Learning to Schedule DAG Tasks

Zhigang Hua  
Ant Group
Sunnyvale, CA 94085  
z.hua@antgroup.com

Feng Qi  
Ant Group
Sunnyvale, CA 94085  
feng.qi@antgroup.com

Gan Liu  
Ant Group
Hangzhou, China  
liugan.lg@antgroup.com

Shuang Yang  
Ant Group
Sunnyvale, CA 94085  
shuang.yang@antgroup.com

Abstract

Scheduling computational tasks represented by directed acyclic graphs (DAGs) is challenging because of its complexity. Conventional scheduling algorithms rely heavily on simple heuristics such as shortest job first (SJF) and critical path (CP), and are often lacking in scheduling quality. In this paper, we present a novel learning-based approach to scheduling DAG tasks. The algorithm employs a reinforcement learning agent to iteratively add directed edges to the DAG, one at a time, to enforce ordering (i.e., priorities of execution and resource allocation) of “tricky” job nodes. By doing so, the original DAG scheduling problem is dramatically reduced to a much simpler proxy problem, on which heuristic scheduling algorithms such as SJF and CP can be efficiently improved. Our approach can be easily applied to any existing heuristic scheduling algorithms. On the benchmark dataset of TPC-H, we show that our learning based approach can significantly improve over popular heuristic algorithms and consistently achieves the best performance among several methods under a variety of settings.

1 Introduction

Scheduling computational tasks, as commonly represented by directed acyclic graphs (DAGs), is an important problem in many areas of computer science ranging from programming language (e.g., compilation), operating systems (e.g., parallel processing), data engineering (e.g., distributed batch/streaming computation topology), to machine learning (e.g., training graphs). Exact algorithms are prohibited due to the exponential complexity – the problem is known to be NP-hard for most of its variants. Current cluster schedulers rely entirely on simple heuristics such as shortest-job-first (SJF), critical path (CP), first-in-first-out (FIFO), and Tetris [1][2][3][4][5]. These heuristics are problem independent, incapable to utilize the dependencies as defined by the DAGs or the resource consumption constraints when scheduling a job. As a result, these methods are often far from optimal.

In this paper, we present a deep reinforcement learning algorithm for DAG scheduling. Our approach is motivated by the observation that unsatisfactory schedules are very often due entirely to the wrong ordering of a few job nodes while the rest is close to optimal. If these “tricky” nodes are correctly ordered, the quality of schedules would be dramatically improved. Moreover, if the correct ordering of these nodes can be given a priori by an oracle, the scheduling tasks would become substantially simpler such that even very simple heuristics are able to find near-optimal solutions. One way to achieve this is to add directed edges to break the ties among tricky job nodes, i.e., to explicitly require that one job node needs to be given priority over another when it comes to execution as well as resource allocation. For example, as shown in Figure 1 after adding directed edges, both SJF and
CP are able to find optimal schedules. By adding directed edges, we simplify DAG scheduling by including additional constraints and convert the original problem to a simpler proxy. In principle, this is similar in spirit to classic OR approaches such as cutting plane or active set.

We present a neural architecture that learns to add directed edges to a given DAG iteratively over time. The proposed model includes a GNN component [6] that is used to effectively encode the problem instance including the topological structure of the DAG as well as the problem configurations such as the runtime and resource requirements of each job node. On top of it, a policy network is designed to select potential directed edges that can be added to the DAG. The network is trained end-to-end using reinforcement learning to minimize the makespan. Our approach can be easily integrated with any existing heuristic algorithms without modification, e.g., SJF, CP, and so on. We test our method on public benchmark TPC-H. Experiment results show that it can effectively improve heuristic algorithms for DAG scheduling.

2 The DAG Scheduling Problem

The DAG scheduling problem is a combination of two well-known NP-hard problems: the minimum makespan problem [7] and the bin packing problem [8][9]. The goal is to find an optimal scheduling order that is executed with minimal makespan. The former features interdependence among tasks, and the latter features one-dimensional or multi-dimensional resource constraints. The Minimum Makespan Scheduling Problem aims at allocating dependent job nodes on limited computation resources with the goal of minimizing the finishing time, aka makespan. The solution can be found by solving an integer programming problem with branch-and-bound [10][11], which is unfortunately intractable for most practical-scale problems. Heuristic approaches such as highest level first, longest job time, critical path, and random priority [12], assign priorities to tasks and then execute tasks when their dependent tasks are finished, which are fast but provide sub-optimal solutions. In a dynamic makespan problem, the DAG jobs are not known beforehand, but arrive dynamically in a stream [13][2]. In a preemptive makespan problem, any job execution can be paused or restarted [14]. In a probabilistic or conditional makespan problem, task branches are executed with uncertainty [15].

There has been a surge of interests recently in finding adaptive data-driven scheduling algorithms using machine learning. For example, [16] and [17] used machine learning to learn near-optimal ordering of job nodes. These studies did not consider the dependencies among the jobs as defined by the DAGs, neither did they exploit the DAG topology when allocating executors and other resources. Decima [2] uses reinforcement learning to select the ordering of DAG jobs as well as the allocation of executors.

We examine DAG scheduling in a more general form. The problem considered in this paper is illustrated in Figure 1 where each DAG’s job node has two values, aka runtime and resource requirement (which is normalized by the total resource as between 0 and 1), and the total available resource is at a unit capacity of 1.0. Given a bunch of DAG jobs under a limited resource, the goal is to minimize the makespan of all DAG while no preemption of any DAG or node is allowed.

3 Learning Algorithm

In the following subsections, we first introduce the reinforcement learning formulation, then the GNN models for graph representations of DAGs, the neural policy networks, and the training and inference algorithms.

3.1 Reinforcement Learning Formulation

Given multiple job DAGs, we merge them into one graph \( G \) by introducing a new root node that connects to existing root nodes of DAGs, as shown in Figure 2 left. We employ deep reinforcement learning algorithm that learns to add edges in \( G \) for better scheduling. The addition of directed edges in a DAG can be formulated as a Markov Decision Process (MDP) with following components:

- **State**: a DAG graph \( G = \{n, N^{(0)}, E^{(0)}\} \), where \( n \) is the number of nodes, \( N^{(0)} \) is the set of \( n \) nodes, and \( E^{(0)} \) is the set of directed edges.
Figure 1: An example of improving DAG scheduling by adding edges. Left: node resource and runtime of a DAG. Middle: DAG’s makespan is 21.0 for both critical path (CP) and shortest job first (SJF), the CP algorithm ranks nodes by the maximum sum of task durations along the path to any of their leaf nodes in a DAG. Right: adding edges (red) helps reduce makespan of CP and SJF to 16.0.

- **Action**: adding a directed edge \( e \) in \( G \) by sequentially selecting a starting node \( a_1 \) and an ending node \( a_2 \) (see Figure 1 right). Here an added edge should not conflict with graph structure of \( G \), and a conflict occurs when there already exists a directed path between \( a_1 \) and \( a_2 \) in \( G \). The selection of starting node \( a_1 \) is conditioned on \( G \), and the selection of ending node \( a_2 \) is conditioned on \( G \) and \( a_1 \). By sequentially selecting the starting and ending nodes, the time complexity of adding an edge in \( G \) is reduced from \( O(n^2) \) to \( O(n) \).
- **Transition**: \( G' \) is composed by adding an edge \( e \) in \( G \).
- **Reward**: in our experiments, we take reward as the difference between makespans of \( G' \) and \( G \) using existing heuristic methods such as SJF, CP, etc. The reward can be easily switched to other measures than makespan, such as average waiting time.

Figure 2: Merge DAGs by adding a new root node that connects to all existing root nodes of DAGs (left), and reverse direction of edges when computing graph embedding for the merged DAG (right).

### 3.2 Graph Neural Network

We employ GNN to compute graph embeddings for DAGs. Given a DAG \( G \), we reverse the direction of all edges in \( G \) to get \( G^T \). The original feature vector of each node in a DAG is comprised of its runtime and required resources, which is transformed into a hidden representation \( e^{(l)}_i \) through a \( L \)-layer neural network with parameters of \( W_{1,l} \) (\( 1 \leq l \leq L \)).
At each iteration of message passing in $G^T$, each node’s embedding is propagated to its neighbors and updated as follows:

$$e_i^{(h)} = \sigma(W_2^{(h)} \cdot \text{Concat}(e_i^{(h-1)}, \sum_{j \in N_i} e_j^{(h-1)})), \forall i \in \{1, \ldots, n\}, \forall h \in \{1, \ldots, H\}$$ (1)

where $\sigma(\cdot)$ stands for activation function, $H$ is the number of message passing iterations and $h$ is the order, $W_2^{(h)}$ is the weight matrix for the $h$-th iteration, $N_i$ represents the set of neighbors in $G^T$ (aka children nodes in $G$). Hence the parameters of the GNN network are:

$$\phi = \{W_1^{(l)}, W_2^{(h)}\}, \forall l \in \{1, \ldots, L\}, \forall h \in \{1, \ldots, H\}$$ (2)

As the output the GNN model, each node is represented as a deep embedding, and the whole DAG graph is represented as an average embedding of all its included nodes.

### 3.3 Neural Policy Network

Our method takes an action of adding an edge $a$ for the DAG graph $G$, which sequentially selects starting node $a^1$ and ending node $a^2$. The joint probability of selecting $a$ is the multiplying product of the probabilities of selecting $a^1$ and $a^2$ as follows:

$$\pi \sim p_{\theta, \phi}(a|G) = p_{\theta_1, \phi}(a^1|G) \cdot p_{\theta_2, \phi}(a^2|G, a^1)$$ (3)

where $\theta = (\theta_1, \theta_2)$, $p_{\theta_1, \phi}(a^1|G)$ is the conditional probability of selecting starting node given $G$, and $p_{\theta_2, \phi}(a^2|G, a^1)$ is the conditional probability of selecting ending node given $G$ and pre-selected $a^1$. We use two deep neural networks to compute these conditional probabilities.

Due to its compelling results we adopt Reset \[18\] to represent two deep policy networks, as shown in Figure 3 that selects starting (left) and ending node (right) for adding an edge. The neural network’s input is encoded as a combination of multiple embeddings, including the graph, the starting node if selecting an ending node, and candidate nodes. As output of the policy networks, the conflicting nodes are masked with probability of 0 at the last softmax layer. It is crucial for a learning method that trains on given graphs and predicts on unseen graphs. This neural architecture is generalized such that it supports heterogeneous DAG structures with different amount of nodes.

### 3.4 Training Algorithm

The GNN and policy networks are improved based on policy gradient algorithm, which is summarized in Appendix \[A.1\]. We discuss its main components as follows:
Policy rollout. Given a DAG graph $G$, we do $N$ rollouts of current policy models and in each rollout we add $M$ directed edges. Based on a commonly used practice of encouraging exploration, we use $\epsilon$-greedy \cite{19} such that the rollout will pick randomly each node with a probability of 0.05 at every timestep. The rollout algorithm is presented in Appendix A.2. At $j$-th timestep of $i$-th rollout, we record a triplet to be used by our training algorithm as follows:

$$\{G_{i,j}, (a_{1,i,j}, a_{2,i,j}), r_{i,j}\}, \forall i \in \{1, ..., N\}, \forall j \in \{1, ..., M\} \quad (4)$$

where $G_{i,j}$ is the updated DAG graph with added edges, $a_{1,i,j}$ and $a_{2,i,j}$ stands for the starting node and ending node of an added edge $a_{i,j}$ respectively, and $r_{i,j}$ is the reward computed as the reduction of makespan of $G_{i,j}$ after an edge $a_{i,j}$ is added.

Reward. At each timestep $j$, the incremental reward is the reduction of makespan of a DAG after an edge is added. To inspire long term reward, the cumulative reward at the $j$-th timestamp is a discounted sum of incremental rewards from current timestep until completion of a rollout:

$$\hat{r}_{i,j} = \sum_{j'=j}^{M} r_{i,j'} \cdot \gamma^{(j'-j)}, \forall i \in \{1, ..., N\}, \forall j \in \{1, ..., M\} \quad (5)$$

where $\gamma$ is the discounting factor, and by default we set it as 1.0 in our experiments.

Baseline. For every $N$ rollouts, we compute the baseline of rewards at each timestep $j$ as shown in Equation (6), which is subtracted from rewards to reduce variance.

$$b_j = \frac{1}{N} \cdot \sum_{i=1}^{N} \hat{r}_{i,j}, \forall j \in \{1, ..., M\} \quad (6)$$

Loss function. The model parameters in the reinforcement learning algorithm are updated after every $N$ rollouts. We use the commonly used policy gradient algorithm to train the parameters in the GNN and policy networks. The joint loss function is represented as follows:

$$\nabla_{\phi, \theta} J(\phi, \theta | G) = \mathbb{E}_{\pi \sim p_{\phi, \theta}(. | G)} (\hat{r} - b) \cdot \nabla \log p_{\phi, \theta}(\pi | G) \quad (7)$$

With $N$ rollouts where $M$ edges are added, Equation (7) can be computed as follows:

$$\nabla J(\phi, \theta_1, \theta_2 | G) = \sum_{i=1}^{N} \sum_{j=1}^{M} (\hat{r}_{i,j} - b_j) \cdot [\nabla \log p_{\phi, \theta_1}(a_{1,i,j} | G_{i,j}) + \nabla \log p_{\phi, \theta_2}(a_{2,i,j} | G_{i,j}, a_{1,i,j})] \quad (8)$$

3.5 Inference Algorithm

We use a beam search method to add edges for DAGs in the inference stage. Suppose the beam size is $K$ (e.g. $K = 10$). The inference algorithm is shown in Appendix A.4. When adding an edge, we first pick up the top $K$ candidate starting nodes based on their probabilities output by the policy network, and then for each of $K$ starting nodes we choose its top ending node with maximal probability. As a result, the edge is selected with the maximal joint probability of the $K$ candidates.

We applied our learning method to two heuristic algorithms of SJF and CP. We tested Tetris \cite{1} and mixed integer linear programming (MILP) for comparison. The CP algorithm ranks nodes by the maximum sum of task durations along the path to any of their connected leaf nodes. The Tetris algorithm ranks nodes by the dot product similarity of two vectors of resource consumption and available resource. The MILP formulation is described in Appendix B. As its scale is large for existing IP solvers, we relax the integer constraints to solve the linear programming problem (LP) with OR-Tools,\footnote{https://developers.google.com/optimization} which might produce sub-optimal results.
Figure 4: The reduction ratios of DAG makespans for SFJ and CP with learning method by varying the number of added edges (from 1 to 5) under two job resource distributions.

Table 1: The average makespan (sec) with real-valued runtime and resource dist of 1.0.

| # dags | SJF Time | SJF Learn | SJF Reduce % | CP Time | CP Learn | CP Reduce % | OR-Tools Time | Tetris Time |
|--------|----------|-----------|--------------|---------|----------|--------------|---------------|-------------|
| 5      | 21.29    | 18.81     | 11.65%       | 18.13   | 17.29    | 4.66%        | 23.05         | 17.73       |
| 10     | 58.66    | 52.66     | 10.23%       | 46.66   | 45.03    | 3.50%        | 59.56         | 45.03       |
| 20     | 87.66    | 80.85     | 7.77%        | 72.35   | 70.01    | 3.23%        | 97.09         | 70.94       |
| 50     | 241.33   | 231.80    | 3.95%        | 203.72  | 191.67   | 5.92%        | -             | 191.47      |
| 100    | 479.54   | 478.19    | 0.28%        | 404.22  | 384.74   | 4.82%        | -             | 382.61      |
| average| 177.70   | 172.46    | 6.78%        | 149.02  | 141.75   | 4.43%        | -             | 141.56      |

Table 2: The average makespan (sec) with real-valued runtime and resource dist of 2/3.

| # dags | SJF Time | SJF Learn | SJF Reduce % | CP Time | CP Learn | CP Reduce % | OR-Tools Time | Tetris Time |
|--------|----------|-----------|--------------|---------|----------|--------------|---------------|-------------|
| 5      | 14.55    | 13.48     | 7.36%        | 11.94   | 11.73    | 1.76%        | 13.49         | 13.26       |
| 10     | 38.45    | 37.15     | 3.37%        | 33.40   | 31.54    | 5.56%        | 37.69         | 33.03       |
| 20     | 61.04    | 59.79     | 2.05%        | 53.71   | 49.72    | 7.44%        | 59.64         | 50.93       |
| 50     | 118.54   | 111.83    | 5.66%        | 98.44   | 97.94    | 0.50%        | -             | 99.46       |
| 100    | 229.05   | 220.81    | 3.60%        | 189.59  | 188.94   | 0.35%        | -             | 189.88      |
| average| 92.33    | 88.61     | 4.41%        | 77.42   | 75.97    | 3.12%        | -             | 77.31       |

Table 3: The average makespan (sec) with real-valued runtime and resource dist of 1/3.

| # dags | SJF Time | SJF Learn | SJF Reduce % | CP Time | CP Learn | CP Reduce % | OR-Tools Time | Tetris Time |
|--------|----------|-----------|--------------|---------|----------|--------------|---------------|-------------|
| 5      | 8.49     | 7.84      | 7.60%        | 7.11    | 7.02     | 1.29%        | 7.70          | 8.77        |
| 10     | 19.39    | 18.59     | 4.15%        | 16.10   | 15.56    | 3.36%        | 17.25         | 16.81       |
| 20     | 29.49    | 28.02     | 4.99%        | 24.06   | 23.47    | 2.44%        | 27.01         | 25.02       |
| 50     | 68.73    | 66.52     | 3.22%        | 60.02   | 59.31    | 1.19%        | -             | 60.85       |
| 100    | 138.21   | 136.93    | 0.93%        | 123.13  | 122.31   | 0.66%        | -             | 122.83      |
| average| 52.86    | 51.58     | 4.18%        | 46.08   | 45.53    | 1.79%        | -             | 46.86       |
Table 4: The average makespan (sec) with uniformly random runtime and resource dist of 1.0.

| # dags | Shortest Job First (SJF) | Critical Path (CP) | OR-Tools | Tetris |
|--------|--------------------------|-------------------|-----------|--------|
|        | Time Learn Reduce %  | Time Learn Reduce % | Time | Time |
| 5      | 9.54 8.29 13.12%       | 8.95 7.91 11.61%   | 9.21  | 7.71  |
| 10     | 20.82 19.70 5.37%      | 19.67 16.76 14.77% | 20.24 | 16.26 |
| 20     | 34.31 31.79 7.35%      | 31.03 28.22 9.05%   | 35.29 | 26.92 |
| 50     | 89.93 87.51 2.69%      | 83.49 73.68 11.76%  | -     | 69.21 |
| 100    | 178.01 176.43 0.89%    | 173.88 148.40 14.66% | -     | 138.60 |
| average| 66.52 64.74 5.88%      | 63.41 54.99 12.37%   | -     | 51.74 |

Table 5: The average makespan (sec) with uniformly random runtime and resource dist of 2/3.

| # dags | Shortest Job First (SJF) | Critical Path (CP) | OR-Tools | Tetris |
|--------|--------------------------|-------------------|-----------|--------|
|        | Time Learn Reduce %  | Time Learn Reduce % | Time | Time |
| 5      | 6.51 6.07 6.72%       | 5.96 5.39 9.49%    | 6.53   | 6.24  |
| 10     | 14.10 13.48 4.42%     | 12.48 11.77 5.70%  | 13.00  | 12.04 |
| 20     | 22.73 21.79 4.12%     | 20.18 19.53 3.21%  | 21.40  | 20.25 |
| 50     | 39.56 39.10 1.17%     | 35.65 35.18 1.33%  | -     | 35.41 |
| 100    | 79.18 78.47 0.89%     | 71.63 70.98 0.91%  | -     | 70.72 |
| average| 32.42 31.78 3.46%     | 29.18 28.37 4.13%  | -     | 28.93 |

Table 6: The average makespan (sec) with uniformly random runtime and resource dist of 1/3.

| # dags | Shortest Job First (SJF) | Critical Path (CP) | OR-Tools | Tetris |
|--------|--------------------------|-------------------|-----------|--------|
|        | Time Learn Reduce %  | Time Learn Reduce % | Time | Time |
| 5      | 4.88 4.82 1.14%       | 4.82 4.82 1.00%   | 4.95   | 5.25  |
| 10     | 7.67 7.07 7.82%      | 6.15 5.90 4.01%   | 6.95   | 6.92  |
| 20     | 11.08 10.69 3.49%    | 9.63 9.28 3.67%   | 10.31  | 11.10 |
| 50     | 25.11 24.85 1.03%    | 23.05 22.59 2.01% | -      | 24.07 |
| 100    | 51.54 51.23 0.60%    | 47.17 46.66 1.08% | -      | 48.32 |
| average| 20.06 19.73 2.82%    | 18.16 17.85 2.15% | -      | 19.13 |

4 Experiments and Results

The TPC-H[^1] is a decision support benchmark that have broad industry-wide relevance. In its DAG datasets, the number of nodes vary from 2 to 18. In the training stage, at each iteration we sample a sequence of DAGs and merge them into one for training. For testing, we built four testsets to measure performance with number of DAGs at 5, 10, 15 and 20. For each testset we sample 10 sequences of DAGs and each sequence is merged into one DAG. The job resource distribution is specified as the ratio of the maximum node resource consumption over total resource, which reflects tightness of resource constraints, and is tuned to 3 values (i.e. 1.0, 2/3 and 1/3) in our experiments. The higher values mean tighter resource constraints.

4.1 Effects of Added Edges

As show in Figure[^4] we test our learning method by varying the number of added edges from 1 to 5. The experiment is conducted under two different resource distributions, e.g. 1.0 and 2/3. The results show that our leaning method can reduce makespan of DAG execution on both SJF and CP algorithms. The two figures in the left side show the reduction ratio of makespan using SJF, where the reduction ratio of makespan is up to about 12%. The two figures in the right side show the reduction ratios of makespan using CP, where the reduction of makespan is up to about 10%. More added edges leads to better reduction of makespan but not always. In the following experiments, we use an ensemble way that chooses the best performance among 1 to 5 added edges in DAGs to measure makespan reduction under different distributions of resource and runtime values.

[^1]: http://www.tpc.org/tpch/
4.2 Resource Distribution

We test our learning algorithm to measure its generalization and robustness under different job resource distributions. We test 4 different resource distributions. Table 1-3 list the comparison of SJF and CP under different resource distributions. Generally, under tighter resource constraints, there are more improvement spaces for learning algorithm to reduce makespans of SJF and CP. Overall the learning algorithm brings good improvements for both of the SJF and CP methods. Under different resource distributions, on average it achieves about 6.03% and 4.30% on the reduction of makespans for SJF and CP, respectively. Originally, CP is more efficient than SJF for DAG scheduling in our experiment, and the overall improvement of makespan for CP (4.30%) is less than SJF (6.03%). In this table, compared to other methods like SJF, Tetris and Or-tools, the learning-based algorithm for CP has consistently achieved the best results under different settings.

4.3 Runtime Distribution

In the above experiments, the runtime of job nodes in DAGs are set as real values in the TPC-H dataset. To test the robustness of our learning algorithm, we further tune the runtime values of DAG nodes using uniform distribution between 0 and 1.0. Table 4-6 show the results of our experiments. Under different settings, on average the learning algorithm can achieve reduction of makespans of 6.0% for SJF and 6.63% for CP, respectively. As shown in the tables, the improvements of CP are more obvious for random runtime (6.63%) than real-valued distribution (4.3%), while for SJF the improvements are less significantly different between uniform runtime (6.0%) and real values (6.03%). The CP algorithm prioritizes the nodes in the critical path, and setting uniform random runtime for DAG nodes offers improvements for these nodes. The learning-based algorithm for CP achieves the overall best performance under all the settings, and Tetris claims the best result under the job resource distribution of 1.

4.4 Convergence Analysis

We study the convergence of our learning algorithm on the test datasets. Figure 5 shows that the learning algorithm helps improve the makespace reduction for SJF and CP when the training iteration starts. It displays the trend of convergence of our learning algorithm on the test datasets for both of the two algorithms, SJF and CP. Within 10,000 iterations, our learning-based method reaches convergence for both SJF and CP. Also from the results it shows that the convergence is more obvious for the testset with larger number of DAGs (e.g. 15 and 20) compared to the testsets with fewer DAGs (e.g. 5 and 10).

5 Conclusions

This paper proposes a novel learning-based approach to improve DAG scheduling by learning to add directional edges in DAGs. We introduce a deep reinforcement learning algorithm on top of a GNN model of DAG structure. Our approach can be easily applied to existing heuristic job scheduling algorithms such as Shortest Job First (SJF), Critical Path (CP), and so on. The experimental results show that it can efficiently improve some heuristic scheduling algorithms for DAG scheduling. As for future work, we plan to extend the support of multi-dimensional resource requirements of DAGs. We will extend the support of other heuristic algorithms such as Tetris and others. Furthermore, it is very interesting to study DAG scheduling under online streaming settings where DAG jobs arrive dynamically over time.

References

[1] Robert Grandl, Ganesh Ananthanarayanan, Srikanth Kandula, Sriram Rao, and Aditya Akella. Multi-resource packing for cluster schedulers. ACM SIGCOMM Computer Communication Review, 44(4):455–466, 2014.

[2] Hongzi Mao, Malte Schwarzkopf, Shaileshh Boja Venkatakrishnan, Zili Meng, and Mohammad Alizadeh. Learning scheduling algorithms for data processing clusters. In Proceedings of the ACM Special Interest Group on Data Communication, pages 270–288. ACM, 2019.
Figure 5: Convergence of test datasets under job resource distribution of 1.0

[3] Craig Chambers, Ashish Raniwala, Frances Perry, Stephen Adams, Robert R. Henry, Robert Bradshaw, and Nathan Weizenbaum. Flumejava: Easy, efficient data-parallel pipelines. ACM SIGPLAN Conference on Programming Language Design and Implementation (PLDI), 2010.

[4] Michael Isard, Mihai Budiu, Yuan Yu, Andrew Birrell, and Fetterly Dennis. Dryad: Distributed data-parallel programs from sequential building blocks. ACM SIGOPS/EuroSys European Conference on Computer Systems (EuroSys), 2007.

[5] Matei Zaharia, Mosharaf Chowdhury, Tathagata Das, Ankur Dave, Justin Ma, Murphy McCauley, Michael J. Franklin, Scott Shenker, and Ion Stoica. Dryad: Distributed data-parallel programs from sequential building blocks. The 9th USENIX Conference on Networked Systems Design and Implementation (NSDI), 2012.

[6] Mikael Henaff, Joan Bruna, and Yann LeCun. Deep convolutional networks on graph-structured data. CoRR abs/1506.05163, 2015.

[7] Vijay V Vazirani. Approximation algorithms. Springer Science & Business Media, 2013.

[8] Eva Hopper and Brian CH Turton. A review of the application of meta-heuristic algorithms to 2d strip packing problems. Artificial Intelligence Review, 16(4):257–300, 2001.

[9] Silvano Martello, David Pisinger, and Daniele Vigo. The three-dimensional bin packing problem. Operations research, 48(2):256–267, 2000.

[10] Jens Clausen. Branch and bound algorithms-principles and examples. Department of Computer Science, University of Copenhagen, pages 1–30, 1999.

[11] Walter H Kohler and Kenneth Steiglitz. Characterization and theoretical comparison of branch-and-bound algorithms for permutation problems. Journal of the ACM, 21(1):140–156, 1974.

[12] Yu-Kwong Kwok and Ishfaq Ahmad. Static scheduling algorithms for allocating directed task graphs to multiprocessors. ACM Computing Surveys (CSUR), 31(4):406–471, 1999.

[13] Michael A Palis, Jing-Chiou Liou, Sanguthevar Rajasekaran, SUNIL SHENDE, and David SL Wei. Online scheduling of dynamic trees. Parallel Processing Letters, 5(04):635–646, 1995.
A Algorithms

Here contains the algorithms for our method.

A.1 Training Algorithm

The training algorithm of our learning method is given in Algorithm 1.

**Algorithm 1** The training algorithm for learning-based DAG scheduling

1: Function Learn($\alpha, \phi, \theta_1, \theta_2, I, N, M, H$)
2: # $\alpha$: learning rate, $\phi$: GNN parameters, $\theta_1$: policy1 parameters, $\theta_2$: policy2 parameters
3: # $I$: num of iterations, $N$: num of rollouts, $M$: num of edges to add, $H$: num of GNN hops
4: for $i \in \{1, ..., I\}$ do
5:     $\text{num}_\text{dags} = \text{Random sample a number from an exponential distribution}$
6:     $\text{dags} = \text{Random sample}\ \text{num}_\text{dags} \ \text{DAGs from a dataset}$
7:     $\text{triplets} = \text{rollout}(\text{dags}, N, M, H, \phi, \theta_1, \theta_2)$
8:     $d_{\phi} = d_{\theta_1} = d_{\theta_2} = 0$
9:     for $(G', (a^1, a^2), \hat{r}) \in \text{triplets}$ do
10:        $\nabla J(\phi, \theta_1, \theta_2|G') = \hat{r} \cdot [\nabla \log p_{\phi, \theta_1}(a^1|G') + \nabla \log p_{\phi, \theta_2}(a^2|G', a^1)]$
11:        $d_{\phi} += \nabla_{\phi} J(\phi, \theta_1, \theta_2|G')$
12:        $d_{\theta_1} += \nabla_{\theta_1} J(\phi, \theta_1, \theta_2|G')$
13:        $d_{\theta_2} += \nabla_{\theta_2} J(\phi, \theta_1, \theta_2|G')$
14:     end for
15:     $\phi = \phi + \alpha \cdot d_{\phi}$
16:     $\theta_1 = \theta_1 + \alpha \cdot d_{\theta_1}$
17:     $\theta_2 = \theta_2 + \alpha \cdot d_{\theta_2}$
18: end for

A.2 Rollout Algorithm

The rollout algorithm of our learning method is listed in Algorithm 2.

A.3 Reward Adjustment Algorithm

The reward adjustment algorithm of our learning method is listed in Algorithm 3.

A.4 Inference Algorithm

The inference algorithm of our learning method is listed in Algorithm 4.
Algorithm 2 The rollout algorithm for collecting actions and rewards in a DAG graph

1: Function Rollout(dags, $N$, $M$, $H$, $\phi$, $\theta_1$, $\theta_2$)
2: # dags: DAG jobs, $N$: num of rollouts, $M$: num of edges to add, $H$: num of GNN hops
3: # $\phi$: GNN parameters, $\theta_1$: parameters for first policy, $\theta_2$: parameters for second policy
4: $G =$ Merge dags into one DAG graph
5: $T_0 =$ MakeSpan($G$) {MakeSpan: calculated with heuristic scheduling algorithm}
6: triplets $= [[[]]] \times N$
7: for $i \in \{1, ..., N\}$ do
8: $G_1 =$ $G.copy()$
9: for $j \in \{1, ..., M\}$ do # add $M$ edges
10: $\text{graph}_em, \text{node}_ems =$ GNN($\phi, G_1, H$) {#Compute graph embeddings}
11: # Compute starting node
12: $\text{qual_nodes}_1 =$ Identify qualified non-conflict starting nodes in $G$
13: $\text{qual_node}_1\_ems =$ Lookup embeddings of $\text{qual_nodes}_1$ from $\text{node}_ems$
14: $\text{qual_node}_1\_probs =$ resnet_policy1($\theta_1, \text{graph}_em, \text{qual_node}_1\_ems$)
15: $\text{node}_1 =$ Sample a node from $\text{qual_node}_1\_probs$ with $\epsilon$-random strategy
16: # Compute ending node
17: $\text{node}_1\_em =$ Lookup embedding of $\text{node}_1$ from $\text{node}_ems$
18: $\text{qual_nodes}_2 =$ Identify qualified non-conflict ending nodes directed by $\text{node}_1$
19: $\text{qual_node}_2\_ems =$ Lookup embeddings of $\text{qual_nodes}_2$ from $\text{node}_ems$
20: $\text{qual_node}_2\_probs =$ resnet_policy2($\theta_2, \text{graph}_em, \text{node}_1\_em, \text{qual_node}_2\_ems$)
21: $\text{node}_2 =$ Sample a node from $\text{qual_node}_2\_probs$ with $\epsilon$-random strategy
22: $G_2 =$ Add a directed edge ($\text{node}_1, \text{node}_2$) in $G_1$
23: $\text{record} =$ ($G_1, (\text{node}_1, \text{node}_2), \text{Makespan}(G_1) - \text{Makespan}(G_2)$)
24: triplets[i].add(record)
25: $G_1 =$ $G_2$
26: end for
27: end for
28: return adjustReward(triplets, $N$, $M$, $T_0$)

Algorithm 3 The algorithm for adjustment of rewards

1: Function adjustReward(triplets, $N$, $M$, $T$)
2: # adjust and normalize rewards on $N$ rollouts and $M$ added edges
3: baseline $= [0.0] \times M$
4: for $i \in \{1, ..., N\}$ do
5: for $j \in \{1, ..., M\}$ do
6: for $k \in \{j + 1, ..., M\}$ do
7: triplets[i][j].reward += triplets[i][k].reward
8: end for
9: baseline[j] += (triplets[i][j].reward / $N$)
10: end for
11: end for
12: for $i \in \{1, ..., N\}$ do
13: for $j \in \{1, ..., M\}$ do
14: triplets[i][j].reward = (triplets[i][j].reward − baseline[j]) / $T$
15: end for
16: end for
17: return triplets
Algorithm 4 The inference algorithm of adding edges in a DAG

1: Function Inference($G, M, K, \phi, \theta_1, \theta_2$)
2: # $G$: graph, $M$: num of edges to add, $K$: num of top candidates
3: # $\phi$: GNN params, $\theta_1$: starting node policy params, $\theta_2$: ending node policy params
4: for $i \in \{1, \ldots, M\}$ do
5:  $\text{graph}_{\text{em}}, \text{node}_{\text{ems}} = \text{GNN}(\phi, G, H)$ (#Compute graph embeddings)
6:  $\text{qual}_{\text{node1}}_{\text{ems}} = \text{Get embeddings from node}_{\text{ems}}$ for qualified starting nodes
7:  $\text{qual}_{\text{node1}}_{\text{probs}} = \text{resnet}_{\text{policy1}}(\theta_1, \text{graph}_{\text{em}}, \text{qual}_{\text{node1}}_{\text{ems}})$
8:  $\text{starting\_nodes} = \text{Pick top K nodes from qual}_{\text{node1}}_{\text{probs}}$
9:  $\text{candidate\_edges} = []$
10: for $(\text{node1}, \text{prob1}) \in \text{starting\_nodes}$ do
11:  $\text{qual}_{\text{node2}}_{\text{ems}} = \text{Get embeddings from node}_{\text{ems}}$ for qualified nodes started by node1
12:  $\text{qual}_{\text{node2}}_{\text{probs}} = \text{resnet}_{\text{policy2}}(\theta_2, \text{graph}_{\text{em}}, \text{node1}_{\text{em}}, \text{qual}_{\text{node2}}_{\text{ems}})$
13:  $\text{node2, prob2} = \text{pick the node with max value in qual}_{\text{node2}}_{\text{probs}}$
14:  $\text{candidate\_edges}.\text{add}((\text{node1}, \text{node2}), \text{prob1} \times \text{prob2})$
15: end for
16: $\text{edge} = \text{Pick (node1, node2) from candidate\_edges having max value of prob}$
17: $G = \text{Add edge in } G$
18: end for
19: return $G$

B MILP Formulation

Here we define a general MILP formulation for DAG scheduling, where there are $N$ task nodes in a DAG, and the dimension of the resource requirement is $K (K \geq 1)$.

B.1 Notations

Below are the coefficients for the MILP problem:

- $t_i$: duration of task $i$, total number of tasks is $N$,
- $r_{ik}$: task $i$ consumption on resource $k$, dimension of resource is $K$,
- $R_k$: total amount of resource in dimension $k$

Below are the decision Variables for the MILP problem:

- $s_i$: start time of task $i$

Below are some predefined operators for the MILP problem:

- $A(i)$: all ancestors of task $i$,
- $D(i)$: all descendants of task $i$,
- $C(i)$: all children of task $i$

B.2 Primal formulation

With task start time $s_i$ as decision variables, two conditions are sufficient for formulating the DAG scheduling problem:

- (1) the staring time of each task is later than then ending time of all its parent nodes, and
- (2) at the start time of each task, the sum of resource consumption of all running tasks is below the maximum resource capacity.

As a result, the DAG scheduling problem can be formulated as $\min$ $\max$ optimization as follows:

$$\begin{align*}
\min \max_{i} (s_i + t_i) \\
\text{s.t.} \quad & s_i + t_i \leq s_j \quad \forall i, j \in C(i) \\
& \sum_{j=1}^{N} I(s_j \leq s_i < s_j + t_j) \cdot r_{jk}^i \leq R_k \quad \forall i, k
\end{align*}$$

(9)
I(·) in the above formula is an indicator function with value of 1 if True and 0 else.

### B.3 Reformulation

The minmax optimization with indicator function is intractable, and we use some intermediate decision variables to reformulate the primal optimization problem.

**Intermediate decision variables:**
- $T$: finishing time of all tasks,
- $y_{ij} \in \{0, 1\}$: start time of task $i$ is later than start time of task $j$,
- $z_{ij} \in \{0, 1\}$: start time of task $i$ is earlier than end time of task $j$,
- $u_{ij} \in \{0, 1\}$: task $j$ is running when task $i$ starts

**Constant:**
- $B$: a sufficiently large positive real number

The reformulation of the primal optimization problem is as follows:

\[
\begin{align*}
\min & \quad T \\
\text{s.t.} & \quad s_i + t_i \leq T \quad \forall i \quad (a) \\
& \quad s_i + t_i \leq s_j \quad \forall i, j \in C(i) \quad (b) \\
& \quad s_i \leq s_j + B y_{ij} \quad \forall i, j \in (D(i) \cup A(j)) \quad (c) \\
& \quad s_j \leq s_i + B(1 - y_{ij}) \quad \forall i, j \in (D(i) \cup A(j)) \quad (d) \\
& \quad s_j + t_j \leq s_i + B z_{ij} \quad \forall i, j \in (D(i) \cup A(j)) \quad (e) \\
& \quad s_i \leq s_j + t_j + B(1 - z_{ij}) \quad \forall i, j \in (D(i) \cup A(j)) \quad (f) \\
& \quad y_{ij} + z_{ij} - 1 \leq B u_{ij} \quad \forall i, j \in (D(i) \cup A(i)) \quad (g) \\
& \quad 2 - y_{ij} - z_{ij} \leq B(1 - u_{ij}) \quad \forall i, j \in (D(i) \cup A(j)) \quad (h) \\
& \quad \sum_j u_{ij} r_j^k + r_i^k \leq R^k \quad \forall i, k \quad (i) \\
& \quad y_{ij}, z_{ij}, u_{ij} \in \{0, 1\} \quad \forall i, j \quad (j)
\end{align*}
\]

In the above formulas, (a)-(b) defines the objective to be the total running time; (c) ensures condition 1 of Primal formulation; (d)-(e) follows the definition of $y_{ij}$; (f)-(g) follows the definition of $z_{ij}$; (h)-(i) follows the definition of $u_{ij}$; and (j) ensures condition 2 of Primal formulation.

In this way, the MILP problem can be formulated and solved with existing solvers. However, this MILP problem for DAG scheduling has a large set of integer variables for even a DAG with tens of nodes, which could not be solved by existing solvers. Here we solve the MILP problem by relaxing integer variables to a corresponding LP problem, and we reserve the order of $s_i$ from the LP solution to execute the DAG given a resource limit.