GRAPH-BASED DETERMINISTIC POLICY GRADIENT FOR REPETITIVE COMBINATORIAL OPTIMIZATION PROBLEMS

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ABSTRACT

We propose an actor-critic framework for graph-based machine learning pipelines with non-differentiable blocks, and apply it to repetitive combinatorial optimization problems (COPs) under hard constraints. Repetitive COP refers to problems to be solved repeatedly on graphs of the same or slowly changing topology but rapidly changing node or edge weights. Compared to one-shot COPs, repetitive COPs often rely on fast heuristics to solve one instance of the problem before the next one arrives, at the cost of a relatively large optimality gap. Through numerical experiments on several discrete optimization problems, we show that our approach can learn reusable node or edge representations to reduce the optimality gap of fast heuristics for independent repetitive COPs, and can optimize the long-term objectives for repetitive COPs embedded in graph-based Markov decision processes. Source code at `https://github.com/XzrTGMu/twin-nphard`.

1 INTRODUCTION

In a general network setting, the network state is captured by a graph $\mathcal{G} = (\mathcal{V}, \mathcal{E}, \mathbf{S})$, that comprises a vertex set $\mathcal{V}$, an edge set $\mathcal{E}$, and a matrix $\mathbf{S}$ representing data supported on $\mathcal{V}$. We aim to optimize the system-level objective $f_{obj}(\mathbf{o})$, which is a known linear combination, $f_{obj} : \mathbb{R}^{|\mathbf{o}|} \to \mathbb{R}$, of a vector $\mathbf{o} \in \mathbb{R}^{|\mathcal{V}|}$ capturing the outcomes (e.g., rewards) on individual nodes of a network process, where

$$\mathbf{o} = f_{net}(\mathcal{G}) \ . \tag{1}$$

In (1), $f_{net}(\cdot)$ is a non-differentiable function that models some network process, such as a network simulator or an operation that involves solving a combinatorial optimization problem (COP).

In this paper, we focus on graph-based repetitive COPs (R-COP) Kraay & Harker (1996) under hard constraints that must be satisfied at all times Kendall (1975), which are often NP-hard. Specifically, we are interested in COPs that need to be solved repeatedly on graphs of the same or slowly changing topology ($\mathcal{V}$ or $\mathcal{E}$) but rapidly changing node weights ($\mathbf{S}$). R-COPs have many real-world applications, such as task scheduling Pinedo (2012), route planning Vogiatzis & Pardalos (2013), link scheduling Joo & Shroff (2012); Paschalidis et al. (2015); Eisen et al. (2019); Zhao et al. (2022a;b) and routing Oliveira et al. (2011) in communication networks, and energy management in smart grids Chau et al. (2018), where a node or edge weight captures varying cost or utility. In practice, $f_{net}(\cdot)$ for R-COP is often subject to restricted runtime and/or distributed execution. For example, in scheduling, network routing, and multi-object tracking in computer vision, COPs need to be solved within tens of milliseconds to a few seconds. Although memory-based approaches can avoid solving each instance from scratch for some applications Kraay & Harker (1996); Wang (2021), in general, R-COPs rely on fast heuristics to meet the strict time constraints, at the cost of relatively large optimality gaps. Moreover, in real-time networked systems, such as communication networks, smart grids, and robot swarms Tolstaya et al. (2020), centralized solvers often suffer from the large communication overhead of gathering the full network state, high computational complexity, and risk of single point of failure. Therefore, distributed solutions Moser & Tardos (2010) are preferred for better scalability and robustness, in which nodes across the network work in parallel to collect and process the information of only their local neighborhoods for decision making.

Depending on the definition of f_{obj}, R-COPs can be categorized as, 1) independent R-COPs, i.e., $\mathbf{S}(t_1)$ and $\mathbf{S}(t_2)$ are considered as independent if $t_1 \neq t_2$, and 2) R-COPs embedded in a graph-based

Markov decision process (MDP). For example, in link scheduling for wireless multiple networks Zhao et al. (2022a;b), the network state $\mathcal{G}(t) = (\mathcal{V}, \mathcal{E}, \mathbf{S}(t))$, where $\mathbf{S}(t)$ captures the packet backlogs of all the links at time t, depends on the schedule of $t-1$ found by solving a maximum weight independent set (MWIS) problem defined on $\mathcal{G}(t-1)$. Scheduling for maximum throughput (number of data packets transmitted on the schedule) is equivalent to optimize each MWIS instance individually Zhao et al. (2022a), which is formulated as an independent R-COP. However, to minimize the average backlog (packets left in the queues by the schedule) across links and *over time*, the transition of network states must be considered and the scheduling is formulated as R-COP in a graph-based MDP Zhao et al. (2022b). Similar MDP formulations can also be found in wireless scheduling for battery lifetime Sikandar et al. (2020), vehicle routing for waste collection Wu et al. (2020), and inventory control in distribution networks Çelebi (2015). However, the 2nd type of R-COPs have rarely been addressed, except in an ad-hoc manner for link scheduling Zhao et al. (2022b). Therefore, a general approach to R-COPs in graph-based MDPs would be of high interest.

1.1 Existing Approaches to COPs

The general approach for exactly solving a COP is to formulate it as a mixed-integer program, and solve it by branch-and-bound Gasse et al. (2019); Nair et al. (2020); Zarpellon et al. (2021) or dynamic programming. Commercial Gurobi solvers LLC (2020) can exactly solve COPs on graphs of hundreds of nodes in reasonable time. For large real-world graphs with certain structural properties, branching with reduction can decrease the input size Lamm et al. (2019). For problems facing large scale or stringent time limit, efficient heuristics are used to approximate the solution; common strategies include greedy algorithms, local search Wang et al. (2018), tabu search, ant colony Jovanovic et al. (2010), and simulated annealing. Many recent works focus on machine learning-based COP solvers. Since it is very hard for a neural network by itself to predict the optimal solution or even satisfy a set of constraints, the general approach is to use graph neural networks (GNNs) (Wu et al., 2021) to guide an algorithmic framework, such as branching Khalil et al. (2016); Gasse et al. (2019); Nair et al. (2020); Zarpellon et al. (2021), tree search Li et al. (2018), greedy algorithms Khalil et al. (2017); Zhao et al. (2022a), and/or local search Hudson et al. (2022), where the latter guarantees that the constraints are always followed. These approaches typically formulate a COP instance as a finite episode of an MDP, in which a state captures the residual graph of an intermediate step, based on which an action of adding one vertex in the residual graph to the partial solution is generated by a GNN, and a solution is built from a sequence of such scalar actions. This formulation has a time complexity of no less than $\mathcal{O}(|\mathcal{V}||\mathcal{E}|)$, since a GNN of time complexity of $\mathcal{O}(|\mathcal{E}|)$ Wu et al. (2021) is called in each intermediate step. Drori et al. (2020); Hottung et al. (2022) lowered the time complexity of vehicle routing problems to $\mathcal{O}(|\mathcal{E}|)$ (typically, $|\mathcal{E}| > |\mathcal{V}|$) by encoding the graph by a GNN only once per COP instance. However, for R-COPs, this formulation is limited by centralized execution and the complexity of a GNN, and does not apply to R-COPs in graph-based MDPs.

Popular distributed approaches to find solutions to COPs include Moser-Tardos algorithm Moser & Tardos (2010) and dynamic programming. The complexity of distributed algorithms is usually measured by local communication complexity, which is the number of rounds of message exchanges between a node and its neighbors Joo & Shroff (2012); Zhao et al. (2022a). On some problems, such as MWIS Joo & Shroff (2012), maximal independent set (MIS) Moser & Tardos (2010), and graph coloring Chung et al. (2017), Moser-Tardos algorithm can converge with high probability with a local communication complexity of $\mathcal{O}(\log^* |V|)$. Message passing-based distributed dynamic programming, e.g. for MWIS Paschalidis et al. (2015), can converge in $\mathcal{O}(|V|)$. However, the lack of global information may cause distributed algorithms to have larger optimality gaps. Topological metrics can be used to reduce the optimality gap, such as edge betweenness for the Steiner tree problem Fujita et al. (2016). Compared to their centralized counterparts, learning-based distributed COP solvers have received less attention. Zhao et al. (2022a) proposed an architecture, GCN-LGS, for a repetitive MWIS problem, in which an L-layer graph convolutional neural network (GCNN) generates a vector $\mathbf{z}$ for a topology $(\mathcal{V}, \mathcal{E})$, and a greedy heuristic solves modified instances $(\mathcal{V}, \mathcal{E}, \mathbf{c}^{(t)} \odot \mathbf{z})$, rather than the original ones $(\mathcal{V}, \mathcal{E}, \mathbf{c}^{(t)})$, for the next N time slots $t \in \{1, \ldots, N\}$, assuming the topology would not change by $t = N$. GCN-LGS can reduce the optimality gap of greedy solvers Joo & Shroff (2012) by ⅓ to ½, with a time complexity of $\mathcal{O}(L|\mathcal{E}|/N + |\mathcal{V}|)$, or can converge in $\mathcal{O}(L/N + \log |V|)$ iterations in a distributed setting. For large N, the overhead of GCNN is negligible. However, the training methods in Zhao et al. (2022a;b) are ad hoc and specific to repetitive MWIS problems, which could not be directly applied to other types of R-COPs.

In this work, we generalize the GCN-LGS architecture in Zhao et al. (2022a;b) to a parameterized network process, $f_{net}(\cdot; \mathbf{Z})$, and propose a unified actor-critic framework to optimize the parameters $\mathbf{Z}$ in broader tasks. We then apply this framework to enhance the heuristics for R-COPs. Rather than using a sequence of scalar actions to solve a COP instance formulated as a finite episode of an MDP, our actor network generates $\mathbf{Z}$ as a high-dimensional action, and the solutions of one or multiple instances of an R-COP are found by the parameterized heuristic $f_{net}(\cdot; \mathbf{Z})$. Under this formulation, distributed heuristics can be used as $f_{net}(\cdot; \mathbf{Z})$, and the long-term objective of R-COPs embedded in a graph-based MDP can be optimized through a sequence of high-dimensional actions, each based on the network state of a time slot. For independent R-COPs, an action $\mathbf{Z}$ encodes the underlying topology shared by N instances, further reducing the overhead of running the GNN from $\mathcal{O}(|\mathcal{E}|)$ Drori et al. (2020); Hottung et al. (2022) to $\mathcal{O}(|\mathcal{E}|/N)$, which is arbitrarily small for a large N. The challenge, however, is that our downstream pipeline contains a non-differentiable block $f_{net}(\cdot; \mathbf{Z})$.

1.2 Learning in Non-differentiable Pipelines

Training with supervised or unsupervised learning methods is challenging in the presence of non-differentiable blocks, such as $f_{net}(\cdot)$ in (1). Reinforcement learning (RL) Sutton & Barto (2018) deals with this problem by treating the non-differentiable block as (part of) the environment Silver et al. (2014); Khalil et al. (2017); Zhao et al. (2022a). Policy gradient Silver et al. (2014) with high-dimensional action space is most suited for the parallel and dynamic nature of networks, whereas the popular Q-learning Watkins & Dayan (1992) is inherently sequential. A major issue in RL for networks is how to assign credit to individual elements based on the system-level reward. For wireless resource allocation with soft constraints (Kendall, 1975), a policy gradient-based primal-dual optimization method was proposed by Eisen et al. (2019). Imitation learning Ross et al. (2011) trains neural networks to mimic existing algorithms, and has been used in GNN-guided search Gasse et al. (2019) and control Tolstaya et al. (2020). However, it requires a good guiding algorithm, which sets the upper limit of the system and could be costly. Zeroth-order optimization (ZOO) Liu et al. (2020) is the last resort for non-differentiable pipelines, as it requires numerous evaluations of $f_{net}(\cdot)$, which could be computationally prohibitive.

To address the aforementioned shortcomings, we propose a graph-based deterministic policy gradient (GDPG-Twin) following the actor-critic method (Sutton & Barto, 2018, ch. 13). The core idea is to train a differentiable twin of $f_{net}(\cdot; \mathbf{Z})$, as part of the critic network, to facilitate the training of the actor network. A similar idea, called differentiable approximation bridges (DAB) was proposed in Ramapuram & Webb (2020) to approximate the *immediate* behavior of a non-differentiable block in standalone systems. We improve DAB from three aspects: we use a twin network to predict the element-wise *expected* outcomes of $f_{net}(\cdot; \mathbf{Z})$, use a GNN to account for the permutation equivariance in network settings, and use random policy sampling for static policy $\mathbf{Z}$ in a fixed topology. Our GDPG-Twin is suitable for network settings with hard constraints, and is more efficient than ZOO. Although we focus on node-related problems, our approach also applies to edge-related problems, e.g., by designing a twin based on simplicial neural networks Roddenberry et al. (2021).

1.3 Contributions

In summary, our proposed framework: 1) can generalize to learning for different COPs without handcrafting the credit assignment strategies as in other schemes of network-based RL Eisen et al. (2019); Zhao et al. (2022a;b), 2) works for R-COPs with hard constraints, 3) requires fewer evaluations of $f_{net}(\cdot; \mathbf{Z})$ than ZOO Liu et al. (2020), and 4) has the advantage of RL schemes in not relying on expensive data labeling as in supervised learning or a computationally intensive supervising algorithm as in imitation learning Ross et al. (2011).

Our contribution contains the following three aspects:

- We propose a general approach to R-COPs under hard constraints. Our approach can reduce the optimality gap of fast and/or distributed heuristics for independent R-COPs, at the cost of only an upfront computation and communication overhead, and can optimize the long-term objectives for R-COPs in a graph-based MDP.
- We propose GDPG-Twin, an actor-critic framework for network settings. The critic comprises a twin network that learns the element-wise expected outcomes of policy $\mathbf{Z}$ applied

to a non-differentiable network process $f_{net}(\cdot; \mathbf{Z})$. This twin-based critic can address the challenge of credit assignment across the network, which is a major roadblock for discrete or mixed-integer network processes.

- We adopt a random policy sampling strategy in the training of the twin network, which enables learning of the static policy $\mathbf{Z}$. Moreover, our twin network can significantly reduce the number of evaluations of the non-differentiable function $f_{net}(\cdot; \mathbf{Z})$ compared to ZOO.

Notation. Upright bold lower-case (upper-case) symbols are used to denote column vectors, e.g., $\mathbf{x}$ (matrices, e.g., $\mathbf{X}$). $\mathbf{x}_i$ denotes the ith element of vector $\mathbf{x}$, $\mathbf{X}_{i,j}$ denotes the element at row i and column j of matrix $\mathbf{X}$, $\mathbf{X}_{i*}$ (or $\mathbf{X}_{*j}$) denotes row i (or column j) of matrix $\mathbf{X}$. Unless otherwise specified, calligraphic upper-case symbols (e.g., $\mathcal{V}$) are used to denote sets. $(\cdot)^\top$ and $\odot$ denote transpose and element-wise product, respectively.

2 Problem Formulation

Many binary discrete COPs have the following formulation,

$$\mathbf{x}^* = \min_{\mathbf{x}} \ \mathbf{c}^\top \mathbf{x} \tag{2a}$$

$$s.t. \ \ \mathbf{x}_i \in \{0, 1\} \ , \forall i \in \{1, \ldots, |\mathcal{V}|\} \ , \tag{2b}$$

$$\text{other problem-specific constraints,} \tag{2c}$$

where $\mathbf{x}$ and $\mathbf{c}$ are respectively the vectors of decisions and weights on nodes. Since many problems in (2) are NP-hard, we seek to develop efficient heuristics to approximate $\mathbf{x}^*$. We define a function space $\mathcal{F}$ as a set of functions that will output solutions satisfying all the constraints of the COP in (2).

2.1 Independent Repetitive COPs

When the instances of an R-COP are independent of each other, the weight $\mathbf{c}$ of each instance is considered to be a random vector drawn from its target sampling distribution $\Omega^{\mathbf{c}}$. We relax the objective function in (2a) to its expectation over $\Omega^{\mathbf{c}}$, and formulate the optimization problem as

$$f^*_{net} = \min_{f_{net} \in \mathcal{F}} \ \mathbb{E}_{\mathbf{c} \sim \Omega^{\mathbf{c}}} (\mathbf{c}^\top \mathbf{x}) \tag{3a}$$

$$s.t. \ \ \mathbf{x} = f_{net}(\mathcal{V}, \mathcal{E}, \mathbf{c}) \ . \tag{3b}$$

Although the optimal solution for (3), $\mathbf{x}^* = f^*_{net}(\mathcal{V}, \mathcal{E}, \mathbf{c})$, is still an exact solver for (2) for every given $\mathbf{c}$, the smoothened objective function in (3a) makes it easier to approximate f^*_{net}, as illustrated in Section 3.

2.2 Repetitive COPs in a Graph-based Markov Decision Process

Given network state $\mathcal{G}(t) = (\mathcal{V}(t), \mathcal{E}(t), \mathbf{S}(t))$, where $\mathbf{S}(t)$ captures features on nodes at time t, our objective is to find a policy, $f_{net} \in \mathcal{F}$, that maximizes the system-level value over time horizon T

$$f^*_{net} = \max_{f_{net} \in \mathcal{F}} \ f_{obj} \left(\mathbb{E}_{t \leq T} \left[\mathbf{o}(t) \right] \right) \ , \tag{4a}$$

$$s.t. \ \ \mathbf{o}(t) = \mathbb{E}_{f_{net}} \left[\sum_{k=0}^{T-t} \gamma^k \mathbf{r}(t+k) \middle| \mathcal{G}(t) \right] \ , \tag{4b}$$

$$\mathbf{r}(t) = f_r(\mathcal{V}(t), \mathcal{E}(t), \mathbf{S}(t), \mathbf{x}(t)) \ , \tag{4c}$$

$$\mathbf{x}(t) = f_{net}(\mathcal{V}(t), \mathcal{E}(t), \mathbf{S}(t)) \ , \tag{4d}$$

$$\mathbf{S}(t+1) = f_s(\mathcal{V}(t), \mathcal{E}(t), \mathbf{S}(t), \mathbf{x}(t)) \ . \tag{4e}$$

In (4), $\mathbf{o}(t)$ is the value vector of current state $\mathcal{G}(t)$ under policy f_{net}, $0 \leq \gamma \leq 1$ is the discount factor, (4a) states that the system-level objective is a linear combination of the value vector, and (4c) and (4e) define the MDP by respectively stating that the reward vector $\mathbf{r}(t)$ and the next state $\mathbf{S}(t+1)$ depend on the current state $\mathbf{S}(t)$ and the decisions $\mathbf{x}(t)$. In general, $f_r(\cdot)$ and $f_s(\cdot)$ in (4) are stochastic functions, capturing some stationary random processes in the environment. The formulation in (4) can capture R-COPs with accumulative objectives, such as latency and battery

lifetime in wireless scheduling, waste level in vehicle routing for waste collection, and inventory in distribution networks. Notice that if $T = t$, $\gamma = 1$, $\mathbf{S}(t) = \mathbf{c}(t)$, $\mathbf{r}(t) = \mathbf{c}(t) \odot \mathbf{x}(t)$, $f_{obj}(\mathbf{o}) = \mathbf{1}^\top \mathbf{o}$, and we set f_s in (4e) as drawing a random vector from Ω^c, then (4) boils down to (3).

3 GRAPH-BASED DETERMINISTIC POLICY GRADIENT

Our downstream pipeline follows the existing methodology of using a neural network to guide a discrete operation, which guarantees the hard constraints, but keeps the neural network outside the iterations of the algorithmic framework for lower complexity Zhao et al. (2022a). In this section, we provide the main solution, whereas the full procedures of optimization for Sections 3.1 and 3.2 are given by Algorithms 1 and 2 in Appendix C. Since (3) and (4) are functional optimization problems, we seek to approximately solve them by parameterizing $f_{net}(\cdot; \mathbf{Z})$ and reformulating (3) and (4) to finding the optimal set of parameters $\mathbf{Z}^*$.

3.1 LEARNING FOR INDEPENDENT REPETITIVE COP

For independent R-COPs, we reformulate (3) as

$$\mathbf{Z}^* = \min_{\mathbf{Z} \in \mathbb{R}^{|\mathbf{Z}|}} \quad \mathbf{1}^\top \mathbf{o} \tag{5a}$$

$$s.t. \quad \mathbf{o} = \mathbb{E}_{\mathbf{c} \sim \Omega^{\mathbf{c}}} \left(\mathbf{c} \odot \mathbf{x} \right) \tag{5b}$$

$$\mathbf{x} = h(\mathcal{V}, \mathcal{E}, \mathbf{w}) \ , h \in \mathcal{F} \ , \tag{5c}$$

$$\mathbf{w}_i = f_{loc}(\mathbf{c}_i; \mathbf{Z}_{i*}) \ , \forall i \in \{1, \ldots, |\mathbf{c}|\} \ . \tag{5d}$$

The objectives in (3a) and (5a) are equal due to the linearity of expectation. Constraints (5c) and (5d) further break the parameterized function $f_{net}(\mathcal{V}, \mathcal{E}, \mathbf{c}; \mathbf{Z})$ in (3b) into a valid heuristic $h(\cdot) \in \mathcal{F}$ and a parameterized local function $f_{loc}(\cdot; \mathbf{Z}_{i*})$, where $\mathbf{Z}_{i*}$ captures the representation on node $i \in \mathcal{V}$. The heuristic $h(\cdot)$ ensures that $f_{net}(\cdot; \mathbf{Z}) \in \mathcal{F}$, whereas the local function $f_{loc}(\cdot; \mathbf{Z}_{i*})$ is parameterized differently for different nodes $i \in \mathcal{V}$. The function $f_{loc}(\cdot; \mathbf{Z}_{i*})$ can be chosen arbitrarily, e.g., it can be a multiplier, a single neuron, or even a small neural network.

To solve the problem formulated in (5), we employ deterministic policy gradient reinforcement learning, in which policy $\mathbf{Z}$ parameterizes $f_{net}(\cdot; \mathbf{Z})$. However, the gradient $\nabla_{\mathbf{Z}} \mathbf{1}^\top \mathbf{o}$ is not available since $f_{net}(\cdot)$ is non-differentiable. To address this problem, we introduce a trainable and differentiable twin network $f_{twin}(\cdot; \mathbf{\Theta}_c)$ to learn the element-wise expected outcome of $f_{net}(\cdot; \mathbf{Z})$. In contrast to the critic in a typical standalone setting, which directly predicts the system-level objective, the twin network works for network settings, where policy and outcome are supported on graphs. The twin can be implemented by a graph or a simplicial neural network Roddenberry et al. (2021), depending on the specific COP. The expected behavior of the twin can be described by

$$\mathbf{o} \approx \hat{\mathbf{o}} = f_{twin}(\mathcal{V}, \mathcal{E}, \bar{\mathbf{c}}, \mathbf{Z}; \mathbf{\Theta}_c^*), \text{ where } \bar{\mathbf{c}} = \mathbb{E}_{\Omega^{\mathbf{c}}}(\mathbf{c}) \ . \tag{6}$$

Based on (5a) and (6), we can estimate the system objective as $\mathbf{1}^\top \hat{\mathbf{o}}$. Based on (6) and the chain rule $\frac{\partial \mathbf{1}^\top \hat{\mathbf{o}}}{\partial \mathbf{Z}} = \mathbf{1}^\top \frac{\partial \hat{\mathbf{o}}}{\partial \mathbf{Z}}$, the policy gradient is estimated as Silver et al. (2014)

$$\widehat{\nabla_{\mathbf{Z}} \mathbf{1}^\top} \mathbf{o} \approx \nabla_{\mathbf{Z}} \mathbf{1}^\top \hat{\mathbf{o}} = \nabla_{\mathbf{Z}} f_{twin}(\mathcal{V}, \mathcal{E}, \mathbb{E}_{\Omega^{\mathbf{c}}}(\mathbf{c}), \mathbf{Z}; \mathbf{\Theta}_c) \mathbf{1} \ . \tag{7}$$

We can update the policy as, $\mathbf{Z} \leftarrow \mathbf{Z} - \alpha_p \nabla_{\mathbf{Z}} \mathbf{1}^\top \hat{\mathbf{o}}$. If the policy is generated by an actor, $\mathbf{Z} = \Psi(\mathcal{V}, \mathcal{E}, \bar{\mathbf{c}}; \mathbf{\Theta}_p)$, we can estimate the gradient $\nabla_{\mathbf{\Theta}_p} \mathbf{1}^\top \hat{\mathbf{o}} = \nabla_{\mathbf{\Theta}_p} \Psi(\mathcal{V}, \mathcal{E}, \bar{\mathbf{c}}; \mathbf{\Theta}_p) \nabla_{\mathbf{Z}} \mathbf{1}^\top \hat{\mathbf{o}}$, and update the parameters of the actor as, $\mathbf{\Theta}_p \leftarrow \mathbf{\Theta}_p - \alpha_p \nabla_{\mathbf{\Theta}_p} \mathbf{1}^\top \hat{\mathbf{o}}$, where $0 \leq \alpha_p \leq 1$ is the policy learning rate.

Given a learning rate $0 \leq \alpha_c \leq 1$, the twin network can be updated by the following gradient descent,

$$\mathbf{\Theta}_c \leftarrow \mathbf{\Theta}_c - \alpha_c \nabla_{\mathbf{\Theta}_c} \ell_{mse}(\hat{\mathbf{o}}, \mathbf{o}) \ , \tag{8}$$

where the loss function $\ell_{mse}(\hat{\mathbf{o}}, \mathbf{o})$ is the mean-square-error (MSE) between $\hat{\mathbf{o}}$ and $\mathbf{o}$. Since $\mathbf{o}$ is an expectation over sampling space $\Omega^{\mathbf{c}}$, we can implement the following stochastic gradient descent

$$\mathbf{\Theta}_c \leftarrow \mathbf{\Theta}_c - \alpha_c \nabla_{\mathbf{\Theta}_c} \ell_{mse}(\hat{\mathbf{o}}, \mathbf{c} \odot \mathbf{x}), \ \ell_{mse}(\hat{\mathbf{o}}, \mathbf{c} \odot \mathbf{x}) = \frac{1}{|\mathbf{x}|} \sum_{i=1}^{|\mathbf{x}|} \left(\hat{\mathbf{o}}_i - \mathbf{c}_i \mathbf{x}_i \right)^2 , \ \mathbf{c} \in \Omega^{|\mathbf{c}|} \ , \tag{9}$$

by minimizing the MSE loss in (9) with an off-the-shelf optimizer. Notice that we need to evaluate $f_{net}(\cdot; \mathbf{Z})$ to get $\mathbf{x}$ in (9). A detailed derivation of (9) is given in Appendix A.

3.1.1 RANDOM SAMPLING AROUND CURRENT POLICY

For static policy $\mathbf{Z}$ on a fixed topology, i.e., not generated by an actor, the twin is likely to be overfitted if we only feed it $\mathbf{Z}$ during training. To address this problem, we feed the twin $f_{twin}(\cdot)$ and $f_{net}(\cdot)$ with random samples around the current policy $\mathbf{Z}^{(j)} = \mathbf{Z} + \mathbf{N}^{(j)}, \mathbf{N}^{(j)}_{m,n} \in \mathbb{U}(-\epsilon, \epsilon)$ where ϵ is the sampling radius. The loss in (9) then becomes $\ell_{mse}(\hat{\mathbf{o}}^{(j)}, \mathbf{c} \odot \mathbf{x}^{(j)})$. This random sampling strategy enables the critic, comprising the twin $f_{twin}(\cdot; \mathbf{\Theta}_c)$ and system-level objective function $f_{obj}(\hat{\mathbf{o}})$, to learn the loss landscape around the current policy $\mathbf{Z}$, thus improve the quality of gradient in (7).

In ZOO, a policy gradient is estimated from at least two random samples around the current policy $\mathbf{Z}$ (including $\mathbf{Z}$ itself) Liu et al. (2020). While fewer policy samples requires fewer evaluations of $f_{net}(\cdot; \mathbf{Z})$, which could be computationally expensive in many applications, it could degrade the convergence by raising the noise floor of the gradient estimate. Compared to ZOO, our twin-based critic can continuously learn, refine, and memorize the loss landscape around the current policy as new samples coming in, leading to better gradient estimate in backpropagation (improved convergence as shown in Figure. 1), and higher policy sampling efficiency, as shown in Sections 4.2 and 4.3.

3.2 LEARNING FOR REPETITIVE COP IN A GRAPH-BASED MARKOV DECISION PROCESS

For R-COPs with state transitions, we parameterize the $f_{net}(\cdot)$ with a heuristic $h(\cdot) \in \mathcal{F}$ taking in an action vector $\mathbf{z}$ generated under the current state, by a deterministic policy network (actor) as $\mathbf{z} = \Psi(\mathcal{V}, \mathcal{E}, \mathbf{S}; \mathbf{\Theta}_p)$. We then reformulate (4) as follows:

$$\mathbf{\Theta}_p^* = \max_{\mathbf{\Theta}_p \in \mathbb{R}^{|\mathbf{\Theta}_p|}} \; f_{obj}\left(\mathbb{E}_{t \le T}\left[\mathbf{o}(t)\right]\right) \;, \tag{10a}$$

$$s.t. \;\; \mathbf{o}(t) = \mathbb{E}_{\mathbf{\Theta}_p}\left[\sum_{k=0}^{T-t} \gamma^k \mathbf{r}(t+k) \middle| \mathcal{G}(t)\right] \;, \tag{10b}$$

$$\mathbf{r}(t) = f_r(\mathcal{V}(t), \mathcal{E}(t), \mathbf{S}(t), \mathbf{x}(t)) \;, \tag{10c}$$

$$\mathbf{x}(t) = h(\mathcal{V}(t), \mathcal{E}(t), \mathbf{z}(t)) \;, \tag{10d}$$

$$\mathbf{z}(t) = \Psi(\mathcal{V}(t), \mathcal{E}(t), \mathbf{S}(t); \mathbf{\Theta}_p) \;, \tag{10e}$$

$$\mathbf{S}(t+1) = f_s(\mathcal{V}(t), \mathcal{E}(t), \mathbf{S}(t), \mathbf{x}(t)) \;. \tag{10f}$$

Similar to (7), we estimate the action gradient $\nabla_{\mathbf{z}(t)} f_{obj}\left(\mathbb{E}_{t \le T}\left[\mathbf{o}(t)\right]\right)$ through a twin network that predicts the value vector in (10b) as $\mathbf{o}(t) \approx \hat{\mathbf{o}}(t) = f_{twin}(\mathcal{V}(t), \mathcal{E}(t), \mathbf{S}(t), \mathbf{z}(t); \mathbf{\Theta}_c)$. Based on the linearity of expectation and that $f_{obj}(\cdot)$ is a linear combination, the policy gradient estimate is Silver et al. (2014)

$$\widehat{\nabla_{\mathbf{\Theta}_p} f_{obj}}\left(\mathbb{E}_{t \le T}\left[\mathbf{o}(t)\right]\right) \approx \mathbb{E}_{t \le T}\left[\nabla_{\mathbf{\Theta}_p} \hat{\mathbf{o}}(t) \nabla_{\hat{\mathbf{o}}(t)} f_{obj}(\hat{\mathbf{o}}(t))\right] \;. \tag{11}$$

Then, we can update the policy network as $\mathbf{\Theta}_p \leftarrow \mathbf{\Theta}_p + \alpha_p \widehat{\nabla_{\mathbf{\Theta}_p} f_{obj}}\left(\mathbb{E}_{t \le T}\left[\mathbf{o}(t)\right]\right)$. According to the detailed derivation in Appendix B, the twin network can be trained by stochastic gradient descent, implemented by minimizing the following loss with an off-the-shelf optimizer:

$$\ell_{mse}(\hat{\mathbf{o}}(t), \mathbf{r}(t) + \gamma \hat{\mathbf{o}}(t+1)) \;, \text{ where } \hat{\mathbf{o}}(t+1) = \mathbf{0}, \; \forall t \ge T \;. \tag{12}$$

4 NUMERICAL RESULTS

4.1 INDEPENDENT R-COPS

We first demonstrate our GDPG-Twin framework on four independent R-COPs, including maximum weighted independent set (MWIS), minimum weighted dominating set (MWDS), node weighted Steiner tree (NWST), and minimum weighted connected dominating set (MWCDS). These problems are all NP-hard, and need to be solved repetitively in a wide range of applications. For example, the MWIS problem appears in various schedulers Pinedo (2012); Joo & Shroff (2012); Paschalidis et al. (2015); Zhao et al. (2022a;b) and multi-object tracking in computer vision. The MWDS problem is encountered in wireless network clustering and covering codes. Multicast routing in communication networks involves the NWST problem Oliveira et al. (2011). The MWCDS problem can establish a virtual backbone network in wireless multihop networks, that covers all the nodes with the lowest cost in energy consumption or security vulnerability Oliveira et al. (2011).

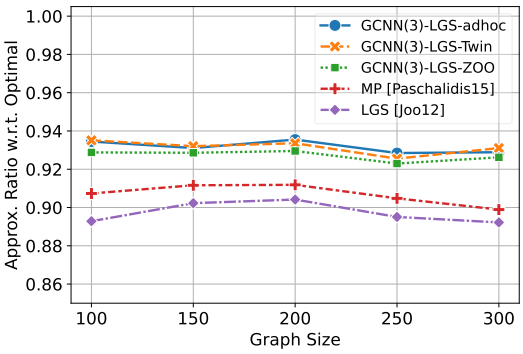

Figure 1: Approximation ratios of the vanilla and GCNN-enhanced distributed heuristics for MWIS problem (max), w.r.t. the optimal solver. Larger is better.

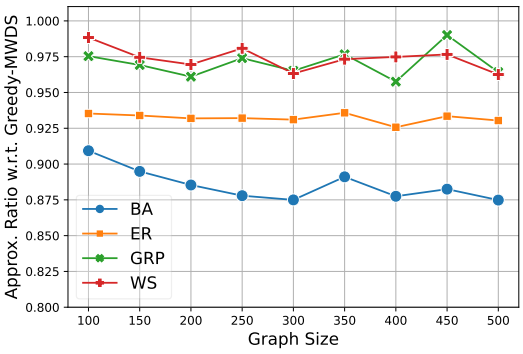

Figure 2: Approximation ratio of the GCNN-enhanced w.r.t. the vanilla Greedy-MWDS for MWDS problem (min) on 4 sets of random graphs. Smaller is better.

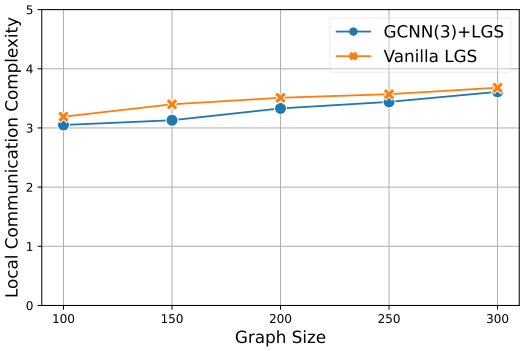

Figure 3: Average local communication complexity of GCNN-enhanced and vanilla LGS-MWIS solvers per instance, in rounds, excluding the GCNN ($N = \infty$).

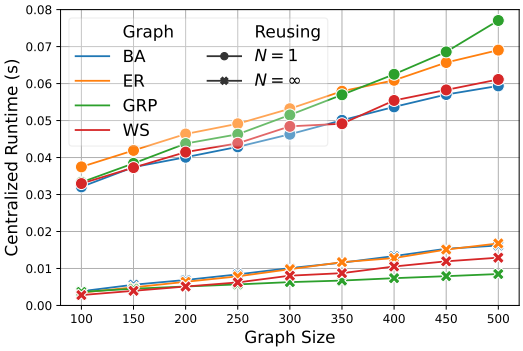

Figure 4: Average runtime of GCNN-enhanced Greedy-MWDS per instance by graph size, in seconds, no reusing $N = 1$ and infinity reusing $N = \infty$ of $\mathbf{Z}$.

We develop four similar ML pipelines respectively for the four R-COPs, in which the actor and twin networks are implemented by L-layer and 5-layer GCNNs, respectively (see Appendix D for the details of GCNN, and Appendix C for the detailed training configurations), the baseline heuristics $h(\cdot)$ in (5c) are selected as centralized or distributed greedy solvers. The details of the four ML pipelines, including brief descriptions of the chosen baseline heuristics, are provided in Appendix F. We aim to demonstrate the effectiveness of our proposed learning framework in closing the optimality gaps of some widely used fast heuristics for R-COPs, at the cost of negligible overhead, e.g., an additional computational complexity of $\mathcal{O}(L|\mathcal{E}|/N)$ or local communication complexity of $\mathcal{O}(L/N)$ per instance on sparse graphs. We do *not* claim smaller optimality gaps than the state-of-the-art (slower and centralized) heuristics, nor that GCNN is the best candidate graph neural architecture for these problems. An appealing characteristic of our framework is its modularity, which allows the GCNNs being replaced by any other (non-convolutional) GNN while our approach is still valid.

The four COPs are widely applied in various wireless networks, involving graphs of up to hundreds of nodes, and runtimes constraints from tens of milliseconds to a few seconds. Due to the dynamic nature and the lack of real-world datasets of wireless network topologies, we follow the norm of wireless research by running our experiments on four sets of synthetic random graphs: Erdős–Rényi (ER) Erdős & Rényi (1959), Barabási–Albert (BA) Albert & Barabási (2002), Gaussian Random Partition (GRP), and connected Watts-Strogatz small-world (WS) graphs. Each test dataset contains 2000 random graphs generated by a graph model with parameters detailed in Appendix E. The optimality of a heuristic is evaluated by the average approximation ratio, $\mathbb{E}_{\Omega'}(\mathbf{c}^\top\mathbf{x}^{(h)}/\mathbf{c}^\top\mathbf{x}^{(b)})$, on a test set Ω', where $\mathbf{x}^{(h)}$ and $\mathbf{x}^{(b)}$ are respectively the solutions from the heuristic of interests and a reference algorithm. Only in MWIS, the optimal solutions from Zhao et al. (2022a) are used as reference, in other COPs, greedy heuristics are the references.

MWIS: An independent (vertex) set for a graph is a subset of vertices not connected by any edges. The MWIS problem is to find an independent set on a vertex weighted graph that maximizes the total weight. The baseline heuristic is a distributed local greedy solver (LGS-MWIS) Joo & Shroff (2012), with a local communication complexity of $\mathcal{O}(\log|\mathcal{V}|)$. We test multiple distributed MWIS solvers,

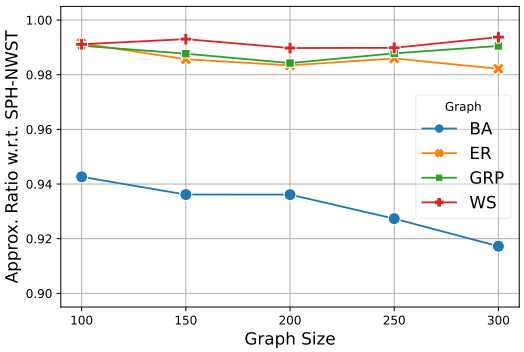

Figure 5: Approximation ratio of the GCNN-enhanced w.r.t. vanilla K-SPH-NWST for NWST problem on 4 sets of random graphs. Smaller is better for a minimization problem.

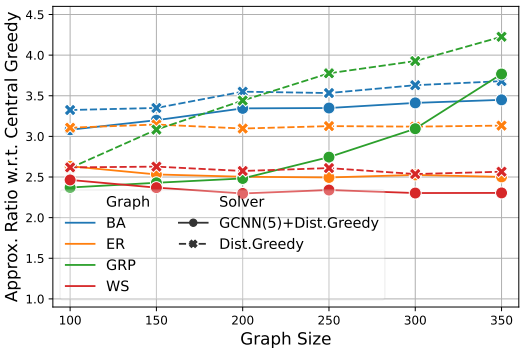

Figure 6: Approximation ratios of the vanilla and GCNN-enhanced distributed heuristics w.r.t. a centralized heuristic for MWCDS problem on 4 sets of random graphs. Smaller is better for a min. problem.

including the GCNN-enhanced and vanilla LGS-MWIS, and a message passing (MP) algorithm Paschalidis et al. (2015) on a set of 500 random ER graphs from Zhao et al. (2022a). 3 GCNNs are respectively trained by ad hoc RL Zhao et al. (2022a), GDPG-Twin, and ZOO Liu et al. (2020), on a set of 6000 ER graphs. The approximation ratios of the tested solvers w.r.t. the optimal solver are shown in Figure 1. GDPG-Twin (93.1%) works equally well as the ad hoc RL (93.2%), and slightly outperforms ZOO (92.7%) with only ⅓ to ½ evaluations of $f_{net}(\cdot; \mathbf{Z})$ (see Section 4.3). The GCNN can reduce the optimality gap of LGS-MWIS (89.7%) by ⅓, beating the MP algorithm (90.7%). Figure 3 shows that GCNN-enhanced and vanilla LGS-MWIS converge in $3 \sim 4$ rounds in this test (MP algorithm converges in $2|\mathcal{V}|$ rounds), where the former is slightly faster for a large N.

MWDS: A dominating set for a graph $\mathcal{G} = (\mathcal{V}, \mathcal{E})$ is a subset $\mathcal{D}$ of $\mathcal{V}$ such that every vertex not in $\mathcal{D}$ is adjacent to at least one member of $\mathcal{D}$. In the MWDS problem, every node is associated with a non-negative weight, and the objective is to find a dominating set of minimum total weight. The baseline heuristic is a centralized greedy algorithm, Greedy-MWDS, as detailed in Appendix F. The approximation ratio of the GCNN-enhanced Greedy-MWDS w.r.t. the vanilla Greedy-MWDS on the 4 sets of random graphs described earlier, are shown in Figure 2. On average, GCNN improves the performance of Greedy-MWDS by 11.42% on BA graphs, 6.8% on ER graphs, 3.0% on GRP graphs, and 2.6% on WS graphs. The improvement is more pronounced on larger graphs. As shown in Figure 4, the average runtime of the GCNN-enhanced Greedy-MWDS on a laptop of 4 CPUs no GPU (detailed in Appendix G) ranges from 32 to 78 milliseconds per instance, and is linear to the graph size, which can be further cut to 2-17 milliseconds for a large reusing factor N.

NWST: In the NWST problem, we are given an undirected graph $\mathcal{G}$ with node cost (non-negative weight) and a subset of nodes called terminals. The goal is to find a minimum cost subgraph of $\mathcal{G}$ that connects the terminals. In the test, the terminals are selected by randomly removing $10\% \sim 50\%$ nodes from a maximal independent set (MIS) on the graph. The baseline heuristic is a distributed greedy algorithm, Kruskal's shortest path heuristic (K-SPH-NWST) Matsuyama (1980); Bauer & Varma (1996). The approximation ratio of the GCNN-enhanced K-SPH-NWST w.r.t. the vanilla K-SPH-NWST on the 4 sets of random graphs, are shown in Figure 5. GCNN can improve K-SPH-NWST by 6.8% on BA graphs, 1.2% on GRP graphs, 1.4% on ER graphs, 0.9% on WS graphs, and 0.9% on a real-world dataset of Internet backbone topology Knight et al. (2011) with $|\mathcal{V}| = 31.23$ on average. The noticeable gain on BA graphs is meaningful to large real-world networks, such as the Internet, World Wide Web, and social networks (Posfai & Barabasi, 2016, Ch. 5).

MWCDS: In MWCDS problem, we are given an undirected and connected graph, and our goal is to find a minimum weighted dominating set that is connected. Our baseline heuristic is a distributed greedy algorithm (Dist.Greedy), whereas the reference algorithm is a centralized greedy heuristic. Both MWCDS heuristics are implemented in two steps Sun et al. (2019): 1) find a MWDS, 2) connect the MWDS by solving a NWST problem where the terminals are the solution of step 1. The approximation ratios of the vanilla and GCNN-enhanced distributed heuristics w.r.t. the centralized greedy heuristic on 4 sets of random graphs, each with 2000 graphs, are shown in Figure 6. Despite the large gap between distributed and centralized greedy algorithms, GCNN can improve the distributed greedy by 17.8% on GRP graphs, 16.0% on ER graphs, 6.6% on WS graphs, and 4.0% on BA graphs.

The average centralized runtimes of GCNN-enhanced distributed solvers for the MWIS, NWST, MWCDS problems are respectively $0.017 \sim 0.05$, $0.07 \sim 1.5$, $0.08 \sim 2.0$ seconds per instance, as

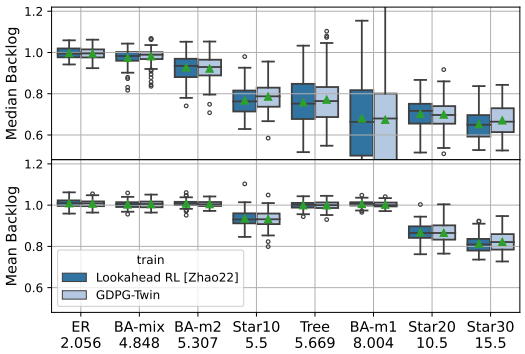

Figure 7: GDPG-Twin achieves similar network-wide mean and medium backlogs (smaller is better) of lookahead RL Zhao et al. (2022b) in training a distributed link scheduler, using only 1/5 evaluations of $h(\cdot)$ of it.

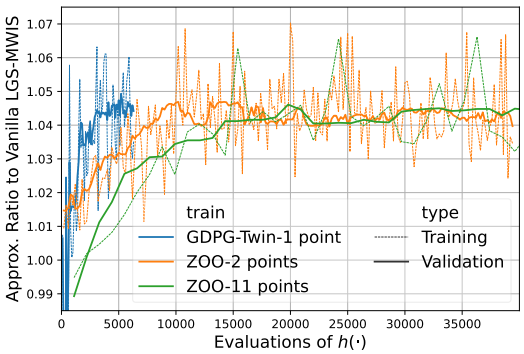

Figure 8: Performance trajectories of GCNN-enhanced LGS-MWIS trained by GDPG-Twin and ZOOs with 2-point and 11-point gradient estimations. Larger is better. GDPG-Twin needs fewer evaluations of $h(\cdot)$.

reported in Appendix G, along with their estimated computational time (not the execution time) in distributed execution, as less than 0.18, 5.1, and 5.8 milliseconds, respectively.

4.2 Repetitive MWIS in a Graph-based Markov Decision Process

GDPG-Twin for R-COP in a graph-based MDP is demonstrated through the delay-oriented distributed link scheduling in Zhao et al. (2022b), in which the distributed scheduler contains a 1-layer GCNN and LGS, and the twin is a 5-layer GCNN. The state feature $\mathbf{S}(t) = \mathbf{q}(t) \odot \mathbf{l}(t)$, where $\mathbf{q}(t)$ captures the queue lengths on wireless links (nodes in conflict graph), and $\mathbf{l}(t)$ captures the link rates. The state transition in (4e) is based on $\mathbf{q}(t+1) = \mathbf{q}(t) + \mathbf{a}(t) - \min(\mathbf{q}(t), \mathbf{l}(t) \odot \mathbf{x}(t))$, where $\mathbf{a}(t)$ captures random packets arrivals, and $\mathbf{x}(t) \in \{0,1\}^{|\mathcal{V}|}$ captures scheduling decisions. The objective is to minimize the average backlog, $\mathbb{E}_{i\in\mathcal{V},t\leq T}\left[\mathbf{q}_i(t)\right]$. As shown in Figure 7, two distributed schedulers respectively trained by 5-step lookahead RL Zhao et al. (2022b) and GDPG-Twin achieve similar performance in terms of the mean and median backlogs on conflict graphs with different levels of centralization, as indicated by the number on the x-axis. However, GPDG-Twin is 5 times faster than lookahead RL, as the former needs only 2 evaluations of $h(\cdot)$ per t, whereas the latter needs 10.

4.3 Comparison with zeroth-order optimization

The trajectories of relative performances of GCNN-enhanced LGS-MWIS (as detailed in Section 4.1) w.r.t. vanilla LGS-MWIS, under different training methods, are illustrated in Figure 8, where x-axis is the number of evaluations of the non-differentiable $h(\cdot)$ (LGS-MWIS). Each point on the curve is the average value of 100 instances. During training, random weights are generated on-the-fly for a training graph, whereas the weights on a validation graph are unchanged. GDPG-Twin and ZOO are configured with the same sampling radius and learning rate. GDPG-Twin converges within only 1/3 to 1/2 evaluations of $h(\cdot)$ required by the fastest ZOO based on 2-point gradient estimation. This result shows that GDPG-twin has a better sampling efficiency than ZOO, by a factor of 2 to 3.

5 Conclusion

We propose to address repetitive combinatorial optimization problems by parameterizing the input node weights of a non-differentiable, fast and/or distributed heuristic, $f_{net}(\cdot)$, through a continuous-valued high-dimensional action generated by an actor GNN. The actor GNN is optimized by graph-based deterministic policy gradient with the help of a critic based on a twin network that can predict the node-wise expected outcomes of $f_{net}(\cdot)$. Through 5 examples, we demonstrate that our approach can: 1) leverage the shared underlying topology of independent R-COPs, to reduce the average optimality gap of the fast and/or distributed heuristics, and 2) optimize the long-term objectives for R-COPs in a graph-based Markov decision process. In terms of limitations, our work has not addressed the variance and worst-case of the optimality gap, which are important for many real-world applications. Our evaluation is based on synthetic rather than real-world graphs. Moreover, the actor and critic networks in our framework would need further design for broader tasks, e.g., edge related R-COPs. In addition, we do not expect our work to have any impact on social equality.

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A APPENDIX: SGD FOR TWIN NETWORK IN INDEPENDENT REPETITIVE COPS

Give MSE loss,

$$\ell_{mse}(\hat{\mathbf{o}}, \mathbf{o}) = \frac{1}{|\mathbf{o}|} \sum_{i=1}^{|\mathbf{o}|} (\hat{\mathbf{o}}_i - \mathbf{o}_i)^2 \ , \tag{13}$$

the partial derivative of $\ell_{mse}(\hat{\mathbf{o}}, \mathbf{o})$ w.r.t. the parameters of the twin network is

$$\frac{\partial \ell_{mse}(\hat{\mathbf{o}}, \mathbf{o})}{\partial \mathbf{\Theta}_c} = \frac{\partial \ell_{mse}(\hat{\mathbf{o}}, \mathbf{o})}{\partial \hat{\mathbf{o}}} \frac{\partial \hat{\mathbf{o}}}{\partial \mathbf{\Theta}_c} \tag{14a}$$

$$= \frac{2}{|\mathbf{o}|} \left[\hat{\mathbf{o}} - \mathbb{E}_{\Omega^{|\mathbf{c}|}}(\mathbf{c} \odot \mathbf{x})\right]^\top \frac{\partial \hat{\mathbf{o}}}{\partial \mathbf{\Theta}_c} \tag{14b}$$

$$= \mathbb{E}_{\Omega^{|\mathbf{c}|}} \left(\frac{2}{|\mathbf{o}|} \left(\hat{\mathbf{o}} - \mathbf{c} \odot \mathbf{x}\right)^\top \frac{\partial \hat{\mathbf{o}}}{\partial \mathbf{\Theta}_c} \right) \ , \tag{14c}$$

where from (14b) to (14c) is based on the linearity of expectation. Based on (14c), by drawing $\mathbf{c} \sim \Omega^{\mathbf{c}}$, we have the following unbiased stochastic gradient estimation:

$$\frac{\partial \ell_{mse}(\hat{\mathbf{o}}, \mathbf{o})}{\partial \mathbf{\Theta}_c} = \mathbb{E}_{\Omega^{\mathbf{c}}} \left[\frac{\partial \widehat{\ell_{mse}(\hat{\mathbf{o}}, \mathbf{o})}}{\partial \mathbf{\Theta}_c} \right] , \tag{15}$$

where

$$\frac{\partial \widehat{\ell_{mse}(\hat{\mathbf{o}}, \mathbf{o})}}{\partial \mathbf{\Theta}_c} = \frac{2}{|\mathbf{o}|} \left(\hat{\mathbf{o}} - \mathbf{c} \odot \mathbf{x} \right)^\top \frac{\partial \hat{\mathbf{o}}}{\partial \mathbf{\Theta}_c} \tag{16a}$$

$$= \frac{\partial \ell_{mse}(\hat{\mathbf{o}}, \mathbf{c} \odot \mathbf{x})}{\partial \mathbf{\Theta}_c} . \tag{16b}$$

Therefore, the stochastic gradient estimation for the parameters of the twin network is

$$\widehat{\nabla_{\mathbf{\Theta}_c} \ell_{mse}}(\hat{\mathbf{o}}, \mathbf{o}) = \nabla_{\mathbf{\Theta}_c} \ell_{mse}(\hat{\mathbf{o}}, \mathbf{c} \odot \mathbf{x}) . \tag{17}$$

B Appendix: SGD for twin network in COPs with state transition

We define a return vector supported on the nodes of the graph as

$$\mathbf{g}(t) = \sum_{k=0}^{T-t} \gamma^k \mathbf{r}(t+k) , \tag{18}$$

which can be expressed in a recursive form

$$\mathbf{g}(t) = \mathbf{r}(t) + \gamma \mathbf{g}(t+1) , \text{ where } \mathbf{g}(t) = \mathbf{0} , \ \forall t > T . \tag{19}$$

The outcome (value) vector of state $\mathcal{G}(t)$ is the expected return vector under policy $\mathbf{\Theta}_p$,

$$\mathbf{o}(t) = \mathbb{E}_{\mathbf{\Theta}_p} \left[\mathbf{g}(t) | \mathcal{G}(t) \right] . \tag{20}$$

The gradient $\nabla_{\mathbf{\Theta}_c} \ell_{mse}(\hat{\mathbf{o}}(t), \mathbf{o}(t))$ can be found by the following partial derivative

$$\frac{\partial \ell_{mse}(\hat{\mathbf{o}}(t), \mathbf{o}(t))}{\partial \mathbf{\Theta}_c} = \frac{\partial \ell_{mse}(\hat{\mathbf{o}}(t), \mathbf{o}(t))}{\partial \hat{\mathbf{o}}(t)} \frac{\partial \hat{\mathbf{o}}(t)}{\partial \mathbf{\Theta}_c} \tag{21a}$$

$$= \frac{2}{|\mathbf{o}(t)|} \Big(\hat{\mathbf{o}}(t) - \mathbb{E}_{\mathbf{\Theta}_p} \left[\mathbf{g}(t) | \mathcal{G}(t) \right] \Big)^\top \frac{\partial \hat{\mathbf{o}}(t)}{\partial \mathbf{\Theta}_c} \tag{21b}$$

$$= \mathbb{E}_{\mathbf{\Theta}_p} \left(\frac{2}{|\mathbf{o}(t)|} \left[\hat{\mathbf{o}}(t) - \mathbf{g}(t) | \mathcal{G}(t) \right]^\top \frac{\partial \hat{\mathbf{o}}(t)}{\partial \mathbf{\Theta}_c} \right) , \tag{21c}$$

where from (21b) to (21c) is based on the linearity of expectation, and that $\hat{\mathbf{o}}(t)$ is a function of $\mathcal{G}(t)$, generated by the twin network, as defined in (12). Based on (19), we have the following unbiased estimation of the partial derivative in (21a)

$$\frac{\partial \ell_{mse}(\hat{\mathbf{o}}(t), \mathbf{o}(t))}{\partial \mathbf{\Theta}_c} = \mathbb{E}_{\mathbf{\Theta}_p} \left[\frac{\partial \widehat{\ell_{mse}(\hat{\mathbf{o}}(t), \mathbf{o}(t))}}{\partial \mathbf{\Theta}_c} \right] , \tag{22}$$

where

$$\frac{\partial \widehat{\ell_{mse}(\hat{\mathbf{o}}(t), \mathbf{o}(t))}}{\partial \mathbf{\Theta}_c} = \frac{2}{|\mathbf{o}(t)|} \left[\hat{\mathbf{o}}(t) - \mathbf{g}(t) | \mathcal{G}(t) \right]^\top \frac{\partial \hat{\mathbf{o}}(t)}{\partial \mathbf{\Theta}_c} \tag{23a}$$

$$= \frac{2}{|\mathbf{o}(t)|} \left[\hat{\mathbf{o}}(t) - \mathbf{r}(t) - \gamma \mathbf{g}(t+1) | \mathcal{G}(t) \right]^\top \frac{\partial \hat{\mathbf{o}}(t)}{\partial \mathbf{\Theta}_c} . \tag{23b}$$

In (23b), $\mathbf{r}(t)$ is the reward vector collected under current state $\mathcal{G}(t)$, as defined in (10c), and $\mathbf{g}(t+1)|\mathcal{G}(t)$ is the return of the next state $\mathcal{G}(t+1)$, evolved from the current state $\mathcal{G}(t)$ according to (10f). The return of the next state $\mathcal{G}(t+1)$ is estimated as $\mathbf{g}(t+1) \approx \hat{\mathbf{o}}(t+1)$ by the twin network, as defined in (12). As a result, we have the following approximation

$$\mathbf{r}(t) + \gamma \mathbf{g}(t+1) | \mathcal{G}(t) \approx \mathbf{r}(t) + \gamma \hat{\mathbf{o}}(t+1) . \tag{24}$$

Plugging (24) to (23b), we have

$$\frac{\partial \widehat{\ell_{mse}(\hat{\mathbf{o}}(t), \mathbf{o}(t))}}{\partial \mathbf{\Theta}_c} \approx \frac{\partial \ell_{mse}(\hat{\mathbf{o}}(t), \mathbf{r}(t) + \gamma \hat{\mathbf{o}}(t+1))}{\partial \mathbf{\Theta}_c} . \tag{25}$$

Therefore, the stochastic gradient estimation for the parameters of the twin network is

$$\widehat{\nabla_{\mathbf{\Theta}_c} \ell_{mse}}(\hat{\mathbf{o}}(t), \mathbf{o}(t)) \approx \nabla_{\mathbf{\Theta}_c} \ell_{mse}(\hat{\mathbf{o}}(t), \mathbf{r}(t) + \gamma \hat{\mathbf{o}}(t+1))) . \tag{26}$$

C APPENDIX: PROCEDURES OF GDPG-TWIN

Algorithm 1 GDPG-Twin for R-COPs with Independent Instances

Input: $\Omega^{\mathbf{c}}, \Omega^{\mathcal{G}}, h(\cdot), \alpha_p, \alpha_c, E, B, \epsilon$
Output: $\mathbf{Z}$ or $\boldsymbol{\Theta}_p, \boldsymbol{\Theta}_c$

Initialize $\mathbf{Z}$ or $\boldsymbol{\Theta}_p, \boldsymbol{\Theta}_c$ randomly or as pretrained models, $\bar{\mathbf{c}} = \mathbb{E}_{\Omega^{\mathbf{c}}}(\mathbf{c})$
for $e \in \{1, 2, \ldots, E\}$ **do**
  $\mathcal{Q}_p = \varnothing, \mathcal{Q}_c = \varnothing$ */* Clear gradient buffers */*
  for $b \in \{1, \ldots, B\}$ **do**
    Draw $\mathcal{G}(\mathcal{V}, \mathcal{E}) \in \Omega^{\mathcal{G}}$, $\mathbf{c} \in \Omega^{\mathbf{c}}$ */* Draw data from training dataset or target distribution */*
    if Actor network is used **then**
      $\mathbf{Z} = \Psi(\mathcal{V}, \mathcal{E}, \bar{\mathbf{c}}; \boldsymbol{\Theta}_p)$
    end if
    $\mathbf{Z}^{(j)} = \mathbf{Z} + \mathbf{N}^{(j)}, \mathbf{N}^{(j)} \in \mathbb{U}(-\epsilon, \epsilon)$ */* Random policy sampling */*
    $\hat{\mathbf{o}} = f_{twin}(\mathcal{V}, \mathcal{E}, \bar{\mathbf{c}}, \mathbf{Z}^{(j)}; \boldsymbol{\Theta}_c^*)$
    $\mathbf{x} = f_{net}(\mathcal{V}, \mathcal{E}, \mathbf{c}; \mathbf{Z}^{(j)})$ based on $h(\cdot)$ in (5c) and $f_{loc}(\cdot)$ in (5d)
    Estimate gradient $\nabla_{\boldsymbol{\Theta}_c} \ell_{mse}(\hat{\mathbf{o}}, \mathbf{c} \odot \mathbf{x})$ for critic
    $\mathcal{Q}_c \leftarrow \mathcal{Q}_c \cup \{\nabla_{\boldsymbol{\Theta}_c} \ell_{mse}(\hat{\mathbf{o}}, \mathbf{c} \odot \mathbf{x})\}$
    Estimate policy gradient $\nabla_{\mathbf{Z}} \mathbf{1}^\top \hat{\mathbf{o}}$ based on (7)
    if Actor network is used **then**
      Estimate gradient $\nabla_{\boldsymbol{\Theta}_p} \mathbf{1}^\top \hat{\mathbf{o}} = \nabla_{\boldsymbol{\Theta}_p} \Psi(\mathcal{V}, \mathcal{E}, \bar{\mathbf{c}}; \boldsymbol{\Theta}_p) \nabla_{\mathbf{Z}} \mathbf{1}^\top \hat{\mathbf{o}}$ for actor
      $\mathcal{Q}_p \leftarrow \mathcal{Q}_p \cup \{\nabla_{\boldsymbol{\Theta}_p} \mathbf{1}^\top \hat{\mathbf{o}}\}$
    else
      $\mathcal{Q}_p \leftarrow \mathcal{Q}_p \cup \{\nabla_{\mathbf{Z}} \mathbf{1}^\top \hat{\mathbf{o}}\}$
    end if
  end for
  $\boldsymbol{\Theta}_c \leftarrow \boldsymbol{\Theta}_c - \alpha_c \mathbb{E}_{\mathcal{Q}_c} \left[\nabla_{\boldsymbol{\Theta}_c} \ell_{mse}(\hat{\mathbf{o}}, \mathbf{c} \odot \mathbf{x})\right]$
  $\mathbf{Z} \leftarrow \mathbf{Z} - \alpha_p \mathbb{E}_{\mathcal{Q}_c} \left(\nabla_{\mathbf{Z}} \mathbf{1}^\top \hat{\mathbf{o}}\right)$ or $\boldsymbol{\Theta}_p \leftarrow \boldsymbol{\Theta}_p - \alpha_p \mathbb{E}_{\mathcal{Q}_p} \left(\nabla_{\boldsymbol{\Theta}_p} \mathbf{1}^\top \hat{\mathbf{o}}\right)$
end for
Output $\mathbf{Z}$ or $\boldsymbol{\Theta}_p, \boldsymbol{\Theta}_c$

For the four demonstrated R-COPs with independent instances, we set the hyperparameters of training procedure in Algorithm 1 as follows: $\alpha_p = \alpha_c = 0.0001$, $E = 25$, $B = 100$, $\epsilon = 0.15$.

Algorithm 2 GDPG-Twin for R-COPs with State Transition

Input: $\Omega^{\mathbf{c}}, \Omega^{\mathcal{G}}, h(\cdot), \alpha_p, \alpha_c, T, E$
Output: $\mathbf{\Theta}_p, \mathbf{\Theta}_c$

Initialize $\mathbf{\Theta}_p, \mathbf{\Theta}_c$ randomly or as pretrained models
for $e \in \{1, 2, \ldots, E\}$ **do**
  $\mathcal{Q}_e = \varnothing, \mathcal{Q}_p = \varnothing, \mathcal{Q}_c = \varnothing$ */* Clear experience & gradient buffers */*
  Initialize state $\mathcal{G}(0) = (\mathcal{V}(0), \mathcal{E}(0), \mathbf{S}(0))$
  for $t \in \{0, \ldots, T\}$ **do**
    $\mathbf{z}(t) = \Psi(\mathcal{V}(t), \mathcal{E}(t), \mathbf{S}(t); \mathbf{\Theta}_p)$
    $\hat{\mathbf{o}}(t) = f_{twin}(\mathcal{V}(t), \mathcal{E}(t), \mathbf{S}(t), \mathbf{z}(t); \mathbf{\Theta}_c^*)$
    Obtain decision vector $\mathbf{x}(t)$ based on (10d)
    Observe reward vector $\mathbf{r}(t)$ according to (10c)
    Update state feature $\mathbf{S}(t+1)$ according to (10f)
    Estimate stochastic policy gradient $\nabla_{\mathbf{\Theta}_p} f_{obj}\left(\hat{\mathbf{o}}(t)\right)$ based on (11)
    $\mathcal{Q}_p \leftarrow \mathcal{Q}_p \cup \{\nabla_{\mathbf{\Theta}_p} f_{obj}\left(\hat{\mathbf{o}}(t)\right)\}$
    $\mathcal{Q}_e \leftarrow \mathcal{Q}_e \cup \{< \mathbf{r}(t), \hat{\mathbf{o}}(t) >\}$
  end for
  for $t \in \{0, \ldots, T\}$ **do**
    Fetch $\mathbf{r}(t), \hat{\mathbf{o}}(t), \hat{\mathbf{o}}(t+1)$ from $\mathcal{Q}_e$
    Estimate stochastic gradient $\nabla_{\mathbf{\Theta}_c} \ell_{mse}(\hat{\mathbf{o}}(t), \mathbf{r}(t) + \gamma \hat{\mathbf{o}}(t+1))$ for critic
    $\mathcal{Q}_c \leftarrow \mathcal{Q}_c \cup \{\nabla_{\mathbf{\Theta}_c} \ell_{mse}(\hat{\mathbf{o}}(t), \mathbf{r}(t) + \gamma \hat{\mathbf{o}}(t+1))\}$
  end for
  $\mathbf{\Theta}_c \leftarrow \mathbf{\Theta}_c - \alpha_c \mathbb{E}_{\mathcal{Q}_c}\left[\nabla_{\mathbf{\Theta}_c} \ell_{mse}(\hat{\mathbf{o}}(t), \mathbf{r}(t) + \gamma \hat{\mathbf{o}}(t+1))\right]$
  $\mathbf{\Theta}_p \leftarrow \mathbf{\Theta}_p + \alpha_p \mathbb{E}_{\mathcal{Q}_p}\left[\nabla_{\mathbf{\Theta}_p} f_{obj}\left(\hat{\mathbf{o}}(t)\right)\right]$ */* Objective maximization */*
end for
Output $\mathbf{\Theta}_p, \mathbf{\Theta}_c$

For the demonstrated delay-oriented link scheduling Zhao et al. (2022b), we use the following hyperparameters in training described in Algorithm 2: $\alpha_p = \alpha_c = 0.0001$, $T = 64$, $E = 200$. The types and mixture of the training graphs, random processes, etc., are identical to Zhao et al. (2022b).

D Appendix: Graph convolutional neural networks

An L-layer GCNN is implemented as follows: Given the input feature $\mathbf{S}^{(0)} = \mathbf{S}$ supported on a graph $\mathcal{G}$, the output is $\mathbf{Z} = \mathbf{S}^{(L)} = f_{GCN}(\mathcal{G}, \mathbf{S}; \mathbf{\Theta})$, where an intermediate lth layer of the GCNN is

$$\mathbf{S}^l = \sigma_l\left(\mathbf{S}^{l-1}\mathbf{\Theta}_0^l + \boldsymbol{\mathcal{L}}\mathbf{S}^{l-1}\mathbf{\Theta}_1^l\right) \ , \ l \in \{1, \ldots, L\} \ . \tag{27}$$

In (27), $\boldsymbol{\mathcal{L}}$ is the normalized Laplacian of graph $\mathcal{G}$, $\mathbf{\Theta}_0^l, \mathbf{\Theta}_1^l \in \mathbb{R}^{g_{l-1} \times g_l}$ are the trainable parameters, g_{l-1} and g_l are the dimensions of the output features of layers $l-1$ and l, respectively, and $\sigma_l(.)$ is an element-wise activation function.

In a distributed system, (27) can be implemented by the following local operation on node $v \in \mathcal{V}$,

$$\mathbf{S}_{v*}^l = \sigma_l\left(\mathbf{S}_{v*}^{l-1}\,\mathbf{\Theta}_0^l + \left[\mathbf{S}_{v*}^{l-1} - \sum_{u \in \mathcal{N}(v)} \frac{\mathbf{S}_{u*}^{l-1}}{\sqrt{d(v)d(u)}}\right]\mathbf{\Theta}_1^l\right) \ , \tag{28}$$

where $\mathbf{S}_{v*}^l \in \mathbb{R}^{1 \times g_l}$ is the vth row of matrix $\mathbf{S}^l$, which captures the features on node v, $d(v)$ is the degree of node v, and $\mathcal{N}(v)$ is the set of neighboring nodes of node v.

E Appendix: Configurations of random graphs for training and testing

$p \in \mathbb{U}(0.15, 0.35)$, $k \in \lfloor \mathbb{U}(10, 30) \rceil$. Training graph size $|\mathcal{V}| \in \{100, 150, 200, 250, 300\}$. Testing graph size $|\mathcal{V}| \in \{100, 150, 200, 250, 300, 350, 400, 450, 500\}$ (varies by problem).

ER: size $|\mathcal{V}|$, edge probability $^{|\mathcal{V}|}/_{k}$. BA: size $|\mathcal{V}|$, number of edges to attach from a new node to existing nodes $m = \lfloor pk \rceil$. WS: size $|\mathcal{V}|$, each node is joined with its k nearest neighbors in a ring topology, p: the probability of rewiring each edge. GRP: size $|\mathcal{V}|$, mean cluster size k, shape parameter $\min(7, k)$, probability of intra-cluster connection p, probability of inter cluster connection $\max(0.1, {}^{p}/_{3})$. For MWIS problem in Section 4.1, the test set of 500 ER graphs and the corresponding optimal solutions are from `https://github.com/zhongyuanzhao/distgcn` Zhao et al. (2022a).

F APPENDIX: ML PIPELINES AND BASELINE HEURISTICS

F.1 MWIS PIPELINE

We adopt the GCN-LGS pipeline in Zhao et al. (2022a) as the actor network, which comprises a 3-layer GCNN followed by a distributed local greedy solver (LGS-MWIS) Joo & Shroff (2012). The twin network is implemented by a 5-layer GCNN. The GCNN outputs vector $\mathbf{z} \in \mathbb{R}^{|\mathcal{V}|}$. The local function in (5d) is instantiated as a multiplier, $f_{loc}(\mathbf{c}_i, \mathbf{z}_i) = \mathbf{c}_i \mathbf{z}_i$. The training takes about an hour on a server with 16 GB memory, 8 CPUs and 1 GPU (Nvidia 1080 Ti).

The basic greedy heuristic first sorts the nodes by their weight in decreasing order, then iteratively adds a node to the solution and removes the node and its neighbors from the sorted list, until the list is empty. The centralized greedy algorithm and LGS-MWIS are detailed in (Zhao et al., 2022a, Algo 1).

The distributed heuristic LGS-MWIS Joo & Shroff (2012) iteratively builds a solution as follows: in an iteration, each node compares its weight with its neighbors; if a node has the maximal weight in the neighborhood, it marks itself as 1, and broadcasts a control message to its neighbors, who then mark themselves as -1; the unmarked nodes enter the next iteration. When all nodes are marked, the solution is the set of nodes marked as 1. LGS-MWIS has an average local communication complexity of $\mathcal{O}(\log |\mathcal{V}|)$ on general graphs.

For MWIS problem in Section 4.1, the test set of 500 ER graphs and the corresponding optimal solutions are from `https://github.com/zhongyuanzhao/distgcn` Zhao et al. (2022a).

F.2 MWDS PIPELINE AND GREEDY-MWIDS

We augment Greedy-MWDS with a 5-layer GCNN and the same local function in the MWIS pipeline in Appendix F.1. The GCNN is trained on randomly generated ER graphs of 100 to 300 nodes. The training takes about an hour on a server with 16 GB memory, 8 CPUs and 1 GPU (Nvidia 1080 Ti)

The greedy algorithm, Greedy-MWDS, iteratively builds a solution by adding to the solution the most cost-effective node from the vertices not yet in the solution, marking its neighbors as covered, until all nodes are either in the solution or covered. A good metric for the cost-effectiveness of node $v \in \mathcal{V}$ is Jovanovic et al. (2010):

$$\omega(v) = \frac{c(v)}{1 + \sum_{u \in \mathcal{N}(v) \cap \mathcal{W}'} c(u)} \ , \mathcal{W}' = \{i | i \in \mathcal{V} \setminus (\mathcal{D}' \cup \mathcal{N}(\mathcal{D}')\} \ , \tag{29}$$

where smaller $\omega(v)$ means better cost-effectiveness, $c(v)$ is the weight of node v, $\mathcal{D}'$ is the partial solution (initialized as $\varnothing$), $\mathcal{N}(\cdot)$ refers to the neighbors of a node or a vertex set, $\mathcal{W}'$ is the set of uncovered nodes.

An alternative greedy algorithm (Greedy-MWIDS) selects the most cost-effective node only from the uncovered vertices in each iteration, which builds an independent dominating set (IDS). Greedy-MWIDS can be implemented by the distributed LGS-MWIS Joo & Shroff (2012), and is used as part of the distributed heuristic for the MWCDS problem in Appendix F.4.

F.3 NWST PIPELINE AND BASELINE HEURISTICS

The GCNN and local function are configured the same as in the MWDS pipeline in Appendix F.2. The input node feature for GCNN is one-hot encoded indicator of whether a node is a terminal. The GCNN is trained on randomly generated GRP graphs with 100 to 300 nodes. The training takes about 5 hours on a server with 16 GB memory, 8 CPUs and 1 GPU (Nvidia 1080 Ti).

Shortest path heuristic (SPH) Matsuyama (1980) initializes the terminals as a set of subtrees; starting from an arbitrary subtree, it iteratively merges with its nearest subtree through the shortest path. The distance of a path is the total cost of nodes on it, where terminals have zero cost. The algorithm terminates when only one tree is left. The shortest path is found by Dijkstra's algorithm Dijkstra et al. (1959). Kruskal's SPH Bauer & Varma (1996) (K-SPH) is a distributed variation of SPH, in which every subtree merges with its nearest subtree until only one tree is left. SPH has an approximation ratio of 2 Matsuyama (1980).

F.4 MWCDS PIPELINE, BASELINE AND REFERENCE HEURISTICS

A low complexity heuristic for MWCDS problem Sun et al. (2019) can be implemented in two steps: 1) find a MWDS, 2) connect the MWDS by solving a NWST problem where the terminals are the solution of step 1. The training takes about 8 hours on a server with 16 GB memory, 8 CPUs and 1 GPU (Nvidia 1080 Ti).

In our baseline heuristic, we choose Greedy-MWIDS in Appendix F.2 for step 1, and K-SPH-NWST in Appendix F.3 for step 2, and treat them as a single distributed greedy heuristic (Dist.Greedy).

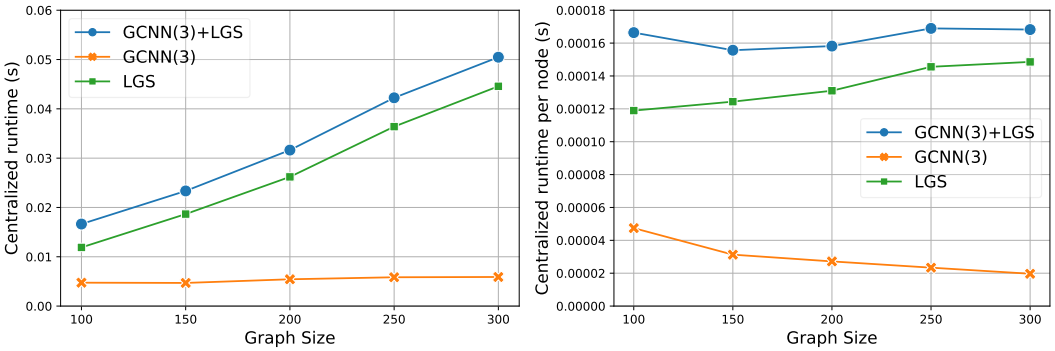
Our reference algorithm is a centralized greedy heuristic, composed of Greedy-MWDS in Appendix F.2 for step 1 and SPH-NWST in Appendix F.3 for step 2.

We use a 5-layer GCNN that outputs $\mathbf{Z} \in \mathbb{R}^{|\mathcal{V}|\times 2}$, and the local function is a single neuron, $f_{loc}(\mathbf{c}_i, \mathbf{Z}_{i*}) = ReLU(\mathbf{Z}_{i,1}\mathbf{c}_i + \mathbf{Z}_{i,2})$. The GCNN is trained on GRP graphs of 100 to 300 nodes.

G APPENDIX: CENTRALIZED RUNTIME IN SECONDS

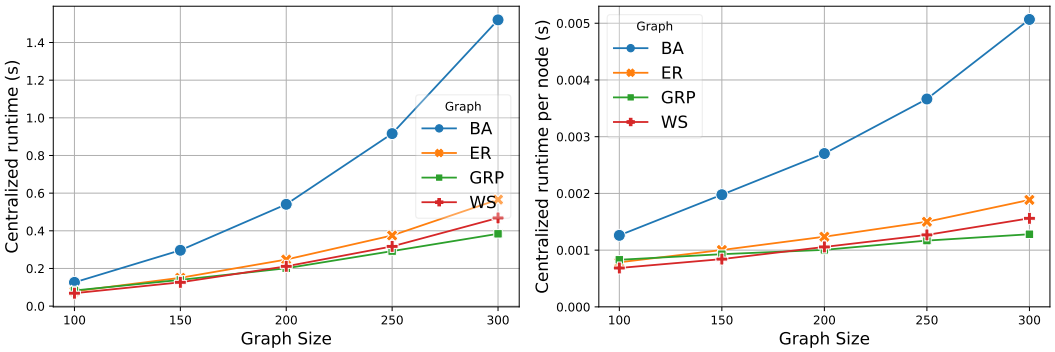
We report the actual runtime of GCNN-enhanced COP solvers demonstrated in Section 4, measured on a laptop computer (Macbook Pro, 16GB memory, 2 GHz Quad-Core Intel Core i5, CPU only). It should be noted that these runtimes are based on our Python code, of which the implementation could be further optimized for running speed.

For the examples demonstrated by distributed COP solvers, the centralized runtime does not represent their distributed runtime. Therefore, we report both the total centralized runtime and the per-node centralized runtime for each distributed solver. The latter represents the estimated computational time in distributed execution. However, the major component of distributed runtime for distributed solvers is the communication time rather than the computational time, which could not be measured in our setting. In general, the GCNN no longer dominate the total runtime for these distributed COP solvers. For MWIS in Figure 9(a) and 9(b), the centralized runtime of distributed COP solvers are still linear to the graph size. For NWST (Figures 10(a) and 10(b)) and MWCDS (Figures 11(a) and 11(b)), the major component of the centralized runtime is Dijkstra's algorithm for the shortest path, which has a time complexity of $\mathcal{O}(|\mathcal{V}|^2)$ or $\mathcal{O}((|\mathcal{V}| + |\mathcal{E}|)\log|\mathcal{V}|)$.



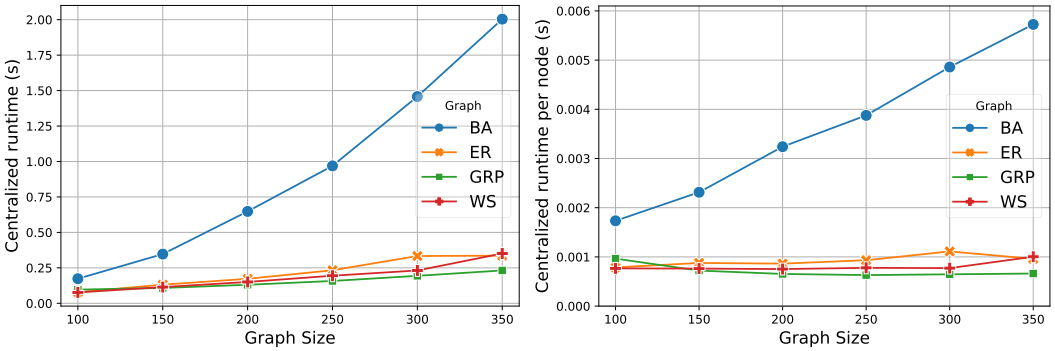
(a) (b)

Figure 9: Average centralized runtime of GCNN-enhanced LGS-MWIS per instance, with a reusing factor $N = 1$. The total runtime is broken down to GCNN(3), as a one time overhead, and LGS, as the runtime for $N = \infty$. (a) Total centralized runtime by graph size, (b) Per node centralized runtime by graph size, representing the estimated computational time in distributed execution. Notice that the major component of distributed runtime is the communication time.



(a) (b)

Figure 10: Average centralized runtime of GCNN-enhanced K-SPH-NWST solver per instance, with a reusing factor $N = 1$. (a) Total centralized runtime by graph size, (b) Per node centralized runtime by graph size, representing the estimated computational time in distributed execution. Notice that the major component of distributed runtime is the communication time.



(a) (b)

Figure 11: Average centralized runtime of GCNN-enhanced MWCDS per instance, with a reusing factor $N = 1$. (a) Total centralized runtime by graph size, (b) Per node centralized runtime by graph size, representing the estimated computational time in distributed execution. Notice that the major component of distributed runtime is the communication time.