Learning Combinatorial Optimization Algorithms over Graphs

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Approach

Input: Graph $G = (V, E)$, weights $w(u, v)$ for $(u, v) \in E$

Algorithm design pattern: Greedy

Feasible solution constructed by successively adding nodes to solution

State representation: Graph embedding

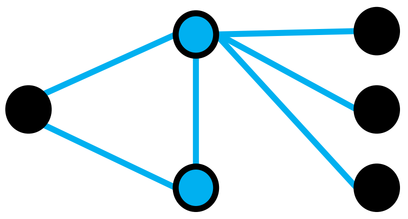
Algorithm training: Fitted Q-learning

Outline

1. **Greedy algorithms**
2. Graph representation
3. RL formulation
4. Q-learning
5. Experiments

Minimum vertex cover

Find smallest vertex subset such that each edge is covered

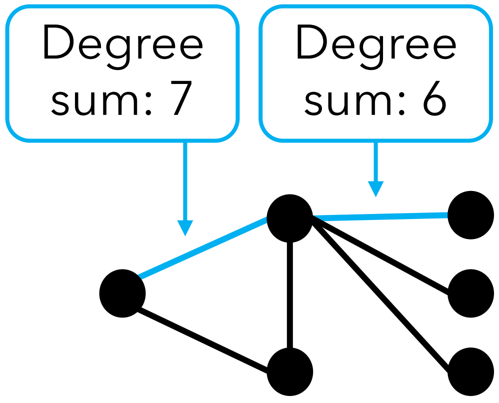


Minimum vertex cover

Find smallest vertex subset such that each edge is covered

2-approximation:

Greedily add vertices of edge with **maximum degree sum**



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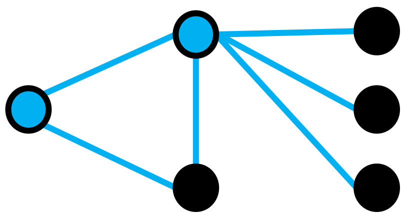
Scoring function that guides greedy algorithm



Maximum cut

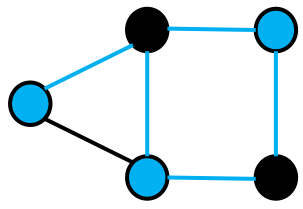
Find partition $(S, V \setminus S)$ of nodes that maximizes

$$\sum_{(u,v)\in C} w(u,v)$$

where $C = \{(u,v) \in E\colon u \in S, v \notin S\}$

If $w(u,v) = 1$ for all $(u,v) \in E$:

$$\sum_{(u,v)\in C} w(u,v) = 5$$



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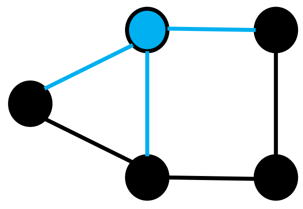
Greedy: move node from one side of cut to the other

Move node that results in the largest improvement in cut weight



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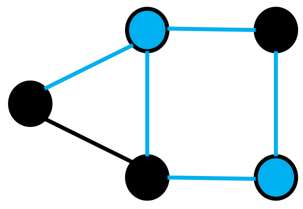
Scoring function that guides greedy algorithm



General greedy algorithm formulation

1. **Partial solution** is an ordered list $S = (v_1, v_2, \dots, v_{|S|}), v_i \in V$
2. ***Helper function*** $h(S)$ maps S to combinatorial structure, eg:
   - **Maxcut:** $h(S)$ returns cut $C = \{(u,v) \in E : u \in S, v \notin S\}$
   - **TSP:** $h(S)$ maintains a partial tour according to order of nodes in S
   - **Min vertex cover:** $h(S)$ does nothing
3. **Quality** of S evaluated by function $c(h(S), G)$, e.g.:
   - **Maxcut:** $c(h(S), G) = \sum_{(u,v) \in C = h(S)} w(u,v)$
   - **TSP:** $c(h(S), G) = -\sum_{i=1}^{|S|-1} w(S[i], S[i+1]) - w\big(S[|S|], S(1)\big)$
   - **Min vertex cover:** $c(h(S), G) = -|S|$

General greedy algorithm formulation

4. Add node that maximizes an evaluation function $Q(h(S), v)$:

$$S \leftarrow (S, v^*) \text{ where } v^* = \operatorname*{argmax}_{v \notin S} Q(h(S), v)$$

5. Terminate based on termination criterion $t\big(h(S)\big)$

This paper: Use RL to learn evaluation function $\hat{Q}(h(S), v; \Theta)$

Model parameters

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Representation: graph embedding

- $x_v = \begin{cases} 1 & \text{if } v \in S \\ 0 & \text{else} \end{cases}$
- Compute embedding over T iterations ($\boldsymbol{\mu}_v^{(0)} = \mathbf{0}$):

$$\boldsymbol{\mu}_v^{(t+1)} \leftarrow \mathrm{relu}\left(\boldsymbol{\theta}_1 x_v + \boldsymbol{\theta}_2 \sum_{u \in N(v)} \boldsymbol{\mu}_u^{(t)} + \boldsymbol{\theta}_3 \sum_{u \in N(v)} \mathrm{relu}\big(\boldsymbol{\theta}_4 w(v,u)\big)\right)$$

Trainable parameters

structure2vec framework of Dai et al. [ICML'16]

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(Usually $T = 4$)
- $\hat{Q}(h(S), v; \Theta) = \boldsymbol{\theta}_5^\top \mathrm{relu}\left(\underbrace{\left[\boldsymbol{\theta}_6 \sum_{u \in V} \boldsymbol{\mu}_u^{(T)}, \boldsymbol{\theta}_7 \boldsymbol{\mu}_u^{(T)}\right]}_{\text{Concatenation}}\right)$

structure2vec framework of Dai et al. [ICML'16]

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Reinforcement learning formulation

State: $\sum_{u \in V} \boldsymbol{\mu}_u^{(T)}$

Action: Choose vertex $v \in V \setminus S$ to add to solution

Transition (deterministic): For chosen $v \in V \setminus S$, set $x_v = 1$

Reinforcement learning formulation

Reward: $r(S, v)$ is objective change when move to $S' = (S, v)$

$$r(S, v) = c(h(S'), G) - c(h(S), G)$$

$c(h(\emptyset), G) = 0$, so cumulative reward of **terminal state** $\hat{S}$ is

$$\sum_{i=1}^{|\hat{S}|} r(S_i, v_i) = c\left(h\left(\hat{S}\right), G\right)$$

Policy (deterministic): $\pi(v|S) = \begin{cases} 1 & \text{if } v = \operatorname{argmax}_{v' \notin S} \hat{Q}(h(S), v'; \Theta) \\ 0 & \text{else} \end{cases}$

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Q-learning

Recall standard (1-step) Q-learning:

$$\min_{\Theta} \left(y - \hat{Q}(h(S_t), v_t; \Theta) \right)^2$$

where $y = r(S_t, v_t) + \gamma \max_{v'} \hat{Q}(h(S_{t+1}), v'; \Theta)$

Challenge:

- Final objective value only revealed after many steps
- 1-step update may be too myopic

Instead, use ***n*-step** Q-learning [Watkins, '89]

n-step Q-learning

$$\min_{\Theta}\left(y-\hat{Q}(h(S_t),v_t;\Theta)\right)^2$$

where $y=\sum_{i=0}^{n-1}\gamma^i r(S_{t+1},v_{t+i})+\gamma^n \max_{v'}\hat{Q}(h(S_{t+n}),v';\Theta)$

Q-learning for the greedy algorithm

initialize set $M = \emptyset$

for episode $e = 1, \ldots, L$:

    sample graph G from underlying distribution D

    initialize state to empty $S_1 = ()$

Q-learning for the greedy algorithm

for episode $e = 1, \dots, L$:

for step $t = 1, \dots, T$:

$$v_t = \begin{cases} \text{random node } v \notin S_t & \text{with probability } \epsilon \\ \operatorname*{argmax}_{v \notin S_t} \hat{Q}(h(S_t), v; \Theta) & \text{otherwise} \end{cases}$$

add v_t to partial solution $S_{t+1} = (S_t, v_t)$

if $t \geq n$:

experience replay

add tuple $(S_{t-n}, v_{t-n}, \sum_{i=1}^{n} R(S_{t-i}, v_{t-i}), S_t)$ to M

sample batch $B \sim M$

update Θ using SGD over B

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5. **Experiments**

Approximation ratio

Results measured in terms of approximation ratio

$$\frac{\text{Algorithm's solution}}{\text{OPT}}$$

Min vertex cover

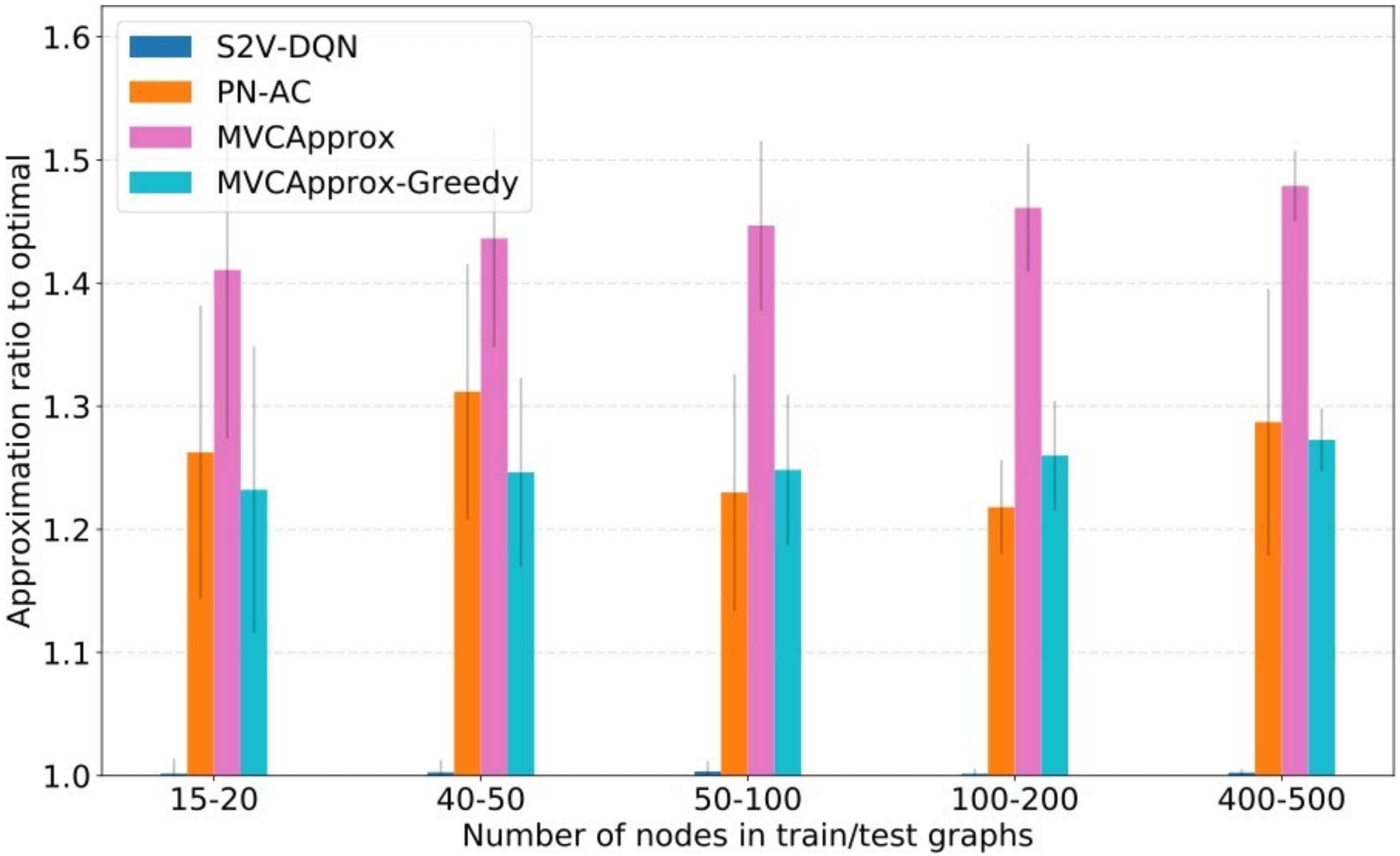
Barabasi-Albert
random graphs

Paper's approach

Another DL approach
[Bello et al., arXiv'16]

2-approximation
algorithm

Greedy algorithm
from first few slides



Max cut

Barabasi-Albert
random graphs

Paper's approach

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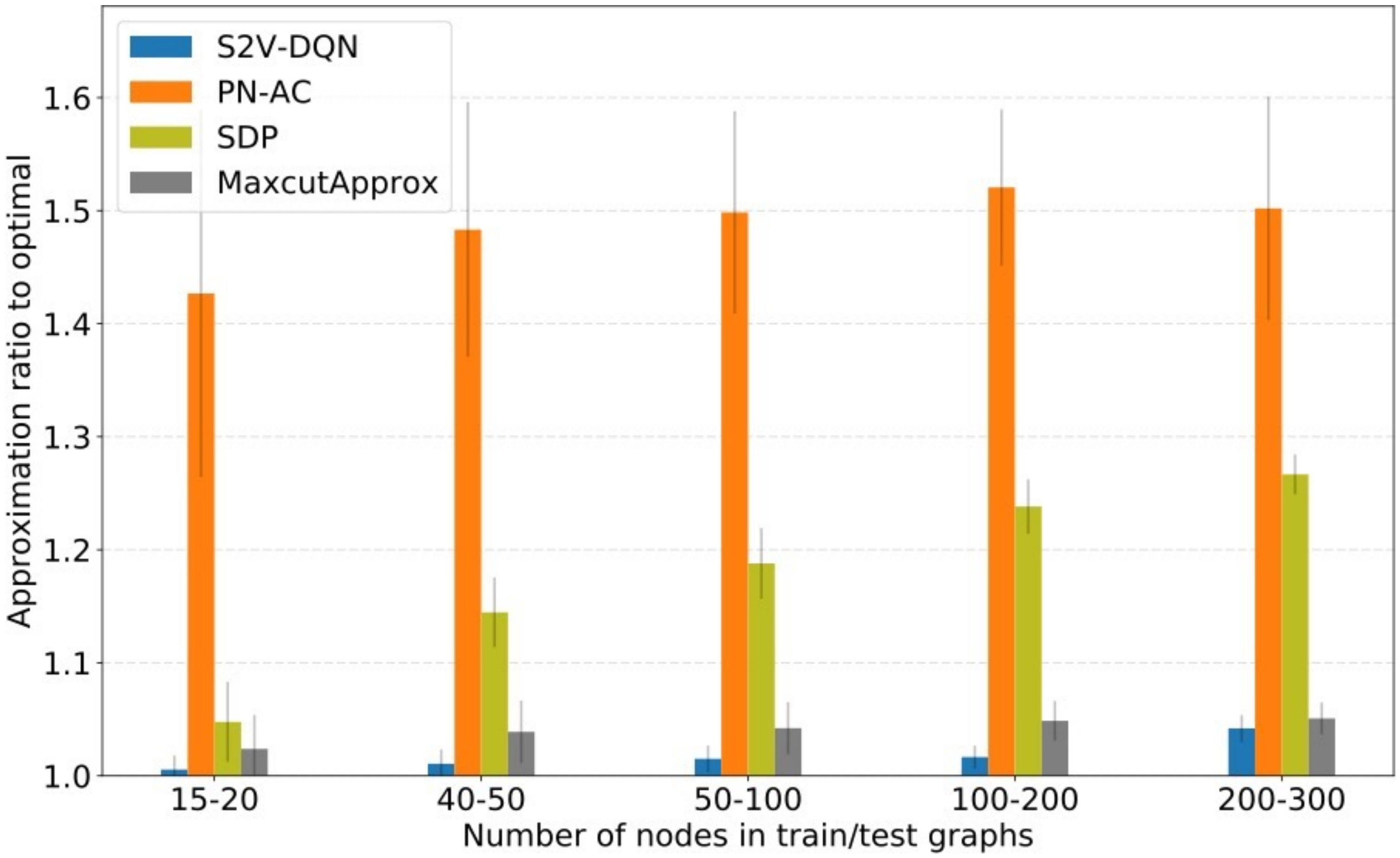
Goemans-Williamson
algorithm

Greedy algorithm
from first few slides



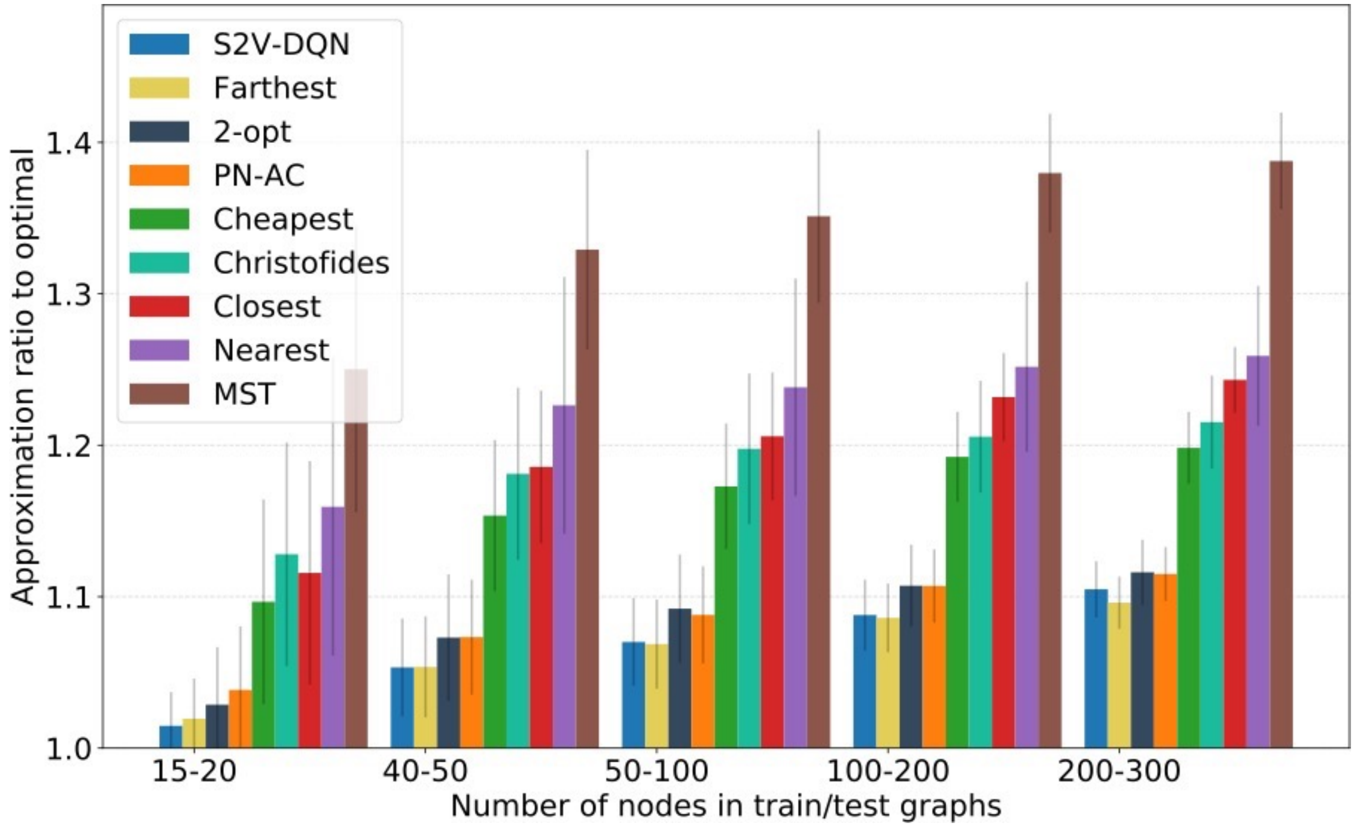
TSP

Uniform random points on 2-D grid

Paper's approach

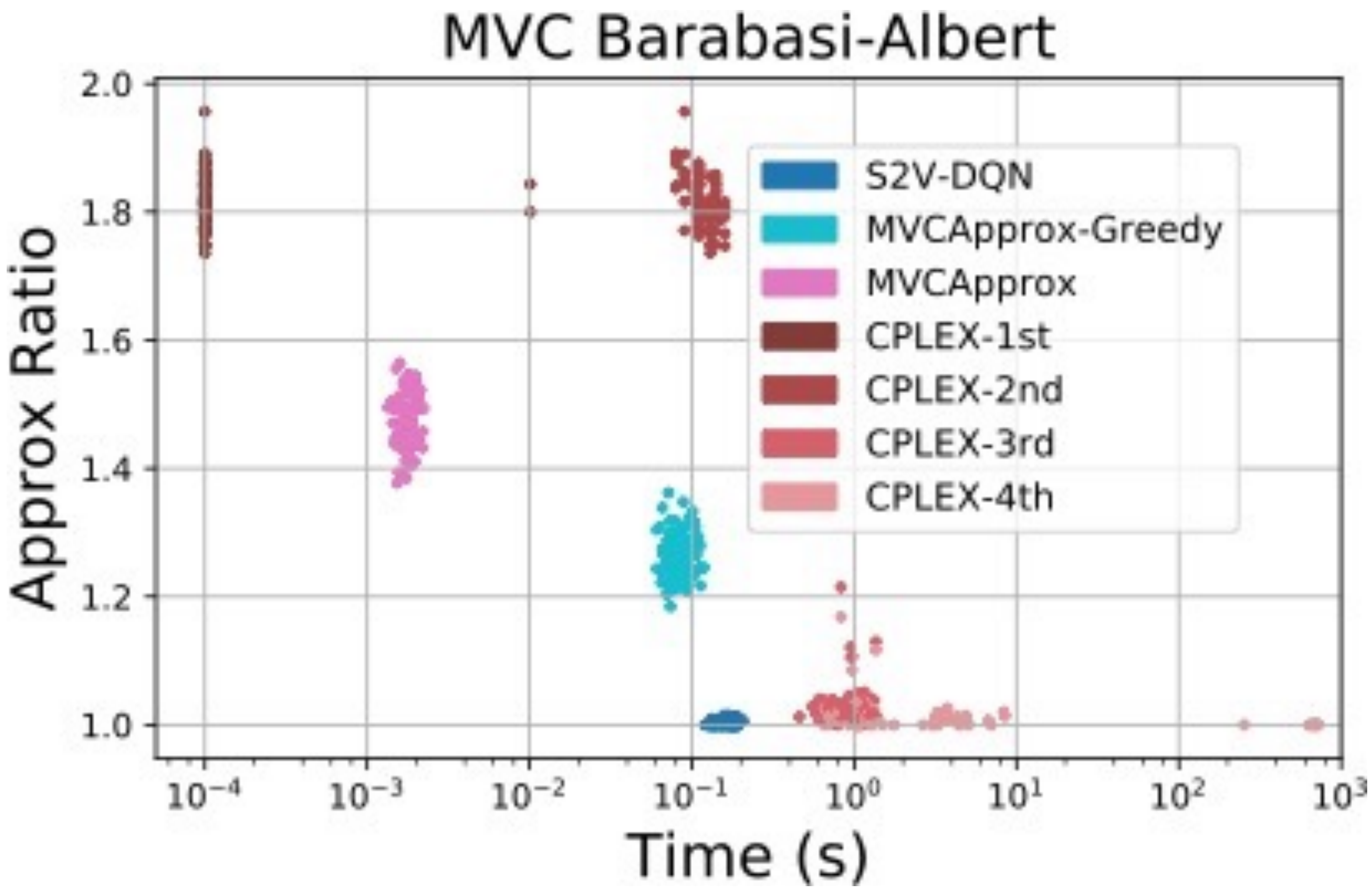
- Initial subtour: 2 cities that are farthest apart
- Repeat the following:
  - Choose city that's *farthest* from any city in the subtour
  - Insert in position where it causes the smallest distance increase

[Rosenkrantz et al., SIAM JoC'77]

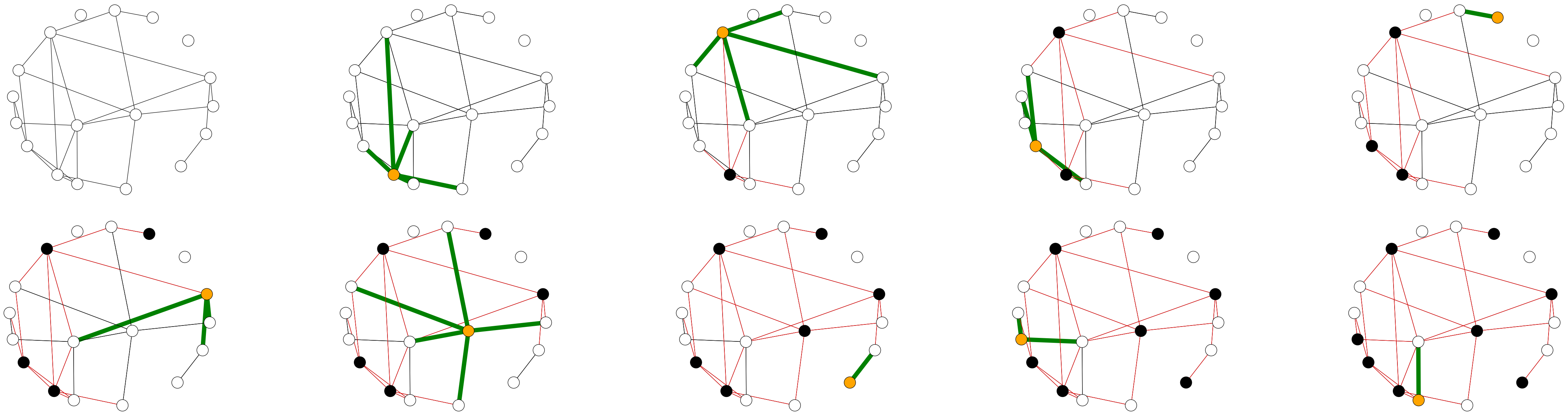


Runtime comparisons

CPLEX-1st: 1st feasible solution found by CPLEX



Min vertex cover visualization



Nodes seem to be selected to balance between:

- Degree
- Connectivity of the remaining graph

Overview

Learn greedy heuristics for hard combinatorial problem

Approach based on graph representation + RL

Suggest approach could be used for **algorithm discovery**

“New and interesting” greedy strategies

“which **intuitively make sense** but have **not been analyzed** before,” thus could be a “good **assistive tool** for discovering new algorithms.”