

SOLVING NP-HARD PROBLEMS ON GRAPHS WITH EXTENDED ALPHAGO ZERO

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ABSTRACT

There have been increasing challenges to solve combinatorial optimization problems by machine learning. Khalil et al. (NeurIPS 2017) proposed an end-to-end reinforcement learning framework, which automatically learns graph embeddings to construct solutions to a wide range of problems. However, it sometimes performs poorly on graphs having different characteristics than training graphs. To improve its generalization ability to various graphs, we propose a novel learning strategy based on AlphaGo Zero, a Go engine that achieved a superhuman level without the domain knowledge of the game. We redesign AlphaGo Zero for combinatorial optimization problems, taking into account several differences from two-player games. In experiments on five NP-hard problems such as MINIMUMVERTEX-COVER and MAXCUT, our method, with only a policy network, shows better generalization than the previous method to various instances that are not used for training, including random graphs, synthetic graphs, and real-world graphs. Furthermore, our method is significantly enhanced by a test-time Monte Carlo Tree Search which makes full use of the policy network and value network. We also compare recently-developed graph neural network (GNN) models, with an interesting insight into a suitable choice of GNN models for each task.

1 INTRODUCTION

There is no polynomial-time algorithm found for NP-hard problems [7], but they often arise in many real-world optimization tasks. Therefore, a variety of algorithms have been developed in a long history, including approximation algorithms [2, 14], meta-heuristics based on local searches such as simulated annealing and evolutionary computation [15, 10], general-purpose exact solvers such as CPLEX¹ and Gurobi [16], and problem-specific exact solvers [1, 25].

Recently, machine learning approaches have been actively investigated to solve combinatorial optimization, with the expectation that the combinatorial structure of the problem can be automatically learned without complicated hand-crafted heuristics. In the early stage, many of these approaches focused on solving specific problems [17, 5] such as the traveling salesperson problem (TSP). Khalil et al. [19] proposed a general framework to solve combinatorial problems by a combination of reinforcement learning and graph embedding, which attracted attention for the following two reasons: It does not require any knowledge on graph algorithms other than greedy selection based on network outputs. Furthermore, it learns algorithms without any training dataset. Thanks to these advantages, the framework can be applied to a diverse range of problems over graphs and it also performs much better than previous learning-based approaches. However, we observed poor empirical performance on some graphs having different characteristics (e.g., synthetic graphs and real-world graphs) than random graphs that were used for training, possibly because of the limited exploration space of their Q-learning method.

In this paper, to overcome its weakness, we propose a novel solver, named CombOpt Zero. CombOpt Zero is inspired by AlphaGo Zero [33], a superhuman engine of Go, which conducts Monte Carlo Tree Search (MCTS) to train deep neural networks. AlphaGo Zero was later generalized to AlphaZero [34] so that it can handle other games; however, its range of applications is limited to two-player games whose state is win/lose (or possibly draw). We extend AlphaGo Zero to a bunch of combinatorial

¹www.cplex.com

problems by a simple normalization technique based on random sampling. In the same way as AlphaGo Zero, CombOpt Zero automatically learns a policy network and value network by self-play based on MCTS. We train our networks for five kinds of NP-hard tasks and test on different instances including standard random graphs (e.g., the Erdős-Renyi model [11] and the Barabási-Albert model [3]), benchmark graphs, and real-world graphs. We show that, with only a greedy selection on the policy network, CombOpt Zero has a better generalization to a variety of graphs than the existing method, which indicates that the MCTS-based training strengthens the exploration of various actions. When more computation time is allowed, using the MCTS at test time with the full use of both the policy network and value network significantly improves the performance. Furthermore, we combine our framework with several graph neural network models [21, 39, 28], and experimentally demonstrate that an appropriate choice of models contributes to improving the performance with a significant margin.

2 BACKGROUND

In this section, we introduce the background which our work is based on.

2.1 MACHINE LEARNING FOR COMBINATORIAL OPTIMIZATION

Machine learning approaches for combinatorial optimization problems have been studied in the literature, starting from Hopfield & Tank [17], who applied a variant of neural networks to small instances of Traveling Salesperson Problem (TSP). With the success of deep learning, more and more studies were conducted including Bello et al. [5], Kool et al. [23] for TSP and Wang et al. [37] for MAXSAT.

Khalil et al. [19] proposed an end-to-end reinforcement learning framework S2V-DQN, which attracted attention because of promising results in a wide range of problems over graphs such as MINIMUMVERTEXCOVER and MAXCUT. Another advantage of this method is that it does not require domain knowledge on specific algorithms or any training dataset. It optimizes a deep Q-network (DQN) where the Q-function is approximated by a graph embedding network, called `structure2vec` (S2V) [9]. The DQN is based on their reinforcement learning formulation, where each action is picking up a node and each state represents the “sequence of actions”. In each step, a partial solution $S \subset V$, i.e., the current state, is expanded by the selected vertex $v^* = \arg \max_{v \in V(h(S))} Q(h(S), v)$ to (S, v^*) , where $h(\cdot)$ is a fixed function determined by the problem that maps a state to a certain graph, so that the selection of v will not violate the problem constraint. For example, in MAXIMUMINDEPENDENTSET, $h(S)$ corresponds to the subgraph of the input graph $G = (V, E)$ induced by $V \setminus (S \cup \mathcal{N}(S))$, where $\mathcal{N}(S)$ is the open neighbors of S . The immediate reward is the change in the objective function. The Q-network, i.e., S2V learns a fixed dimensional embedding for each node.

In this work, we mitigate the issue of S2V-DQN’s generalization ability. We follow the idea of their reinforcement learning setting, with a different formulation, and replace their Q-learning by a novel learning strategy inspired by AlphaGo Zero. Note that although some studies combine classic heuristic algorithms and learning-based approaches (using dataset) to achieve the state-of-the-art performance [26, 12], we stick to learning without domain knowledge and dataset in the same way as S2V-DQN.

2.2 ALPHAGO ZERO

AlphaGo Zero [35] is a well-known superhuman engine designed for use with the game of Go. It trains a deep neural network f_θ with parameter θ by reinforcement learning. Given a state (game board), the network outputs $f_\theta(s) = (p, v)$, where p is the probability vector of each move and $v \in [-1, 1]$ is a scalar denoting the state value. If v is close to 1, the player who takes a corresponding action from state s is very likely to win.

The fundamental idea of AlphaGo Zero is to enhance its own networks by self-play. For this self-play, a special version of Monte Carlo Tree Search (MCTS) [22], which we describe later, is used. The network is trained in such a way that the policy imitates the enhanced policy by MCTS π , and the value imitates the actual reward from self play z (i.e. $z = 1$ if the player wins and $z = -1$ otherwise).

More formally, it learns to minimize the loss

$$\mathcal{L} = (z - v)^2 + \text{CrossEntropy}(\mathbf{p}, \boldsymbol{\pi}) + c_{\text{reg}} \|\boldsymbol{\theta}\|_2^2, \quad (1)$$

where c_{reg} is a nonnegative constant for L_2 regularization.

MCTS is a heuristic search on game trees. In AlphaGo Zero, the search tree is a rooted tree, where each node corresponds to a state and the root is the initial state. Each edge (s, a) denotes action a at state s and stores a tuple $(N(s, a), W(s, a), Q(s, a), P(s, a))$, where $N(s, a)$ is the visit count, $W(s, a)$ and $Q(s, a)$ are the total and mean action value respectively, and $P(s, a)$ is the prior probability. One iteration of MCTS consists of three parts: *select*, *expand*, and *backup*. First, from the root node, we keep choosing an action that maximizes an upper confidence bound

$$Q(s, a) + c_{\text{puct}} P(s, a) \frac{\sqrt{\sum_{a'} N(s, a')}}{1 + N(s, a)}, \quad (2)$$

where c_{puct} is a non-negative constant (*select*). Once it reaches to unexplored node s , then the edge values are initialized using the network prediction $(\mathbf{p}, v) = f_{\theta}(s)$ (*expand*). After expanding a new node, each visited edge is traversed and its edge values are updated (*backup*) so that Q maintain the mean of state evaluations over simulations: $Q(s, a) = \frac{1}{N(s, a)} \sum_{s' | s, a \rightarrow s'} v_{s'}$, where the sum is taken over those states reached from s after taking action a . After some iterations, the probability vector $\boldsymbol{\pi}$ is calculated by $\pi_a = \frac{N(s_0, a)^{1/\tau}}{\sum_b N(s_0, b)^{1/\tau}}$ for each $a \in A_{s_0}$, where τ is a temperature parameter.

AlphaGo Zero defeated its previous engine AlphaGo [33] with 100-0 score without human knowledge, i.e., the records of the games of professional players and some known techniques in the history of Go. We are motivated to take advantage of the AlphaGo Zero technique in our problem setting since we also aim at training deep neural networks for discrete optimization without domain knowledge. However, we cannot directly apply AlphaGo Zero, which was designed for two-player games, to combinatorial optimization problems. Section 3.2 and 3.3 explains how we resolve this issue.

2.3 GRAPH NEURAL NETWORK

A Graph Neural Network (GNN) is a neural network that takes graphs as input. Kipf & Welling [21] proposed the *Graph Convolutional Network* (GCN) inspired by spectral graph convolutions. Because of its scalability, many variants of spatial based GNN were proposed. Many of them can be described as a Message Passing Neural Network (MPNN) [13]. They recursively aggregate neighboring feature vectors to obtain node embeddings that capture the structural information of the input graph. The *Graph Isomorphism Network* (GIN) [39] is one of the most expressive MPNNs in terms of graph isomorphism. Although they have a good empirical performance, some studies point out the limitation of the representation power of MPNNs [39, 30]. Maron et al. [27] proposed an Invariant Graph Network (IGN) using tensor representations of a graph and was shown to be universal [29, 18]. Since it requires a high-order tensor in middle layers, which is impractical, Maron et al. [28] proposed 2-IGN+, a scalable and powerful model.

All of these models, as well as S2V [9] used in S2V-DQN, are compared in the experiments to test the difference in the performance for combinatorial optimization. The detail of each model is described in Appendix B.

3 METHOD

In this section, we give a detailed explanation of our algorithm to solve combinatorial optimization problems over graphs. First, we introduce our reinforcement learning formulation for NP-hard problems. Then, we explain the basic ideas of our proposed CombOpt Zero in light of the difference between 2-player games and our formulation. Finally, we describe the whole algorithm.

3.1 REDUCTION TO MDP

Following S2V-DQN [19], we reduce graph problems into a reinforcement learning setting. Here, we introduce our formulation based on a Markov Decision Process (MDP) [4]. A deterministic MDP is defined as (S, A_s, T, R) , where S is a set of states, A_s is a set of actions from the state $s \in S$,

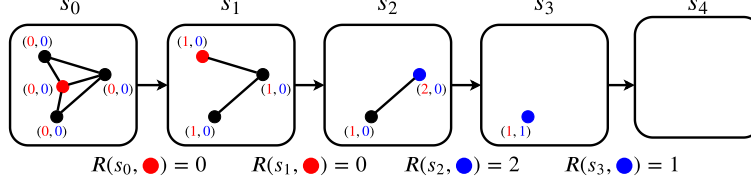


Figure 1: **Example of MaxCut MDP transitions.** In the transition sequence, the upper left and center node are colored in ●, the right and lower left node are colored in ●, resulting in the cumulative reward 3.

$T : S \times A_s \rightarrow S$ is a deterministic state transition function, and $R : S \times A_s \rightarrow \mathbb{R}$ is an immediate reward function. In our problem setting on graphs, each state $s \in S$ is represented as a *labeled* graph, a tuple $s = (G, d)$. $G = (V, E)$ is a graph and $d : V \rightarrow L$ is a node-labeling function, where L is a label space.

For each problem, we have a set of terminal states S_{end} . Given a state s , we repeat selecting an action a from A_s and transiting to the next state $T(s, a)$, until $s \in S_{\text{end}}$ holds. By this process, we get a sequence of states and actions $[s_0, a_0, s_1, a_1, \dots, a_{N-1}, s_N]$ of N steps where $s_N \in S_{\text{end}}$, which we call a trajectory. For this trajectory, we can calculate the simple sum of immediate rewards $\sum_{n=0}^{N-1} R(s_n, a_n)$, and we define $r^*(s)$ be the maximum possible sum of immediate rewards out of all trajectories from state s . Let Init be a function that maps the input graph to the initial state. Our goal is to, given graph G_0 , obtain the maximum sum of rewards $r^*(\text{Init}(G_0))$.

Many combinatorial optimization problems can be accommodated in this framework by appropriately defining L , A_s , T , R , Init , and S_{end} (see Appendix G). Now we take MAXCUT as an example. Let $C \subset E$ be a cut set between $V' \subset V$ and $V \setminus V'$, i.e., $C = \{(u, v) \in E \mid u \in V', v \in V \setminus V'\}$. MAXCUT asks for a subset V' that maximizes the size of cut set C . Below, we explain our MDP formulation of MAXCUT.

In each action, we color a node by 0 or 1 and remove it while each node keeps track of how many adjacent nodes have been colored with each color. $A_s = \{(x, c) \mid x \in V, c \in \{0, 1\}\}$ denotes a set of possible coloring of a node, where (x, c) means coloring node x with color c . $L = \mathbb{N}^2$, representing the number of colored (and removed) nodes in each color (i.e., l_0 is the number of (previously) adjacent nodes of x colored with 0, and same for l_1 , where $l = d(x)$). Init uses the same graph as G_0 and sets $d(x) = (0, 0)$ for all $x \in V$. $T(s, (x, c))$ increases the c -th value of $d(x')$ by one for $x' \in N(x)$ and removes x and neighboring edges from the graph. S_{end} is the states with the empty graphs. $R(s, (x, c))$ is the $(1 - c)$ -th (i.e., 1 if $c = 0$ and 0 if $c = 1$) value of $d(x)$, meaning the number of edges in the original graph which has turned out to be included in the cut set (i.e., colors of the two nodes are different).

Figure 1 shows some possible MDP transitions for MAXCUT. It is easy to check that finding a sequence that maximizes the sum of rewards is equivalent to solving the original problem. One of the important differences from the formulation of Khalil et al. [19] is that we do not limit the action space to a set of nodes. This flexibility enables the above formulation, where actions represent *a node coloring*. See Appendix F for the details.

3.2 EXTENDING ALPHAGO ZERO

We have seen that many combinatorial optimization problems can be reduced to the deterministic MDP formulation, which is similar to the problem setting of AlphaGo Zero. However, since AlphaGo Zero is designed exclusively for Go (or AlphaZero for two-player games), it still can not be directly applied for our MDP settings. Here, we explain how to extend AlphaGo Zero to our MDP formulation of combinatorial problems with respect to three main differences from Go.

Graph Input In our problem setting, the states are represented by (labeled) graphs of different sizes, while the boards of Go can be represented by 19×19 fixed-size matrix. This can be addressed easily

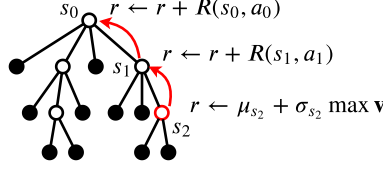


Figure 2: **Backup.** After estimating the reward of the expanded node, we iteratively update the rewards of its ancestors.

by adopting GNN instead of convolutional neural networks in AlphaGo Zero, just like S2V-DQN. The whole state $s = (G, d)$ can be given to GNN, where the coloring d is used as the node feature.

Range of Final Results While the final result of Go is only win or lose (or possible draw), the answer to combinatorial problems can take any integer or even real number. AlphaGo Zero models the state value with the range of $[-1, 1]$, meaning that the larger the value is, the more likely the player is to win. A naive extension of this is to directly predict the maximum possible sum of rewards $r^*(s)$. That may, however, grow infinitely in our problem setting usually depending on the graph size, which causes issues. In our preliminary experiments, it did not work well due to difficulty in balancing the scale in equation 1 or in equation 2. For example, in equation 2, the first term could be too large when the answer is large, causing less focus on $P(s, a)$ and $N(s, a)$. To mitigate these issues, we propose a reward normalization technique. Given a state s , the network outputs $(\mathbf{p}, \mathbf{q}) = f_\theta(s)$. While \mathbf{p} is the same as AlphaGo Zero (action probabilities), \mathbf{q} is a *vector* representing a *normalized* state action value instead of a scalar state value. Intuitively, \mathbf{q}_a predicts “how good the reward is compared to the solution obtained by random actions” when taking action a from state s . Formally, we train the network so that \mathbf{q}_a predicts $(R(s, a) + r^*(T(s, a)) - \mu_s) / \sigma_s$, where μ_s and σ_s are the mean and the standard deviation of the cumulative rewards by random plays from state s . Similarly, we also let $W(s, a)$ and $Q(s, a)$ hold the sum and mean of *normalized* action value estimations over the MCTS iterations. By virtue of this normalization, we no longer need to care about the difference of scales in equation 1 and equation 2. When we estimate the state value of s , we consider taking action a which maximizes \mathbf{q}_a and restoring the unnormalized value by μ_s and σ_s :

$$r_{\text{estim}}(s) = \begin{cases} 0 & (s \in S_{\text{end}}), \\ \mu_s + \sigma_s \cdot (\max_{a \in A_s} \mathbf{q}_a) & (\text{otherwise}). \end{cases} \quad (3)$$

Various Immediate Rewards Since the immediate reward of Go is always zero, the *backup* phase of AlphaGo Zero is simple: Update each edge value so that $Q(s, a)$ keeps the mean of state value predictions over expanded states from s after taking action a . Although we have various immediate rewards in our MDP formulations, all of these can be handled easily. Each time we go back to the parent node in the *backup*, we add the immediate reward of the edge to the current reward: $r \leftarrow r + R(s, a)$ when going up path (s, a) . Note that since we use normalization technique, r is initialized by equation 3. Figure 2 illustrates the process. We can apply the same strategy when calculating the normalized cumulative reward in data generation (See Section 3.3 for the details).

3.3 ALGORITHMS

Based on the discussion so far, now we are ready to introduce the whole algorithm of our proposed CombOpt Zero.

MCTS Each edge stores a tuple $(N(s, a), W(s, a), Q(s, a), P(s, a))$ in the same way as AlphaGo Zero. Additionally, each node s stores a tuple (μ_s, σ_s) , the mean and the standard deviation of the results by random plays. Given an initial state s_0 , we repeat the iterations of the three parts: *select*, *expand*, and *backup*. *Select* is same as AlphaGo Zero (keep selecting a child node that maximizes equation 2). Once we reach unexpanded node s , we *expand* the node. $(\mathbf{p}, \mathbf{q}) = f_\theta(s)$ is evaluated and each edge value is updated as $N(s, a) = 0$, $W(s, a) = 0$, $Q(s, a) = 0$, and $P(s, a) = \mathbf{p}_a$ for $a \in A_s$. At the same time, (μ_s, σ_s) is estimated by random sampling from s . In *backup*, for each node s' and the corresponding action a' in a backward pass, $N(s', a')$ is incremented by one in the same way as AlphaGo Zero. The difference is that $Q(s', a')$ is updated to hold the estimation of the

normalized mean reward from s' . We approximate the non-normalized state value by equation 3 and calculate the estimated cumulative reward from s' by adding the immediate reward each time we move back to the parent node (Figure 2 illustrates this process). After sufficient iterations, π is calculated from $N(s_0, a)$ in the same way as AlphaGo Zero. While the number of the iterations is fixed in AlphaGo Zero, in our proposed CombOpt Zero, since the size of action space differs by states, we make it proportional to the number of actions: $c_{\text{iter}}|A_s|$. Following AlphaGo Zero, we add Dirichlet noise to the prior probabilities only for the initial state s_0 to explore the various initial actions. The pseudocode is available in Algorithm 1 in Appendix A.

Training Following AlphaGo Zero, the training of CombOpt Zero is composed of three roles: *data generators*, *learners*, and *model evaluators*. The model that has performed best so far is shared among all of these three components. The *data generator* repeats generating self-play records for a randomly generated graph input, by the MCTS based on the current best model. The records are the sequence of (s, a, π, z') , which means action a was taken from s depending on the MCTS-enhanced policy π and the normalized final cumulative reward was z' . z' can be calculated in the same way as *backup* in MCTS: after generating the self-play trajectory, it first calculates the cumulative sum of immediate rewards for each state s in reverse order and normalizes them with μ_s and σ_s . The pseudocode of the data generator is available in Algorithm 2 in Appendix A. The *learner* randomly samples mini-batches from the generator’s data and updates the parameter of the best model so that it minimizes the loss

$$\mathcal{L} = (z' - q_a)^2 + \text{CrossEntropy}(\mathbf{p}, \boldsymbol{\pi}) + c_{\text{reg}} \|\theta\|_2^2. \quad (4)$$

We train q_a to be closer to the normalized cumulative reward z' . The *model evaluator* compares the updated model with the best one and stores the better one. Since we can not put two players in a match, the evaluator generates random graph instances each time and compare the performance on them.

4 EXPERIMENTS

In this section, we show some brief results of our experiments mainly on MINIMUMVERTEXCOVER, MAXCUT, and MAXIMUMCLIQUE. Refer to Appendix I for the full results and Appendix H for further analyses for each problem.

Competitors Since we aim at solving combinatorial optimization problems without domain knowledge or training dataset, S2V-DQN is our main competitor. Additionally, for each problem, we prepared some known heuristics or approximation algorithms to compare with. For instance, for MINIMUMVERTEXCOVER, we implemented a simple randomized 2-approximation algorithm (2-approx) and an interger programming by CPLEX solver. For MAXCUT, we used a randomized algorithm by semidefinite programming [14] and two heuristics, non-linear optimization with local search [6] and cross-entropy method with local search [24] from MQLib [10]. See Appendix H for competitors of other problems and the details.

Training and Test We trained the models for two hours to make the training of both CombOpt Zero and S2V-DQN converge (Only 2-IGN+ was trained for four hours due to its slow inference). Note that CombOpt Zero was trained on 4 GPUs while S2V-DQN uses a single GPU because of its implementation, which we discuss in Section 4.4. For the hyperparameters of the MCTS, we referred to the original AlphaGo Zero and its reimplementation, ELF OpenGo [36]. See Appendix C for the detailed environment and hyperparameters. Since we sometimes observed extremely poor performance for a few models both in S2V-DQN and CombOpt Zero when applied to large graphs, we trained five different models from random parameters and took the best value among them at the test time. Throughout the experiments, all models were trained on randomly genrated Erdős-Renyi (ER) [11] graphs with $80 \leq n \leq 100$ nodes and edge probability $p = 0.15$ except for MAXCUT, where nodes were $40 \leq n \leq 50$ and for MAXIMUMCLIQUE, where edge probability was $p = 0.5$. As the input node feature of MAXCUT, we used a two-dimensional feature vector that stores the number of adjacent nodes of color 1 and color 2. For the other problems, we used a vector of ones. In tests, to keep the fairness, CombOpt Zero conducted a greedy selection on network policy output \mathbf{p} , which is the same way as S2V-DQN works (except for Section 4.2 where we compared the greedy selection and MCTS).

Table 1: **Generalization Comparison between CombOpt Zero and S2V-DQN.** COZ and DQN are short for CombOpt Zero and S2V-DQN respectively. Smaller is better for MINIMUMVERTEXCOVER and larger is better for MAXCUT. Three sections stand for Erdős-Renyi models, other synthetic graphs such as BA graphs and Watts-Strogatz graphs, and real-world graphs.

	MVC		MAXCUT			MVC		MAXCUT	
	COZ	DQN	COZ	DQN		COZ	DQN	COZ	DQN
er100_15	76	76	494	527					
er1000_5	900	898	12561	14424					
er5000_1	4484	4482	63389	71909					
ba100_5	63	63	337	343	cora	1258	1258	4260	4243
ba1000_5	592	594	3492	3465	citeseer	1462	1461	3933	3893
ba5000_5	2920	2927	17381	16870	web-edu	1451	1451	4712	4289
ws100_2	49	49	98	97	web-spam	2299	2319	20645	21027
ws100_10	78	78	335	335	road-min...	1324	1329	3080	3015
ws1000_2	492	496	999	973	bio-yeast	456	457	1769	1751
ws1000_4	635	636	1536	1327	bio-SC-...	1039	1053	10893	11890
ws1000_10	787	784	3312	3287	rt_dama...	369	369	3698	3667
reg_100_5	63	64	207	205	soc-wiki...	407	406	2119	2064
reg_1000_5	632	634	2051	2046	socfb-bo...	1796	1793	42063	37140
tree100	44	44	99	98					
tree1000	439	440	999	982					

Table 2: **Improvement by test-time MCTS for MAXIMUMCLIQUE.** Larger is better. Results with test-time MCTS are shown in the parentheses. Bold values means the best solution among learning based approaches (COZ and S2V-DQN). Underlined values are the best among all methods.

	CombOpt Zero						S2V-DQN	CPLEX
	2-IGN+	GIN	GCN	S2V				
cora	4 (5)	4 (5)	3 (5)	4 (5)		4		5
citeseer	4 (6)	5 (6)	4 (6)	4 (6)		4		6
web-edu	16 (30)	16 (30)	16 (16)	16 (30)		16		30
web-spam	10 (20)	16 (17)	7 (17)	16 (17)		16		20
soc-wiki-vote	5 (7)	6 (7)	6 (7)	6 (7)		6		7
socfb-bowdoin47	14 (23)	15 (23)	7 (22)	13 (23)		14		23

Dataset We generated ER and Barabási-Albert (BA) graphs [3] of different sizes for testing. ER100_15 denotes an ER graph with 100 nodes and edge probability $p = 0.15$ and BA100_5 denotes a BA graph with 100 nodes and 5 edges addition per node. Also, we used 10 real-world graphs from Network Repository [32], including citation networks, web graphs, bio graphs, and road map graphs, all of which were handled as unlabeled and undirected graphs. Refer to Appendix H for the full results on these 10 graphs. For MINIMUMVERTEXCOVER and MAXIMUMINDEPENDENTSET, we additionally tested on DIMACS², difficult artificial instances. We generated other synthetic instances in Section 4.1.

4.1 COMPARISON OF GENERALIZATION ABILITY

We compared the generalization ability of CombOpt Zero and S2V-DQN to various kinds of graphs. To see the pure contribution of CombOpt Zero, here CombOpt Zero incorporated the same graph representation model as S2V-DQN, namely S2V. Table 1 shows the performance for MINIMUMVERTEXCOVER and MAXCUT on various graph instances (see Appendix C for the explanation of each graph). While S2V-DQN had a better performance on ER graphs, which were used for training, CombOpt Zero showed a better generalization ability to the other synthetic graphs such as BA graphs, Watts-Strogatz graphs [38], and regular graphs (i.e., graphs with the same degree of nodes). It was interesting that CombOpt Zero successfully learned the optimal solution of MAXCUT on trees (two-coloring of a tree puts all the edges into the cut set), while S2V-DQN does not. Appendix E

²https://turing.cs.hbg.psu.edu/txn131/vertex_cover.html

visualizes how CombOpt Zero achieves the optimal solution on trees. CombOpt Zero also generalized better to real-world graphs although S2V-DQN performed better on a few instances, which might be because some real-world graphs have similar characteristics as ER random graphs.

4.2 TEST-TIME MCTS

The greedy selection in Sections 4.1 and 4.3 does not make full use of CombOpt Zero. When more computational time is allowed in test-time, CombOpt Zero can explore better solutions using the MCTS. Since the MCTS on large graphs takes a long time, we chose MAXIMUMCLIQUE as a case study because solution sizes and the MCTS depths are much smaller than the other problems. We used the same algorithm as in the training (Algorithm 1) with the same iteration coefficient ($c_{\text{iter}} = 4$) and $\tau = 0$, and selected an action based on the enhanced policy π . In all the instances, the MCTS finished in a few minutes on a single process and a single GPU, thanks to the small depth of the MCTS tree. The improvements are shown in Table 2. Note that the solutions by CPLEX except for scfb-bowdoin was optimal since the execution finished within the cut-off time. Considering this fact, CombOpt Zero with test-time MCTS gaining the same result as CPLEX on all the instances, while S2V-DQN on no instances, is promising.

4.3 COMBINATION WITH DIFFERENT GNN MODELS

We compared the performance of CombOpt Zero with four different GNN models (2-IGN+, GIN, GCN, and S2V). See Appendix H for all the results of the 5 problems. One interesting insight was that the best GNN models were different across the problems. For example, while GIN had the best performance in MAXCUT, GCN performed slightly better in MINIMUMVERTEXCOVER. Although GCN performed significantly worse in MAXCUT, it did almost the best for the other four NP-hard problems. 2-IGN+, a theoretically more expressive GNN, did not work well except for MAXIMUMCLIQUE. Since we observed that the performance on training instances did not significantly differ among different GNN models, the test performance difference is possibly because of the generalization ability of each GNN for specific combinatorial structure, which we put as future research. Overall, CombOpt Zero was strongly enhanced with a proper GNN model. Also, it is worth noting that, in a few instances, CombOpt Zero outperformed CPLEX on MINIMUMVERTEXCOVER or SOTA heuristic solvers on MAXCUT (see Table 5 and Table 6 in Appendix I).

4.4 TRADEOFFS BETWEEN COMBOPT ZERO AND S2V-DQN

Here, we summarize some characteristics of CombOpt Zero and S2V-DQN. During the training, CombOpt Zero used 32 processes and four GPUs as described in Appendix C, while S2V-DQN used a single process and GPU because of its implementation. CombOpt Zero takes a longer time to generate self-play data than S2V-DQN due to the MCTS process. For this reason, CombOpt Zero needs a more powerful environment to obtain stable training. On the other hand, since CombOpt Zero is much more sample-efficient than S2V-DQN (see Appendix D), the bottleneck of the CombOpt Zero training is the data generation by the MCTS. This means that it can be highly optimized with an enormous GPU or TPU environment as in Silver et al. [35], Silver et al. [34], and Tian et al. [36].

By its nature, S2V-DQN can be also combined with other GNN models than S2V. However, S2V-DQN is directly implemented with GPU programming, it is practically laborious to combine various GNN models. On the other hand, CombOpt Zero is based on PyTorch framework [31] and it is relatively easy to implement different GNN models.

5 CONCLUSION

In this paper, we presented a general framework, CombOpt Zero, to solve combinatorial optimization on graphs without domain knowledge. We showed that CombOpt Zero worked well for combinatorial problems in relatively small computational resources (four GPUs) compared to the original AlphaGo Zero. The Monte Carlo Tree Search (MCTS) in the training time successfully helped the wider exploration than the existing method and enhanced the generalization ability to various graphs. Another advantage of our method is that the test-time MCTS significantly strengthened the performance if more computation time is allowed.

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A PSEUDOCODE

Algorithm 1 MCTS

Require: Network f_θ , root node s_0

Ensure: Return π , enhanced policy

```

while  $\sum_{a \in A_{s_0}} N(s_0, a) \leq c_{\text{iter}} |A_{s_0}|$  do
   $s = s_0$ 
  {select}
  while  $s$  is expanded before and  $s \notin S_{\text{end}}$  do
     $a = \arg \max_{b \in A_s} \left( Q(s, b) + c_{\text{puct}} P(s, b) \frac{\sqrt{\sum_{b'} N(s, b')}}{1 + N(s, b)} \right)$ 
     $s \leftarrow T(s, a)$ 
  end while
  {expand}
  if  $s \notin S_{\text{end}}$  then
     $(\mathbf{p}, \mathbf{v}) = f_\theta(s)$ 
    initialize  $(N(s, a) = 0, W(s, a) = 0, Q(s, a) = 0, P(s, a) = \mathbf{p}_a)$  for each  $a \in A_s$ 
    Calculate  $(\mu_s, \sigma_s)$  by random sampling
  end if
  {backup}
   $r = r_{\text{estim}}(s)$ 
  while  $s$  is not  $s_0$  do
     $a = \text{previous action}$ 
     $s \leftarrow \text{parent of } s$ 
     $r \leftarrow r + R(s, a)$ 
     $r' = (r - \mu_s) / \sigma_s$ 
     $W(s, a) \leftarrow W(s, a) + r'$ 
     $N(s, a) \leftarrow N(s, a) + 1$ 
     $Q(s, a) \leftarrow \frac{W(s, a)}{N(s, a)}$ 
  end while
end while
Compute  $\left( \pi_a = \frac{N(s_0, a)^{1/\tau}}{\sum_b N(s_0, b)^{1/\tau}} \right)$  for each  $a$ 
return  $\pi$ 

```

Algorithm 2 Self-play Data Generation

Require: Network f_θ , Initial graph G_0

Ensure: Return self-play data records

```

{self-play}
 $s = \text{Init}(G_0)$ 
records = {}
while  $s \notin S_{\text{end}}$  do
   $\pi = \text{MCTS}(s)$ 
   $a = \text{sampled action according to probability } \pi$ 
   $s \leftarrow T(s, a)$ 
  Add  $(s, a, \pi)$  to records
end while
{calculate  $z'$ }
 $z = 0$ 
for all  $(s, a, \pi)$  in records (reversed order) do
   $z \leftarrow z + R(s, a)$ 
   $z' = (z - \mu_R(s)) / \sigma_R(s)$ 
  Replace  $(s, a, \pi)$  with  $(s, a, \pi, z')$ 
end for
return records

```

B GRAPH NEURAL NETWORKS

In this section, we review several Graph Neural Network (GNN) models and explain some modifications for our problem setting. Given a graph and input node feature $H^{(0)} \in \mathbb{R}^{n \times C_0}$, we aim at obtaining $y \in \mathbb{R}^{n \times C_{\text{out}}}$ which represents node feature as an output. L denotes a number of layers.

B.1 STRUCTURE2VEC

In `structure2vec` (S2V) [9], the feature is propagated by

$$H_v^{(l+1)} = \text{relu}\left(\theta_1 H_v^{(0)} + \theta_2 \sum_{u \in \mathcal{N}(v)} H_u^{(l)}\right),$$

where $\theta_1 \in \mathbb{R}^{p \times C_0}$, $\theta_2 \in \mathbb{R}^{p \times p}$ for some fixed integer p . The edge propagation term is ignored since we don't handle weighted edges in this work. In the last layer, the features of every node are aggregated to encode the whole graph:

$$y_v = \theta_3^T \text{relu}\left([\theta_4 \sum_{u \in V} H_u^{(L)}, \theta_5 H_v^{(L)}]\right),$$

where $\theta_3 \in \mathbb{R}^{C_{\text{out}} \times 2p}$, $\theta_4, \theta_5 \in \mathbb{R}^{p \times p}$ and $[\cdot, \cdot]$ is the concatenation operator.

B.2 GRAPH CONVOLUTIONAL NETWORK

Graph Convolutional Network (GCN) [21] follows the layer-wise propagation rule:

$$H^{(l+1)} = \sigma(\tilde{D}^{-1/2} \tilde{A} \tilde{D}^{-1/2} H^{(l)} \theta^{(l)}). \quad (5)$$

$\tilde{A} = A + I_n$ where I_n is the identity matrix of the size n and expresses an adjacency matrix with self-connections. Multiplying $H^{(l)}$ by \tilde{A} means passing each node's feature vector to its neighbors' feature vectors in the next layer. \tilde{D} is the degree matrix of \tilde{A} , such that $\tilde{D}_{ii} = \sum_j \tilde{A}_{ij}$ for diagonal elements and 0 for the other elements. $\tilde{D}^{-1/2}$ is multiplied to normalize \tilde{A} . θ^l is a trainable weight matrix in l -th layer.

B.3 GRAPH ISOMORPHISM NETWORK

The propagation rule of Graph Isomorphism Network (GIN) [39] is as follows:

$$H^{(l+1)} = \text{MLP}^{(l)}(\tilde{A} H^{(l)}),$$

where MLP^l refers to the multi-layer perceptron in the l -th layer. It takes the simple sum of features among the neighbors and itself by multiplying \tilde{A} . We adopt a similar suffix as the original paper:

$$y_v = \text{MLP}(\text{CONCAT}(H_v^{(l)} \mid l = 0, 1, \dots, L)) \quad (6)$$

B.4 2-IGN+

Different from message passing GNNs, each block of 2-IGN+ [28] takes a tensor as an input. It follows the propagation rule:

$$\mathbf{X}^{(l+1)} = B_l(\mathbf{X}^{(l)}). \quad (7)$$

$\mathbf{X}^{(l)} \in \mathbb{R}^{n \times n \times C_l}$ is a hidden tensor of the l -th block. $\mathbf{X}^{(0)} \in \mathbb{R}^{n \times n \times (C_0+1)}$ is initialized as the concatenation of the adjacency matrix and a tensor with node feature in its diagonal elements (other elements are 0). B_l is the l -th block of 2-IGN+ and consists of three MLPs: $m_1^{(l)}, m_2^{(l)} \in \mathbb{R}^{C_l} \rightarrow \mathbb{R}^{C'_l}$ and $m_3^{(l)} \in \mathbb{R}^{C_l+C'_l} \rightarrow \mathbb{R}^{C'_l}$. After applying the two MLPs independently, we perform feature-wise matrix multiplication: $\mathbf{W}_{::,j}^{(l)} = m_1^{(l)}(\mathbf{X}^{(l)})_{::,j} \cdot m_2^{(l)}(\mathbf{X}^{(l)})_{::,j}$. The output of the block is the last MLP over the concatenation with $\mathbf{X}^{(l)}$: $\mathbf{X}^{(l+1)} = m_3^{(l)}([\mathbf{X}^{(l)}, \mathbf{W}^{(l)}])$. In our problem

setting, we adopt equivariant linear layer instead of invariant linear layers to obtain the output tensor $y \in \mathbb{R}^{n \times C_{\text{out}}}$. We also adopt the suffix mentioned in the original paper:

$$y = \sum_{l=1}^L h^{(l)}(X^{(l)}), \quad (8)$$

where $h^{(l)} \in \mathbb{R}^{n \times C_l} \rightarrow \mathbb{R}^{n \times C_{\text{out}}}$ is an equivariant linear layer of l -th block.

C EXPERIMENT SETTINGS

In this section, we explain the detailed settings of experiments.

C.1 ENVIRONMENT

The experiments were run on Intel Xeon E5-2695 v4, with four NVIDIA Tesla P100 GPUs. Libraries were compiled with GCC 5.4.0 and CUDA 9.2.148.

C.2 COMPETITORS

Our main competitor was S2V-DQN, the state-of-the-art reinforcement learning solver of NP-hard problems. We also tested some heuristics and approximation algorithms for specific problems. Note that a fair setting of the running environment is difficult since they do not use GPUs nor training time. Therefore, they were referred to just for checking how successfully CombOpt Zero learned combinatorial structure and algorithms for each problem. For MINIMUMVERTEXCOVER, MAXIMUMINDEPENDENTSET, MINIMUMFEEDBACKVERTEXSET and MAXCUT, we compared our algorithm to randomized algorithms. The results of the randomized algorithm were the best objective among 100 runs. For MAXCUT, we tried two heuristics solvers from MQLib [10]. We set the time limit of 10 minutes for these algorithms and used the best found solution as the results. We also used CPLEX to solve the integer programming formulation of MINIMUMVERTEXCOVER and MAXIMUMINDEPENDENTSET. Only CPLEX was run on MacBook Pro 2.4 GHz Quad-Core Intel Core i5. It was executed on 8 threads with the time limit of 10 minutes.

C.3 HYPERPARAMETERS

Some of the hyperparameters are summarized in Table 3.

Graph Neural Networks For S2V, we used the same hyperparameters as the ones used in S2V-DQN [19]: we set embedding dimension $p = 64$ and the number of iterations $L = 5$. For GCN, we used a 5-layer network with a hidden dimension of size 32. For GIN, the network consisted of 5 layers of hidden dimension of size 32. Each MLP consisted of 5 layers also and the size of a hidden dimension was 16. Lastly, for 2-IGN+, we used a 2-block network with a hidden dimension of size 8. Each MLP had 2 layers with a hidden dimension of size 8.

MCTS We followed the implementation of AlphaGo Zero [35] and ELF [36]. We set $c_{\text{puct}} = 1.5$. In training phase and test-time MCTS, we added Dirichlet noise $\boldsymbol{\eta} \sim \text{Dir}(\mathbf{0.03})$ to the first move to explore a variety of actions. More specifically, the policy \mathbf{p} for the first action is modified to $\mathbf{p} \leftarrow (1 - \varepsilon)\mathbf{p} + \varepsilon\boldsymbol{\eta}$, where $\varepsilon = 0.25$. We set $c_{\text{iter}} = 4$, i.e., ran MCTS for $c_{\text{iter}}|A_{s_0}|$ times, for MAXCUT, MAXIMUMCLIQUE, MAXIMUMINDEPENDENTSET. We set $c_{\text{iter}} = 3$ for MINIMUMVERTEXCOVER and MINIMUMFEEDBACKVERTEXSET because they took relatively longer time due to larger solution sizes. We set the temperature as $\tau = 1$ during the training phase, and $\tau = 0$ in the test-time MCTS. $\tau = 0$ means to take an action whose visit count is the maximum (if there are multiple possible actions, choose one at random). When a new node is visited in MCTS, we calculated the mean and standard deviation of the reward from its corresponding state. We approximated these value from 20 random plays.

Training Each *learner* sampled 20 trajectories from the self-play records and ran stochastic gradient descent by Adam, where the learning rate is 0.001, weight decay is 0.0001, and batch size is 16. After

Table 3: **Part of hyperparameters.** For each of the five problems, some important hyperparameters are summarized. $\min n$, $\max n$, p regard ER graphs, c_{iter} is for MCTS, and keep denotes the duration (minutes) to keep trajectories.

	$\min n$	$\max n$	p	c_{iter}	keep
MVC	80	100	0.15	3	10
MAXCUT	40	50	0.15	4	5
MAXCLIQUE	80	100	0.5	4	5
MIS	80	100	0.15	4	5
FVS	80	100	0.15	3	10

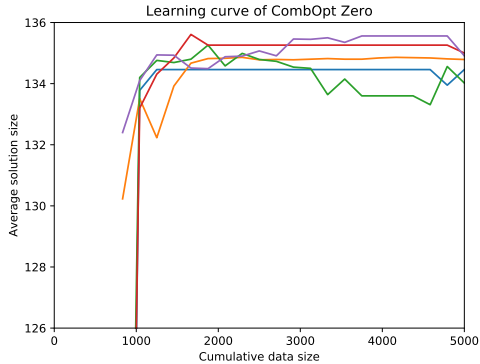


Figure 3: **Training curve for CombOpt Zero on MAXCUT.** Data for five models with the same hyperparameters are shown. The horizontal axis is the cumulative number of generated trajectories during 2 hours. Since, CombOpt Zero saves the best models after 15 minutes from start, its learning curve is not shown for the first 15 minutes.

repeating this routine for 15 times, the *learner* saved the new model. The number of *data generators* was 24 except when 2-IGN+ was used. In that case, the number was 20. The number of *learners* and *model evaluators* were set to 6 and 2, respectively. Each *model evaluator* generated 50 test ER graphs with $n = 100$ and $p = 0.15$ ($n = 50$ for MAXCUT and $p = 0.5$ for MAXIMUMCLIQUE) each time. It compared the performance of the best model and a newly generated model by the cumulative objective and managed the best model. Each trajectory was removed after 5 minutes (10 minutes for MINIMUMVERTEXCOVER and MINIMUMFEEDBACKVERTEXSET) since it was generated.

D TRAINING CONVERGENCE

Here, we show the learning curves of CombOpt Zero and S2V-DQN for MAXCUT. For CombOpt Zero, we chose S2V as the network. Figure 3 and Figure 4 are the learning curves for CombOpt Zero and S2V-DQN respectively. As explained in Section 4, we trained both CombOpt Zero and S2V-DQN for 2 hours. The horizontal axes show the number of trajectories generated during this 2 hours. The vertical axes correspond to the average cut size found on 100 fixed random ER graphs of size 50. Since CombOpt Zero starts to log the best models after 15 minutes from the beginning, and updates the log each 5 minutes after that, data for the first 15 minutes is not shown on the chart. Unlike S2V-DQN, if the newly generated models do not perform better than the current one, the best model is not updated and hence the learning curve remains flat for some intervals.

While S2V-DQN generated about 225000 data in two hours on a single GPU, CombOpt Zero generated only 5000 data on four GPUs. This is because the MCTS, which CombOpt Zero executes to generate self-play data, takes time. On the other hand, S2V-DQN requires about 50000 data for training to converge, while CombOpt Zero requires only about 2000 data, meaning that the training of CombOpt Zero is much more sample-efficient.

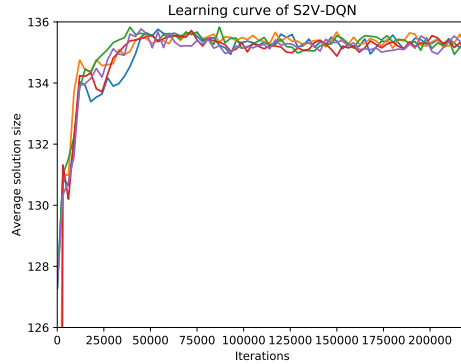


Figure 4: **Training curve for S2V-DQN on MAXCUT.** Data for five models with the same hyperparameters are shown. The horizontal axis shows the total number of generated trajectories during 2 hours (on average, S2V-DQN generates one trajectory per iteration).

E VISUALIZATION

In this section, we illustrate how CombOpt Zero finds solutions for MAXCUT. As described in Section 4, CombOpt Zero found an optimal solution for trees and its overall performance was comparable to the state-of-the-art heuristic solvers. Figure 5 shows the sequence of actions by CombOpt Zero on an ER graph. Starting from one node, CombOpt Zero colors surrounding nodes one by one with the opposite color. Figure 6 shows the sequence of actions on a tree. The order of actions was similar to the order of visiting nodes in the depth-first-search. Since an optimal two coloring for MAXCUT on a tree can be obtained by the depth-first-search, we can say that CombOpt Zero successfully learned the effective algorithm for MAXCUT on a tree from the training on random graphs.

It is also interesting that CombOpt Zero sometimes skips the neighbors and colors a two-hop node by the same color as the current node. This is possible because the L -layer (5 in our case) message passing GNN can catch information of the L -hop neighbors. This flexibility possibly affected the good performance on other graph instances than trees.

F COMPARISON OF REDUCTION RULES

Here, we discuss some differences of reinforcement learning formulation between S2V-DQN and CombOpt Zero. The first difference is their states. While S2V-DQN’s state keeps both the original graph and selected nodes, CombOpt Zero’s state is a single current (labeled) graph and its size usually gets smaller as the state proceeds. Since the GNN inference of smaller graphs is faster, it’s more efficient to give small graphs as an input. Although S2V-DQN implicitly reduces the graph size in most of its implementation, our formulation is more explicit.

The second difference is that while S2V-DQN limits action space to a selection of one vertex, CombOpt Zero does not. Thanks to this, as stated in 3.1, MAXCUT can be formulated as a node coloring by two colors with more intuitive termination criteria: finish coloring all the nodes. This also allows the application to a wider range of problems. For example, K-COLORING by defining the action space by $\{(x, c) \mid x \in V, c \in \mathbb{N}, 0 \leq c \leq K\}$, where (x, c) represents the coloring of node x by color c .

G OTHER NP-HARD PROBLEMS AND MDP FORMULATION

Here, we introduce four more NP-hard problems except for MAXCUT that we used in the experiments and their MDP formulations. We use $G = (V, E)$ to denote an undirected and unlabelled graph, where V is the set of vertices and E is the set of edges. Since v is used to represent a state value in AlphaGo Zero, we often use x, y, \dots to denote a node of a graph. $V(G)$ indicates the set of vertices of graph G . $\mathcal{N}(x)$ means the set of 1-hop neighbors of node x .

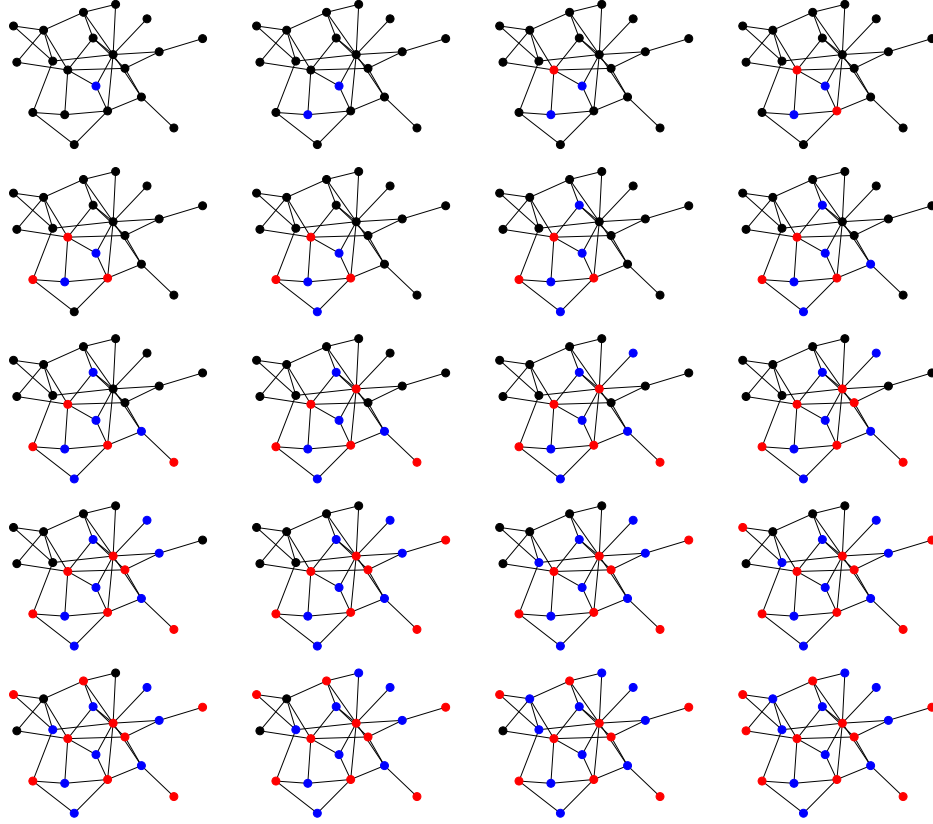


Figure 5: **Order of actions of CombOpt Zero for MAXCUT on a ER graph.** Although the order of selecting nodes and the coloring is arbitrary, CombOpt Zero learned to color neighbors one by one with the opposite color.

G.1 MINIMUM VERTEX COVER

A subset of nodes $V' \subset V$ is called a vertex cover if all edges are covered by V' ; for all $(x, y) \in E$, $x \in V'$ or $y \in V'$ holds. MINIMUMVERTEXCOVER asks a vertex cover whose size is minimum.

Since we do not need a label of the graph for this problem, we set d to a constant function on any set L (e.g., $L = \mathbb{R}$, $d(s) = 1$). Actions are represented by selecting one node ($A_s = V$). Init uses the same graph as G_0 and d defined above. $T(s, x)$ returns the next state, corresponding to the graph where edges covered by x and isolated nodes are deleted. S_{end} is the states with the empty graphs. $R(s, x) = -1$ for all s and x because we want to minimize the number of transition steps in the MDP.

G.2 MAXIMUM CLIQUE

A subset of nodes $V' \subset V$ is called a clique if any two nodes in V' are adjacent in the original graph; for all $x, y \in V'$ ($x \neq y$), $(x, y) \in E$. MAXIMUMCLIQUE asks for a largest clique.

d , A_s , Init, and S_{end} are the same as MINIMUMVERTEXCOVER. $T(s, x)$ return the next state whose corresponding graphs is the induced subgraph of $\mathcal{N}(x)$; 1-hop neighbors of x . $R(s, x) = 1$ because we want to maximize the number of transition steps of the MDP.

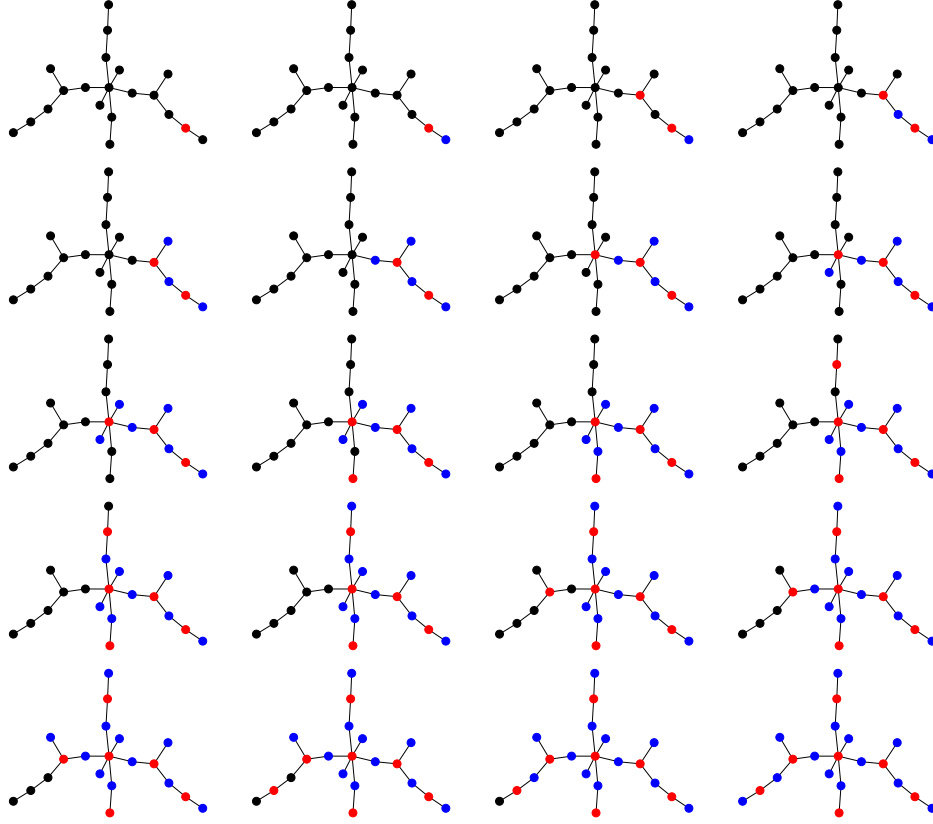


Figure 6: **Order of actions of CombOpt Zero for MAXCUT on a tree.** It successfully found an optimal solution. The order of actions is similar to the order of visiting nodes in the depth-first-search.

G.3 MAXIMUM INDEPENDENT SET

A subset of nodes $V' \subset V$ is called an independent set if no two nodes in V' are adjacent; for all $(x, y) \in E$, $x \notin V'$ or $y \notin V'$ holds. **MAXIMUMINDEPENDENTSET** asks for an independent set whose size is maximum.

d , A_s , Init , and S_{end} are the same as **MINIMUMVERTEXCOVER**. $T(s, x)$ returns the next state, corresponding to the graph where x and its adjacent nodes are deleted. $R(s, x) = 1$ because we want to maximize the number of transition steps of the MDP.

G.4 MINIMUM FEEDBACK VERTEX SET

A subset of nodes $V' \subset V$ is called a feedback vertex set if the induced graph $G[V \setminus V']$ is cycle-free. **MINIMUMFEEDBACKVERTEXSET** asks a feedback vertex set whose size is minimum.

d , A_s , $T(s, x)$, $R(s, x)$ and Init are the same as **MINIMUMVERTEXCOVER**. S_{end} is the states with cycle-free graphs.

H PERFORMANCE COMPARISON OF COMBOPT ZERO AND OTHER APPROACHES

In this section, we show the full results of our experiments. We compared CombOpt Zero to some simple randomized algorithms and state-of-the-art solvers, in addition to S2V-DQN. For each of the five problems, we first explain the characteristics of the problem and some famous approaches, then we show the comparison of the performances.

Algorithm 3 A Simple Randomized Algorithm for MINIMUMVERTEXCOVER

Require: Graph $G = (V, E)$
Ensure: Size of a vertex cover r

```

 $r \leftarrow 0$ 
while  $G$  is not empty do
  if  $G$  has a degree-1 vertex then
     $v \leftarrow$  uniformly randomly chosen degree-1 vertex
  else
     $v \leftarrow$  uniformly randomly chosen vertex
  end if
   $r \leftarrow r + 1$ 
   $G \leftarrow$  delete  $v$  and its neighbor(s)
end while

```

H.1 MINIMUM VERTEX COVER

Approximability There is a simple 2-approximation algorithm for MINIMUMVERTEXCOVER. It greedily obtains a maximal (not necessarily maximum) matching and outputs the nodes in the matching as a solution. Under Unique Games Conjecture [20], MINIMUMVERTEXCOVER cannot be approximated better than this.

Randomized Heuristics Regardless of the hardness of approximation of MINIMUMVERTEXCOVER, there are some practical algorithms to solve this (and equivalently, MAXIMUMINDEPENDENTSET) [25, 1]. These state-of-the-art algorithms usually iteratively *kernelize* the graph, i.e., reduce the size of the problem, and search better solutions, either in an exact way or in an approximated way. We adopted the easiest reduction rule to design a simple randomized algorithm (Algorithm 3) for MINIMUMVERTEXCOVER; if the input graph has a degree-1 vertex v , there is always a vertex cover that does not contain v . Although theoretically, this reduction rule does not improve the approximation ratio, i.e., the approximation is still 2, it is effective because we can cut off trivial solutions and make the size of the problem smaller.

Analysis Table 5 shows the full results for MINIMUMVERTEXCOVER. Although both CombOpt Zero and S2V-DQN failed to find an optimal solution for the ER graph of 200 nodes (er200_10), both of them found near-optimal solutions for large cases even though they were trained on small random graphs. Remarkably, some models of CombOpt Zero found better solutions than CPLEX for large random graphs. However, for some large sparse real-world networks, they performed worse than a simple 2-approximation algorithm. A hybrid approach that mixes the reduction rules and machine learning, as done in [26], may be effective in such sparse networks, but our work focuses on a method without domain knowledge. Theoretically, 2-IGN+ is stronger than GIN or GCN in terms of discriminative power [28], its performance on large instances was not good although they successfully learned er100_15. One reason could be because we reduced the size of the network to fasten the training. Also, since 2-IGN+ is not a message passing neural network, its tendency of learning could be different from other GNNs. We leave the empirical and theoretical analyses on the characteristics of learning by 2-IGN+ as future work.

H.2 MAX CUT

Approximability MAXCUT has a famous 0.878-approximation randomized algorithm by SDP (semidefinite programming) [14]. Similarly to MINIMUMVERTEXCOVER, this approximation ratio is best under Unique Games Conjecture [20].

Competing Algorithms Although the randomized algorithm mentioned above has a polynomial-time complexity and the best approximation ratio, they are rarely applied for graphs of thousands of nodes due to the large size of the SDP. We only applied this algorithm to graphs that have no more than 200 nodes. Instead, we compared the performance with a MAXCUT solver by Dunning et al. [10].

Analysis Table 6 shows the full results for MAXCUT. We compared CombOpt Zero, S2V-DQN, the SDP approximation algorithm and heuristics. Unlike MINIMUMVERTEXCOVER, CombOpt Zero with GCN had poor performance. CombOpt Zero with GIN had the best performance and it overperformed S2V-DQN. CombOpt Zero even overperformed state-of-the-art heuristics for some instances such as citeseer and rt_damascus. It is also remarkable that all of the results by CombOpt Zero with GIN overperformed 0.878-approximation SDP algorithm (note that SDP did not finish for large instances).

H.3 MAXIMUM CLIQUE

For MAXIMUMCLIQUE, we compared CombOpt Zero and S2V-DQN. For CombOpt Zero, since the solution sizes were relatively small, we also tested test-time MCTS.

Although MAXIMUMCLIQUE is equivalent to MAXIMUMINDEPENDENTSET on complement graphs, since the number of edges in the complement graphs of sparse networks becomes too large, it is usually difficult to solve MAXIMUMCLIQUE by algorithms designed for MINIMUMVERTEXCOVER.

Analysis Full results for MAXIMUMCLIQUE is given in Table 4. CombOpt Zero with GIN worked the best among four models and outperformed S2V-DQN especially on random graphs. We can also observe that the performance is strongly enhanced by test-time MCTS. For example, although the performance of CombOpt Zero with GCN or 2-IGN+ was relatively poor than other GNNs, by test-time MCTS, its performance became much stabler and solutions were also improved. Since test-time MCTS requires n times larger time complexity, where n is the number of nodes, it is hard to apply test-time MCTS on large instances when solution size is too large or time limit is too short.

H.4 MAXIMUM INDEPENDENT SET

Randomized Algorithm We also compared our methods and S2V-DQN to a randomized algorithm for MAXIMUMINDEPENDENTSET. We adopt the randomized algorithm developed in 3 with a slight change: for a degree-1 vertex v , there is always a maximum independent set that includes v . Therefore, instead, we include v to the current solution and erase v and its neighbors from the original graph. Note that although MINIMUMVERTEXCOVER and MAXIMUMINDEPENDENTSET are theoretically equivalent, when solved by CombOpt Zero or S2V-DQN, their difficulties are different. For example, in the first stage of the training, the sizes of independent sets obtained are usually much greater than the complements of vertex covers (usually, they tend to select almost all nodes as vertex cover at the beginning).

Analysis Please refer to Table 7 for the full results for MAXIMUMINDEPENDENTSET. Similarly to MINIMUMVERTEXCOVER, even a simple randomized algorithm with recursive reductions could obtain near-optimal solutions for large sparse networks, its performance on ER graphs were much weaker than both CombOpt Zero and S2V-DQN. This is because, in ER graphs, there were only a few trivial vertices to be selected. Notably, CombOpt Zero with GIN reached to a better solution than CPLEX on one of the DIMACS instances.

H.5 MINIMUM FEEDBACK VERTEX SET

Randomized Algorithm Similarly to MINIMUMVERTEXCOVER, a 2-approximation algorithm is known for MINIMUMFEEDBACKVERTEXSET [2]. In this experiment, we implemented a parameterized algorithm that runs in time $4^k n^{O(1)}$ [8], where k is the size of the solution, instead, which would work well for real-world sparse networks.

Analysis Full results for MINIMUMFEEDBACKVERTEXSET is given in Table 8. For the randomized parameterized algorithm, we ran it for 100 times and took the best objective as the score. Although in this problem, we could not observe a significant superiority of CombOpt Zero against S2V-DQN, we can see a significant difference of solution sizes for some of the datasets such as web-edu, bio-SC-LC, and socfb-bowdoin47. This is probably because all of the five S2V-DQN models converged into local optima. Interestingly even the performances were significantly poor on certain instances, they still sometimes overperformed CombOpt Zero on other instances. The

randomized algorithm effectively worked on large real-world networks where the degrees were biased. On the other hand, on ER graphs, since the degrees of nodes were not as variant as social networks, CombOpt Zero and S2V-DQN performed much better than the randomized algorithm.

I FULL RESULTS

Table 4: **Performance comparison on MAXIMUMCLIQUE**. Larger is better. Results with test-time MCTS are shown in the parentheses. Bold values are the best values among reinforcement learning approaches (CombOpt Zero and S2V-DQN). Underlined values are the best solution size among all methods. Empty cells mean execution did not finish within 2 hours.

	V	2-IGN+	CombOpt Zero		GIN		GCN		S2V	S2V-DQN	CPLEX
er100_15	100	<u>4</u> (4)	<u>4</u> (4)	<u>4</u> (4)	<u>4</u> (4)	<u>4</u> (4)	<u>4</u> (4)	<u>4</u> (4)	<u>4</u> (4)	3	<u>4</u>
er200_10	200	<u>4</u> (4)	<u>4</u> (4)	<u>4</u> (4)	<u>4</u> (4)	<u>4</u> (4)	<u>4</u> (4)	<u>4</u> (4)	<u>4</u> (4)	3	<u>4</u>
er1000_5	1000	<u>4</u> (4)	<u>4</u> (4)	<u>4</u> (4)	<u>4</u> (4)	<u>4</u> (4)	<u>4</u> (4)	<u>4</u> (4)	<u>4</u> (4)	3	<u>4</u>
er5000_1	5000	3 (4)	3 (4)	3 (4)	3 (4)	3 (4)	3 (4)	3 (4)	3 (4)	3	<u>4</u>
ba100_5	100	<u>5</u> (5)	<u>5</u> (5)	<u>5</u> (5)	<u>5</u> (5)	<u>5</u> (5)	<u>5</u> (5)	<u>5</u> (5)	<u>5</u> (5)	3	<u>5</u>
ba200_5	200	<u>5</u> (5)	<u>5</u> (5)	<u>5</u> (5)	4 (5)	<u>5</u> (5)	<u>5</u> (5)	<u>5</u> (5)	<u>5</u> (5)	3	<u>5</u>
ba1000_5	1000	<u>5</u> (5)	<u>5</u> (5)	<u>5</u> (5)	<u>5</u> (5)	<u>5</u> (5)	<u>5</u> (5)	<u>5</u> (5)	<u>5</u> (5)	3	<u>5</u>
ba5000_5	5000	4 (5)	4 (5)	4 (5)	4 (5)	4 (5)	4 (5)	4 (5)	4 (5)	3	<u>5</u>
cora	2708	4 (5)	4 (5)	3 (5)	3 (5)	4 (5)	4 (5)	4 (5)	4 (5)	4	<u>5</u>
citeseer	3327	4 (6)	5 (6)	4 (6)	4 (6)	4 (6)	4 (6)	4 (6)	4 (6)	4	<u>6</u>
web-edu	3031	16 (30)	16 (30)	16 (16)	16 (16)	16 (16)	16 (30)	16 (30)	16 (30)	16	<u>30</u>
web-spam	4767	10 (20)	16 (17)	7 (17)	7 (17)	16 (17)	16 (17)	16 (17)	16 (17)	16	<u>20</u>
road-minnesota	2642	2 (2)	2 (3)	2 (3)	2 (3)	<u>3</u> (3)	<u>3</u> (3)	<u>3</u> (3)	<u>3</u> (3)	<u>3</u>	<u>3</u>
bio-yeast	1458	3 (6)	4 (6)	2 (6)	2 (6)	3 (6)	3 (6)	3 (6)	3 (6)	4	<u>6</u>
bio-SC-LC	2004	12 (29)	<u>29</u> (29)	3 (29)	3 (29)	<u>29</u> (29)	<u>29</u> (29)	<u>29</u> (29)	<u>29</u> (29)	<u>29</u>	<u>29</u>
rt_damascus	3052	3 (4)	3 (4)	3 (4)	3 (4)	<u>4</u> (4)	<u>4</u> (4)	<u>4</u> (4)	<u>4</u> (4)	3	<u>4</u>
soc-wiki-vote	889	5 (7)	6 (7)	6 (7)	6 (7)	6 (7)	6 (7)	6 (7)	6 (7)	6	<u>7</u>
socfb-bowdoin47	2252	14 (23)	15 (23)	7 (22)	7 (22)	13 (23)	<u>23</u> (23)	<u>23</u> (23)	<u>23</u> (23)	14	<u>23</u>

Table 5: **Performance comparison on MINIMUMVERTEXCOVER**. Smaller is better.

	V	2-IGN+	CombOpt Zero		GIN		GCN		S2V	S2V-DQN	2-approx	CPLEX
er100_15	100	77	77	76	76	76	76	76	76	76	83	<u>76</u>
er200_10	200	160	160	161	160	160	160	160	160	160	174	<u>159</u>
er1000_5	1000	907	900	893	893	893	893	893	893	893	954	<u>894</u>
er5000_1	5000	-	4479	4448	4448	4448	4448	4448	4448	4448	4793	<u>4480</u>
ba100_5	100	63	63	63	63	63	63	63	63	63	69	<u>63</u>
ba200_5	200	121	120	120	120	120	120	120	120	120	134	<u>118</u>
ba1000_5	1000	745	592	591	591	591	591	591	591	591	670	<u>589</u>
ba5000_5	5000	-	2920	2905	2905	2905	2905	2905	2905	2905	3374	<u>2932</u>
cora	2708	-	1257	1258	1258	1258	1258	1258	1258	1258	1274	<u>1257</u>
citeseer	3327	-	1460	1462	1462	1462	1462	1462	1462	1462	1475	<u>1460</u>
web-edu	3031	-	1451	1451	1451	1451	1451	1451	1451	1451	1451	<u>1451</u>
web-spam	4767	-	2305	2298	2298	2298	2298	2298	2298	2298	2420	<u>2297</u>
road-minnesota	2642	-	1322	1323	1324	1324	1324	1324	1324	1324	1330	<u>1319</u>
bio-yeast	1458	702	456	456	456	456	456	456	456	456	457	<u>456</u>
bio-SC-LC	2004	1471	1041	1046	1039	1039	1039	1039	1039	1039	1245	<u>1036</u>
rt_damascus	3052	370	369	369	369	369	369	369	369	369	369	<u>369</u>
soc-wiki-vote	889	413	406	406	406	406	406	406	406	406	406	<u>406</u>
socfb-bowdoin47	2252	2187	1793	1792	1792	1792	1792	1792	1792	1792	2052	<u>1792</u>
dimacs-frb30-15-1	450	436	427	426	426	426	426	426	426	426	436	<u>421</u>
dimacs-frb50-23-1	1150	1132	1115	1111	1111	1111	1111	1111	1111	1111	1130	<u>1107</u>

Table 6: **Performance comparison on MAXCUT.** Larger is better.

	V	CombOpt Zero				S2V-DQN	SDP	Heuristics	
		2-IGN+	GIN	GCN	S2V			Burer	Laguna
er100_15	100	516	526	390	494	527	521	528	528
er200_10	200	1194	1269	974	1221	1262	1266	<u>1289</u>	<u>1289</u>
er1000_5	1000	12278	14787	8596	12561	14424	-	<u>15164</u>	15140
er5000_1	5000	-	73275	42860	63389	71909	-	<u>75601</u>	75406
ba100_5	100	324	343	282	337	343	341	<u>344</u>	<u>344</u>
ba200_5	200	639	694	576	687	698	693	<u>703</u>	<u>703</u>
ba1000_5	1000	2595	3485	2941	3492	3465	-	<u>3589</u>	3580
ba5000_5	5000	-	17643	15015	17381	16870	-	<u>17997</u>	17911
cora	2708	-	4268	3945	4260	4243	-	<u>4394</u>	4383
citeseer	3327	-	3929	3477	3933	3893	-	3927	3927
web-edu	3031	-	4705	4243	4712	4289	-	4679	<u>4714</u>
web-spam	4767	-	23882	20498	20645	21027	-	25001	<u>25070</u>
road-minnesota	2642	-	3079	2856	3080	3015	-	<u>3091</u>	3024
bio-yeast	1458	714	1769	1582	1769	1751	-	<u>1770</u>	1761
bio-SC-LC	2004	7967	14358	11589	10893	11890	-	<u>14586</u>	14583
rt_damascus	3052	-	3694	3439	3698	3667	-	3617	3683
soc-wiki-vote	889	1645	2116	1730	2119	2064	-	<u>2175</u>	2163
socfb-bowdoin47	2252	41741	47426	20002	42063	37140	-	<u>48639</u>	48636

Table 7: **Performance comparison on MAXIMUMINDEPENDENTSET.** Larger is better.

	V	CombOpt Zero				S2V-DQN	randomized	CPLEX
		2-IGN+	GIN	GCN	S2V			
er100_15	100	<u>24</u>	<u>24</u>	23	<u>24</u>	<u>24</u>	23	<u>24</u>
er200_10	200	40	40	39	<u>41</u>	40	37	<u>41</u>
er1000_5	1000	106	107	108	105	106	89	107
er5000_1	5000	-	544	538	544	551	435	544
ba100_5	100	37	37	37	37	37	37	<u>37</u>
ba200_5	200	81	81	80	82	82	79	<u>82</u>
ba1000_5	1000	400	407	403	408	409	394	<u>411</u>
ba5000_5	5000	-	2079	2062	2085	2078	1960	<u>2090</u>
cora	2708	-	1450	1448	1451	1448	1439	<u>1451</u>
citeseer	3327	-	1818	1817	1819	1817	1860	<u>1867</u>
web-edu	3031	-	1580	1580	1580	1580	<u>1580</u>	<u>1580</u>
web-spam	4767	-	2464	2456	2463	2441	2434	<u>2470</u>
road-minnesota	2642	-	1318	1300	1316	1321	1313	<u>1323</u>
bio-yeast	1458	990	1000	1001	1002	1002	<u>1002</u>	<u>1002</u>
bio-SC-LC	2004	945	959	953	964	948	936	<u>968</u>
rt_damascus	3052	-	2673	2683	2679	2683	<u>2683</u>	<u>2683</u>
soc-wiki-vote	889	481	483	482	483	482	<u>483</u>	<u>483</u>
socfb-bowdoin47	2252	445	456	457	443	426	392	<u>461</u>
dimacs-frb30-15-1	450	26	26	26	27	26	24	<u>28</u>
dimacs-frb50-23-1	1150	41	<u>44</u>	43	40	41	39	43

Table 8: **Performance comparison on MINIMUMFEEDBACKVERTEXSET**. Smaller is better.

	V	2-IGN+	CombOpt GIN	Zero GCN	S2V	S2V-DQN	randomized
er100_15	100	64	63	69	63	63	72
er200_10	200	143	137	150	137	136	156
er1000_5	1000	917	844	868	848	874	909
er5000_1	5000	-	4201	4339	4229	4359	4567
ba100_5	100	44	40	44	38	37	46
ba200_5	200	91	70	77	69	69	88
ba1000_5	1000	828	341	367	328	330	445
ba5000_5	5000	-	1753	1879	1692	1678	2265
cora	2708	-	527	571	545	509	565
citeseer	3327	-	447	471	457	450	<u>430</u>
web-edu	3031	-	525	479	540	859	<u>247</u>
web-spam	4767	-	1514	1587	1486	1461	1601
road-minnesota	2642	-	401	523	478	415	<u>316</u>
bio-yeast	1458	794	153	168	186	144	<u>122</u>
bio-SC-LC	2004	1596	856	859	796	1591	895
rt_damascus	3052	1424	120	150	132	286	<u>98</u>
soc-wiki-vote	889	677	205	204	204	201	227
socfb-bowdoin47	2252	2066	1773	1741	1619	2175	1763