# ScheduleNet: Learn to solve multi-agent scheduling problems with reinforcement learning

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#### **Abstract**

We propose ScheduleNet, a RL-based real-time scheduler, that can solve various types of multi-agent scheduling problems. We formulate these problems as a semi-MDP with episodic reward (makespan) and learn ScheduleNet, a decentralized decision-making policy that can effectively coordinate multiple agents to complete tasks. The decision making procedure of ScheduleNet includes: (1) representing the state of a scheduling problem with the agent-task graph, (2) extracting node embeddings for agent and tasks nodes, the important relational information among agents and tasks, by employing the type-aware graph attention (TGA), and (3) computing the assignment probability with the computed node embeddings. We validate the effectiveness of ScheduleNet as a general learning-based scheduler for solving various types of multi-agent scheduling tasks, including multiple salesman traveling problem (mTSP) and job shop scheduling problem (JSP).

# 1 Introduction

Optimal assignments of multiple autonomous agents for sequential completion of distributed tasks is necessary to solve various types of scheduling problems in logistics, transportation, and manufacturing. Finding the optimal delivery plans for vaccines, customer pickup order for ride sharing services, and machine operation sequence in modern manufacturing facilities are some examples of such scheduling problems. As the size of the problems increase, it is imperative to design an effective scheduler to solve these complex problems.

Solving large-scale scheduling problems using mathematical programming is infeasible/ineffective due to (1) the expensive computational cost, and (2) the inability to modify the scheduling action during real-time execution. As a remedy, learning-based approaches, especially reinforcement Learning (RL), have been proposed to solve the traveling salesman problem (TSP) and the vehicle routing problem (VRP) [3, 20, 19, 28]. Although recent works show the promising performances, they have been limited to solve only single-agent scheduling problems. RL-based approaches that solve multi-agent scheduling problems (mSP) are underrepresented in the research community, even though mSP poses greater scientific challenges and covers a broader set of real-world problems.

**Objective**. In this paper, we propose ScheduleNet, a RL-based real-time decentralized multi-agent scheduler. ScheduleNet builds solution sequentially by accommodating for current partial solution and actions of other agents. ScheduleNet attempt to achieve following three goals:

• General scheduler that can effectively solve various types mSPs.

- Cooperative scheduler that can effectively induce coordination among multiple agents to minimize the total completion time (makespan) of distributed tasks.
- Scalable scheduler that can solve the large-scale mSPs in a computationally efficient way.

**Formulation**. To achieve these goals, we formulate mSPs as a semi Markov decision process (MDP) with episodic reward (e.g. makespan) and seek to derive a decentralized decision making policy that can be shared by all agents. In the proposed semi-MDP, the state is defined as the current status (partial solution) of a target mSP, and the action is defined as an assignment of an idle agent to one of the remaining and feasible tasks. The proposed formulation has following advantages:

- Direct optimization of scheduling objective (makespan). This formulation alleviates the need for devising dense reward functions, which can be very challenging for complex problems and do not guarantee an optimal cooperative behavior of agents.
- Decentralization of scheduling policy that can be transferred to any sized problems. ScheduleNet allows each agent chooses its destination independently while using its local observations and incorporating other agents' assignments. This decentralization ensures that the learned policy can solve problems with any number of agents and tasks in a scalable manner.

**Solution construction method**. ScheduleNet constructs the solution using a sequential decision-making framework. At every step, ScheduleNet accepts the MDP state as an input and assigns an idle agent to one of the feasible tasks. The decision-making procedure of ScheduleNet is as follows:

- ScheduleNet first represents the MDP state as a agent-task graph, which is both effective in capturing complex relationships among the entities and general enough to be applied to various types of mSPs.
- ScheduleNet then employs the type-aware graph attention (TGA) to extract important relational features among agents and tasks in a computationally efficient manner.
- Lastly, ScheduleNet computes the agent-task assignment probability by utilizing the computed node embeddings.

**Training Method.** Although makespan (shared team reward) is the most direct and general reward design for solving mSPs, training a decentralized scheduling policy using this reward is extremely difficult due to the credit assignment issues [34, 12]. Additionally, makespan is highly volatile due to the combinatorial aspect of mSPs' solution space; a small change in a solution can drastically alter the outcome. Thus, training the decentralized scheduling policy is an extremely challenging task. To overcome these difficulties, we propose a RL training scheme, which empirically increases the stability of learning and asymptotic performance of ScheduleNet.

**Validation**. We validate the effectiveness of ScheduleNet on two types of mSPs: multiple traveling salesmen problem (mTSP) and jop-shop scheduling problem (JSP). From a series of experiments on random mSP instances and benchmark datasets, we empirically show that ScheduleNet can outperform other heuristic approaches and existing deep RL approaches. Furthermore, ScheduleNet demonstrates its exceptional effectiveness on large and practical problems.

# 2 Related Works

Solving single-agent routing (scheduling) problems with RL. According to [26], the RL approaches to solving agent routing problems can be categorized into: (1) improvement heuristics learns to rewrite the complete solution iteratively to obtain a better solution [43, 5, 4, 24]; (2) construction approach learns to construct a solution by sequentially assigning idle agents to unvisited cities until the full routing schedule (sequence) is constructed [3, 28, 20, 19], and (3) hybrid approaches blending both approaches [17, 7, 21, 1]. Typically, learning-based improvement or hybrid approaches have shown good performance since these can iteratively update the best solution until reaching the best one. However, these approaches usually require a longer computational time. In addition, since these approaches run in a centralized manner, they are hard to be expanded to multi-agent seating where agents need to be operated in a decentralized manner.

**Learned mTSP solvers.** There are only few RL approaches for solving mTSP. [18] proposed a variant of transformer [41] that trains the policy assigning a agent to a city using the mTSP solutions computed by integer linear programming solvers (imitation learning). [14] applies RL to train

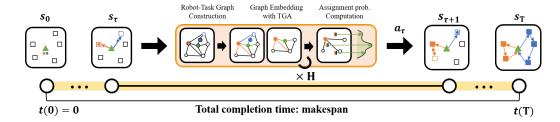


Figure 1: Solving mSP with ScheduleNet. At every event of the semi-MDP, ScheduleNet constructs the agent-task graph  $\mathcal{G}_{\tau}$  from  $s_{\tau}$ , then computes the node embedding of  $\mathcal{G}_{\tau}$  using TGA, and finally computes the agent-task assignment probabilities from the node embedding.

the clustering algorithm to group cities and applied (1) trained RL-policy for solving TSP or (2) strong TSP heuristics (OR-Tool) to optimize the sub-tour in each cluster. Being different from these approaches, we focus on deriving a complete *end-to-end* learned heuristic that constructs a feasible solution from "scratch" without relying on any existing solvers. For this reason, We did not consider [18], and [14] as baseline algorithms since they use 2-stage approaches, relying on learned or well known TSP heuristics.

**Learned JSP solvers.** Some RL methods have also been proposed for solving JSP. For example, [9, 23] have proposed to learn scheduling policy for each agent and hence, it requires an additional training to solve JSPs with a different number of agents from the training cases. Recently, [30, 45] have proposed to learn a shared scheduling policy for all agents while utilizing the disjunctive graph representation of JSP. Unlike these methods utilizing well-designed dense reward, we directly use the makespan reward to train a policy.

### 3 Problem Formulation

We formulate mSP as a semi-MDP with sparse reward and aim to derive a decentralized scheduling decision-making policy that can be shared by all agents. The semi-MDP is defined as:

**State**. We define state  $s_{\tau}$  as the  $\tau$ -th partial solution of mSP (i.e., the completed/uncompleted tasks, the status of agents, and the sequence of the past assignments). The initial  $s_0$  and terminal state  $s_{\rm T}$  are defined as an empty and a complete solution respectively.

**Action**. We define action  $a_{\tau}$  as the act of assigning an idle agent to one of the feasible tasks (unassigned tasks). We refer to  $a_{\tau}$  as the agent-to-task assignment.<sup>1</sup>

**Transition**. The proposed MDP is formulated with an *event*-based transition. An event is defined as the the case where any agent finishes the assigned task (e.g. a salesman reaches the assigned city in mTSP). Whenever an event occurs, the idle agent is assigned to a new task, and the status of the agent and the target task are updated accordingly. We enumerate the event with  $\tau$  to avoid confusion from the elapsed time of the problem;  $t(\tau)$  is a function that returns the time of event  $\tau$ .

**Reward**. The proposed MDP uses the minus of makespan (i.e. total completion time of tasks) as a reward, i.e.,  $r(s_T) = -t(T)$ , that is realized only at  $s_T$ .

#### 3.1 Example: MDP formulation of mTSP

Let us consider the single-depot mTSP with two types of entities: m salesmen (i.e. m agents) and N cities (i.e. N tasks) to visit. All salesmen start their journey from the depot and come back to the depot after visiting all cities (each city can be visited by only one salesman). A solution to mTSP is considered to be complete when all the cities have been visited and all salesmen have returned to the depot. The semi-MDP formulation for mTSP is similar to that of the general mSP. The specific definitions of the state and reward for mTSP are as follows:

<sup>&</sup>lt;sup>1</sup>When the multiple agents are idle at the same time t, we randomly choose one agent and assign an action to the agent and repeat the process until no agent is idle. Note that such randomness do not alter the resulting solutions, since the agents are considered to be homogeneous and the scheduling policy is shared.

**State.** We define  $s_{\tau} = (\{s_{\tau}^i\}_{i=1}^{N+m}, s_{\tau}^{\text{env}})$  is composed of two types of states: entity state  $s_{\tau}^i$  and environment state  $s_{\tau}^{\text{env}}$ .

- $s_{\tau}^{i} = (p_{\tau}^{i}, \mathbf{1}_{\tau}^{\text{active}}, \mathbf{1}_{\tau}^{\text{assigned}})$  is the state of *i*-th entity.  $p_{\tau}^{i}$  is the position of *i*-th entity at the  $\tau$ -th event.  $\mathbf{1}_{\tau}^{\text{active}}$  indicates whether the *i*-th worker/task is active (worker is working/ task is not visited) or not. Similarly,  $\mathbf{1}_{\tau}^{\text{assigned}}$  indicates whether worker/task is assigned or not.
- $s_{\tau}^{\text{env}}$  contains the current time of the environment, and the sequence of cities visited by each salesman.

**Reward.** We use makespan of mTSP as a reward, which is sparse and episodic. The reward  $r(s_{\tau}) = 0$  for all non-terminal events, and  $r(s_{\rm T}) = -t({\rm T})$ , where T is the index of the terminal state.

#### 4 ScheduleNet

In this section, we explain how ScheduleNet recommends a scheduling action  $a_{\tau}$  of an idle agent from input  $s_{\tau}$  (partial solution) by (1) constructing the agent-task graph  $\mathcal{G}_{\tau}$ , (2) embedding  $\mathcal{G}_{\tau}$  using TGA, and (3) computing the assignment probabilities. Figure 1 illustrates the decision-making process of ScheduleNet.

## 4.1 Constructing agent-task graph

ScheduleNet constructs the agent-task graph  $\mathcal{G}_{\tau}$  that reflects the complex relationships among the entities in  $s_{\tau}$ . Specifically, ScheduleNet constructs a directed complete graph  $\mathcal{G}_{\tau} = (\mathbb{V}, \mathbb{E})$  out of  $s_{\tau}$ , where  $\mathbb{V}$  is the set of nodes and  $\mathbb{E}$  is the set of edges. The nodes and edges, and their associated features are defined as:

- $v_i$  denotes the *i*-th node representing either a agent or a task.  $v_i$  contains the node feature  $x_i = (s_\tau^i, k_i)$ , where  $s_\tau^i$  is the state of entity *i*, and  $k_i$  is the type of  $v_i$ . For example, if the entity *i* is *agent* and its  $\mathbf{1}_\tau^{active} = 1$ , then the  $k_i$  becomes *active-agent* type. For the full list of the node types, refer to Appendix C.1.2.
- $e_{ij}$  denotes the edge between the source node  $v_j$  and the destination node  $v_i$ . The edge feature  $w_{ij}$  is equal to the Euclidean distance between the two nodes.

In the following subsections, we omit the event iterator  $\tau$  for notational brevity, since the action selection procedure is only associated with the current event index  $\tau$ .

# 4.2 Graph embedding using TGA

ScheduleNet computes the node embeddings from the agent-task graph  $\mathcal G$  using the type-aware graph attention (TGA). The embedding procedure first encodes the features of  $\mathcal G$  into the initial node embeddings  $\{h_i^{(0)}|v_i\in\mathbb V\}$ , and the initial edge embeddings  $\{h_{ij}^{(0)}|e_{ij}\in\mathbb E\}$ . ScheduleNet then performs TGA embedding H times to produce final node embeddings  $\{h_i^{(H)}|v_i\in\mathbb V\}$ , and edge embeddings  $\{h_{ij}^{(H)}|e_{ij}\in\mathbb E\}$ . To be specific, TGA embeds the input graph using the type-aware edge update, type-aware message aggregation, and the type-aware node update as explained in the following paragraphs.

**Type-aware edge update**. Given the node embedding  $h_i$  and edge embedding  $h_{ij}$ , TGA computes the type-aware edge embedding  $h'_{ij}$  and the attention logit  $z_{ij}$  as follows:

$$h'_{ij} = TGA_{\mathbb{E}}([h_i, h_j, h_{ij}], k_j)$$

$$z_{ij} = TGA_{\mathbb{A}}([h_i, h_j, h_{ij}], k_j)$$
(1)

where  $TGA_{\mathbb{E}}$  and  $TGA_{\mathbb{A}}$  are the type-aware edge update function and the type-aware attention function, respectively.

 $TGA_{\mathbb{E}}$  and  $TGA_{\mathbb{A}}$  are parameterized as Multilayer Perceptron (MLP) where the first layer is the Multiplicative Interaction (MI) layer [16]. The MI layer, which is a bilinear instantiation of hypernetwork [11], adaptively generates parameters of  $TGA_{\mathbb{E}}$  and  $TGA_{\mathbb{A}}$  based on the type  $k_j$ . This allows us to use  $TGA_{\mathbb{E}}$  and  $TGA_{\mathbb{A}}$  for all types of nodes, and thus reduces the number of embedding functions to be learned while maintaining the good representational power of GNN.

**Type-aware message aggregation**. Each entity in the agent-task graph interacts differently with the other entities, depending on the type of the edge between them. To preserve the different relationships

between the entities during the graph embedding procedure, TGA gathers messages  $h'_{ij}$  via the type-aware message aggregation.

First, TGA aggregates messages for each node type (per-type) and produces the per-type message  $m_i^k$  as follows:

$$m_i^k = \sum_{j \in \mathcal{N}_k(i)} \alpha_{ij} h_{ij}' \tag{2}$$

where  $\mathcal{N}_k(i) = \{v_l | k_l = k, \forall v_l \in \mathcal{N}(i)\}$  is the type k neighborhood of  $v_i$ , and  $\alpha_{ij}$  is the attention score that is computed using  $z_{ij}$ :

$$\alpha_{ij} = \frac{\exp(z_{ij})}{\sum_{j \in \mathcal{N}_k(i)} \exp(z_{ij})}$$
(3)

TGA then concatenates the per-type messages to produce the aggregated message  $m_i$  as:

$$m_i = \operatorname{concat}(\{m_i^k | k \in \mathbb{K}\}) \tag{4}$$

where  $\mathbb{K}$  is the set of node types. Since the number of node types is fixed, the size of  $m_i$  is fixed regardless of the size of problems.

**Type-aware node update.** The aggregated message  $m_i$  is then used to compute the updated node embedding  $h'_i$  as follows:  $h'_i = \text{TGA}_{\mathbb{V}}([h_i, m_i], k_i)$  (5)

where  $TGA_{\mathbb{V}}$  is the type-aware node update function that is parametrized with MLP. The first layer

where  $TGA_{\mathbb{V}}$  is the type-aware node update function that is parametrized with MLP. The first layer of  $TGA_{\mathbb{V}}$  is MI Layer, similar to the edge updater. The detailed architectures of  $TGA_{\mathbb{E}}$ ,  $TGA_{\mathbb{A}}$ , and  $TGA_{\mathbb{V}}$  are provided in Appendix A.

### 4.3 Computing assignment probability

Using the computed final node embeddings  $\{h_i^{(H)}|v_i\in\mathbb{V}\}$  and edge embeddings  $\{h_{ij}^{(H)}|e_{ij}\in\mathbb{E}\}$ , ScheduleNet selects the best assignment action  $a_{\tau}$  for the target agent.

ScheduleNet computes the assignment probability of the target idle agent i to the unassigned task j as follows:

$$l_{ij} = \text{MLP}_{actor}(h_i^{(H)}, h_j^{(H)}, h_{ij}^{(H)})$$

$$p_{ij} = \text{softmax}(\{l_{ij}\}_{j \in \mathbb{A}(\mathcal{G}_\tau)})$$
(6)

where  $h_i^{(H)}$  is the final node embedding for  $v_i$ , and  $h_{ij}^{(H)}$  is the final edge embeddings for  $e_{ij}$ . In addition,  $\mathbb{A}(\mathcal{G}_{\tau})$  denote the set of feasible actions defined as  $\{v_j|k_j=U \text{ nassigned-task}\ \forall j\in\mathbb{V}\}$ .

Note that ScheduleNet learns how to process local information of the state and make the decentralized action for each agent. This allows ScheduleNet to compute the assignment probabilities for mSPs with *arbitrarily* numbered agents and tasks in a *scalable* manner.

## 5 Training ScheduleNet

We utilize sparse team reward (makespan) as the direct reward signal to train the decentralized scheduler (ScheduleNet) for having multiple agents to complete tasks as quickly as possible. Even though this team reward is the most direct signal that can be used for solving various types of mSPs, training a decentralized cooperative policy using a single sparse and delayed reward is notoriously difficult [34, 12]. The high variance of the reward signal due to the combinatorial nature of mSPs' solution space adds an additional difficulty. To handle such difficulties, we employ two training stabilizers, reward normalization, and Clip-REINFORCE, while training ScheduleNet.

## 5.1 Reward normalization

We denote the makespan induced by policy  $\pi_{\theta}$  as  $M(\pi_{\theta})$ . We observe that  $M(\pi_{\theta})$  is highly volatile depending on the problem size (N, m) and  $\pi_{\theta}$ . To reduce the variance of the reward incurred from

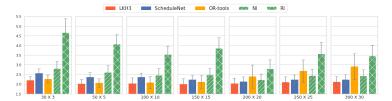


Figure 2: Scheduling performance on random  $(N \times m)$  mTSP datasets (smaller is better). The y-axis shows the normalized makespans. The red, blue and orange bar charts demonstrate the performance of LKH3, SchdeduleNet and OR-tools respectively. The green bars show the performance of two-phase heuristics. The error bars shows  $\pm 1.0$  standard deviation of the makespans.

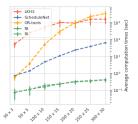


Figure 3: Inference time of ScheduleNet and the baselines

the problem sizes, we propose to use the normalized makespan  $\bar{M}(\pi_{\theta}, \pi_{b})$  computed as:

$$\bar{M}(\pi_{\theta}, \pi_b) = \frac{M(\pi_{\theta}) - M(\pi_b)}{M(\pi_b)} \tag{7}$$

where  $\pi_b$ , a baseline policy, is the current policy  $\pi$  in greedy (test) mode.  $\bar{M}(\pi_{\theta}, \pi_b)$  measures the relative scheduling performance of  $\pi_{\theta}$  to  $\pi_b$ . Obviously,  $\bar{M}(\pi_{\theta}, \pi_b)$  has smaller variance than  $M(\pi_{\theta})$ , especially when the number of agent m changes.

Using  $\bar{M}(\pi_{\theta}, \pi_{b})$ , we compute the normalized return  $G_{\tau}(\pi_{\theta}, \pi_{b})$  as follows:

$$G_{\tau}(\pi_{\theta}, \pi_{b}) \triangleq -\gamma^{T-\tau} \bar{M}(\pi_{\theta}, \pi_{b}) \tag{8}$$

where T is the index of the terminal state, and  $\gamma$  is the discount factor of MDP. The minus sign is for minimizing the makespan. Note that, in the early phase of mSP (when  $\tau$  is small), it is difficult to estimate the makespan. Thus, we place a smaller weight (i.e,  $\gamma^{T-\tau}$ ) for  $G_{\tau}$  evaluated when  $\tau$  is small.

#### 5.2 Clip-REINFORCE

Even a small change in a single assignment can result in a dramatic change to make span due to the combinatorial nature of the solution. Hence, training value function that predicts the  $G_{\tau}$  reliably is difficult. See Appendix D for more information. We thus propose to utilize the Clip-REINFORCE (CR), a variant of PPO [36], without the learned value function for training ScheduleNet. The objective of the Clip-REINFORCE is given as follows:

$$\mathcal{L}(\theta) = \underset{(\mathcal{G}_{\tau}, a_{\tau}) \sim \pi_{\theta}}{\mathbb{E}} \left[ \min(\text{clip}(\rho_{\tau}, 1 - \epsilon, 1 + \epsilon) G_{\tau}, \rho_{\tau} G_{\tau}) \right] \tag{9}$$

where  $G_{\tau}$  is a shorthand notation for  $G_{\tau}(\pi_{\theta}, \pi_{b})$  and  $\rho_{\tau} = \pi_{\theta}(a_{\tau}|\mathcal{G}_{\tau})/\pi_{b}(a_{\tau}|\mathcal{G}_{\tau})$  is the ratio between the target and baseline policy.

# 6 Experiments

In this section, we evaluate the performance of ScheduleNet on mTSP and JSP. To calculate the inference time, we run all experiements on the server equipped with a NVIDIA Titan X GPU and AMD Threadripper 2990WX CPU. we use the GPU to evaluate ScheduleNet, and single CPU core for all other baseline algorithms. In the testing phase, the action with the highest probability is selected greedily and used. No further solution refinement techniques such as beam search and random shooting, are applied to test ScheduleNet.

**Performance metrics**. It is computationally infeasible to obtain the optimal solution for mTSP with MILP solvers (e.g. CPLEX) even for the small-sized problems. Therefore, when the optimal solution is unknown, we define the *scheduling performance* of scheduler  $\pi$  as  $M(\pi)$ . On the other hand, when the optimal solution is known, we report the scheduling performance as the optimality gap, which is defined as  $M(\pi)/M^*$ , where  $M^*$  is the optimal makespan.

Table 1: **mTSPLib results.** The CPLEX results with \* are optimial solutions. Otherwise, the known-best upper bound of CPLEX results are reported [27]. Population based metaheuristics results are reproduced from Lupoaie et al. [25].

Instance		eil.	51			berl	in52			eil'.	76			rai	99		Gap
m	2	3	5	7	2	3	5	7	2	3	5	7	2	3	5	7	
CPLEX	222.7*	159.6	124.0	112.1	4110.2	3244.4	2441.4	2440.9	280.9*	197.3	150.3	139.6	728.8	587.2	469.3	443.9	1.00
LKH3	222.7	159.6	124.0	112.1	4110.2	3244.4	2441.4	2440.9	280.9*	197.3	150.3	139.6	728.8	587.2	469.3	443.9	1.00
OR-Tools	243.3	170.5	127.5	112.1	4665.5	3311.3	2482.6	2440.9	318.0	212.4	143.4	128.3	762.2	552.1	473.7	442.5	1.03
ScheduleNet	259.7	172.2	118.9	112.4	4816.3	3372.1	2615.6	2576.0	334.1	226.5	168.0	151.3	790.0	579.3	502.5	471.7	1.08
SOM	278.4	210.3	157.7	136.8	5350.8	4197.6	3461.9	3125.2	364.0	278.6	210.7	183.1	927.4	756.1	624.4	564.1	1.31
ACO	248.8	180.6	135.1	120.0	4389.0	3468.9	2733.6	2510.1	308.5	224.6	163.9	146.9	767.2	620.5	525.5	492.1	1.09
EA	276.6	208.2	151.2	123.9	5038.3	3865.5	2853.6	2543.7	365.7	285.4	211.9	177.8	896.7	739.4	596.9	534.9	1.24
NI	271.3	202.9	183.5	129.7	5941.0	3811.5	2972.6	2972.6	363.2	302.1	191.4	173.8	916.6	802.8	668.6	554.2	1.30
RI	265.9	195.9	150.5	127.7	5785.0	4133.9	4108.6	2998.2	395.2	276.6	185.8	155.5	890.9	843.0	675.4	565.1	1.31

## 6.1 mTSP experiments

**Training.** We denote  $(N \times m)$  as the mTSP with N cities (tasks) and m salesmen (agents). To generate a random mTSP instance, we sample N and m from U(20,25) and U(2,5), respectively. Similarly, the Euclidean coordinates of N cities are sampled uniformly at random from the unit square. ScheduleNet is trained on random mTSP instances that are generated on-the-fly. For all experimental results, we evaluate the performance of a single trained ScheduleNet model. Please refer to Appendix C.1.3 for more information.

**Results on random mTSP datasets**. To investigate the generalization capacity of ScheduleNet to various problem sizes, we evaluate ScheduleNet on the randomly generated mTSP datasets. Each  $(N \times m)$  dataset consists of 100 random uniform mTSP instances.

The baseline algorithms we considered are:

- Lin-Kernighan-Helsgaun 3 (LKH3) [13], a state-of-the-art heuristic solver, that are known to find the optimal solutions for the mTSP problems with the identified optimal solutions. We use the makespans computed by LKH3 as the proxies for the optimal solutions of the test mTSP instances.
- Google OR-Tools[32], a highly optimized meta-heuristic library.
- NI and RI, two-phase mTSP heuristics, that first group the cities with K-means clustering (where K=m) and then apply the well-known TSP heuristics, i.e., Nearest Insertion (NI) and Random Insertion (RI), per cluster.

From Figure 2, in the small-sized maps (N < 200), we can notice that the scheduling performances of ScheduleNet better than that of the two-phase heuristics and worse than that of OR-tools. In the larger maps ( $N \ge 200$ ), on the other hand, ScheduleNet outperforms OR-tools and the two-phase heuristics as well. ScheduleNet exhibits small standard deviations of makespans for all problem sizes. In addition, Figure 3 compares the average inference time and the standard deviation per problem size, clearly indicating that ScheduleNet is significantly faster especially for large size mTSP instances.

**Results on Public Benchmarks**. Next, to explore the generalization of ScheduleNet to problems that come from completely different distributions (i.e. real-world data), we present the results on the mTSPLib dataset defined by Necula et al. [29]. mTSPLib consists of four small-to-medium- sized problems from TSPLib [33], each of which extended to multi-agent setup where m equals to 2, 3, 5, and 7.

The baseline algorithms are: (1) exact solver CPLEX, (2) LKH3 whose stopping criteria set to be the known best solutions, (3) OR-Tools, (4) population-based meta-heuristics Self-organization map (SOM), Ant-colony optimization (ACO), Evolutionary algorithm (EA) [25], and (5) the two-phase heuristics (NI and RI). From Table 1, we can observe that, at small-to-medium scale, OR-Tools produces near-optimal solutions, followed by ScheduleNet and ACO. However, the two-phase heuristics show drastic performance degradation, which is most likely due to the non-uniform distribution of the cities. From this experiment, we can observe that the ScheduleNet policy is equally effective in solving both generated and real-world mTSPs problems.

**Graph sparsity ablation**. From the aforementioned performance results, we can conclude that ScheduleNet is specifically effective in solving large scale problems. However, as the problem

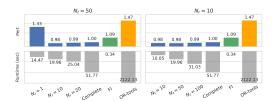


Figure 4: Scheduling performance (top) and computational time (bottom) on the sparse graphs. The left figure shows the scheduling performance w.r.t.  $N_r$ . The right figure w.r.t.  $N_t$ . We normalize the makespan of each scheduling algorithm with the ScheduleNet makespan with complete graph.

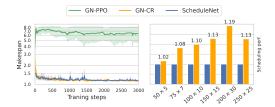


Figure 5: **Training ablation.** Makespan over the training steps (left) and scheduling performance on uniform random test datasets (right). The blue, orange, and green curves show the normalized makespan of ScheduleNet, CR-GN, and PPO-GN resepctively.

size increases, the computational complexity for processing a complete graph will also increase in  $\mathcal{O}(N^2+m^2)$ . We hypothesize that a smaller value of  $N_r$  (number of agent connection) and  $N_t$  (number of task connection) reduce the computational cost significantly without losing performance a lot. To verify this idea, we evaluate the same ScheduleNet that is trained on small complete graphs (random mTSPs) on large mTSP instances (300  $\times$  30). The graph embedding procedure for the described sparse graph has complexity  $\mathcal{O}((m+N)(N_r+N_t))$ .

Figure 4 shows the scheduling performance (colored) and the computational time (gray) of ScheduleNet for different values of  $N_r$  and  $N_t$ , i.e. the level of sparsity. The results show that the performance of the scheduleNet does not deteriorate significantly even with the limited information scope. These results imply that ScheduleNet can be used to solve very large real-world mTSPs in a fast and computationally efficient manner with local information. We also evaluate ScheduleNet on random mTSPs of size  $(500 \times 50)$  and  $(750 \times 70)$  (see Appendix C.1.4).

**RL** training ablation. To investigate the effectiveness of each ScheduleNet component (TGA and the training stabilizers), we train the following ScheduleNet variants:

- GN-PPO is a variant of ScheduleNet that has Attention-GN layers<sup>2</sup> for graph embedding (instead of TGA) and is trained by the PPO.
- GN-CR is a variant of ScheduleNet that has Attention-GN layers and is trained by Clip-REINFORCE with the normalized makespan.
- TGA-CR is the ScheduleNet setting.

Figure 5 (left) visualizes the validation performance of ScheduleNet and its variants over the training steps. It can be seen that GN-PPO fails to learn meaningful scheduling policy, which indicates that solving mSP with the standard Actor-Critic methods can be a challenging. We see the same trend for TGA-PPO (result is omitted). In contrast, the model trained with the stabilizers (GN-CR and ScheduleNet) exhibit stable training, and converge to a similar performance level on the validation dataset. In addition, as shown in Figure 5 (right), TGA-CR (ScheduleNet) consistently shows better performance than GN-CR over the random test datasets, showing that TGA plays an essential role in generalizing to larger mTSPs.

# 6.2 JSP experiments

We employ ScheduleNet to solve JSP, another type of mSP, to evaluate its generalization capacity in terms of solving various types of mSPs. The goal of the JSP is to schedule machines (i.e. agents) in a manufacturing facility to complete the jobs that consist of a series of operations (tasks), while minimizing the total completion time (makespan). Solving JSP is considered to be challenging since it imposes additional constraints that scheduler must obey: precedence constraints (i.e. an operation of a job cannot be processed until its precedence operation is done) and agent-sharing constraints (i.e. each agent has a unique set of feasible tasks).

<sup>&</sup>lt;sup>2</sup>AttentionGN does not use MI layer uses different message aggregation scheme. AttentionGN computes attention scores w.r.t. *all incoming edges*, in type agnostic manner. In contrast, TGA attention scores are computed w.r.t. edge types with inter-type and intra-type aggregations. For more details about AttentionGN, refer to Algorithm 3 in Appendix D.

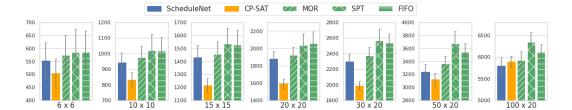


Figure 6: Scheduling Performance on random  $(N \times m)$  JSP datasets (smaller is better). Each dataset contains 100 instances. The blue and orange bar charts demonstrate the performance of SchdeduleNet and CP-SAT respectively. The green bars show the performance of JSP heuristics.

Table 2: **The average scheduling gaps of ScheduleNet and the baseline algorithms.** The gaps are measured with respect to the optimal (or the best-known) makespan [42, 40].

TA Instances	15×15	20×15	20×20	30×15	30×20	50×15	50×20	100×20    Mean Gap
ScheduleNet	1.153	1.194	1.172	1.180	1.187	1.138	1.135	1.066    1.154
[30]	1.171	1.202	1.228	1.189	1.254	1.159	1.174	1.070   1.181
[45]	1.259	1.300	1.316	1.319	1.336	1.224	1.264	1.136   1.269
MOR	1.205	1.236	1.217	1.249	1.173	1.177	1.092	1.092   1.197
FIFO	1.239	1.314	1.275	1.319	1.310	1.206	1.239	1.136   1.255
SPT	1.258	1.329	1.278	1.349	1.344	1.241	1.256	1.144   1.275

**Formulation**. We formulate JSP as a semi-MDP where  $s_{\tau}$  is the partial solution of JSP,  $a_{\tau}$  is agent-task assignment (i.e. assigning an idle machine to one of the feasible operations), and reward is the minus of makespan. Please refer to Appendix C.2.1 for the detailed formulation of semi-MDP and agent-task graph construction.

**Training.** We train ScheduleNet using the random JSP instances  $(N \times m)$  that have N jobs and m machines.We sample N and m from U(7,14) and U(2,5) respectively to generate the training JSP instances. We randomly shuffle the order of the machines in a job to generate machine sharing constraints. Please refer to Appendix C.2.3 for more information.

Results on random JSP datasets. To investigate the generalization capacity of ScheduleNet to various problem sizes, we evaluate ScheduleNet on the randomly generated JSP datasets. We compare the scheduling performance with the following baselines: exact solver CP-SAT [32] with one hour time-limit, and three JSP heuristics that known to work well in practice, Most Operation Remaining (MOR), First-in-first-out (FIFO), and Shortest Processing Time (SPT). As shown in Figure 6, ScheduleNet always outperforms the baseline heuristics for all sizes of the maps and even outperforms CP-SAT for the larger maps. The result confirms that ScheduleNet has good generalization capacity in terms of the problem size.

Results on Public Benchmarks. We evaluate the scheduling performance to verify ScheduleNet's generalization capacity to unseen JSP distributions on the Taillard's 80 dataset [39]. We compare against two deep RL baselines [30, 45], as well as the mentioned heuristics (MOR, FIFO, and SPT). Both baseline RL methods were specifically designed to solve JSP by utilizing the well-known disjunctive JSP graph representation [35] and well-engineered dense reward functions. Nevertheless, we can observe that ScheduleNet outperforms all baselines in all of the cases while utilizing only a sparse episodic reward (see Table 2). Please refer to Appendix C.2.5 for the extended benchmark results, including ORB [2], SWV [38], FT [6], LA [22], YN [44].

### 7 Conclusion

In this work, we proposed ScheduleNet, which is a RL-based scheduler that can solve various types of multi-agent scheduling problems (mSPs) in a decentralized manner. We evaluated the scheduling performance on random and benchmark instances of mTSP and JSP, and verified that ScheduleNet is an effective *general scheduler* that can solve various mSPs, a *cooperative scheduler* that induces multi-agent coordination to achieve a common objective, and a *scalable scheduler* that can solve large scale and practical scheduling problems.

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# A Details of Type-aware Graph Attention

In this section, we thoroughly describe the computation procedures of type-aware graph attention (TGA). Similar to the main body, We overload notations for the simplicity of notation such that the input node and edge feature as  $h_i$  and  $h_{ij}$ , and the embedded node and edge feature  $h_i'$  and  $h_{ij}'$ , respectively.

The proposed TGA performs graph embedding with the following three phases: (1) type-aware edge update, (2) type-aware message aggregation, and (3) type-aware node update.

**Type-aware edge update.** The edge update scheme is designed to reflect the complex type relationship among the entities while updating edge features. First, the *context* embedding  $c_{ij}$  of edge  $e_{ij}$  is computed using the source node type  $k_j$  such that:

$$c_{ij} = \text{MLP}_{etype}(k_j) \tag{10}$$

where  $MLP_{etype}$  is the edge type encoder. The source node types are embedded into the context embedding  $c_{ij}$  using  $MLP_{etype}$ . Next, the type-aware edge encoding  $u_{ij}$  is computed using the Multiplicative Interaction (MI) layer [16] as follows:

$$u_{ij} = \mathbf{MI}_{edge}([h_i, h_j, h_{ij}], c_{ij}) \tag{11}$$

where  $MI_{edge}$  is the edge MI layer. We utilize the MI layer, which dynamically generates its parameter depending on the context  $c_{ij}$  and produces type-aware edge encoding  $u_{ij}$ , to effectively model the complex type relationships among the nodes. Type-aware edge encoding  $u_{ij}$  can be seen as a dynamic edge feature which varies depending on the source node type. Then, the updated edge embedding  $h'_{ij}$  and its attention logit  $z_{ij}$  are obtained as:

$$h'_{ij} = \text{MLP}_{edge}(u_{ij}) \tag{12}$$

$$z_{ij} = \text{MLP}_{attn}(u_{ij}) \tag{13}$$

where  $MLP_{edge}$  and  $MLP_{attn}$  is the edge updater and logit function, respectively. The edge updater and logit function produce updated edge embedding and logits from the type-aware edge.

The computation steps of Equation 10, 11, and 12 are defined as  $TGA_{\mathbb{E}}$ . Similarly, the computation steps of Equation 10, 11, and 13 are defined as  $TGA_{\mathbb{A}}$ .

**Type-aware message aggregation.** We first define the type-k neighborhood of  $v_i$  as  $\mathcal{N}_k(i) = \{v_l | k_l = k, \forall v_l \in \mathcal{N}(i)\}$ , where  $\mathcal{N}(i)$  is the in-neigborhood set of  $v_i$ . The proposed type-aware message aggregation procedure computes attention score  $\alpha_{ij}$  for the  $e_{ij}$ , which starts from  $v_j$  and heads to  $v_i$ , such that:

$$\alpha_{ij} = \frac{\exp(z_{ij})}{\sum_{l \in \mathcal{N}_{k_j}(i)} \exp(z_{il})}$$
(14)

Intuitively speaking, The proposed attention scheme normalizes the attention logits of incoming edges over the types. Therefore, the attention scores sum up to 1 over each type-k neighborhood. Next, the type-k neighborhood message  $m_i^k$  for node  $v_i$  is computed as:

$$m_i^k = \sum_{j \in \mathcal{N}_k(i)} \alpha_{ij} h'_{ij} \tag{15}$$

In this aggregation step, the incoming messages of node i are aggregated per type. All incoming type neighborhood messages are concatenated to produce (inter-type) aggregated message  $m_i$  for  $v_i$ , such that:

$$m_i = \operatorname{concat}(\{m_i^k | k \in \mathbb{K}\}) \tag{16}$$

**Type-aware node update.** Similar to the edge update phase, the context embedding  $c_i$  is computed first for each node  $v_i$ :

$$c_i = \text{MLP}_{ntype}(k_i) \tag{17}$$

where  $MLP_{ntype}$  is the node type encoder. Then, the updated hidden node embedding  $h'_i$  is computed as below:

$$h_i' = \text{MLP}_{node}(h_i, u_i) \tag{18}$$

where  $u_i = \text{MI}_{node}(m_i, c_i)$  is the type-aware node embedding that is produced by  $\text{MI}_{node}$  layer using aggregated messages  $m_i$  and the context embedding  $c_i$ .

The computation steps of Equation 17, and 18 are defined as  $TGA_{\mathbb{E}}$ .

## **B** Extended discussion for reward normalization scheme

In this section, we further discuss the effect of the proposed reward normalization scheme and its variants to the performance of ScheduleNet. The proposed reward normalization (i.e. normalized makespan)  $m(\pi, \pi_b)$  is given as follows:

$$m(\pi, \pi_b) = \frac{M(\pi_\theta) - M(\pi_b)}{M(\pi_b)} \tag{19}$$

where  $\pi_b$  is the baseline policy.

Effect of the denominator.  $m(\pi, \pi_b)$  measures the relative scheduling supremacy of  $\pi$  to the  $\pi_b$ . Similar reward normalization scheme, but without  $M(\pi_b)$  division, is employed to solve single-agent scheduling problems [20]. We empirically found that the division leads in much stable learning when the scale of makespan change (e.g. the area of map change from the unit square to different geometries).

Effect of the baseline selection. A proper selection of  $\pi_b$  is essential to assure stable and asymptotically better learning of ScheduleNet. Intuitively speaking, choosing too strong baseline (i.e. policy having smaller makespan such as OR-tools) can makes the entire learning process unstable since the normalized reward tends to have larger values. On the other hand, employing too weak baseline can leads in virtually no learning since the  $m(\pi, \pi_b)$  becomes nearly zero.

We select  $\pi_b$  as Greedy( $\pi$ ). This baseline selection has several advantages from selecting a fixed/preexisting scheduling policy: (1) Entire learning process becomes independent from existing scheduling methods. Thus ScheduleNet is applicable even when the cheap-and-performing  $\pi_b$  for some target mSP does not exist. (2) Greedy( $\pi$ ) serves as an appropriate  $\pi_b$  (either not too strong or weak) during policy learning. We experimentally confirmed that the baseline section Greedy( $\pi$ ) results in a better scheduling policy as similar to the several literature [20, 37].

# **C** Experiments

### C.1 mTSP experiments

#### C.1.1 semi-MDP formulation

The formulated mTSP semi-MDP is event-based. Here we discuss the further details about the event-based transitions of mTSP MDP. Whenever all agents are assigned to cities, the environment transits in time, until any of the workers arrives to the city (i.e. completes the task). Arrival of the worker to the city triggers an event, meanwhile the other assigned salesman are still on the way to their correspondingly assigned cities. We assume that each worker transits towards the assigned city with unit speed in the 2D Euclidean space, i.e. the distance travelled by each worker equals the time past between two consecutive MDP events.

It is noteworthy that multiple events can happen at the same time, typically when time stamp t=0. If the MDP has multiple available workers at the same time, we repeatedly choose an arbitrary idle agent and assign it to the one of an idle task until no agent is idle, while updating event index  $\tau$ . This random selections do not alter the resulting solutions since we do not differentiate each agent (i.e. agents are homogeneous agents).

### C.1.2 Agent-task graph formulation

In this section, we present the list of all possible node types in  $\mathcal{G}_{\tau}$ : (1) assigned-agent, (2) unassigned-agent, (3), (4) assigned-task, (5) unassigned-task, (5) depot. Here, we do not include already visited cities (i.e. inactive tasks) to the graph. Thus, the set of active agents/tasks is defined by the union of assigned and unassigned agents/tasks. Our empirical experiments showed no performance difference between the graph with inactive nodes included versus the graph with active-only nodes. All nodes in the  $\mathcal{G}_{\tau}$  are fully connected.

## C.1.3 Training details

**Network parameters.** ScheduleNet is composed of two TGA layers. Each TGA layer (*raw-to-hidden* and *hidden-to-hidden*) has same MLP parameters, as shown in Table 3. The node and edge

Table 3: ScheduleNet TGA Layer parameters.

Encoder name	MLP hidden dimensions	Hidden activation	Output activation
$\mathrm{MLP}_{etype}$	[32]	ReLU	Identity
$\mathrm{MLP}_{edge}$	[32, 32]	ReLU	Identity
$\mathrm{MLP}_{attn}$	[32, 32]	ReLU	Identity
$\mathrm{MLP}_{ntype}$	[32]	ReLU	Identity
$\mathrm{MLP}_{node}$	[32, 32]	ReLU	Identity
$MLP_{\it actor}$	[256, 128]	ReLU	Identity

encoders input dimensions for the first *raw-to-hidden* TGA layer is 4 and 7, respectively, the output node, edge dimensions of the first TGA layer is 32, 32, which is used as input dimensions for the *hidden-to-hidden* TGA layer. The embedded node and edge features are used to calculate the action embeddings via MLP<sub>actor</sub> with parameters described in Table 3.

**Training.** In this section, we presents a pseudocode for training ScheduleNet. We smooth the evaluation policy  $\pi_{\theta}$  with the Polyak average as studied [15] for the further stabilization of training process.

```
Algorithm 2: ScheduleNet Training
```

```
input: Training policy \pi_{\theta}
   output: Smoothed policy \pi_{\phi}
 1 Initialize the smoothed policy with parameters \phi \leftarrow \theta.
 2 for update step do
        Generate a random mTSP instance I
         \pi_b \leftarrow \text{Greedy}(\pi_\theta)
 4
        for number of episodes do
 5
              Construct mTSP MDP from the instance I
              Collect samples with \pi_{\theta} and \pi_{b} from the mTSP MDP.
 7
        end
 8
        for inner updates K do
 9
         \theta \leftarrow \theta + \alpha \nabla_{\theta} \mathcal{L}(\theta)
10
        end
11
        \phi \leftarrow \beta \phi + (1 - \beta)\theta
12
13 end
```

We set the MDP discounting factor  $\gamma$  to 0.9, and the polyak smoothing coefficient  $\beta$  as 0.1, and the clipping parameter  $\epsilon$  to 0.2.

## C.1.4 Details of Random mTSP experiments

**OR-Tools implementation.** The Google OR-Tools routing module [32] is a set of highly optimized and also practically working meta-heuristics for solving various routing problems (e.g. mTPS, mVRP). It first finds the initial feasible solution and then iteratively improves the solution with local search heuristics (e.g. Greedy Descent, Simulated Annealing, Tabu Search) until certain termination condition is satisfied. We achieve the scheduling results of the baseline OR-tools algorithm with the official implementation mTSP provided by Google.

We further tune the hyperparameters of OR-Tools to achieve better scheduling results on large mTSP instances (n>200 and m>20) by applying different initial solution search and solution improvement schemes. However, such tuning results in virtually no improvements in scheduling performances.

**Two-phase heuristics implementations.** The 2-phase heuristics for mTSP is an extension of well-known TSP heuristics to the m > 1 cases. First, we perform K-means clustering (where K = m) of

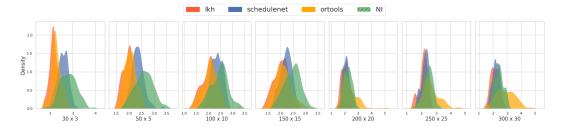


Figure 7: **Histogram of makespans on random**  $(N \times m)$  **mTSP datasets.** The x-axis demonstrates the makespans. The y-axis shows the density of makespans.

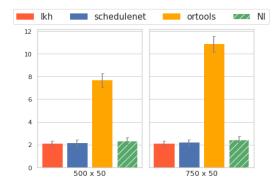


Figure 8: Scheduling performances on large random ( $N \times m$ ) mTSP datasets. The y-axis shows the makespans.

cities in the mTSP instance by utilizing scikit-learn [31]. Next, we apply TSP insertion heuristics, Nearest Insertion, Farthest Insertion, Random Insertion, and Nearest Neighbour Insertion, for each cluster of cities. It should be noted that, performance of the 2-phase heuristics is highly depended on the spatial distribution of the cities on the map. Thus 2-phase heuristics perform particularly well on uniformly distributed random instances, where K-means clustering can obtain clusters with approximately same number of cities per cluster.

## C.1.5 Qualitative analysis

The histogram of scheduling performances on random mTSP datasets. ScheduleNet averagely shows higher makespans than OR-tools on the small (M < 200) random mTSP datasets as discussed in Section 6.1. However, we observe that, even on the small mTSP problems, ScheduleNet can outperform OR-tools as visualized in Figure 7.

**Extended results of sparse graph experiments.** We provide the scheduling performance of ScheduleNet and baseline algorithms on random mTSPs of size  $(500 \times 50)$  and  $(750 \times 70)$ . See Figure 8 for the results.

## C.2 JSP experiments

Job-shop scheduling problem (JSP) is a mSP that can be applied in various industries including the operation of semi-conductor chip fabrication facility and railroad system. The objective of JSP is to find the sequence of machine (agent) allocations to finish the jobs (a sequence of operations; tasks) as soon as possible. JSP can be seen as an extension of mTSP with two additional constraints: (1) precedence constraint that models a scenario where an operation of a job becomes processable only after all of its preceding operations are done; (2) agent-sharing (disjunctive) constraint that confines the machine to process only one operation at a time. Due to these additional constraints, JSP is considered to be a more difficult problem when it is solved via mathematical optimization techniques. A common representation of JSP is the disjunctive graph representation. As shown in Figures 9, 10 and 11, JSP contains the set of jobs, machines, precedence constraints, and disjunctive constraints as

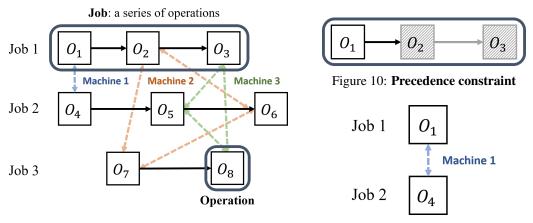


Figure 9: Disjunctive graph representation of JSP

Figure 11: Agent-sharing constraint

its entities. In the following subsections, we provide the details of the proposed MDP formulation of JSP, training details of ScheduleNet, and experiment results.

#### C.2.1 semi-MDP formulation

The semi-MDP formulation of JSP is similar to that of mTSP. The specific definitions of the state and action for JSP are as follows:

**State.** We define  $s_{\tau}=(\{s_{\tau}^i\}_{i=1}^{N+m},s_{\tau}^{\rm env})$  which is composed of two types of states: entity state  $s_{\tau}^i$ 

- and environment state  $s_{\tau}^{\text{env}}$ .

    $s_{\tau}^{i} = (p_{\tau}^{i}, \mathbf{1}_{\tau}^{\text{processable}}, \mathbf{1}_{\tau}^{\text{assigned}}, \mathbf{1}_{\tau}^{\text{accessible}}, \mathbf{1}_{\tau}^{\text{waiting}})$  is the state of the *i*-th entity.  $p_{\tau}^{i}$  is the processing time of the *i*-th entity at the  $\tau$ -th event.  $\mathbf{1}_{\tau}^{\text{processable}}$  indicates whether the *i*-th task is processable by the target agent or not. Similar to mTSP,  $1_{\tau}^{\text{assigned}}$  indicates whether an agent/task is assigned.
- $s_{\pi}^{\text{env}}$  contains the current time of the environment, the sequence of tasks completed by each agent (machine), and the precedence constraints of tasks within each job.

**Action.** We define the action space at the  $\tau$ -th event as a set of operations that is both processable and currently available. Additionally, we define the waiting action as a reservation of the target agent (i.e. the unique idle machine) until the next event. Having waiting as an action allows the adaptive scheduler (e.g. ScheduleNet) to achieve the optimal scheduling solution (and also makespan) from the JSP MDP, where the optimal solution contains waiting (idle) time intervals.

#### C.2.2 Agent-task graph formulation

ScheduleNet constructs the agent-task graph  $\mathcal{G}_{\tau}$  that reflects the complex relationships among the entities in  $s_{\tau}$ . ScheduleNet constructs a directed graph  $\mathcal{G}_{\tau} = (\mathbb{V}, \mathbb{E})$  out of  $s_{\tau}$ , where  $\mathbb{V}$  is the set of nodes and  $\mathbb{E}$  is the set of edges. The nodes and edges and their associated features are defined as:

- $v_i$  denotes the i-th node and represents either an agent or a task.  $v_i$  contains the node feature  $x_i = (s_\tau^i, k_i)$ , where  $s_\tau^i$  is the state of entity i, and  $k_i$  is the type of  $v_i$  (e.g. if the entity i is a task and its  $1_{\tau}^{processable} = 1$ , then the  $k_i$  becomes a processable-task type.)
- $e_{ij}$  denotes the edge between the source node  $v_i$  and the destination node  $v_i$ . The edge feature  $w_{ij}$ is a binary feature which indicates whether the destination node  $v_i$  is processable by the source node  $v_i$ .

All possible node types in  $\mathcal{G}_{\tau}$  are: (1) assigned-agent, (2) unassigned-agent, (3) assigned-task, (4) processable-task, and (5) unprocessable-task. We do not include completed tasks in the graph. Thus, the currently active tasks are the union of the assigned tasks, processable-tasks, and unprocessabletasks. The full list of node features are as follows:

- $\mathbf{1}_{\tau}^{\text{agent}}$  indicates whether the node is a agent or a task.
- $\mathbf{1}_{\tau}^{\text{target-agent}}$  indicates whether the node is a target-agent (unique idle agent that needs to be assigned).

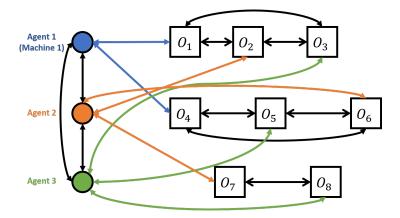


Figure 12: JSP agent-task graph representation

- $\mathbf{1}_{\tau}^{\text{assigned}}$  indicates whether the agent/task is assigned.
- $\mathbf{1}_{\tau}^{\text{waiting}}$  indicates whether the node is an agent in waiting state.
- $\mathbf{1}_{\tau}^{\text{processable}}$  indicates whether the node is a task that is *processable* by the target-agent.
- $\mathbf{1}_{\tau}^{\text{accessible}}$  indicates whether the node is processable by the target-agent and is available.
- Task wait time indicates the amount of time passed since the operation became accessible.
- Task processing time indicates the processing time of the operation.
- *Time-to-complete* indicates the amount of time it will take to complete the task, i.e. the time-distance to the given task.
- *Remain ops.* indicates the number of remaining operations to be completed for the job where the task belongs to.
- Job completion ratio is the ratio of completed operations within the job to the total amount of
  operations in the job.

**JSP graph connectivity**. Figure 12 visualizes the proposed agent-task graph. From Figure 12, each agent is fully connected to the set of processable tasks by that agent, and vice versa. Each task is fully connected to the other tasks (operations) that belong to the same job. Each agent is fully connected to the other agents.

## C.2.3 Training details

The TGA layer hyperparameters are set according to Table 3. We use same training hyperparameters as in Appendix C.1.3. The node and edge encoder input dimensions for the first *raw-to-hidden* TGA layer is 12 and 4 respectively. The output node and edge dimensions of the first TGA layer is 32 and 32 respectively, which are used as the input dimensions for the *hidden-to-hidden* TGA layer.

# C.2.4 Random JSP experiments

**CP-SAT implementation.** CP-SAT is one of the state-of-the-art constraint programming solver that is implemented as a module of Google OR-Tools [32]. We employ CP-SAT with a one hour time-limit as a baseline algorithm for solving JSP. Our implementation of CP-SAT is directly adopted from the official JSP solver implementation provided by Google, which is considered to be highly optimized to solve JSP. The official implementation can be found in https://developers.google.com/optimization/scheduling/job\_shop.

**JSP heuristic implementations.** Priority dispatching rules (PDR) is one of the most common JSP solving heuristics. PDR computes the priority of the feasible operations (i.e. the set of operations whose precedent operation is done and, at the same time, the target machine is idle) by utilizing the dispatching rules. As the JSP heuristic baselines, we consider the following three dispatching rules:

• Most Operation Remaining (MOR) sets the highest priority to the operation that has the most remaining operations to finish its corresponding job.

- First-in-first-out (FIFO) sets the highest priority to the operation that joins to the feasible operation set first.
- Shortest Processing Time (SPT) sets the highest priority to the operation that has the shortest processing time.

## C.2.5 Extended public benchmark JSP results

We provide the detailed JSP results for the following public datasets: TA [39] (Tables 4 and 5), ORB [2], FT [6], YN [44] (Table 6), SWV [38] (Table 7), and LA [22] (Table 8).

### D Details of the Ablation studies

#### D.1 Details of ablation models

In this section, we explain the details of ScheduleNet variants GN-CR, GN-PPO. Both variants employ the attention GN blocks (layer) to embed  $\mathcal{G}_{\tau}$ . The attention GN block takes a set of node embeddings  $\mathbb{V}$  and edge embeddings  $\mathbb{E}'$  by utilizing three trainable modules (edge function  $f_e(\cdot)$ , attention function  $f_a(\cdot)$  and node function  $f_n(\cdot)$ ) and one aggregation function  $\rho(\cdot)$ . The computation procedure of the attention GN block is given in Algorithm 3.

#### **Algorithm 3:** Attention GN block

```
input: set of edges features \mathbb{E}
                set of nodes features V
                edge function f_e(\cdot)
                attention function f_a(\cdot)
                node function f_n(\cdot)
                edge aggregation function \rho(\cdot)
 1 \mathbb{E}', \mathbb{V}' \leftarrow \{\}, \{\};
                                                                                          // Initialize empty sets
 2 for e_{ij} in \mathbb{E} do
         e'_{ij} \leftarrow f_e(e_{ij}, v_i, v_j);
                                                                                            // Update edge features
        z_{ij} \leftarrow f_a(e_{ij}, v_i, v_j) ;
\mathbb{E}' \leftarrow \mathbb{E}' \cup \{e'_{ij}\}
                                                                                     // Compute attention logits
 6 end
 7 for v_i in \mathbb{V} do
         w_{ji} \leftarrow softmax(\{z_{ji}\}_{j \in \mathcal{N}(i)});
                                                                                // Normalize attention logits
         m_i \leftarrow \rho(\{w_{ji} \times e'_{ji}\}_{j \in \mathcal{N}(i)});
                                                                               // Aggregate incoming messages
         v_i' \leftarrow f_n(v_i, m_i) ;

\mathbb{V}' \leftarrow \mathbb{V}' \cup \{v_i'\}
                                                                                            // Update node features
10
11
    return : Updated node features V' and edge E' features
```

#### **Details of GN-CR**

- Network architecture. GN-CR is composed of two attention GN layers. The first GN layer encodes the raw node/edge features to the hidden embedding. Each GN layer's encoders  $f_e$ ,  $f_a$ , and  $f_n$  has the same parameters as  $\text{MLP}_{edge}$ ,  $\text{MLP}_{attn}$ ,  $\text{MLP}_{node}$  respectively, as shown in Table 3. We use  $\rho(\cdot)$  as the average operator. The second GN layer has the same architecture as the first GN layer but the input and output dimensions of  $f_e$ ,  $f_a$ , and  $f_n$  are 32, 32, and 32 respectively. All hidden action are ReLU, and output activations are indentity function.
- Action assignments. Similar to ScheduleNet, we perform raw feature encoding with the first GN layer and *H*-rounds of hidden embedding with the second GN layer. We use the same MLP architecture of ScheduleNet to compute the assignment probabilities from the embedded graph.
- Training. Same as ScheduleNet.

#### Details of GN-PPO.

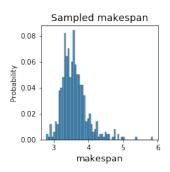


Figure 13: makespan distribution

- Network architecture. Actor (policy) is the same as GN-CR. Critic (value function) utilize the same GNN architecture to embed the input graph  $\mathcal{G}_{\tau}$ . On the embedded graph, we perform the average readout function to readout the embedded information. All other MLP parameters are the same as GN-CR.
- **Training.** We use proximal policy gradient (PPO) [36] to train GN-PPO with the default PPO hyperparameters of the stable baseline PPO2 implementation. The hyperparameters can be found in https://stable-baselines.readthedocs.io/en/master/modules/ppo2.html.

#### D.2 Extended discussion on Actor-Critic approach.

As explained in Section 6.1, the model trained with PPO (GN-PPO) results in lower scheduling performance as compared to the models trained with Clip-REINFORCE (ScheduleNet and GN-CR). We hypothesize that this phenomenon is because of the high volatility and multi-modality of the critic's training target (sampled makepsan) as visualized in Figure 13. This may cause inaccurate state-value predictions of the critic. The value prediction error would deteriorate the policy due to the bellman error propagation in the actor-critic setup as discussed in [8].

## E Limitations and future works.

ScheduleNet is an end-to-end learned heuristic that constructs feasible solutions from "scratch" without relying on existing solvers and/or effective local search heuristics. ScheduleNet builds a complete solution sequentially by accounting for the current partial solution and actions of other agents. This poses a challenge for cooperative decision-making with sparse and episodic team-reward. As we use only a single-shared scheduling policy (ScheduleNet) for all agents, it can be effectively transferred to solve extremely large mSPs. We propose ScheduleNet not only to achieve the best performance in mathematically well-defined scheduling problems, but also to address the challenging research question: "Learning to solve various large-scale multi-agent scheduling problems in a sequential, decentralized and cooperative manner". The following are the limitations of the current study and the future research direction to overcome these limitations.

Towards improving the performance of ScheduleNet. The RL approaches for routing problems can be categorized into: (1) *improvement heuristics* which learns to revise a complete solution iteratively to obtain a better solution; and (2) *construction heuristics* learns to construct a solution by sequentially assigning idle vehicles to unvisited cities until the full routing schedule (sequence) is constructed. The improvement heuristics typically can obtain better performance than the construction heuristics as they find the best solution iteratively through the repetitive solution revising/searching process. However, improvement heuristics require expensive computations than construction heuristics. Moreover, such solution revising processes can be a computational bottleneck when the size of multi-agent scheduling problems becomes larger (i.e., many agents and tasks). In this regard, this study expands the construction heuristics to a multi-agent setting to design a computationally efficient and scalable solver. While focusing on providing general schemes to solve various mSPs, ScheduleNet does not have the most competitive performance than the algorithms that are specially designed to solve specific target problems.

We can also employ the structure of the existing scheduling methods, which eventually attains better solutions after a series of computations. For instance, the learnable Monte-Carlo tree search (MCTS) [10] learns the tree traversing heuristics and empirically shows better tree search performance than UBT/UCT based MCTS. We can also borrow the structure of existing scheduling algorithms (e.g., LKH3, Branch & Bound, N-opt) to construct improvement-guaranteed policy-learning schemes.

**Towards more realistic mSP solver.** The proposed MDP formulation framework allows modeling more realistic/complex mSPs. Nowadays, the consideration of the random task demand and agent supply are necessitated for real-life mSP applications (e.g., robot taxi service with autonomous vehicles). In this study, we only aim to solve classical mSP problems, which are mathematically well-studied and have baseline heuristics to confirm the potential of the proposed SchdeduleNet framework. We expect that the current ScheduleNet framework can cope with such real-world scenarios by reformulating the state and reward definition appropriately.

Table 4: Job-shop scheduling makespans on TA dataset (Part 1)

Instance	$\mathbf{N} \times \mathbf{m}$	SPT	FIFO	MOR	Park et al. [30]	Zhang et al. [45]	ScheduleNet	OPT
Ta01	$15 \times 15$	1462	1486	1438	1389	1443	1452	1231
Ta02	$15 \times 15$	1446	1486	1452	1519	1544	1411	1244
Ta03	$15 \times 15$	1495	1461	1418	1457	1440	1396	1218
Ta04	$15 \times 15$	1708	1575	1457	1465	1637	1348	1175
Ta05	$15 \times 15$	1618	1457	1448	1352	1619	1382	1224
Ta06	$15 \times 15$	1522	1528	1486	1481	1601	1413	1238
Ta07	$15 \times 15$	1434	1497	1456	1554	1568	1380	1227
Ta08	$15 \times 15$	1457	1496	1482	1488	1468	1374	1217
Ta09	$15 \times 15$	1622	1642	1594	1556	1627	1523	1274
Ta10	$15 \times 15$	1697	1600	1582	1501	1527	1493	1241
Ta11	20 × 15	1865	1701	1665	1626	1794	1612	1357
Ta12	$20 \times 15$	1667	1670	1739	1668	1805	1600	1367
Ta13	$20 \times 15$	1802	1862	1642	1715	1932	1625	1342
Ta14	$20 \times 15$	1635	1812	1662	1642	1664	1590	1345
Ta15	$20 \times 15$	1835	1788	1682	1672	1730	1676	1339
Ta16	$20 \times 15$	1965	1825	1638	1700	1710	1550	1360
Ta17	$20 \times 15$	2059	1899	1856	1678	1897	1753	1462
Ta18	$20 \times 15$	1808	1833	1710	1684	1794	1668	1396
Ta19	$20 \times 15$	1789	1716	1651	1900	1682	1622	1332
Ta20	$20 \times 15$	1710	1827	1622	1752	1739	1604	1348
Ta21	$20 \times 20$	2175	2089	1964	2199	2252	1921	1642
Ta22	$20 \times 20$	1965	2146	1905	2049	2102	1844	1600
Ta23	$20 \times 20$	1933	2010	1922	2006	2085	1879	1557
Ta24	$20 \times 20$	2230	1989	1943	2020	2200	1922	1644
Ta25	$20 \times 20$	1950	2160	1957	1981	2201	1897	1595
Ta26	$20 \times 20$	2188	2182	1964	2057	2176	1887	1643
Ta27	$20 \times 20$	2096	2091	2160	2187	2132	2009	1680
Ta28	$20 \times 20$	1968	1980	1952	2054	2146	1813	1603
Ta29	$20 \times 20$	2166	2011	1899	2210	1952	1875	1625
Ta30	$20 \times 20$	1999	1941	2017	2140	2035	1913	1584
Ta31	$30 \times 15$	2335	2277	2143	2251	2565	2055	1764
Ta32	$30 \times 15$	2432	2279	2188	2378	2388	2268	1784
Ta33	$30 \times 15$	2453	2481	2308	2316	2324	2281	1791
Ta34	$30 \times 15$	2434	2546	2193	2319	2332	2061	1829
Ta35	$30 \times 15$	2497	2478	2255	2333	2505	2218	2007
Ta36	$30 \times 15$	2445	2433	2307	2210	2497	2154	1819
Ta37	$30 \times 15$	2664	2382	2190	2201	2325	2112	1771
Ta38	$30 \times 15$	2155	2277	2179	2151	2302	1970	1673
Ta39	$30 \times 15$	2477	2255	2167	2138	2410	2146	1795
Ta40	$30 \times 15$	2301	2069	2028	2007	2140	2030	1669

Table 5: Job-shop scheduling makespans on TA dataset (Part 2)

Instance	$\mathbf{N} \times \mathbf{m}$	SPT	FIFO	MOR	Park et al. [30]	Zhang et al. [45]	ScheduleNet	ОРТ
Ta41	$30 \times 20$	2499	2543	2538	2654	2667	2572	2005
Ta42	$30 \times 20$	2710	2669	2440	2579	2664	2397	1937
Ta43	$30 \times 20$	2434	2506	2432	2737	2431	2310	1846
Ta44	$30 \times 20$	2906	2540	2426	2772	2714	2456	1979
Ta45	$30 \times 20$	2640	2565	2487	2435	2637	2445	2000
Ta46	$30 \times 20$	2667	2582	2490	2681	2776	2541	2004
Ta47	$30 \times 20$	2620	2508	2286	2428	2476	2280	1889
Ta48	$30 \times 20$	2620	2541	2371	2440	2490	2358	1941
Ta49	$30 \times 20$	2666	2550	2397	2446	2556	2301	1961
Ta50	$30 \times 20$	2429	2531	2469	2530	2628	2453	1923
Ta51	$50 \times 15$	3856	3590	3567	3145	3599	3382	2760
Ta52	$50 \times 15$	3266	3365	3303	3157	3341	3231	2756
Ta53	$50 \times 15$	3507	3169	3115	3103	3186	3083	2717
Ta54	$50 \times 15$	3142	3218	3265	3278	3266	3068	2839
Ta55	$50 \times 15$	3225	3291	3279	3142	3232	3078	2679
Ta56	$50 \times 15$	3530	3329	3100	3258	3378	3065	2781
Ta57	$50 \times 15$	3725	3654	3335	3230	3471	3266	2943
Ta58	$50 \times 15$	3365	3362	3420	3469	3732	3321	2885
Ta59	$50 \times 15$	3294	3357	3117	3108	3381	3044	2655
Ta60	$50 \times 15$	3500	3129	3044	3256	3352	3036	2723
Ta61	$50 \times 20$	3606	3690	3376	3425	3654	3202	2868
Ta62	$50 \times 20$	3639	3657	3417	3626	3722	3339	2869
Ta63	$50 \times 20$	3521	3367	3276	3110	3536	3118	2755
Ta64	$50 \times 20$	3447	3179	3057	3329	3631	2989	2702
Ta65	$50 \times 20$	3332	3273	3249	3339	3359	3168	2725
Ta66	$50 \times 20$	3677	3610	3335	3340	3555	3199	2845
Ta67	$50 \times 20$	3487	3612	3392	3371	3567	3236	2825
Ta68	$50 \times 20$	3336	3471	3251	3265	3680	3072	2784
Ta69	$50 \times 20$	3862	3607	3526	3798	3592	3535	3071
Ta70	$50 \times 20$	3801	3784	3590	3919	3643	3436	2995
Ta71	$100 \times 20$	6232	6270	5938	5962	6452	5879	5464
Ta72	$100 \times 20$	5973	5671	5639	5522	5695	5456	5181
Ta73	$100 \times 20$	6482	6357	6128	6335	6462	6052	5568
Ta74	$100 \times 20$	6062	6003	5642	5827	5885	5513	5339
Ta75	$100 \times 20$	6217	6420	6212	6042	6355	5992	5392
Ta76	$100 \times 20$	6370	6183	5936	5707	6135	5773	5342
Ta77	$100 \times 20$	6045	5952	5829	5737	6056	5637	5436
Ta78	$100 \times 20$	6143	6328	5886	5979	6101	5833	5394
Ta79	$100 \times 20$	6018	6003	5652	5799	5943	5556	5358
Ta80	$100 \times 20$	5848	5763	5707	5718	5892	5545	5183

Table 6: Job-shop scheduling makespans on ABZ, FT, ORB, and YN datasets.

Instance	$\mathbf{N} \times \mathbf{m}$	SPT	FIFO	MOR	Park et al. [30]	ScheduleNet	ОРТ
abz5	$10 \times 10$	1352	1467	1336	1353	1336	1234
abz6	$10 \times 10$	1097	1045	1031	1043	981	943
abz7	$20 \times 15$	849	803	775	887	791	656
abz8	$20 \times 15$	929	877	810	843	787	665
abz9	$20 \times 15$	887	946	899	848	832	678
ft06	$6 \times 6$	88	65	59	71	59	55
ft10	$10 \times 10$	1074	1184	1163	1142	1111	930
ft20	$20 \times 5$	1267	1645	1601	1338	1498	1165
orb01	10 × 10	1478	1368	1307	1336	1276	1059
orb02	$10 \times 10$	1175	1007	1047	1067	958	888
orb03	$10 \times 10$	1179	1405	1445	1202	1335	1005
orb04	$10 \times 10$	1236	1325	1287	1281	1178	1005
orb05	$10 \times 10$	1152	1155	1050	1082	1042	887
orb06	$10 \times 10$	1190	1330	1345	1178	1222	1010
orb07	$10 \times 10$	504	475	500	477	456	397
orb08	$10 \times 10$	1107	1225	1278	1156	1178	899
orb09	$10 \times 10$	1262	1189	1165	1143	1145	934
orb10	$10 \times 10$	1113	1303	1256	1087	1080	944
yn1	$20 \times 20$	1196	1113	1045	1118	1027	884
yn2	$20 \times 20$	1256	1148	1074	1097	1037	904
yn3	$20 \times 20$	1042	1135	1100	1083	1046	892
yn4	$20 \times 20$	1273	1194	1267	1258	1216	968

Table 7: Job-shop scheduling makespans on SWV datasets.

Instance	$\mathbf{N} \times \mathbf{m}$	SPT	FIFO	MOR	Park et al. [30]	ScheduleNet	ОРТ
swv01	$20 \times 10$	1737	2154	1971	1761	1913	1407
swv02	$20 \times 10$	1706	2157	2158	1846	1998	1475
swv03	$20 \times 10$	1806	2019	1870	1892	1830	1398
swv04	$20 \times 10$	1874	2015	2026	1908	1971	1464
swv05	$20 \times 10$	1922	2003	2049	1796	1922	1424
swv06	$20 \times 15$	2140	2519	2287	2068	2216	1671
swv07	$20 \times 15$	2146	2268	2101	2194	2037	1594
swv08	$20 \times 15$	2231	2554	2480	2191	2255	1752
swv09	$20 \times 15$	2247	2498	2553	2278	2196	1655
swv10	$20 \times 15$	2337	2352	2431	2141	2279	1743
swv11	$50 \times 10$	3714	4427	4642	3989	4390	2983
swv12	$50 \times 10$	3759	4749	4821	4136	4532	2977
swv13	$50 \times 10$	3657	4829	4755	4008	4602	3104
swv14	$50 \times 10$	3506	4621	4740	3758	4387	2968
swv15	$50 \times 10$	3501	4620	4905	3860	4402	2885
swv16	$50 \times 10$	3453	2951	2924	2924	2924	2924
swv17	$50 \times 10$	3082	2962	2848	2840	2794	2794
swv18	$50 \times 10$	3191	2974	2852	2852	2852	2852
swv19	$50 \times 10$	3161	3095	3060	2961	2992	2843
swv20	$50 \times 10$	3125	2853	2851	2823	2823	2823

Table 8: Job-shop scheduling makespans on LA datasets.

Instance	$  \mathbf{N} \times \mathbf{m}  $	SPT	FIFO	MOR	Park et al. [30]	ScheduleNet	ОРТ
la01	$10 \times 5$	751	772	763	805	680	666
la02	$10 \times 5$	821	830	812	687	768	655
la03	$10 \times 5$	672	755	726	862	734	597
la04	$10 \times 5$	711	695	706	650	698	590
la05	$10 \times 5$	610	610	593	593	593	593
la06	$15 \times 5$	1200	926	926	926	926	926
la07	$15 \times 5$	1034	1088	1001	931	1008	890
la08	$15 \times 5$	942	980	925	863	863	863
la09	$15 \times 5$	1045	1018	951	951	951	951
la10	$15 \times 5$	1049	1006	958	966	958	958
la11	$20 \times 5$	1473	1272	1222	1276	1254	1222
la12	$20 \times 5$	1203	1039	1039	1039	1039	1039
la13	$20 \times 5$	1275	1199	1150	1150	1150	1150
la14	$20 \times 5$	1427	1292	1292	1292	1292	1292
la15	$20 \times 5$	1339	1587	1436	1282	1395	1207
la16	$10 \times 10$	1156	1180	1108	1134	1047	945
la17	$10 \times 10$	924	943	844	953	888	784
la18	$10 \times 10$	981	1049	942	1049	947	848
la19	$10 \times 10$	940	983	1088	880	963	842
la20	$10 \times 10$	1000	1272	1130	1042	989	902
la21	$15 \times 10$	1324	1265	1251	1309	1261	1046
la22	$15 \times 10$	1180	1312	1198	1158	1027	927
la23	$15 \times 10$	1162	1354	1268	1085	1145	1032
la24	$15 \times 10$	1203	1141	1149	1129	1088	935
la25	$15 \times 10$	1449	1283	1209	1308	1117	977
la26	$20 \times 10$	1498	1372	1411	1553	1458	1218
la27	$20 \times 10$	1784	1644	1566	1624	1516	1235
la28	$20 \times 10$	1610	1474	1477	1438	1357	1216
la29	$20 \times 10$	1556	1540	1437	1582	1320	1152
la30	$20 \times 10$	1792	1648	1565	1649	1490	1355
la31	30 × 10	1951	1918	1836	1817	1906	1784
la32	$30 \times 10$	2165	2110	1984	1977	1850	1850
la33	$30 \times 10$	1901	1873	1811	1795	1731	1719
la34	$30 \times 10$	2070	1925	1853	1895	1784	1721
la35	$30 \times 10$	2118	2142	2064	2041	1969	1888
la36	15 × 15	1799	1516	1492	1489	1449	1268
la37	$15 \times 15$	1655	1873	1606	1623	1653	1397
la38	$15 \times 15$	1404	1475	1455	1421	1444	1196
la39	$15 \times 15$	1534	1532	1540	1555	1430	1233
la40	$15 \times 15$	1476	1531	1358	1570	1357	1222