Attention-based Reinforcement Learning for Combinatorial Optimization: Application to Job Shop Scheduling Problem

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Abstract

Job shop scheduling problems represent a significant and complex facet of combinatorial optimization problems, which have traditionally been addressed through either exact or approximate solution methodologies. However, the practical application of these solutions is often challenged due to the complexity of real-world problems. Even when utilizing an approximate solution approach, the time required to identify a near-optimal solution can be prohibitively extensive, and the solutions derived are generally not applicable to new problems. This study proposes an innovative attention-based reinforcement learning method specifically designed for the category of job shop scheduling problems. This method integrates a policy gradient reinforcement learning approach with a modified transformer architecture. A key finding of this research is the ability of our trained learners within the proposed method to be repurposed for larger-scale problems that were not part of the initial training set. Furthermore, empirical evidence demonstrates that our approach surpasses the results of recent studies and outperforms commonly implemented heuristic rules. This suggests that our method offers a promising

avenue for future research and practical application in the field of job shop scheduling problems.

Index terms— Combinatorial optimization, Job shop scheduling problem, Reinforcement learning, Attention

1 Introduction

Job shop scheduling problem (JSSP) is a well-known and one of the hardest classes of combinatorial optimization problems in operations research, computer science, and industrial engineering. It has a long history as a research topic and is still being actively studied because of its applicability in numerous industrial areas, such as manufacturing and production domains (Gao et al., 2020).

JSSP has been tackled in mainly two ways, by exact solution approaches and approximate approaches (Zhang et al., 2019; Kwon et al., 2021; Xie et al., 2019). Exact solution approaches with mathematical programming have been widely adopted (Ku and Beck, 2016; Pei et al., 2020; Wang et al., 2018; Zhang and Wang, 2018); however, it may take a prohibitive amount of time to find an optimal solution, or the problems can be infeasible to find an optimal solution. This can be problematic for real-world JSSP, where a large number of jobs or machines would be associated. This has led researchers and practitioners to turn their attention to approximate methods, which aim to achieve near-optimal solutions instead. Various heuristic approaches have been applied to solve JSSP (Gonçalves et al., 2005; Park et al., 2003; Peng et al., 2015; Kawaguchi and Fukuyama, 2016; Chakraborty and Bhowmik, 2015; Cruz-Chávez et al., 2017; Nagata and Ono, 2018; Shi et al., 2020).

Although the above mentioned approaches have gained success in addressing JSSP and are recognized as effective means to solve this particular problem type, solutions by those methods are subject to the constraints that are assumed when solving the problems. For example, solutions using the above methods are for the particular problems where the methods are applied, and thus, the solutions are not applicable to other problems in general. New problems are solved anew even with the same approach. Considering the shortcomings of classical solution approaches, it is essential to have a framework that can effectively solve

large-scale problems without needing model adjustments or human intervention.

To address those challenges, we propose a learning method that is capable of providing solutions to unseen problems. In particular, we employ attention mechanisms (Bahdanau et al., 2014) and integrate them with reinforcement learning (Sutton and Barto, 2018) and the transformer architecture (Vaswani et al., 2017). We show that our trained learners can be reused to solve problems not only of the same size but also of larger sizes without retraining and demonstrate that our proposed approach outperforms the results in recent studies and widely adopted heuristic rules.

Building on this foundation, we highlight the principal contributions of our study:

- The suggested model introduces a novel approach for representing the characteristics operations in JSSP by utilizing a revised transformer architecture, two independent transformer encoders attending operations in same job groups and machine sharing operations, respectively.
- The proposed model is agnostic to problem size. A trained policy in simpler scenarios, like 6 jobs and 6 machines, can effectively solve unseen, more complex problem instances than used in training.
- A trained policy with the proposed model outperforms popularly used dispatching heuristics and other proposed models employing RL frameworks.
- We conducted extensive testing on synthetic and the seven most recognized benchmark instances of varying complexities to demonstrate the proposed model's broad applicability and performance.

The remainder of the paper proceeds as follows. Related work is provided in Section 2, the problem is defined in Section 3, details of our methodologies are proposed in Section 4, the experiments are described, and the results are provided in Section 5, and the study is concluded in Section 6.

2 Related Work

In recent years, the application of machine learning and deep learning methods has expanded to the field of combinatorial optimization problems (COPs), providing innovative approaches to tackle problems that have traditionally been considered challenging due to their complexity and computational demands. Vinyals et al. (2015) proposed the Pointer Network, a sequence-to-sequence model to generate a permutation of the input sequence instead of a sequence from a fixed-size dictionary. This allows the model to select and order elements from the input sequence. In the original work of Vinyals et al. (2015), the traveling salesman problem (TSP) was studied. However, the model is trained with supervised learning and optimal solutions obtained from alternative methods such as the Held-Karp (Held and Karp, 1962) algorithm for TSP. The study introduced the potential for implementing a learning-based approach in addressing COPs. A critical challenge, however, arises from its dependency on supervised learning, which requires optimal solutions for model training, but it is not possible to get optimal solutions for complex instances in most cases.

To address this issue, Bello et al. (2017) introduced a reinforcement learning (RL) framework as an alternative to supervised learning to train models. Like Vinyals et al. (2015), they also employed the Pointer Network architecture and studied TSPs in their research. The RL framework trains the model to learn an effective policy via a trial-and-error process, interacting with the problem environment to gradually improve its solution-finding capabilities. Unlike supervised learning used in Vinyals et al. (2015)'s approach, it does not require an optimal solution for model training, making it a practical approach for solving COPs.

Kool et al. (2018) applied a transformer architecture (Vaswani et al., 2017) with a transformer encoder and a point network type of decoder to solve TSPs and vehicle routing problems (VRPs). The proposed model, leveraging the Transformer architecture, captures the complex inter-relationships among inputs more effectively than the model by Bello et al. (2017), which employs Long Short-Term Memory (LSTM) (Hochreiter and Schmidhuber, 1997). This advantage is attributed to the Transformer's superior ability to represent long-range dependencies (Vaswani et al., 2017). Nazari et al. (2018) proposed a modified encoder architecture by replacing the LSTM unit with 1D convolutional layers to have a model that is

invariant to the input sequence order, handling the dynamic state changes to solve extended the VRPs. Subsequent studies followed the RL framework with different architectures and training methods to solve combinatorial optimization COPs, mainly for TSPs and VRPs (Miki et al., 2018; Deudon et al., 2018; Ma et al., 2019; Kwon et al., 2020; Xu et al., 2021).

Beginning with well-known TSPs and VRPs, research efforts have extended to JSSP with a similar framework. Zhang et al. (2020) proposed a model that uses deep reinforcement learning to prioritize an operation from a set of possible operations. They used the Graph Neural Network (GNN) to represent operations' states in a disjunctive graph. One advantage of using GNN to represent states is that the proposed model is agnostic to the size of the problem, i.e., the model will not be dependent on the number of jobs and machines of the problem instances. However, a drawback of their model lies in the reward function's reliance on an estimated makespan instead of the actual makespan, potentially degrading the model's performance.

Numerous studies Park et al. (2021a,b); Chen et al. (2022); Yuan et al. (2023) have adopted graph neural networks or variants to embed operations similarly to Zhang et al. (2020) with different reward functions, training algorithms, masking technique, and model structures. A motivation for using GNN is to represent the inter-relationships of operations in a disjunctive graph effectively. In a disjunctive graph, each operation is characterized by two main attributes: its relationship within a specific job group (via conjunctive edges) and its use of shared machines (via disjunctive edges). Potentially, keeping these attributes separate would help accurately represent the unique characteristics of each operation. However, a disjunctive graph is connected by both conjunctive and disjunctive edges, which results in a mixture of these important details.

Apart from using a graph neural network, Tassel et al. (2021) proposed an RL framework with seven designed scalar variables to capture the current state of individual jobs. However, their framework is subject to the problem size and requires retraining or adjustments to the model to solve new problems of different sizes.

Liu et al. (2020) introduced another RL framework based on a convolutional neural network architecture for feature extraction. One notable drawback of the proposed model is employing too simple action space, selecting the next operation by three different dispatching

rules such as first-in-first-out (FIFO), shortest processing time first (SPT), and longest processing time first (LPT). These simplistic action spaces could restrict candidates for the operations that can be scheduled and potentially degrade the quality of the solutions.

3 Problem Definition

A JSSP contains a set of J jobs, for $j=1,2,\ldots,J$, which are to be processed in a shop that consists of M machines for $m=1,2,\ldots,M$. Each job is comprised of M operations, O_{jm} for for $j=1,2,\ldots,J$ and $m=1,2,\ldots,M$, where each operation O_{jm} can be processed on specific machine m. Additionally, each operation O_{jm} has a predefined order t in the sequence of operations. That is, O_{jm}^t can be processed if and only if all the prior operations, O_{jm}^t , where t' < t, have been completed. One machine processes exactly one operation at a time without interruption. The time to complete an operation, O_{jm} , is called the processing time, denoted as p_{jm} . Completion of all the element operations completes a job. A valid sequence of job assignments to machines generates a feasible schedule. The objective is to learn a schedule or a scheduling policy that optimizes a function of feasible schedules, e.g., the minimization of makespan or the maximization of machine utilization.

4 Attention-based Reinforcement Learning for JSSP

We propose a transformer-based reinforcement learning scheduler (ARLS) with enhancements on top of the original transformer architecture (Vaswani et al., 2017). ARLS specifically aims to capture the characteristics of operations better, focusing on job groups and machine-sharing aspects using two independent transformer encoders.

The input vector of each operation is encoded by linear projection, which is then transformed into embedding by the encoder using a self-attention mechanism. Two independent encoders produce two different operation embeddings from the same initial encoding. The decoder applies encoder-decoder attention using embeddings from both encoders and the decoder input. More details about this will be provided in subsequent sections.

4.1 Input

The input vectors \mathbf{o}_n , for n=1,2,...,JM+1, are concatenated from four vectors: 1) job index, 2) operation order in the job sequence, 3) machine index of the operation, and 4) processing time of the operation. The operation index n=JM+1 accounts for the cases when no operation is assigned. i.e., the machine is left idle.

The operations are initially encoded via the linear projection of the input as shown in equation 1.

$$\boldsymbol{h}^{(0)} = \mathbf{W}^{(0)} \boldsymbol{o}_n + \boldsymbol{b}^{(0)} \tag{1}$$

where o_n , for n = 1, 2, ..., JM + 1, are the input vectors, $\mathbf{W}^{(0)}$ is the weight matrix, and $\boldsymbol{b}^{(0)}$ is the bias vector.

4.2 Encoder

We have modified the original transformer encoder to effectively represent the characteristics of operations. In contrast to the traditional transformer encoder, ARLS has two separate encoders that both take the same initial input encoding, denoted as $\boldsymbol{h}^{(0)}$ as input. The input encodings are transformed from the initial encoding $\boldsymbol{h}^{(0)}$ to the embedding $\boldsymbol{h}^{(L)}$ through multiple, e.g., L, encoder layers.

The original transformer employs simple masked attention in its encoder layers to prevent the model from attending to padding, which is used to equalize the lengths of input tokens in natural language processing (NLP). In contrast to NLP, COPs have inputs of identical length, eliminating the need for padding. Instead, ARLS employs two distinct attention mechanisms in each encoder layer. These mechanisms are designed to focus attention specifically on operations within the same job group and operations sharing machines, respectively.

Consider the scaled dot-product attention function

Attention
$$(Q, K, V) = \operatorname{softmax}\left(\frac{QK^{\mathsf{T}}}{\sqrt{d_K}}\right)V$$
 (2)

where Q, K, V are each head's query, key, and value matrices, respectively, and d_K is the dimension for each head's query and key matrices. Let each element $c_{i,j} = \mathbf{q}_i \mathbf{k}_j^T / \sqrt{d_K}$ where \mathbf{q}, \mathbf{k} are *i*th and *j*th columns of the query and key matrices, Q and K, respectively.

We apply two different masking schemes to $c_{i,j}$, one for the jobs, denoted as $c_{i,j}^{(\mathcal{J})}$, and another for the machines, $c_{i,j}^{(\mathcal{M})}$, and integrate the two encoder results at the end of the encoder. In particular, the values of the elements $c_{i,j}^{(\mathcal{J})} = -\infty$ are masked if operations i and j are not in the same job sequence, and similarly, $c_{i,j}^{(\mathcal{M})} = -\infty$ if operations i and j are not processed by the same machine.

The embedding of operations from the last layer of the encoder $\boldsymbol{h}^{(L)}$ is computed as a convex combination of the two embeddings $\boldsymbol{h}_{\mathcal{J}}^{(L)}$ and $\boldsymbol{h}_{\mathcal{M}}^{(L)}$ as

$$\boldsymbol{h}^{(L)} = \lambda \boldsymbol{h}_{\mathcal{J}}^{(L)} + (1 - \lambda) \boldsymbol{h}_{\mathcal{M}}^{(L)} \tag{3}$$

where $0 \le \lambda \le 1$ controls the importance of each embedding.

4.3 Decoder

The decoder has L^* identical attention layers similar to the original transformer model (Vaswani et al., 2017). However, masking is performed respective to the operations that were already assigned. Let $\mathcal{O}_t^- \subset \mathcal{O}$ be the set of operations that were already assigned by time t. The complement is $\mathcal{O}_t^+ = \mathcal{O} \setminus \mathcal{O}_t^-$. Also, h_{t-1} denotes the encoder embedding of the operation assigned at the previous time step t-1.

For decoder attention, which is also a masked, multi-head attention with scaled dotproduct, we use the encoder embedding of the last assigned operation h_{t-1} for query vector, q, and the encoder embeddings from the previous time step $h^{(L)}$ for keys K and values V

An action selection module generates a probability distribution over possible operations on the top of the decoder. Attention scores are calculated using the decoder output at time t, denoted as $\mathbf{q}_{(t)}$ for query, and the previous encoder embeddings $\mathbf{h}^{(L)}$ for keys K to generate probabilities p_o over the possible operations \mathcal{O}^+ . Nonlinear activation function tanh is applied with the clipping technique (Li, 2023) before the softmax function is applied.

$$p_{o} = \begin{cases} \text{softmax} \left(C \tanh \left(\mathbf{q}_{(t)} \mathbf{k}_{o}^{\mathsf{T}} / \sqrt{d_{K}} \right) \right), & \text{if operation } j \notin \mathcal{O}^{-} \\ 0 & \text{otherwise} \end{cases}$$

$$(4)$$

where C is the clipping constant. The probability p_o is used to choose operation at time step t.

4.4 Training

We modify the Monte-Carlo policy gradient method (Sutton and Barto, 2018; Bahdanau et al., 2016) for training. The performance of learned policy was estimated by a Monte-Carlo method using observed makespans. The average of the makespans respective to the same problem is used as the baseline. Observed makespans minus the baseline generate the advantages used for gradient updates

$$\nabla_{\theta} J(\pi_{\theta}) = \mathop{\mathbf{E}}_{\tau \sim \pi_{\theta}} \left[\sum_{t=0}^{T} \nabla_{\theta} \ln \pi_{\theta}(a_{t}|s_{t}) \left(R(\tau) - b \right) \right]$$
 (5)

where τ is a trajectory of an episode, $R(\tau)$ is the Monte-Carlo episodic reward, i.e., makespan of a trajectory, and b is a baseline to reduce variance.

Preferred by researchers, as cited in works by (Mnih et al., 2013; Schulman et al., 2015; Haarnoja et al., 2018; Reda et al., 2020), the baseline b is typically derived from the value network. Unlike the typical RL model, our proposed model does not have a value network but takes a different strategy compared to the typical Monte-Carlo Policy Gradient, which generates multiple trajectories. Our multi-trajectory strategy offers several advantages compared to employing a value network. More problem instances are expected to increase the scheduling performance robustness. Furthermore, for each problem instance, the learner is expected to improve with more diverse scheduling solutions.

Let \mathcal{T} denote the set of all trajectories, that is, all the feasible solutions for a JSSP instance. Let each $\tau_n \in \mathcal{T}$ be a sampled trajectory, and $\mathcal{T}_N = \{\tau_1, \dots, \tau_N\}$ be the set of N sampled trajectories for a JSSP instance, with which we make minibatch updates for the weights throughout the training as follows.

$$\nabla_{\theta} J(\pi_{\theta}) = \frac{1}{N} \sum_{n=1}^{N} \left(\underbrace{\mathbf{E}}_{\tau \sim \pi_{\theta}} \left[\sum_{t=0}^{T} \nabla_{\theta} \ln \pi_{\theta}(a_{t}|s_{t}) \left(R(\tau_{n}) - b \right) \right] \right)$$
 (6)

where $R(\tau_n)$ is the Monte-Carlo episodic reward of trajectory n, and $b = \frac{1}{N} \sum_{n=1}^{N} R(\tau_n)$, which is the average of the N episodic rewards obtained from the same problem instance in parallel.

5 Experimental Results

The training and testing approach for ARLS prioritizes rapid model learning in simplified settings. A key objective is a learner design that effectively scales to greater problem instance sizes and maintains high performance. ARLS is trained with synthetic data with 6 jobs and 6 machines. In total 36 operations, with processing times randomly selected uniformly in the range between 1 and 15, similar to the prior study Zhang et al. (2020). The Adam optimization (Kingma and Ba, 2014) was employed for weight updates. ARLS uses a relatively low complexity transformer architecture with only three encoder layers and a single decoder layer, the model dimension is 256, the number of heads is 16, and the fully connected feed-forward neural networks dimension is 512. Further design studies might improve performance.

Training generated 100,000 replicate synthetic 6 jobs \times 6 machines problem instances. A mini-batch update (Yang et al., 2019) is applied. The objective is to minimize the schedule's makespan. To evaluate ARLS performance, the average optimality gap is used

$$opt_{gap} = \frac{obj - obj^*}{obj^*}$$

where obj is the makespan obtained from the ARLS, and obj^* is either the optimal or best-known solution. For synthetic instances, the optimal solutions are derived using constraint programming with Cplex (IBM Decision Optimization, 2024).

The generalized performance of ARLS is tested with varying sizes of synthetic and benchmark instances, including problem instance sizes greater than seen in training. To evaluate, we use three synthetic datasets with sizes configured as follows: the first dataset has 6 jobs and 6 machines, the second dataset consists of 10 jobs and 10 machines, and the third dataset comprises 15 jobs and 15 machines. Additionally, seven well-known benchmark sets from Shylo (2010) are tested for comparison.

Table 1 shows the test results on synthetic data. The average optimality gap is obtained from 1,000 instances for each problem size. To the best of our knowledge, the comparable test on synthetic instances is the study by Zhang et al. (2020)(Z20). Our model is trained on only 6 jobs and 6 machine settings. In contrast, Zhang et al., (Zhang et al., 2020) trained their model separately with samples from the three problem sizes. On average, ARLS outperforms

their results by a substantial margin of 12.5%.

Table 1: Performance of our ARLS model compared with Z20 (Zhang et al., 2020) on three different synthetic datasets. Performance is evaluated by the optimality gap in percentage

Jobs	Machines	Instances	ARLS (Ours)	Z20
6	6	1000	4.8	17.7
10	10	1000	10.9	22.3
15	15	1000	13.5	26.7

ARLS was tested with seven benchmark datasets of varying sizes in the number of jobs (ranging from 6 to 100) and machines (ranging from 5 to 20). Table 2 shows ARLS's performance compared to work by Zhang et al. (2020) denoted as Z20, Park et al. (2021a) as P21a, Park et al. (2021b) as P21b, Chen et al. (2022) as C22, and Yuan et al. (2023) and Y23, and popularly adopted heuristic rules, such as first-in-first-out (FIFO), shortest processing time (SPT), and most work remaining (MWKR). Here, instead of the optimality gap, the best-known gap, which is the relative difference to the best-known makespan, is used as optimal makespans are unknown for some of the problems. Problems with multiple instances show average results. Our ARLS model showed the best performance on all but 4 problem sizes out of 26 problem classes despite being trained in the simplest setting of 6 jobs and 6 machines.

Table 2: Performance of our ARLS model compared with heuristic rules and other studies on benchmark datasets. Performance is evaluated by the best known gap in percentage (with averages for multiple instances). Results by Zhang et al. (2020) denoted as Z20, Park et al. (2021a) as P21a, Park et al. (2021b) as P21b, Chen et al. (2022) as C22, and Yuan et al. (2023) and Y23, and popularly adopted heuristic rules, such as first-in-first-out (FIFO), shortest processing time (SPT), and most work remaining (MWKR).

ABZ	Dataset	Jobs	Machines	Instances	FIFO	SPT	MWKR	Z20	P21a	P21b	C22	Y23	Ours
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DMU 20 20 10 26.4 64.6 32.4 37.7 23.6 17.3 20.7 20.7 20.7 20.7 20.7 20.7 20.7 20.7		100	20	10	8.8	14.4	12.8	13.6	6.7	9.2	18.0	8.9	9.3
DMU	DMU	20	15	10	30.5	64.1	37.2	39.0	-	-	-	26.6	18.9
DMU 30 20 10 32.2 65.9 36.6 39.5 29.2 22.6 40 15 10 31.2 55.9 35.1 35.4 24.5 20.2 40 20 10 33.2 63.0 39.7 39.4 30.1 24.8 50 15 10 31.0 50.4 34.7 36.2 24.9 18.8		20	20	10	26.4	64.6	32.4	37.7	-	-	-	23.6	17.3
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		40	20	10	33.2	63.0	39.7	39.4	-	-	_	30.1	24.8
50 20 10 35.3 62.2 41.4 38.4 29.5 21.8		50	15	10	31.0	50.4	34.7	36.2	-	-	_	24.9	18.8
		50	20	10	35.3	62.2	41.4	38.4	-	-	-	29.5	21.8



Figure 1: Generalized Performance of our ARLS model compared with heuristic rules and other studies on benchmark datasets, ABZ, FT, YN, SWVM, and ORB. Results by Zhang et al. (2020) denoted as Z20, Park et al. (2021a) as P21a, Park et al. (2021b) as P21b and Yuan et al. (2023) and Y23, and popularly adopted heuristic rules, such as first-in-first-out (FIFO), shortest processing time (SPT), and most work remaining (MWKR).

On average, ARLS outperformed other algorithms in all cases, as shown in Figures 1 and 2. ARLS was exceeded only in a few problem classes in TA. Even then, the P21a algorithm was trained on problem instances about 67% greater than the training size for ARLS.

Although ARLS was exceeded by P21a for three TA classes: TA(30, 15), TA(50, 20), and TA(100, 20) when ARLS trained in the 6 jobs and 6 machines scenario, ARLS outperformed P21a when trained on datasets of the equivalent size of P21a, resulting smaller optimality gaps, with 16.8% vs. 19.1% for TA(30,15), 9.96% vs. 13..5% for TA(50,20), and 4.4% vs. 6.7% for TA(100,20), respectively.

6 Conclusions

We developed an attention-based reinforcement learner for job shop scheduling problems with a modified transformer architecture. A key point of our model is that it enables the learner to scale with problem instance size. The learner was trained with synthetic problem instances of relatively small size in the number of jobs and machines and scaled to new problems of

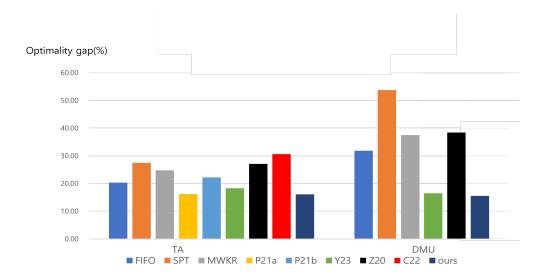


Figure 2: Generalized Performance of our ARLS model compared with heuristic rules and other studies on benchmark datasets, TA and DMU. Results by Zhang et al. (2020) denoted as Z20, Chen et al. (2022) as C22, and Yuan et al. (2023) and Y23, and popularly adopted heuristic rules, such as first-in-first-out (FIFO), shortest processing time (SPT), and most work remaining (MWKR).

various larger sizes with both synthetic and benchmark datasets. We have obtained generally outperforming results compared to recent studies and widely adopted heuristic rules. The model architecture is new, but the transformer is low in complexity (few layers), and further work might improve results with larger transformer architectures.

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