# Efficient Neural Neighborhood Search for Pickup and Delivery Problems

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#### **Abstract**

In this paper, an efficient Neural Neighborhood Search (N2S) method is proposed to solve Pickup and Deliver Problems (PDPs). Specifically, a robust synthetic attention is designed that allows vanilla self-attention to synthesize various types of features about routing solutions. In addition, two decoders are leveraged that automatically learn to perform removal and reinsertion of a pick-deliver node pair to address precedence constraint. Furthermore, a diversity enhancement scheme is utilized to further improve the performance of N2S. Experimental studies on two standard PDP variants show that it can produce state-of-the-art results among existing neural methods. Finally, it even outperforms the well-known LKH3 solver on the more constrained PDP variant.

**Keywords:** Neural Neighborhood Search, Pickup and Deliver Problems, diversity enhancement.

## 1 Introduction

Combinatorial optimization problems with NP-hardness have the characteristics of discrete search space and computational difficulty in finding the optimal solution. As a fundamental combinatorial optimization problem in logistics, the vehicle routing problem (VRP)<sup>[1]</sup> is concerned with the optimal cost of delivering items by vehicle from a warehouse to a geographically dispersed set of customers. It has been studied extensively over the decades and finds a wide range of real-world applications, such as garbage collection<sup>[2]</sup>, calling a car<sup>[3]</sup> and express delivery<sup>[4]</sup>.

Efficient neighborhood search is a key component of a powerful heuristic for the Pickup and Delivery Problem (PDPs)<sup>[5]</sup>. It involves an iterative search process that converts a solution to another candidate in its current neighborhood, hopefully in an efficient manner. The design of the neighborhood and search rules often determines the efficiency or even the success of the solver. However, they are usually problem-specific and manually designed with extensive trial and error, which requires redesign when constraints or objectives change. These limitations may hamper application in rapidly evolving industries.

On the other hand, recent neural approaches for VRP have emerged as promising alternatives to traditional heuristics (e.g., paper<sup>[6]</sup>). They are often faster and, more importantly, can automatically design heuristics for new variants where no handcrafted rules are available<sup>[7]</sup>. However, the current popular neural methods mainly focus on the Traveling Salesman Problem (TSP) or the Capable Vehicle Routing Problem (CVRP), and there are less researches on effective solution methods for the PDP problem. PDP is ubiquitous in logistics, robotics, and food delivery services<sup>[5]</sup>, which optimizes the routing of pickup and delivery requests, and is characterized by precedence constraints (pickup before delivery). Although the first attempt in<sup>[6]</sup> learned a construction method

to build a PDP solution (route) in a few seconds, it still a considerable gap comparable to traditional heuristics in solution quality.

To reduce the gap, this paper proposed an efficient Neural Neighborhood Search (N2S) method based on a novel Transformer-style policy network with an encoder-decoder structure. The most similar existing policy network to N2S is DACT in<sup>[6]</sup>. As an improvement method, DACT learns to encode the current solution and transform it into another solution using a 2-opt, insertion or exchange decoder. Among them, the 2-opt decoder considering inverting a segment solution performs best for TSP and CVRP. However, since segment inversion can easily violate precedence constraints, it is not suitable for PDP. While insertion decoders perform well on small PDPs, which consider the removal and reinsertion of individual nodes, performance degrades significantly on large-scale or highly constrained PDPs. In contrast, N2S more efficiently addresses the precedence constraint by allowing a pair of pickup-delivery nodes to simultaneously operate in neighborhood search through two removal and reinsertion decoders, as shown in Figure 1.

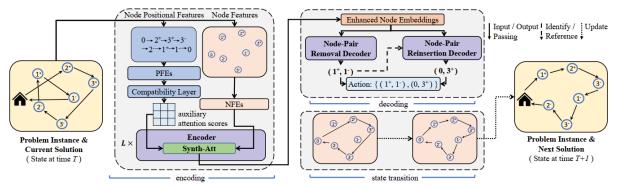


Figure 1: An example of a PDTSP-7 instance to illustrate our N2S approach.

Another challenge lies in the design of the encoder. Paper<sup>[6]</sup> nicely reveals that the vanilla Transformer encoder<sup>[8]</sup> fails to correctly encode routing solutions because the embedding of node features (i.e., coordinates) and node position features (i.e., node positions) involves two different aspects of the routing solution, not directly compatible during coding. Therefore, they propose Dual Aspect Co-Attention (DAC-Att) to learn dual representations for each feature aspect. In this paper, a simple yet powerful Synthesis Attention (Synthetic-Att) is proposed, where attention scores from different types of node feature embeddings can be combined to obtain a synthetic representation. Not only does it have the potential to encode more aspects than DAC-Att, but it also reduces computational cost while maintaining competitive performance.

Moreover, this paper design a diversity enhancement scheme to further improve the performance of the system. The proposed N2S method is trained by reinforcement learning<sup>[6]</sup>, and it is evaluated on two typical problems in the PDP family, the Pickup and Delivery Traveling Salesman Problem (PDTSP) and its variant with last-in-first-out constraint (PDTSP-LIFO) to validate N2S's design. Experimental results show that N2S outperforms the state-of-the-art in solving synthetic PDP instances, becoming the first neural method to surpass the well-known LKH3 solver<sup>[9]</sup>.

## 2 Related works

#### 2.1 Neural Methods for VRPs

In this paper, current neural methods are divided into construction methods and improvement methods. Construction methods, e.g., papers<sup>[10-12]</sup>, learn distributions over selection nodes to autoregressively build solutions from scratch. Although fast, they lack the ability to search for (near) optimal solutions, even when equipped with sampling (e.g., [12], local search (e.g., paper [13]) or Monte Carlo Luo tree search (eg, paper [14]). Among them, POMO [7] explores different rollouts and data augmentations and is considered the best construction method. The difference is that the improvement method usually depends on the neighborhood search process, such as node exchange [15], destruction and repair [16], and 2-opt. Paper [6] extended the transformer-style model of work [17] to Dual Aspect Collaborative Transformer (DACT) and achieved state-of-the-art performance, which is also competitive with hybrid neural approaches, e.g. with a combined approach of differential evolution [18] and dynamic programming [19]. Although the above methods have been successful on CVRP or TSP, they have not been verified on precedence constrained PDP. Although literature [20] made the first attempt to learn a constructed solver for PDP by introducing heterogeneous attention [12], the resulting solution quality is still far from optimal.

#### 2.2 Neighbourhood Search for PDPs

Various heuristics based on neighborhood search have been proposed for PDP. For PDTSP, literature<sup>[21]</sup> studied k-exchange neighborhoods. Later, paper<sup>[22]</sup> proposed the ruin-repair neighborhood, which was further extended in<sup>[23]</sup> with various perturbation methods. In addition to PDTSP, other PDP variants have been studied, usually by designing new problem-specific neighborhoods<sup>[5]</sup>, for example, literature<sup>[24]</sup> proposed five neighborhoods to address the PDTSP. Among them, the PDTSP-LIFO algorithm has attracted much attention because of its limited search space. To address this issue, paper<sup>[25]</sup> introduced additional communities such as double bridges and shake. In work<sup>[26]</sup>, a tree-structured neighborhood is further proposed. Different from the PDP solvers mentioned above, the well-known LKH3 solver<sup>[9]</sup> incorporates a neighborhood restriction strategy to achieve more efficient local search and can solve various VRPs with excellent performance. Recently, LKH3 was extended to handle several PDP variants, including PDTSP and PDTSP-LIFO, and provided comparable performance to paper<sup>[23]</sup> and paper<sup>[26]</sup> on PDTSP and PDTSP-LIFO, respectively. Also considering the nature of open source, LKH3 is use as the baseline heuristic in this paper.

#### 3 Method

#### 3.1 Encoder and Synth-Att

Node feature and node location feature are used as inputs to learn to represent the embedding of the current solution. Like DACT, the two features are first mapped into two embedding sets, namely node feature embeddings(NFEs) and positional feature embeddings (PFEs). NFEs is treated as the primary embeddings and PFEs as the auxiliary embed set. The encoder is the same as the Transformer encoder except that the multi-head attention part is replaced with Synth-Att.

#### 3.2 Decoder

**Node-Pair Removal Decoder.** Given an enhanced embedding (all global representations of the embeddings are aggregated into each individual), the removal decoder outputs a classified distribution of n removal actions. Firstly, a fraction i is calculated for each node  $x_i$  to represent the closeness between node  $x_i$  and its neighbors. Then select the node pair according to the score to remove operation.

**Node-Pair Reinsertion Decoder.** Given a pickup-delivery node pair for removal, the reinserting decoder outputs the joint distribution to reinsert the two nodes into the solution. First, two scores are defined for node  $x_a$ , representing the degree of preference of accepting a node  $x_b$  as its new predecessor and successor nodes, respectively. Based on the score, MLP is used by the decoder to predict the distribution of inserting node  $i^+$  after node j and node  $i^-$  after node k. Finally, sampling is performed according to the result distribution to obtain a node pair (j, k) as an insertion action, which means that the node pairs  $(i^-, i^+)$  is inserted into the solution.

## 3.3 Diversity Enhancement

The basic principle is that an instance can be transformed into a different instance for searching while preserving the same optimal solution, for example, rotating the positions of all nodes by  $\pi$  /2 radians.

## 4 Implementation details

## 4.1 Comparing with released source codes

As shown in Figure 2, N2S is a learning based improvement framework for solving the pickup and delivery problems based on DAC-Att<sup>[6]</sup>. Specifically, In the left of Figure 2, the DAC-Att, where each embedding set computes the attention score independently and shares another aspect to learn the dual-aspect representation. As shown in the right of Figure 2, N2S proposes a simple and general mechanism combined with multi-layer perception (MLP). In addition to the original self-attention score (orange box), multiple auxiliary attention scores learned from other feature embeddings (blue box) are utilized and fed into a in an element-wise MLP, thus enabling it to synthesize heterogeneous attention relations into a synthetic attention relation.

Therefore, my implementation of N2S of this paper is based on the code of DAC-Att<sup>[6]</sup>. Specifically, I add a MLP into DAC-Att and enable it to synthesize heterogeneous attention relations into a synthetic attention relation.

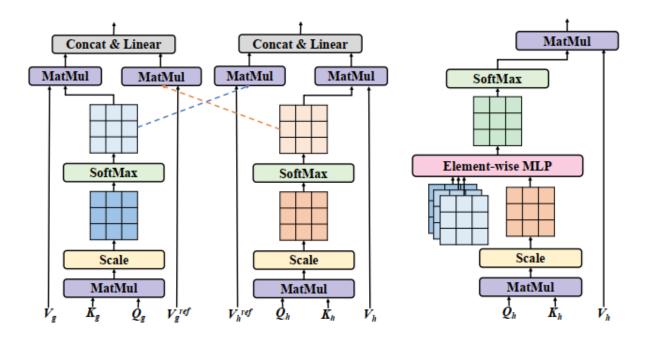


Figure 2: The left is attention module for VRPs in DAC-Att<sup>[6]</sup>; The right is the attention module of this paper

## 4.2 Experimental environment setup

I use the platform named Pycharm 2021.2.2 for the implementation of the algorithm. To study the performance of N2S I implement, it is compared with original result in the paper of N2S. Then, two experiments can demonstrate the superiority of the implementation of N2S. According to the experiments, the effectiveness of my implementation can be verified.

In this paper, N2S is evaluated on PDTSP and PDTSP-LIFO with three sizes |V| = 21; 51; 101 following the conventions in papers<sup>[6-7]</sup>. Please note that other parameters in the benchmark suites and the algorithm are set the same as suggested in original references. Meanwhile, the distance of the solution is adopted as the performance indicator.

#### 4.3 Main contributions

- An efficient N2S method is proposed for PDP that can automatically learn the removal and reinsertion of pickup-delivery node pairs.
- The Synth-Att is proposed, which allows the vanilla self-attention mechanism to synthesizing node relations from various feature embeddings, and achieves better expressive power with less computational cost compared to DAC-Att.
- A diversity enhancement scheme is explored, which further enables N2S be the first neural method with little domain knowledge to outperform the LKH3 solver on synthetic PDP instances (when there is no significant distributional shift compared to r.t training instances).

# 5 Results and analysis

The experimental results obtained by N2S implemented by me and the results from original paper are presented in Table I, in which the best result compared with the others is highlighted in bold. As observed from Table I, the results of the original paper and the implemented N2S get the best results on the PDTSP and PDTSP-

LIFO of three dimensions, respectively. Therefore, we can reasonably conclude that My implementation of N2S is successful.

Table 1: Comparison results for solving PDTSP and PDTSP-LIFO

Problem	n	Result of original paper	Implemented N2S
PDTSP	21	4.563	4.618
	51	6.865	7.145
	101	9.475	9.472
PDTSP-LIFO	21	5.539	5.538
	51	10.135	10.356
	101	16.806	16.792

## 6 Conclusion and future work

In this paper, an efficient N2S method for PDP is propose. It leverages a novel Synth-Att to synthesize various types of node relations for solving features, and exploits node pair removal and reinsertion decoders to address precedence constraint. Extensive experiments on PDTSP and PDTSP-LIFO validate the design, where N2S achieves state-of-the-art performance among existing neural methods. Further equipped with a diversity enhancement scheme, it even becomes the first neural method to outperform LKH3 on synthetic PDP instances.

In the future, we will 1) deploy N2S in the hierarchical framework of as a low-level agent for dynamic PDP, and 2) combine N2S with a similar divide-and-conquer strategy for larger instances, 3) enhances out-of-distribution generalization to outperform LKH3 on instances of arbitrary distribution.

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