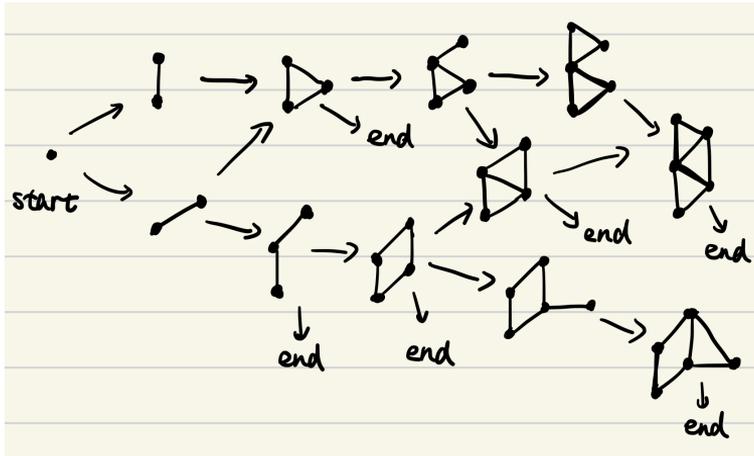# Let the Flows Tell:
Solving Graph Combinatorial Optimization Problems with GFlowNets

NeurIPS 2023 spotlight
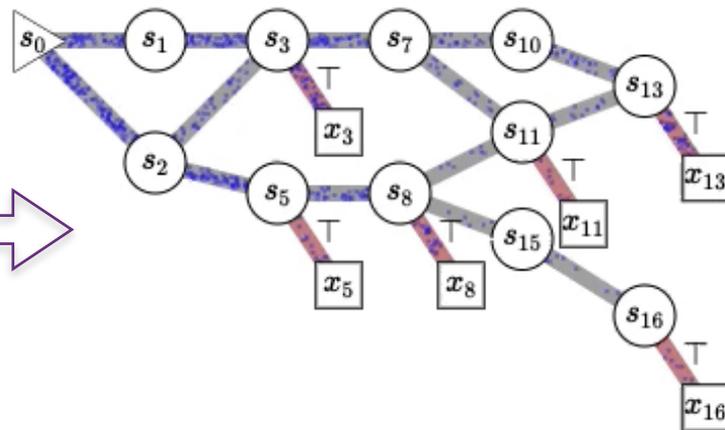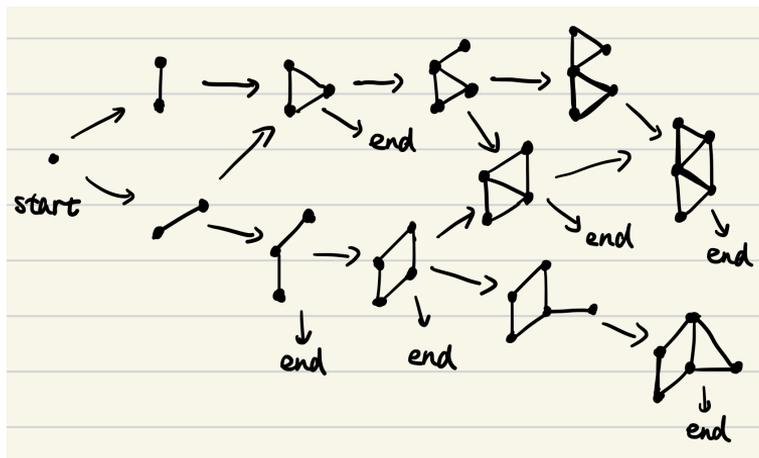
Dinghuai Zhang, Hanjun Dai, Nikolay Malkin, Aaron Courville, Yoshua Bengio, Ling Pan
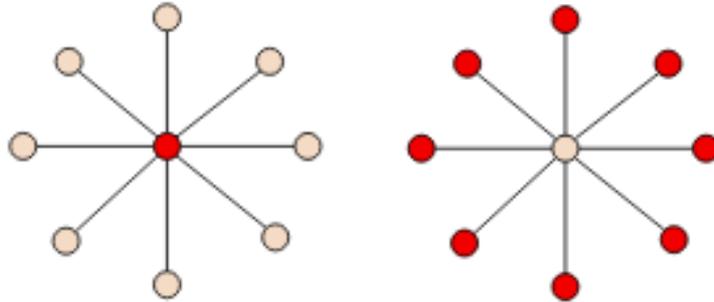
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Abstract the graph generation example…

Abstract the graph generation example...

Emmanuel Bengio, blog of "Flow Network based Generative Models for Non-Iterative Diverse Candidate Generation"

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Maximum independent set (MIS)

- Given an undirected graph g, an independent set is a set of vertices x where every pair of vertices are not neighbours

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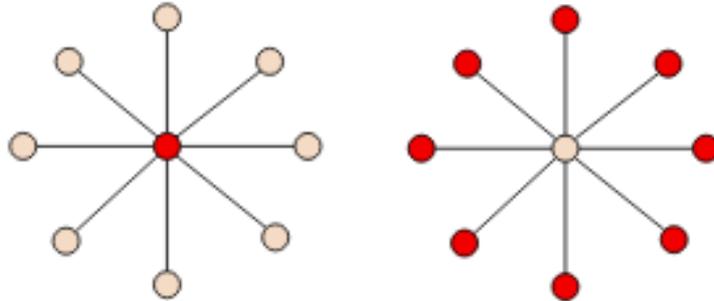
Maximum independent set (MIS)

- Given an undirected graph g, an independent set is a set of vertices x where every pair of vertices are not neighbours

- MIS: find largest independent set x

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Optimization as probabilistic inference

- $R(x|g) \leftarrow$ exponential of "number of vertices in x"
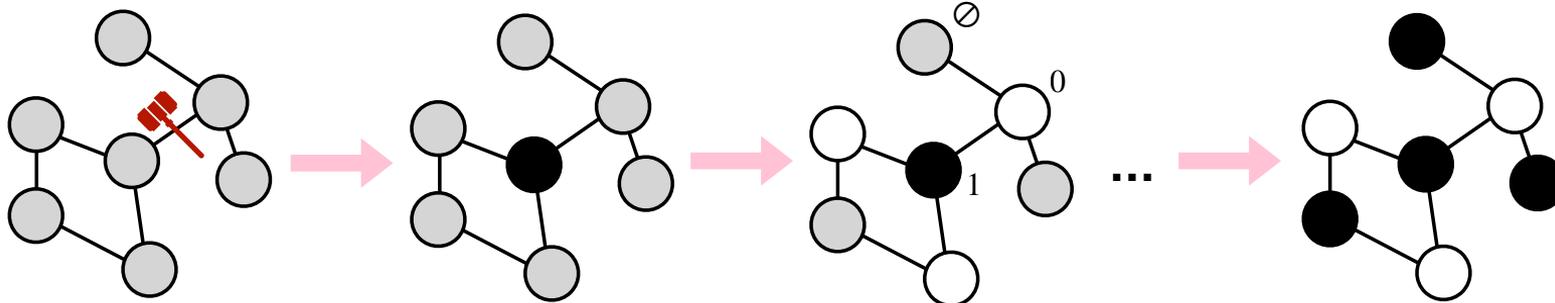
Optimization as probabilistic inference

- $R(x|g) \leftarrow$ exponential of "number of vertices in x"
- Instead of maximize $R(x|g)$

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Optimization as probabilistic inference

- $R(x|g) \leftarrow$ exponential of "number of vertices in x"
- Instead of maximize $R(x|g)$
- train a GFlowNet to sample prop to (tempered) reward

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Designing MDPs for GFlowNets
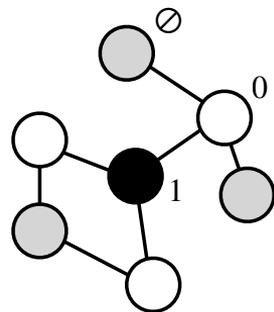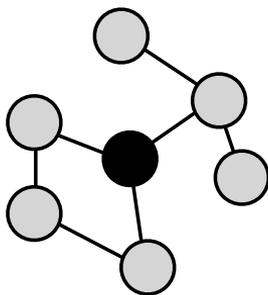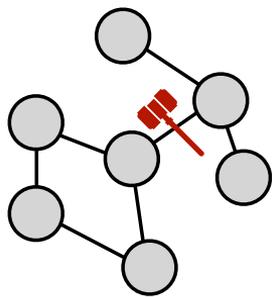
GFlowNet conditional
on graph structure *g*

Designing MDPs for GFlowNets

GFlowNet conditional
on graph structure g

intermediate state
$s \in \{0, 1, \oslash\}^{|V|}$

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Designing MDPs for GFlowNets

GFlowNet conditional on graph structure g

intermediate state $s \in \{0,1,\oslash\}^{|V|}$

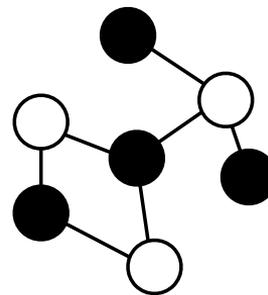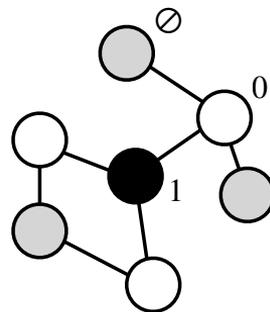terminating state $x \in \{0,1\}^{|V|}$

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Designing MDPs for GFlowNets

GFlowNet conditional on graph structure g

intermediate state $s \in \{0,1,\oslash\}^{|V|}$

terminating state $x \in \{0,1\}^{|V|}$

action

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Designing MDPs for GFlowNets

GFlowNet conditional on graph structure g

intermediate state $s \in \{0, 1, \oslash\}^{|V|}$

terminating state $x \in \{0, 1\}^{|V|}$

action

transition

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Designing MDPs for GFlowNets
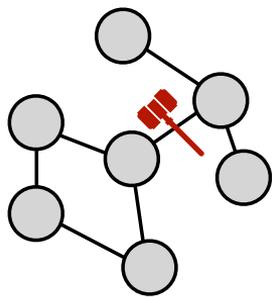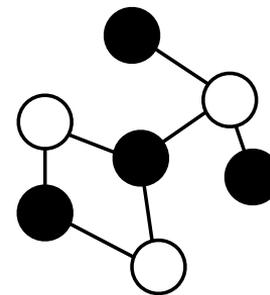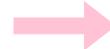

GFlowNet conditional on graph structure g

intermediate state $s \in \{0,1,\oslash\}^{|V|}$

terminating state $x \in \{0,1\}^{|V|}$
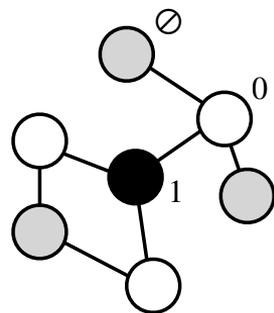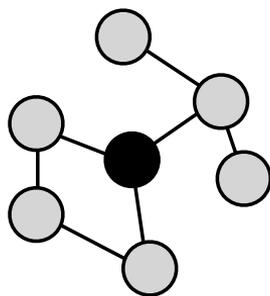
action

transition

reward / energy: number of black nodes

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Designing MDPs for GFlowNets

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Factors affecting training efficiency

- large scale problems
  - GPU memory not enough
    for trajectory-level loss

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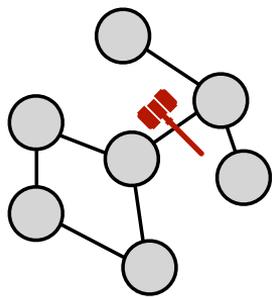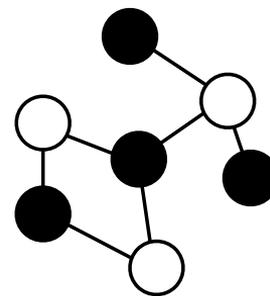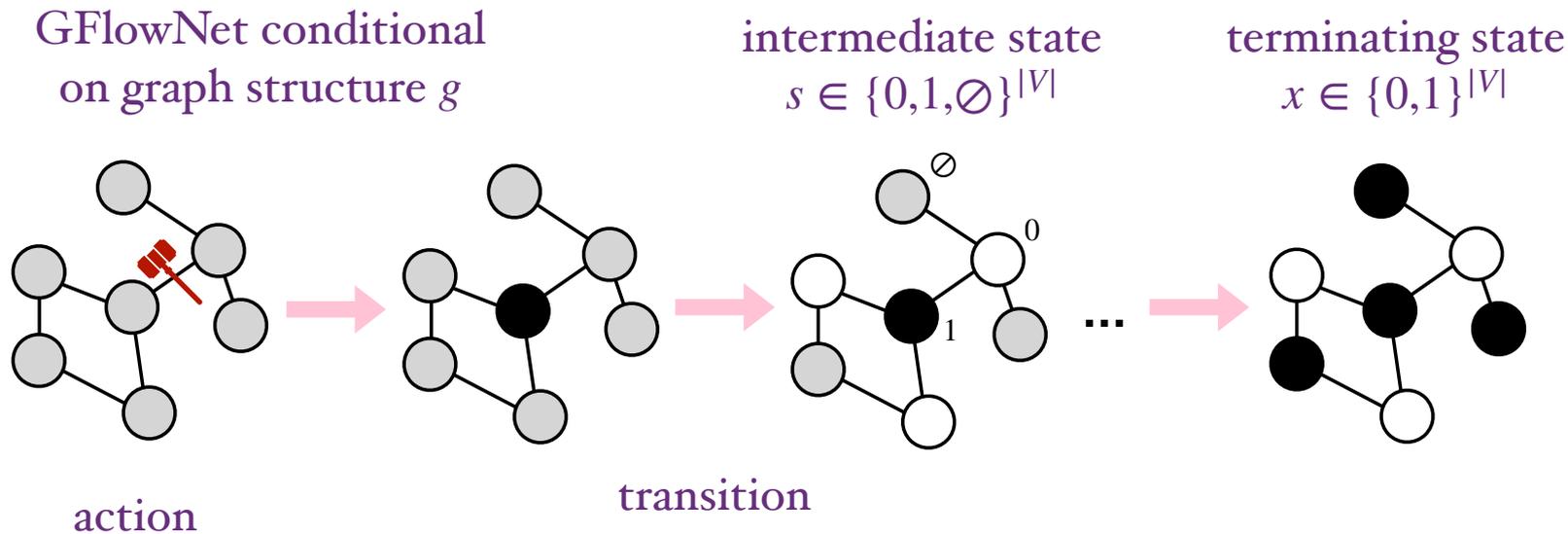
Factors affecting training efficiency

- large scale problems
  - GPU memory not enough for trajectory-level loss

$$\mathscr{L}(\tau; \theta) = \frac{1}{n} \sum_{t=0}^{n-1} \ell_{\mathrm{DB}}(s_t, s_{t+1}; \theta)$$

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Factors affecting training efficiency

- large scale problems
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- Transition-based training

Deleu, et al. Bayesian Structure Learning with Generative Flow Networks. UAI 2022.

Factors affecting training efficiency

- large scale problems
  - GPU memory not enough for trajectory-level loss
- Transition-based training
  - $\mathscr{L}(\theta) = \dfrac{1}{B} \sum\limits_{b=1}^{B} \ell_{\mathrm{DB}}(s^b, s'^b; \theta)$

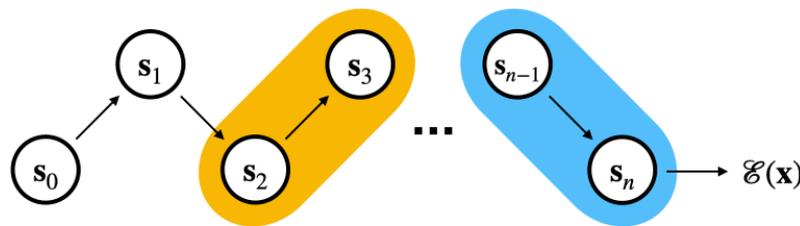Deleu, et al. Bayesian Structure Learning with Generative Flow Networks. UAI 2022.

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Factors affecting training efficiency

- large scale problems
  - GPU memory not enough for trajectory-level loss
- Transition-based training
  - $$\mathscr{L}(\theta) = \frac{1}{B} \sum_{b=1}^{B} \ell_{\mathrm{DB}}(s^b, s'^b; \theta)$$
- Intermediate signals
  - forward-looking (FL)

Deleu, et al. Bayesian Structure Learning with Generative Flow Networks. UAI 2022.

Pan, et al. Better Training of GFlowNets with Local Credit and Incomplete Trajectories. ICML 2023.

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Factors affecting training efficiency

- large scale problems
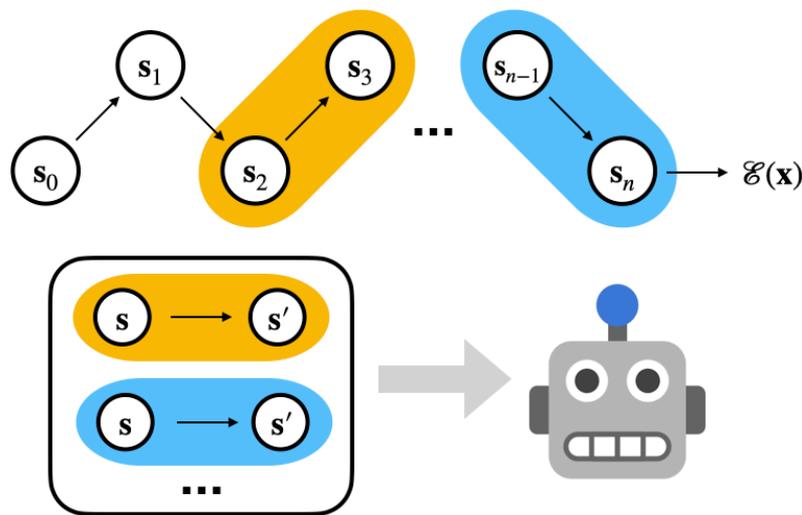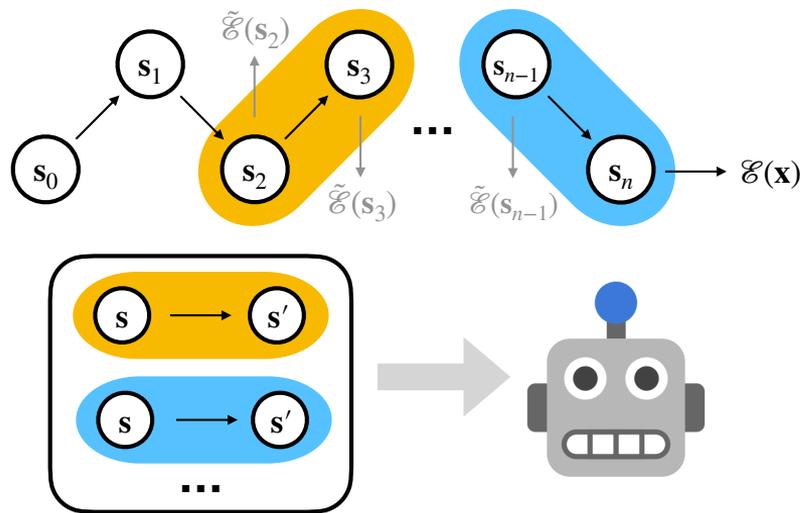 - GPU memory not enough for trajectory-level loss
- Transition-based training

  - $$\mathscr{L}(\theta) = \frac{1}{B} \sum_{b=1}^{B} \ell_{\mathrm{DB}}(s^b, s'^b; \theta)$$

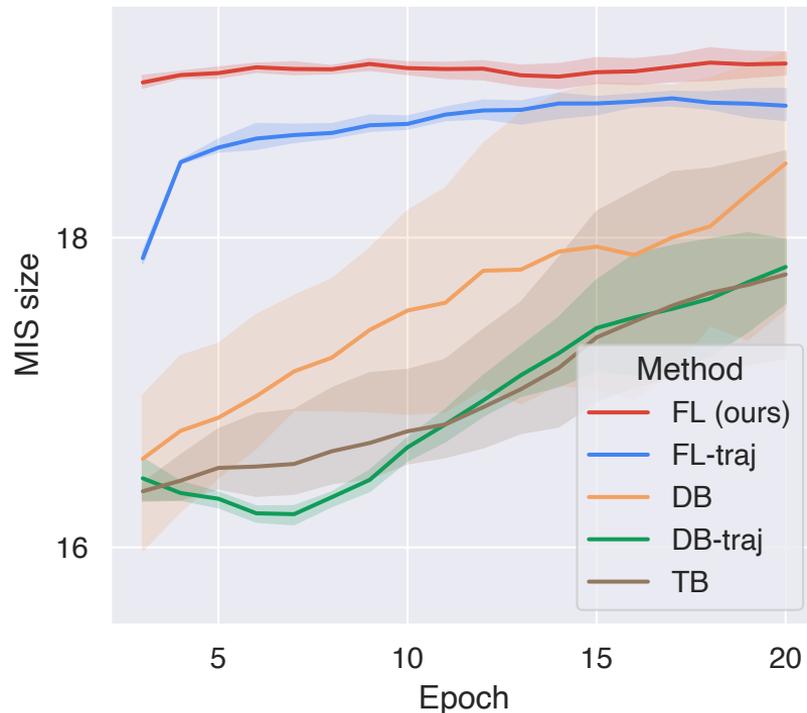- Intermediate signals
  - forward-looking (FL)

Deleu, et al. Bayesian Structure Lear
Pan, et al. Better Training of GFlow

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MIS results

Method	Type	Small			Large			SATLIB		
		Size ↑	Drop ↓	Time ↓	Size ↑	Drop ↓	Time ↓	Size ↑	Drop ↓	Time ↓
Gurobi	OR	19.98	0.01%	47:34	40.90	5.21%	2:10:26	425.95	0.00%	3:43:19
KaMIS	OR	20.10	0.00%	1:24:12	43.15	0.00%	2:03:36	425.96	0.00%	4:15:41
PPO	UL	19.01	5.42%	1:17	32.32	25.10%	7:33	421.49	1.05%	13:12
Intel	SL	18.47	8.11%	13:04	34.47	20.12%	20:17	—	—	—
DGL	SL	17.36	13.61%	12:47	34.50	20.05%	23:54	—	—	—
Ours	UL	**19.18**	4.57%	0:32	**37.48**	13.14%	04:22	**423.54**	0.57%	23:13

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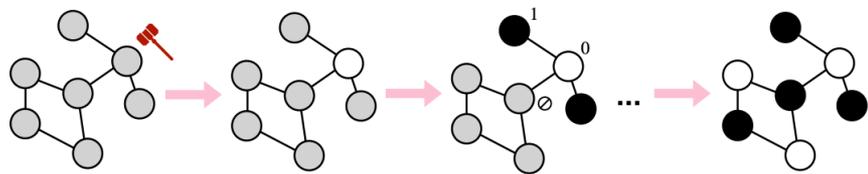# Other CombOpt problems
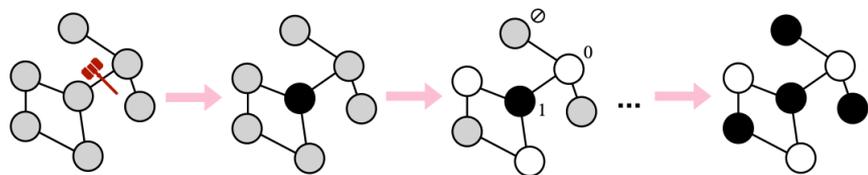
(a) Independent set
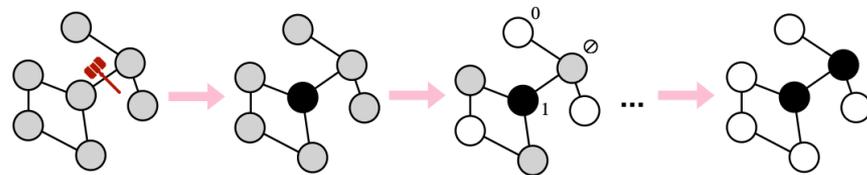
(b) Clique

(c) Dominating set

(d) Cut

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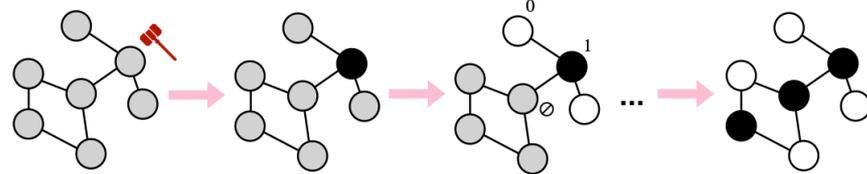
Other problem results

METHOD	TYPE	MC			MDS			MCUT		
		SIZE ↑	DROP ↓	TIME ↓	SIZE ↓	GAP ↓	TIME ↓	SIZE ↑	DROP ↓	TIME ↓
GUROBI	OR	19.05	0.00%	1:55	27.89	0.00%	1:47	732.47	0.00%	13:04
SDP	OR	—	—	—	—	—	—	700.36	4.38%	35:47
GREEDY	H	13.53	28.98%	0:25	37.39	25.41%	2:13	688.31	6.03%	0:13
MFA	H	14.82	22.15%	0:27	36.36	23.29%	2:56	**704.03**	3.88%	1:36
ERDOS	UL	12.02	36.90%	0:41	30.68	9.09%	1:00	693.45	5.33%	0:46
ANNEAL	UL	14.10	25.98%	0:41	29.24	4.62%	1:01	696.73	4.88%	0:45
OURS	UL	**16.24**	14.75%	0:42	**28.61**	2.52%	2:20	**704.30**	3.85%	2:57

Thank you for listening!

https://github.com/zdhNarsil/Awesome-GFlowNets