn2branch>



Slides: www.pgupta.info/talks

To enable **CPU-based discrete optimization solvers** to **use deep learning models** without sacrificing runtime performance.

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Outline

Problem formulation

Our approach: Hybrid Models

Conclusion

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Discrete Optimization

Branch-and-Bound

The Branching Problem

Learning to branch

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Mixed-Integer Linear Program (MILP)

$$\arg \min_{\mathbf{x}} \quad \mathbf{c}^T \mathbf{x}$$

- ▶ $\mathbf{c} \in \mathbb{R}^n$ the objective coefficients

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NP-hard problem.

Applications

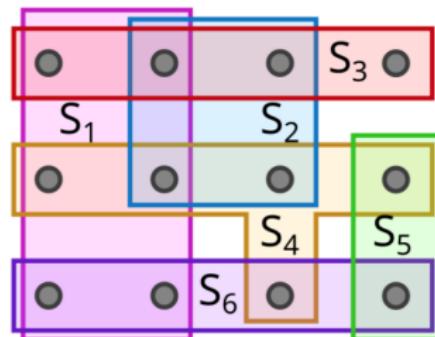
Combinatorial Auctions

Facility location-Allocation

Maximum Indendent Set

Set Covering

and many more ...



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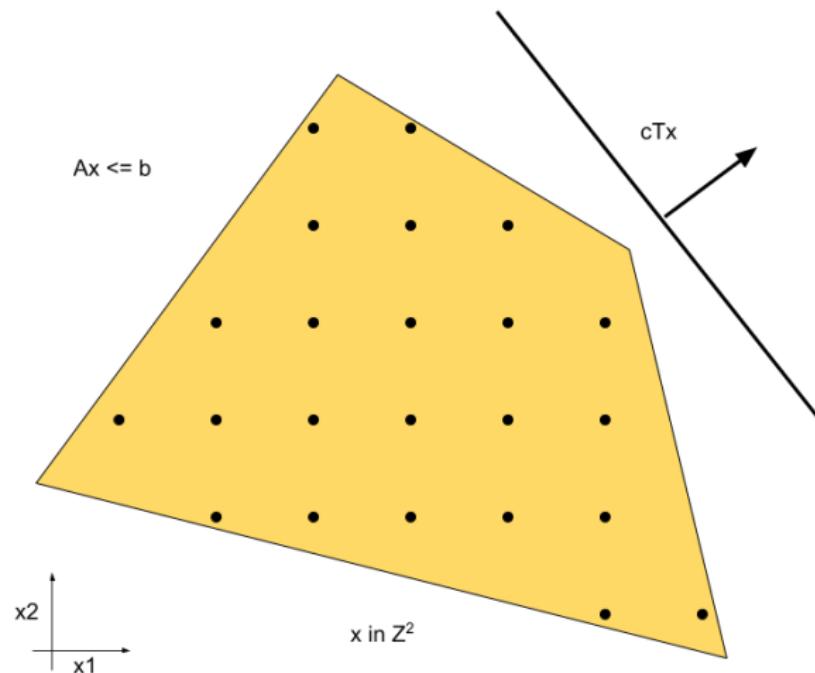


Image credit: Maxime Gasse

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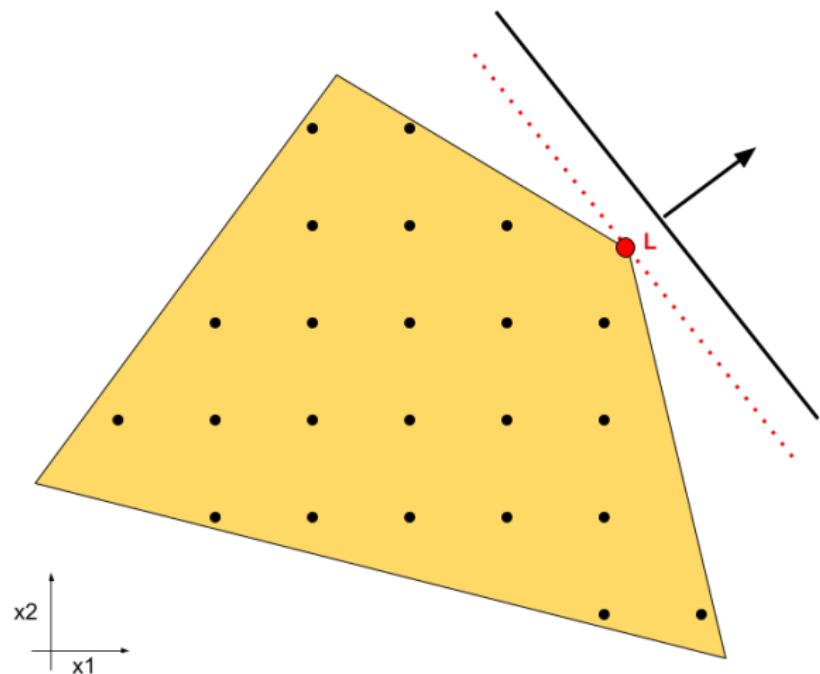
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- ▶ $\mathbf{l}, \mathbf{u} \in \mathbb{R}^n$ the lower and upper variable bounds
 - Polynomially solvable
 - Yields lower bounds to the original MILP

LP Relaxation of a MILP



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Branch-and-Bound (B&B)

B&B ([Land et al., 1960](#)) is the widely used to solve MILPs.

It consists of two steps



Each node in branch-and-bound is a new MIP

Image source: <https://www.gurobi.com/resource/mip-basics/>

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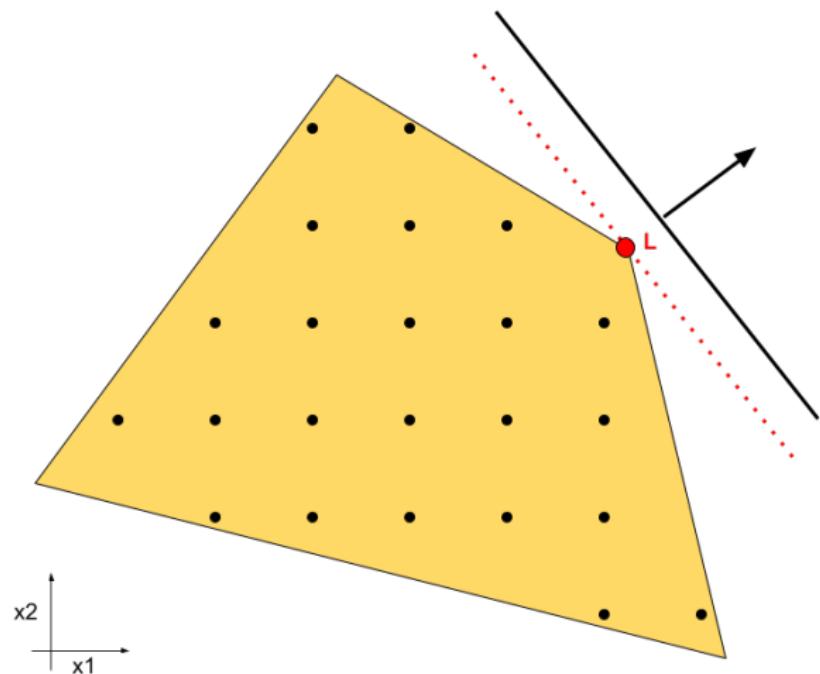
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- ▶ **Branching** - Select variable to split the problem into two
- ▶ **Bounding** - Solve the LP relaxation of resulting problem to obtain optimization guarantees on the solution

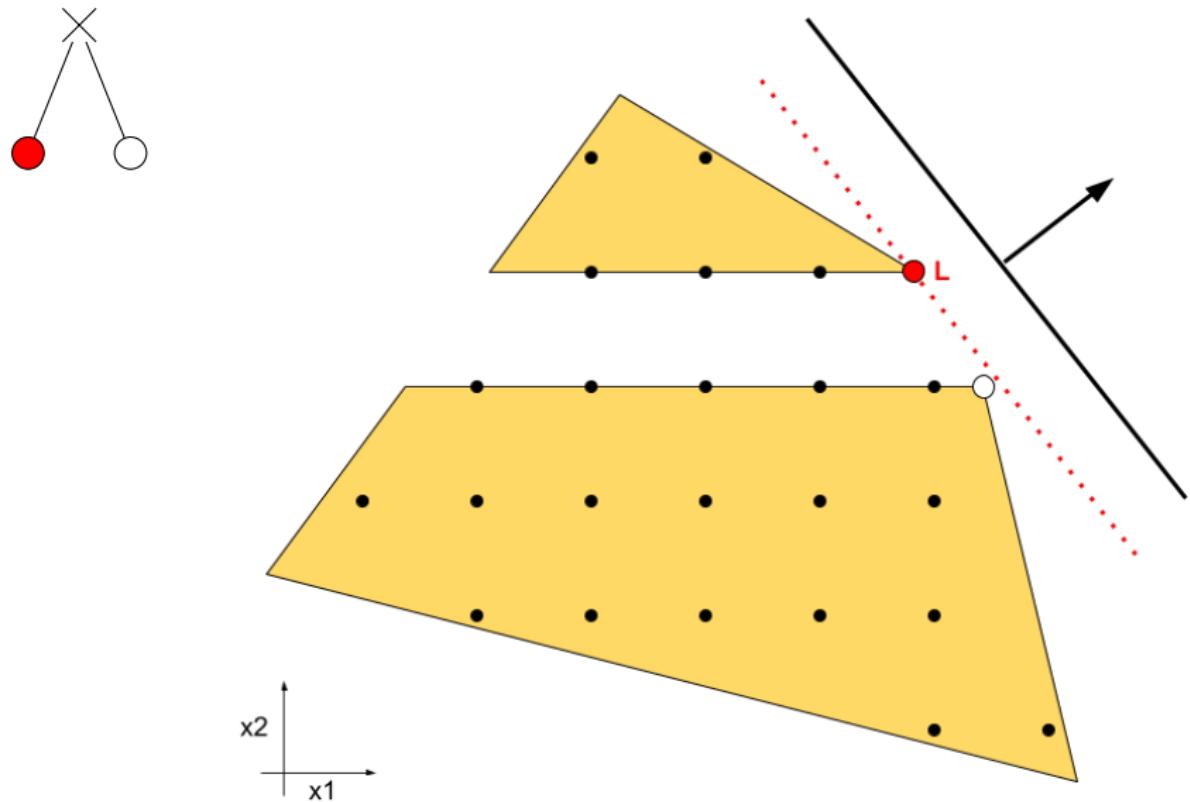


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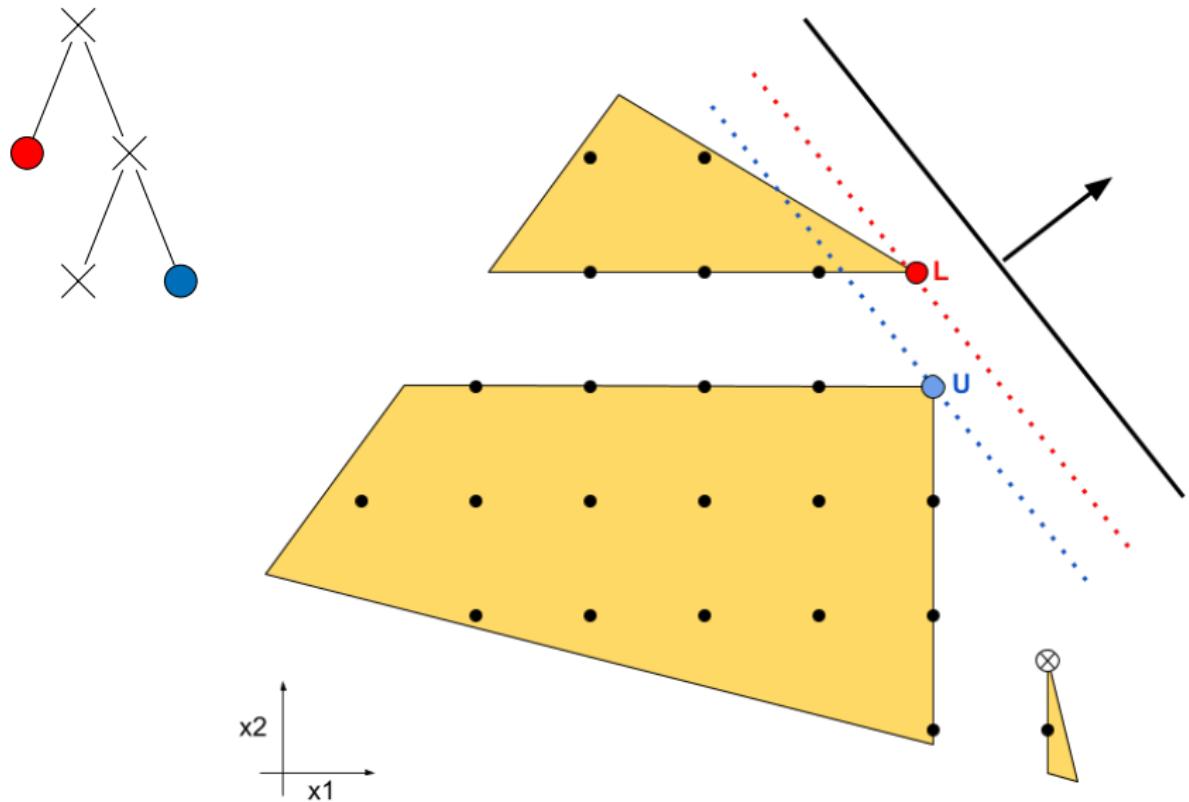
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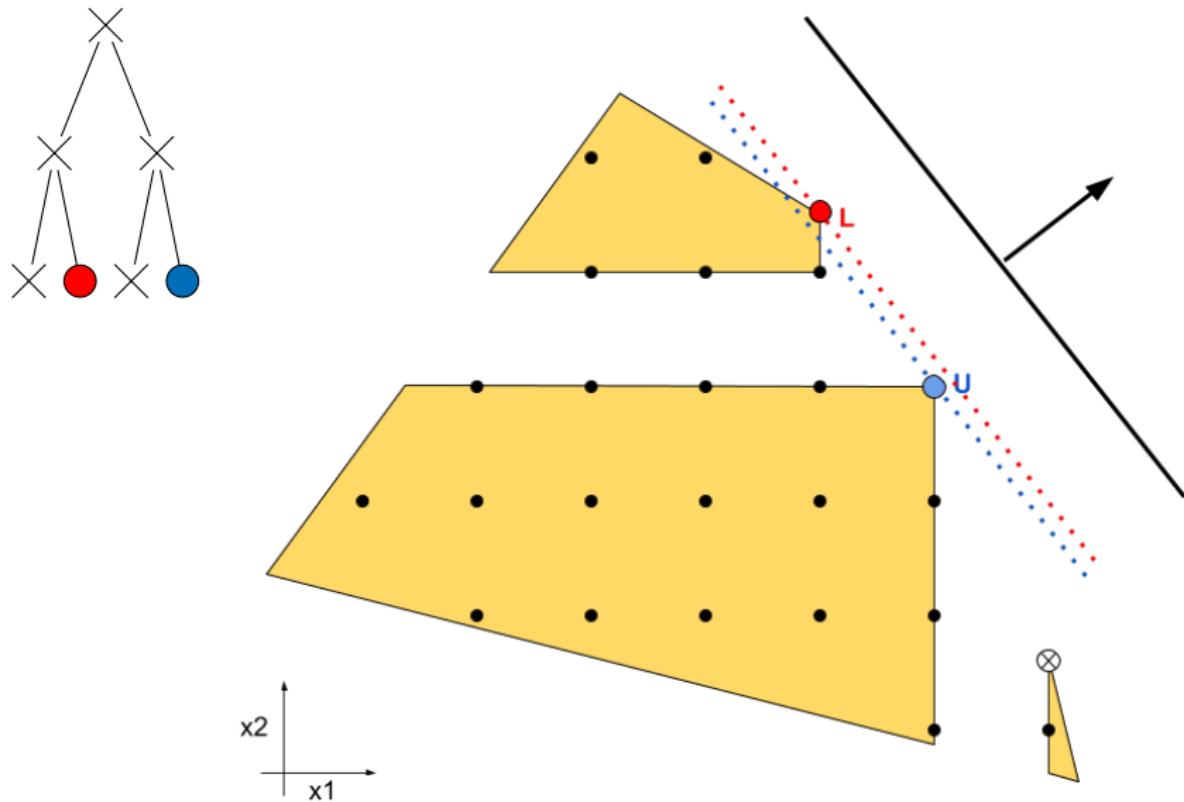
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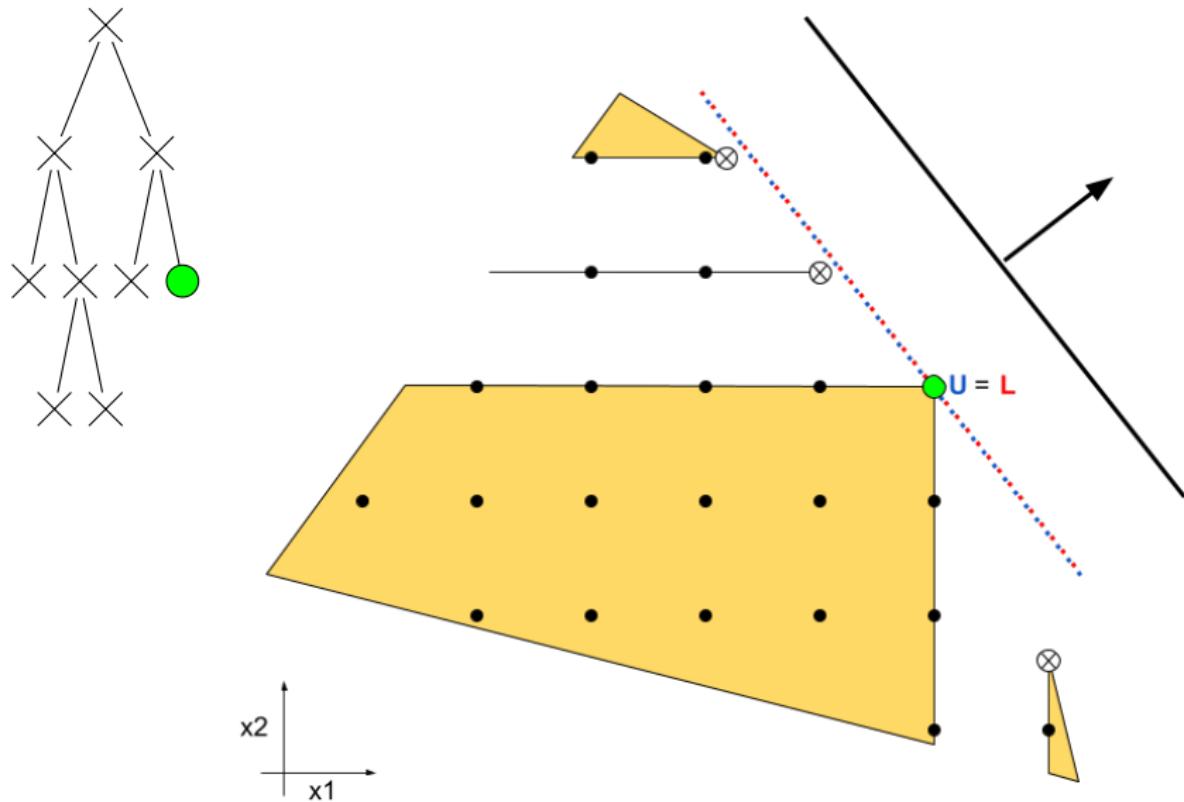
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Branch: Split the LP recursively over a non-integral variable, i.e.

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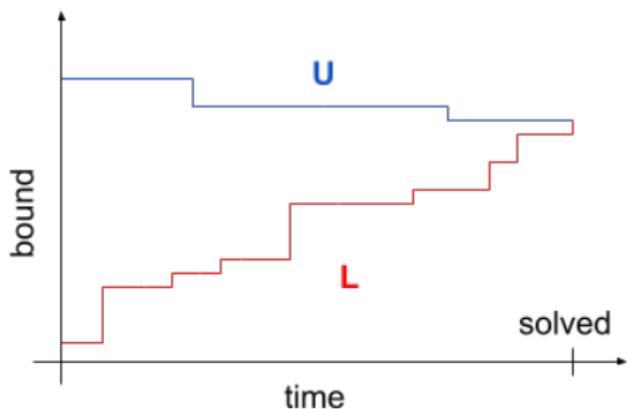
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Note: A time limit is used to ensure termination.

Branch-and-bound: a sequential process

Sequential decisions:

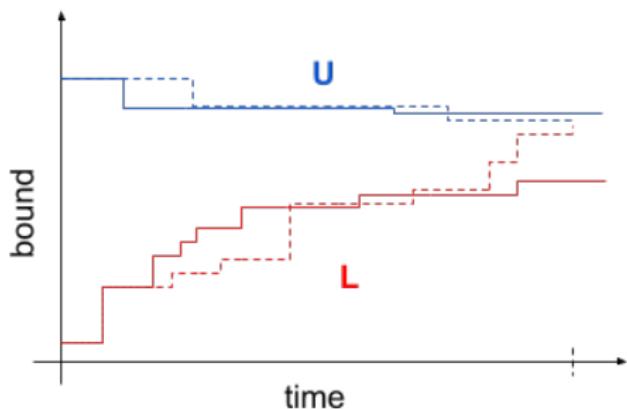
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(branching)
- ▶ node selection
- ▶ cutting plane selection
- ▶ primal heuristic selection
- ▶ simplex initialization
- ▶ ...



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Branching Policy

It is also called as **variable selection policy**.

Policy Objective: Given a B&B node i.e. MILP, select a variable $i \leq p \mid x_i^* \notin \mathbb{Z}$ so that the final size of the tree is minimum (a proxy for running time).

A gold standard: Strong Branching (impractical)

Strong branching¹: one-step forward looking (greedy)

- ▶ solve both LPs for each candidate variable
- ▶ select the variable resulting in tightest relaxation
- + small trees
- computationally expensive

¹D. Applegate et al. (1995). Finding cuts in the TSP. Tech. rep. DIMACS; J. Linneroth et al. (May 1999). A Computational Study of Search Strategies for Mixed Integer Programming.

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$$i_{SB}^* = \arg \max_i \text{score}_{SB,i}$$

Expert branching rules: state-of-the-art

Strong branching: one-step forward looking (greedy)

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Pseudo-cost branching (PB): backward looking

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

Reliability pseudo-cost branching (RPB): best of both worlds

- ▶ compute SB scores at the beginning
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Learning to branch

Objective:

Given a distribution of problem sets, find a branching policy that yields a shortest tree on an average.

Exploits statistical correlation across problem sets.

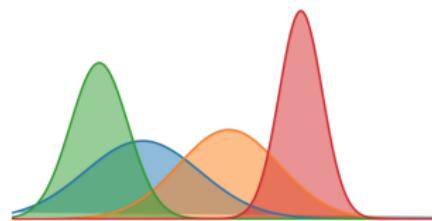


Figure: Application specific distribution

Learning to branch

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Well studied problem (not an exhaustive list)

- ▶ Khalil et al., 2016 \implies "online" imitation learning
- ▶ Balcan et al., 2018 \implies theoretical results
- ▶ Gasse et al., 2019 \implies offline imitation learning using GCNN

Learning to branch: SVMs

Khalil et al., 2016 uses Support Vector Machines (SVM) to imitate the strong branching policy *through learning-to-rank framework*

- + adapts to the problem instance instead of the distribution
- + computationally inexpensive once the SVM weights are learned
- less representational power as compared to GNNs

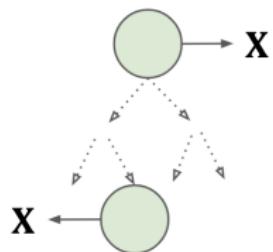
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Model inputs

Inputs to the SVM model are hand-designed features: X



Learning to branch: GNNs

Gasse et al., 2019 uses Graph Neural Networks to imitate the strong branching policy *through classification framework*

- + superior representation power
- + best overall accuracy
- requires GPUs for best running times

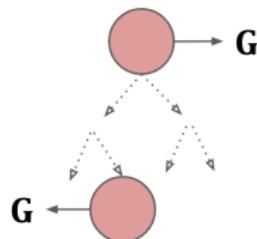
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bipartite-representation of MILP: G



GNNs: Bipartite Representation of MILPs

Natural representation : variable / constraint bipartite graph

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GNNs: Bipartite Representation of MILPs

Natural representation : variable / constraint bipartite graph

$$\begin{array}{ll} \arg \min_{x} & c^T x \\ \text{subject to} & Ax \leq b, \\ & l \leq x \leq u, \\ & x \in \mathbb{Z}^p \times \mathbb{R}^{n-p}. \end{array}$$

The diagram shows three nodes labeled v_0 , v_1 , and v_2 arranged vertically on the right side of the equation block. Each node is enclosed in a small circle.

- ▶ v_i : variable features (type, coef., bounds, LP solution...)

GNNs: Bipartite Representation of MILPs

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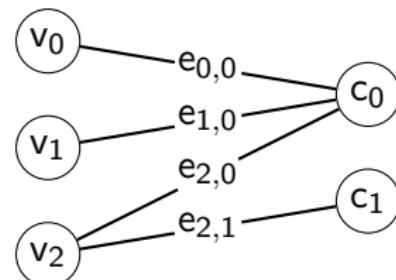


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- ▶ $e_{i,j}$: non-zero coefficients in A

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MILP Solvers



MILP solvers do not use GPUs.

Use of GNNs can get infeasible in the following scenarios

- ▶ No GPUs: It will be infeasible to incorporate GNNs as a branching policy in any of the available solvers
- ▶ Parallel MILP solving: As a single GPU can only fit a limited number of GNNs, when several 100s of MILPs need to be solved in parallel, GNNs can get infeasible

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Data Extraction

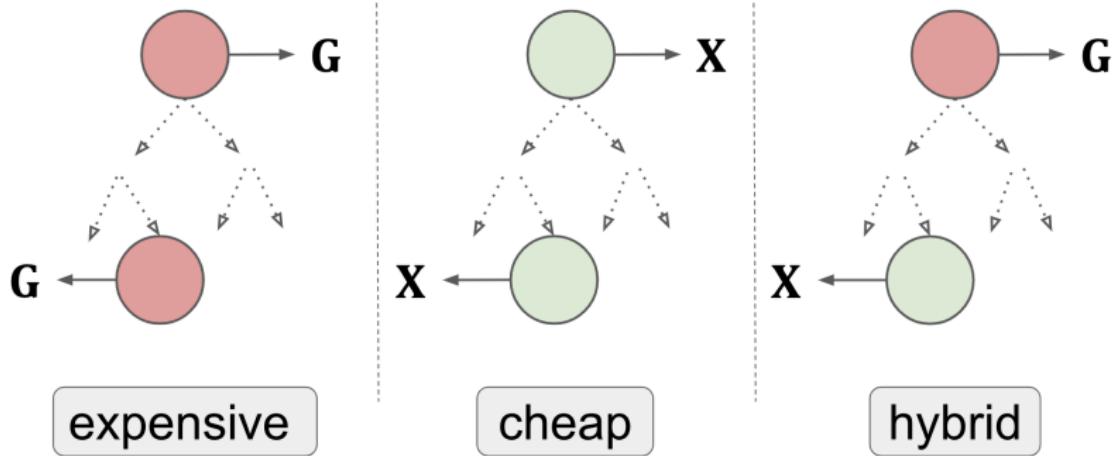


Figure: Data extraction strategies: bipartite graph representation **G** at every node (expensive); candidate variable features **X** at every node (cheap); bipartite graph at the root node and variable features at tree node (hybrid).

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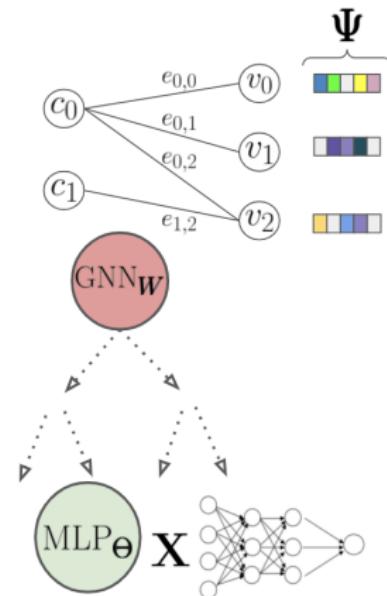
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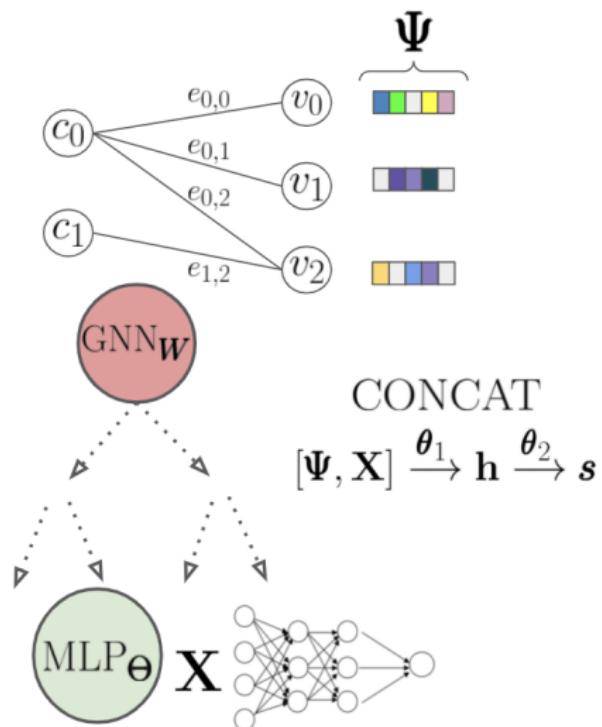
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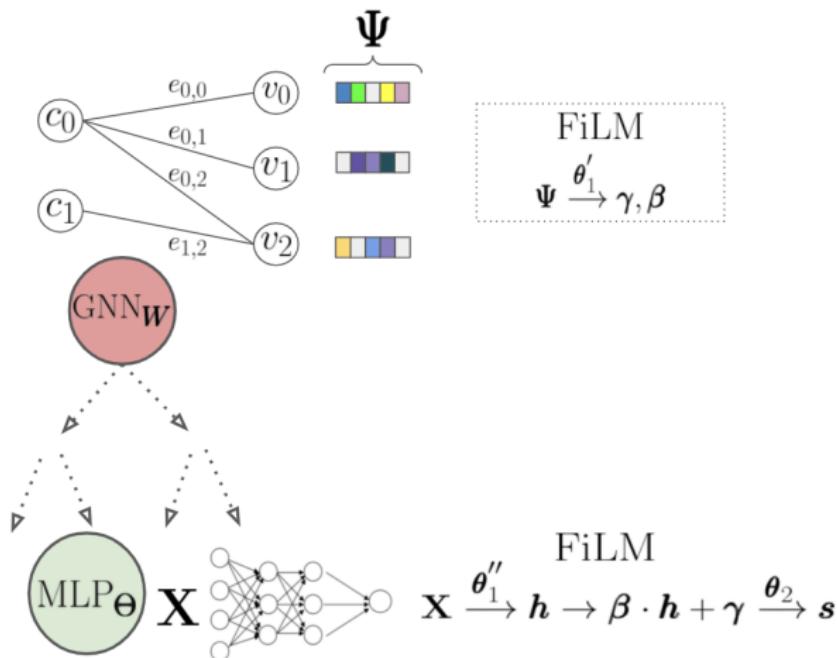


Model Architecture: CONCAT



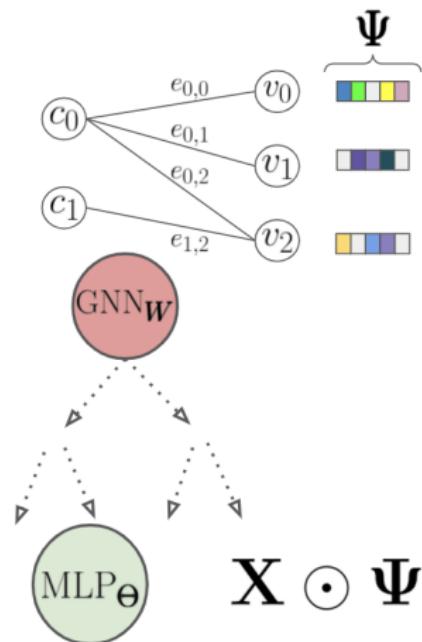
Perez et al., 2018 first proposed FiLM for visual question answering task

Model Architecture: FiLM



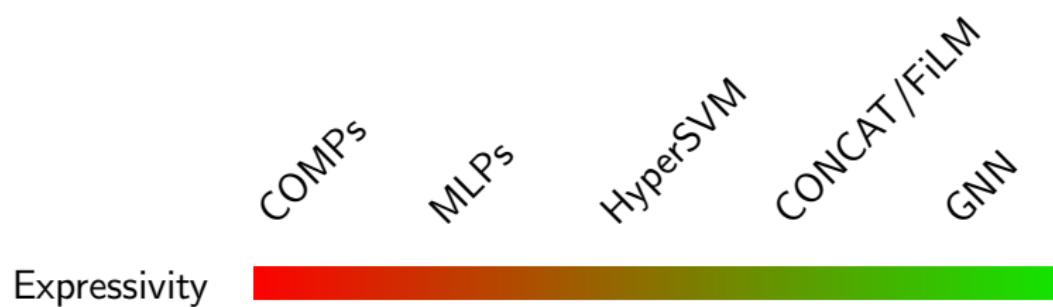
Perez et al., 2018 first proposed FiLM for visual question answering task

Model Architecture: HyperSVM

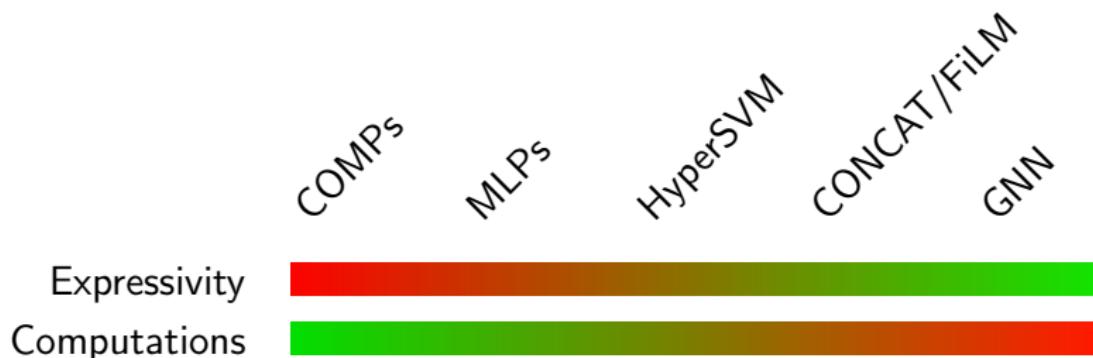


Perez et al., 2018 first proposed FiLM for visual question answering task

Model Architecture



Model Architecture



Model Architecture: Performance

End-to-end training

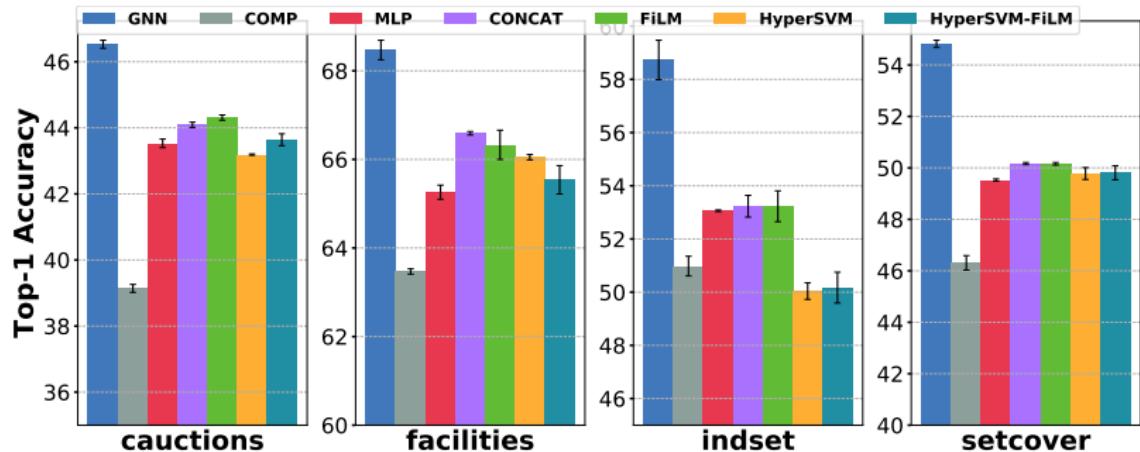


Figure: Test accuracy of the different models, with a simple e2e training protocol.

Outline

Problem formulation

Our approach: Hybrid Models

Model Architecture

Training Protocols

Conclusion

Training Protocols

To enhance the generalization power of the learned models on the bigger instances

Training Protocols: Loss weights

A good decision closer to the root node is more important than the ones far away from it.

Table: Effect of different sample weighting schemes on combinatorial auctions (big) instances, with a simple MLP model. $z \in [0, 1]$ is the ratio of the depth of the node and the maximum depth observed in a tree.

Type	Weighting scheme	Nodes	Wins
Constant	1	9678	10/60
Exponential decay	$e^{-0.5z}$	9793	10/60
Linear	$(e^{-0.5} - 1) * z + 1$	9789	12/60
Quadratic decay	$(e^{-0.5} - 1) * z^2 + 1$	9561	14/60
Sigmoidal	$(1 + e^{-0.5}) / (1 + e^{z-0.5})$	9534	14/60

Training Protocols: Knowledge Distillation

Knowledge distillation (KD):² Use the output of an expert GNN from [Gasse et al., 2019](#) as a target for the model.

KD reweights the samples so that the student doesn't attempt to sharply classify samples that even the teacher didn't succeed with (i.e. the logits have higher entropy for the more difficult samples) [Phuong et al., 2019](#).

Table: Test accuracy of FiLM, using different training protocols.

	cautions	facilities	indset	setcover
Pretrained GNN	44.12 ± 0.09	65.78 ± 0.06	53.16 ± 0.51	50.00 ± 0.09
e2e	44.31 ± 0.08	66.33 ± 0.33	53.23 ± 0.58	50.16 ± 0.05
e2e & KD	44.10 ± 0.09	66.60 ± 0.21	53.08 ± 0.3	50.31 ± 0.19

²[G. Hinton et al. \(2015\)](#). Distilling the knowledge in a neural network.

Training Protocols: Auxiliary Task

Auxiliary Task (AT): No additional data required. We force the variable representations to be far apart from each other.

- ▶ ED : Maximum distance between these representations in euclidean space
- ▶ MHE³ : Uniform distribution of these representations over a unit hypersphere

Table: Test accuracy of FiLM, using different training protocols.

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Pretrained GNN	44.12 ± 0.09	65.78 ± 0.06	53.16 ± 0.51	50.00 ± 0.09
e2e	44.31 ± 0.08	66.33 ± 0.33	53.23 ± 0.58	50.16 ± 0.05
e2e & KD	44.10 ± 0.09	66.60 ± 0.21	53.08 ± 0.3	50.31 ± 0.19
e2e & KD & AT	44.56 ± 0.13	66.85 ± 0.28	53.68 ± 0.23	50.37 ± 0.03

³W. Liu et al. (2018). Learning towards minimum hyperspherical energy.

B&B Performance (Runtime)

Finally, the learned models are used as a branching policy in SCIP solver⁴.

Hybrid models have a better runtime performance on average than other baselines as evaluated on CPU only machines.

Model	Time	Easy			Medium			Hard		
		Wins	Nodes	Time	Wins	Nodes	Time	Wins	Nodes	
FSB	42.5	1 / 60	13	313.3	0 / 59	75	997.2	0 / 51	50	
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FiLM (ours)	24.7	51 / 60	109	136.4	51 / 60	325	531.7	46 / 57	295	
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B&B Performance (Runtime)

Model	Time	Small		Medium		Big	
		Wins	Nodes	Wins	Nodes	Wins	Nodes
FSB	42.53	1 / 60	13	313.33	0 / 59	75	997.23
PB	31.35	4 / 60	139	177.69	4 / 60	384	712.45
RPB	36.86	1 / 60	23	213.99	1 / 60	152	794.80
COMP	30.37	3 / 60	120	172.51	4 / 60	347	633.42
GNN	39.18	0 / 60	112	209.84	0 / 60	314	748.85
FiLM (ours)	24.67	51 / 60	109	136.42	51 / 60	325	531.70
GNN-GPU	28.91	– / 60	112	150.11	– / 60	314	628.12
Capacitated Facility Location							
FSB	27.16	0 / 60	17	582.18	0 / 45	116	2700.00
PB	10.19	0 / 60	286	94.12	0 / 60	2451	2208.57
RPB	14.05	0 / 60	54	94.65	0 / 60	1129	1887.70
COMP	9.83	3 / 60	178	89.24	0 / 60	1474	2166.44
GNN	17.61	0 / 60	136	242.15	0 / 60	1013	2700.17
FiLM (ours)	8.73	57 / 60	147	63.75	60 / 60	1131	1843.24
GNN-GPU	8.26	– / 60	136	53.56	– / 60	1013	1535.80
Set Covering							
FSB	6.12	0 / 60	6	132.38	0 / 60	71	2127.35
PB	2.76	1 / 60	234	25.83	0 / 60	2765	393.60
RPB	4.01	0 / 60	11	26.36	0 / 60	714	210.95
COMP	2.76	0 / 60	82	29.76	0 / 60	930	494.59
GNN	2.73	1 / 60	71	22.26	0 / 60	688	257.99
FiLM (ours)	2.13	58 / 60	73	15.71	60 / 60	686	217.02
GNN-GPU	1.96	– / 60	71	11.70	– / 60	688	121.18
Combinatorial Auctions							
FSB	673.43	0 / 53	47	1689.75	0 / 20	10	2700.00
PB	172.03	2 / 57	5728	753.95	0 / 45	1570	2685.23
RPB	59.87	5 / 60	603	173.17	11 / 60	205	1946.51
COMP	82.22	1 / 58	847	383.97	1 / 52	267	2393.75
GNN*	44.07	15 / 60	331	625.23	1 / 50	599	2330.95
FiLM* (ours)	52.96	37 / 55	376	131.45	47 / 54	264	1823.29
GNN-GPU*	31.71	– / 60	331	63.96	– / 60	599	1158.59
Maximum Independent Set							

B&B Performance (Optimality Gap)

Hybrid models also have the least optimality gap at the end of the time limit as compared to other baselines as evaluated on CPU only machines.

Table: Mean optimality gap (lower the better) of commonly unsolved "big" instances (number of such instances in brackets).

	setcover (33)	indset (39)
FSB	0.1709	0.0755
PB	0.0713	0.0298
RPB	0.0628	0.0252
COMP	0.0740	0.0252
GNN	0.1039	0.0341
Film	0.0597	0.0187

Runtime performance

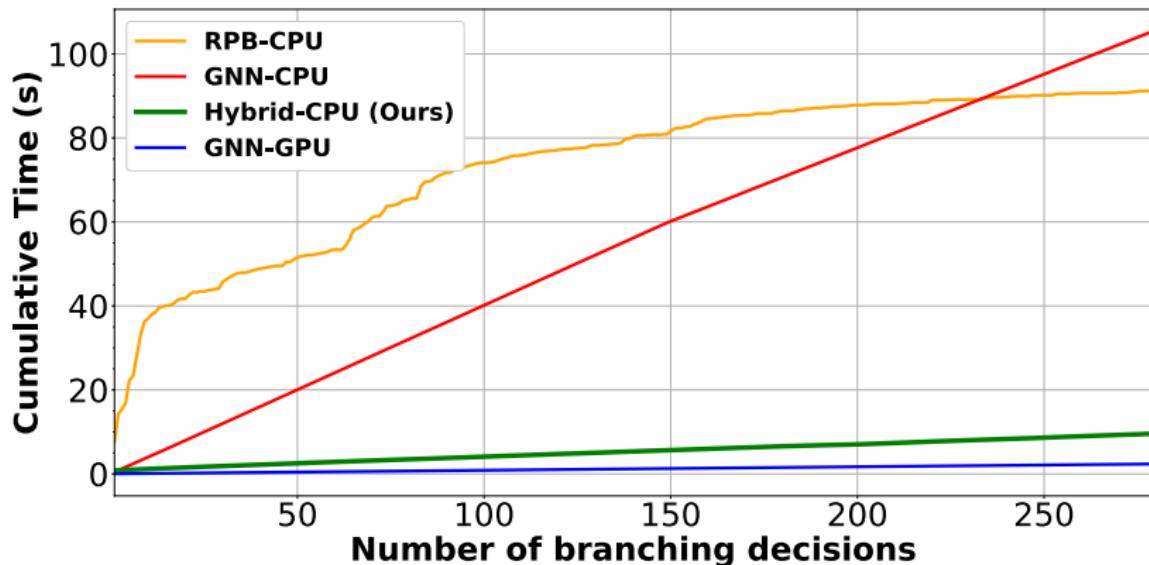


Figure: Cumulative time cost of different branching policies: (i) the default internal rule RPB of the SCIP solver; (ii) a GNN model (using a GPU or a CPU); and (iii) our hybrid model. Clearly the GNN model requires a GPU for being competitive, while our hybrid model does not. (Measured on a capacitated facility location problem, medium size).

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Conclusion

- ▶ We **propose hybrid models** as branching policies that can be easily integrated with any discrete optimization solvers without needing any access to GPU machines
- ▶ We **explored various training protocols** to enhance both the Top-1 accuracy as well as the runtime B&B performance of these hybrid models
- ▶ We **recommend** training protocol as FiLM (e2e & KD & AT) only when these models have significantly better accuracy than FiLM (e2e & KD).

Open questions

- ▶ scaling to the real-world problems
- ▶ reinforcement learning: still a lot of challenges
- ▶ interpretation: which variables are chosen? Why ?
- ▶ learning in collaboration with other heuristics, e.g, cut selection, node selection, etc.
- ▶ meta-learning to transfer to unseen instances



Paper: <https://arxiv.org/abs/2006.15212>



Code: <https://github.com/pg2455/Hybrid-learn2branch>



Slides: www.pgupta.info/talks

QR Codes generated via <https://www.qr-code-generator.com/>

Hybrid Models for Learning to Branch

Thank you!

Prateek Gupta*, Maxime Gasse, Elias B. Khalil,
M. Pawan Kumar, Andrea Lodi, Yoshua Bengio

