Learning to Branch

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Slides

Slides: `www.pgupta.info/talks`

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To **improve** the extent to which neural networks can **imitate** a *computationally expensive but accurate heuristic* to solve mixed-integer linear programming (MILP) problems.

Outline

Problem formulation

Hybrid Models for Learning to Branch
(NeurIPS 2020)

Lookback for Learning to Branch
(TMLR 2022)

Outline

Problem formulation
- Discrete Optimization
- Branch-and-Bound
- The Branching Problem
- Learning to branch

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Mixed-Integer Linear Program (MILP)

$$\arg\min_{x} \quad c^\top x$$

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

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- $p \leq n$ integer variables

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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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- 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 framework 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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- **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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LP Relaxation of a MILP

Branch-and-Bound

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

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

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Note: A time limit is used to ensure termination.

Branch-and-bound: a sequential process

Sequential decisions:

- variable selection (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 branching[1]: one-step forward looking (greedy)

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

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

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Strong branching decision

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

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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

Objective: Given a dataset of MILPs

- learn an inexpensive function f
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$$i^\star_{SB} = \arg\max_{i \in \mathcal{C}} \text{score}_{SB,i} \qquad i^\star_f = \arg\max_{i \in \mathcal{C}} \text{score}_{f_\theta,i},$$

where $s^i_{f_\theta}$ is the score for $i \leq p$ variable as estimated by f_θ.

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$$\theta^* = \arg\min_\theta \mathcal{L}(f_\theta(MILP), i^\star_{SB})$$

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Well studied problem (not an exhaustive list)

- Gasse et al., 2019 $\implies$ offline imitation learning using GCNN
- Nair et al., 2020 $\implies$ uses GCNNs to design other heuristics
- Chen et al., 2022 $\implies$ studies the limitations of existing GNNs to represent MILPs

Learning to branch: GNNs

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

+ superior representation power
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Model inputs

Inputs to the GNN is a **bipartite-representation of MILP**: G

GNNs: Bipartite Representation of MILPs

Natural representation : variable / constraint bipartite graph

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v_0

v_1

v_2

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

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− requires GPUs for best running times (Gupta, Gasse, et al., 2020)
? Can we further improve the performance? (Gupta, Khalil, et al., 2022)

Hybrid Models for Learning to Branch (NeurIPS 2020)

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- Model Architecture
- Training Protocols

Lookback for Learning to Branch (TMLR 2022)

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

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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Model Architecture

Model Architecture: CONCAT

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

Model Architecture: FiLM

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Model Architecture: HyperSVM

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Model Architecture

Model Architecture

Model Architecture: Performance

End-to-end training

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

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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.

	cauctions	facilities	indset	setcover
Pretrained GNN	44.12 $\pm$ 0.09	65.78 $\pm$ 0.06	53.16 $\pm$ 0.51	50.00 $\pm$ 0.09
e2e	44.31 $\pm$ 0.08	66.33 $\pm$ 0.33	53.23 $\pm$ 0.58	50.16 $\pm$ 0.05
e2e & KD	44.10 $\pm$ 0.09	66.60 $\pm$ 0.21	53.08 $\pm$ 0.3	50.31 $\pm$ 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
- MHE[3] : Uniform distribution of these representations over a unit hypersphere

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e2e & KD & AT	**44.56 $\pm$ 0.13**	**66.85 $\pm$ 0.28**	**53.68 $\pm$ 0.23**	**50.37 $\pm$ 0.03**

[3] W. 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 solver[4].

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

	Easy			Medium			Hard		
Model	Time	Wins	Nodes	Time	Wins	Nodes	Time	Wins	Nodes
FSB	42.5	1 / 60	13	313.3	0 / 59	75	997.2	0 / 51	50
PB	31.4	4 / 60	139	177.7	4 / 60	384	712.6	3 / 56	309
RPB	36.9	1 / 60	**23**	214.0	1 / 60	**152**	794.8	2 / 54	**99**
COMP	30.4	3 / 60	120	172.5	4 / 60	347	633.4	6 / 57	294
GNN	39.2	0 / 60	112	209.8	0 / 60	314	748.8	0 / 54	286
FiLM (ours)	**24.7**	**51** / 60	109	**136.4**	**51** / 60	325	**531.7**	**46** / 57	295
GNN	28.9	– / 60	112	150.1	– / 60	314	628.1	– / 56	286

Capacitated Facility Location

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RPB	36.9	1 / 60	**23**	214.0	1 / 60	**152**	794.8	2 / 54	**99**
COMP	30.4	3 / 60	120	172.5	4 / 60	347	633.4	6 / 57	294
GNN	39.2	0 / 60	112	209.8	0 / 60	314	748.8	0 / 54	286
FiLM (ours)	**24.7**	**51** / 60	109	**136.4**	**51** / 60	325	**531.7**	**46** / 57	295
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Capacitated Facility Location

[4] A. Gleixner et al. (July 2018). The SCIP Optimization Suite 60. Technical Report. Optimization Online

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B&B Performance (Runtime)

Model	Small Time	Small Wins	Small Nodes	Medium Time	Medium Wins	Medium Nodes	Big Time	Big Wins	Big Nodes
FSB	42.53	1 / 60	13	313.33	0 / 59	75	997.23	0 / 51	50
PB	31.35	4 / 60	139	177.69	4 / 60	384	712.45	3 / 56	309
RPB	36.86	1 / 60	**23**	213.99	1 / 60	**152**	794.80	2 / 54	**99**
COMP	30.37	3 / 60	120	172.51	4 / 60	347	633.42	6 / 57	294
GNN	39.18	0 / 60	112	209.84	0 / 60	314	748.85	0 / 54	286
FILM (ours)	**24.67**	**51** / 60	109	**136.42**	**51** / 60	325	**531.70**	**46** / 57	295
GNN-GPU	28.91	– / 60	112	150.11	– / 60	314	628.12	– / 56	286
				Capacitated Facility Location					
FSB	27.16	0 / 60	17	582.18	0 / 45	116	2700.00	0 / 0	n/a
PB	10.19	0 / 60	286	94.12	0 / 60	2451	2208.57	0 / 23	82 624
RPB	14.05	0 / 60	**54**	94.65	0 / 60	1129	1887.70	7 / 27	48 395
COMP	9.83	3 / 60	178	89.24	0 / 60	1474	2166.44	0 / 21	52 326
GNN	17.61	0 / 60	136	242.15	0 / 60	**1013**	2700.17	0 / 0	n/a
FILM (ours)	**8.73**	**57** / 60	147	**63.75**	**60** / 60	1131	**1843.24**	**20** / 26	**37 777**
GNN-GPU	8.26	– / 60	136	53.56	– / 60	1013	1535.80	– / 36	31 662
				Set Covering					
FSB	6.12	0 / 60	6	132.38	0 / 60	71	2127.35	0 / 28	318
PB	2.76	1 / 60	234	25.83	0 / 60	2765	393.60	0 / 59	13 719
RPB	4.01	0 / 60	**11**	26.36	0 / 60	714	**210.95**	**29** / 60	4701
COMP	2.76	0 / 60	82	29.76	0 / 60	930	494.59	0 / 54	5613
GNN	2.73	1 / 60	71	22.26	0 / 60	688	257.99	6 / 60	**3755**
FILM (ours)	**2.13**	**58** / 60	73	**15.71**	**60** / 60	**686**	217.02	25 / 60	4315
GNN-GPU	1.96	– / 60	71	11.70	– / 60	688	121.18	– / 60	3755
				Combinatorial Auctions					
FSB	673.43	0 / 53	47	1689.75	0 / 20	10	2700.00	0 / 0	n/a
PB	172.03	2 / 57	5728	753.95	0 / 45	1570	2685.23	0 / 1	38 215
RPB	59.87	5 / 60	603	173.17	11 / 60	**205**	1946.51	9 / 21	2461
COMP	82.22	1 / 58	847	383.97	1 / 52	267	2393.75	0 / 6	5589
GNN*	**44.07**	15 / 60	**331**	625.23	1 / 50	599	2330.95	0 / 10	**687**
FILM* (ours)	52.96	**37** / 55	376	**131.45**	**47** / 54	264	**1823.29**	**12** / 15	1201
GNN-GPU*	31.71	– / 60	331	63.96	– / 60	599	1158.59	– / 27	685
				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).

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`

Peer-reviews: `http://bit.ly/3XU9E8W`

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

Lookback for Learning to Branch
(TMLR 2022)

Outline

Problem formulation

Hybrid Models for Learning to Branch (NeurIPS 2020)

Lookback for Learning to Branch (TMLR 2022)
- Lookback condition
- Loss target
- Regularizer
- Evaluation
- Conclusion

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Lookback condition in strong branching

Strong branching heuristic exhibits the following condition:
Parent's second best choice is *often* the **child's best choice**.

Frequency of Lookback condition

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Instances	Description	number of parent-child pairs collected	number of parent-child pairs exhibiting the lookback property	Frequency of the lookback property
CORLAT	Corridor planning in wildlife management	5082	1765	34.73%
RCW	Red-cockaded woodpecker diffusion conservation	5115	1952	38.16%

Frequency of the lookback property in the real-world instances is as prevalent as in the synthetic instances considered in the main paper. These instances are made available by Dilkina et al., 2017.

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Loss targets

We consider two types of targets
($\mathcal{Z}$ is the set of all the second best branching variables)

Original one-hot encoded target,

$$\mathrm{y}$$

$$\mathrm{y}_i = \begin{cases} 1, & i = i^*_{SB} \\ 0, & \text{otherwise} \end{cases}$$

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Second-best ϵ-smoothed target, z

$$z_i = \begin{cases} 1-\epsilon, & i = i^*_{SB} \\ \frac{\epsilon}{|\mathcal{Z}|}, & i \in \mathcal{Z} \\ 0, & \text{otherwise} \end{cases}$$

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$$\text{loss}_{PAT} = 1\{Lookback_i\} \cdot CE(f_\theta(\mathcal{G}_i), f_\theta(\mathcal{G}_i^{parent})[\mathcal{C}_i]),$$

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Performance evaluation

We will consider three different set of parameters

- Choice of the target:
  - One-hot encoded, y
  - Second-best ϵ-smoothed, z
- Strength of the PAT regularizer, $\lambda_{PAT} \in \{0, 0.01, 0.1, 0.2, 0.3\}$
- Strength of the $l2$-regularizer, $\lambda_{l2} \in \{0.0, 0.01, 0.1, 1.0\}$

Performance evaluation

$$\theta_y = \arg\min_{\theta, \lambda_{l2}} \frac{1}{N} \sum_{k=1}^{N} CE(f_\theta(\mathcal{G}_k), \mathrm{y}_k) + \lambda_{l2} \cdot ||\theta||_2$$

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$$\theta_{PAT} = \arg\min_{\theta,\mathrm{v},\lambda_{l2},\lambda_{PAT}} \frac{1}{N} \sum_{k=1}^{N} CE(f_\theta(\mathcal{G}_k), \mathrm{v}) + \lambda_{l2} \cdot ||\theta||_2 + \lambda_{PAT} \cdot \mathrm{loss}_{PAT}$$

Performance evaluation: Instances

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- **Small** instances are used to *collect training data* of parent-child nodes by solving these instances using the strong branching heuristic as the variable selection policy in the solver
- **Medium** instances are used for *hyperparameter selection* incorporating harder-to-formulate criterion in the objective function
- **Big** instances are used to *report performance* evaluation

Model selection criterion: Validation accuracy

Top-1 accuracy (1-standard deviation) on validation dataset.

Model selection criterion: Out-of-distribution performance

We solve 100 **medium** instances and collect the following metrics

- Wins: Number of times a model solved the instance fastest
- Time: 1-shifted geometric mean of time taken to solve each instance
- Nodes: 1-shifted geometric mean of nodes taken in the B&B tree of the *commonly solved instances*

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We plot the range-normalized (range is specified in parenthesis) Time and Node performance of the selected models. The centered "X" black mark shows the final models that were selected to be used for evaluating the performance on Big instances. The points with a red outline show the performance of the models selected according to the best validation accuracy (Note that we omit such models for indset as it distorts the scale of the plot.)

Final performance

Model	Time	Time (c)	Wins	Solved	Nodes (c)
FSB*	n/a	n/a	n/a	n/a	n/a
RPB	626.81	434.92	1	80	17 979
TUNEDRPB	644.20	450.06	0	80	18 104
GNN	507.06	333.59	14	80	17 145
GNN-PAT (ours)	**477.26**	**310.22**	**69**	**84**	**16 388**
Combinatorial Auction (Bigger)					

Figure: Evaluation metrics on Big instances with a time budget of 30 minutes per instance

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Optimality gap on commonly unsolved instances

Figure: Mean optimality gap of the *commonly unsolved instances*

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- Our proposed models outperform the SOTA results

Open questions

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

Peer-reviews: https://openreview.net/forum?id=EQpGkw5rvL

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Learning to Branch

Thank you!

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M. Pawan Kumar, Andrea Lodi, Yoshua Bengio

Slides

Slides: `www.pgupta.info/talks`

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