A GRAPH NEURAL NETWORK ASSISTED MONTE CARLO TREE SEARCH APPROACH TO TRAVELING SALESMAN PROBLEM

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ABSTRACT

We present a graph neural network assisted Monte Carlo Tree Search approach for the classical traveling salesman problem (TSP). We adopt a greedy algorithm framework to construct the optimal solution to TSP by adding the nodes successively. A graph neural network (GNN) is trained to capture the local and global graph structure and give the prior probability of selecting each vertex every step. The prior probability provides a heuristics for MCTS, and the MCTS output is an improved probability for selecting the successive vertex, as it is the feedback information by fusing the prior with the scouting procedure. Experimental results on TSP up to 100 nodes demonstrate that the proposed method obtains shorter tours than other learning-based methods.

1 INTRODUCTION

Traveling Salesman Problem (TSP) is a classical combinatorial optimization problem and has many practical applications in real life, such as planning, manufacturing and genetics (Applegate et al., 2006b). The goal of TSP is to find the shortest route that visits each city once and ends in the origin city, which is well-known as an NP-hard problem (Papadimitriou, 1977). In the literature, approximation algorithms were proposed to solve TSP (Lawler et al., 1986; Goodrich & Tamassia, 2015). In particular, many heuristic search algorithms were made to find a satisfactory solution within a reasonable time. However, the performance of heuristic algorithms depends on handcrafted heuristics to guide the search procedure to find competitive tours efficiently, and the design of heuristics usually requires substantial expertise of the problem (Johnson & McGeoch, 1997; Dorigo & Gambardella, 1997).

Recent advances in deep learning provide a powerful way of learning effective representations from data, leading to breakthroughs in many fields such as speech recognition (Lecun et al., 2015). Efforts of the deep learning approach to tackling TSP has been made under the supervised learning and reinforcement learning frameworks. Vinyals *et al.* (Vinyals et al., 2015) introduced a pointer network based on the Recurrent Neural Network (RNN) to model the stochastic policy that assigns high probabilities to short tours given an input set of coordinates of vertices. Dai *et al.* (Dai et al., 2017) tackled the difficulty of designing heuristics by Deep Q-Network (DQN) based on strcuture2vec (Dai et al., 2016), and a TSP solution was constructed incrementally by the learned greedy policy. Most recently, Kool *et al.* (Kool et al., 2019) used Transformer-Pointer Network (Vaswani et al., 2017) to learn heuristics efficiently and got close to the optimal TSP solution for up to 100 vertices. These efforts made it possible to solve TSP by an end-to-end heuristic algorithm without special expert skills and complicated feature design.

In this paper, we present a new approach to solving TSP. Our approach combines the deep neural network with the Monte Carlo Tree Search (MCTS), so that takes advantage of the powerful feature representation and scouting exploration. The central component is a static edge graph neural network (SE-GNN) that is trained to capture the local and global graph structure and predict the prior probability, for each vertex, of whether this vertex is part of the tour sequence. Compared with basic GNN (Hamilton et al., 2017), we integrate edge information into each update-layer in order to extract features efficiently from the problem whose solution relies on the edge weight.

Similar to above-learned heuristic approaches that greedily select the vertex according to the biggest prior probability, the algorithm may fall into the local optimal because the algorithm has only one shot to compute the optimal tour and never goes back and reverses the decision. To overcome this problem, we introduce a graph neural network assisted Monte Carlo Tree Search (GNN-MCTS) to make the decision more reliable by a large number of scouting simulations. The trained SE-GNN is used to guide the MCTS procedure that effectively reduces the complexity of the search space. Experimental results on TSP up to 100 vertices demonstrate that the proposed method obtains shorter tours than other learning-based methods. The specific contributions of this paper are as follows,

- We introduce a SE-GNN that has access to the full graph context and generates the prior probability of each vertex being in the optimal tour.

- We introduce a GNN-MCTS, which obtains an improved probability by scouting simulations, to avoid being stuck into local optimum. Furthermore, we design a value function based on the prior probability to evaluate nodes during the MCTS procedure. The experimental results show that GNN-MCTS and value function play an important role in solving TSP efficiently.

The remainder of the paper is organized as follows: After reviewing related work in Section 2, we briefly give a preliminary introduction to TSP in Section 3. Our approach is formulated in Section 4. Experimental results are given in Section 5, followed by the conclusion in Section 6.

2 Related Work

The TSP is a well studied combinatorial optimization problem, and many learning-based algorithms have been proposed. In 1985, Hopfield *et al.* proposed a neural network to solve the TSP (Hopfield & Tank, 1985). This is the first time that researchers attempted to use neural networks to solve combinatorial optimization problems. Since the impressive results produced by this approach, many researchers have made efforts on improving the performance (Bout & Miller, 1988; Brandt et al., 1988). Many shallow network architectures were also proposed to solve the combinatorial optimization problem (Favata & Walker, 1991; Fort, 1988; Angniol et al., 1988; Kohonen, 1982).

Recent years, deep neural networks have been adopted to solve the TSP. Vinyals *et al.* (Vinyals et al., 2015) introduce a neural architecture called Pointer Network (Ptr-Net), which is based on a recurrent neural network (RNN) and trained in a supervised manner. They introduces an attention mechanism to output a permutation of the given input. Two flaws exist in the method. First, Ptr-Net can only be applied to solve problems of small scale. If the number of vertices reaches 40, the performance of the algorithm suffers greatly. Second, the beam search procedure might generate invalid routes. Bello *et al.* (Bello et al., 2016) introduce an Actor-Critic algorithm to train the Ptr-Net without supervised solutions. They solve the problem of invalid paths by adding a glimpse at the embeddings, masking vertices already visited. They get close to the results by Ptr-Net on small instances ($n = 20$) and improve the performance for $n = 50$ and additionally include results for $n = 100$. Instead of using RNN for designing encoder and decoder, Deudon *et al.* (Deudon et al., 2018) present a model for TSP using a Transformer architecture (Vaswani et al., 2017) and further enhance the solution approach with the well-known 2-opt heuristics. Kool *et al.* (Kool et al., 2019) introduce a reinforcement learning method, which uses the policy gradient with a rollout baseline, to solve the TSP. They also integrate Transformer architecture into their approach, where the encoder computes the embedding of vertices, and the decoder outputs the probability of selecting a vertex at every step. They improve the state-of-art performance among 20, 50, and 100 vertices.

Nowak *et al.* propose a supervised manner to directly output a tour as an adjacency matrix based on a graph neural network (GNN) and then convert the matrix into a feasible solution by beam search (Nowak et al., 2017). The author only reports an optimality gap of 2.7% for $n = 20$. Dai *et al.* (Dai et al., 2017) propose an approach which trains a deep Q-network (DQN) to construct solutions for combinatorial optimization problems incrementally.

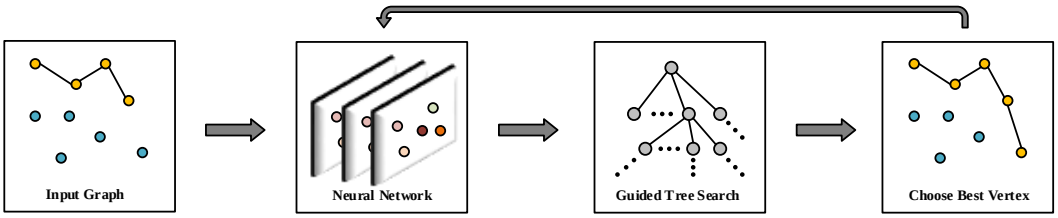

Figure 1: Approach overview. First, the graph is fed into the graph neural network, which captures global and local graph structure and generates a prior probability that indicates how likely each vertex being in the tour sequence. Then, with the help of the graph neural network, a developed MCTS outputs an improved probability by scouting simulations. Lastly, we visit the best vertex among unvisited vertices according to the improved probability. The above process will loop until all vertices are visited.

3 PRELIMINARIES

TRAVELING SALESMAN PROBLEM

Let $G(V, E, w)$ denotes a weighted graph, where V is the set of vertices, E the set of edges and $w : E \to R^+$ the edge weight function, i.e., $w(u, v)$ is the weight of edge $(u, v) \in E$. We use $S = \{v_1, v_2, ..., v_i\}$ to represent an ordered tour sequence that starts with v_1 and ends with v_i, and $\bar{S} = V \setminus S$ the set of candidate vertices for addition, condition on S. The target of TSP is to find a tour sequence with the lowest cost, i.e., $c(G, S) = \sum_{i=1}^{|S|-1} w(S(i), S(i + 1)) + w(S(|S|), S(1))$ when $|S| = |V|$.

4 PROPOSED APPROACH

For a graph, our goal is to construct a tour solution by adding vertices successively. A natural approach is to train a deep neural network of some form to decide which vertex being added to the tour sequence at each step. That is, a neural network f would take the graph G and the partial tour sequence S as input, and the output $f(G|S)$ would be a prior probability that indices how likely each vertex to be selected. Intuitively, we can use the prior probability in a greedy way, i.e., selecting vertex with the biggest probability, to generate the tour sequence incrementally. However, deriving tours in this way might fall into the local optimum because the algorithm has only one shot to compute the optimal tour and never goes back and reverses the decision. To overcome this problem, we enhance the policy-decisions by MCTS assisted with the deep neural network.

We begin in Section 4.1 by introducing how to transform TSP into a Markov Decision Process (MDP). Then in Section 4.2, we propose a new GNN architecture for parameterizing $f(G|S)$. Finally, Section 4.3 describes GNN-MCTS for combinatorial optimization problems, especially the TSP. The overall approach is illustrated in Figure 1.

4.1 TRAVELING SALESMAN PROBLEM AS MARKOV DECISION PROCESS

We present TSP as a MDP as follows,

- ***States***: a state s is an ordered sequence of visited vertices on a graph G and the terminal state is that all vertices have been visited.
- ***Transition***: transition is deterministic in the TSP, and corresponds to adding one vertex $v \in \bar{S}$ to S.
- ***Actions***: an action a is selecting a vertex of G from the vertices candidate set $\bar{S}$.
- ***Rewards***: the reward function $r(s, a)$ at state s is defined as the change of cost after taking action a and transitioning to a new state s', i.e., $r(s, a) = -w(v_m, v_n)$, where v_m and v_n are the last vertex in partial tour sequence S and S' respectively.

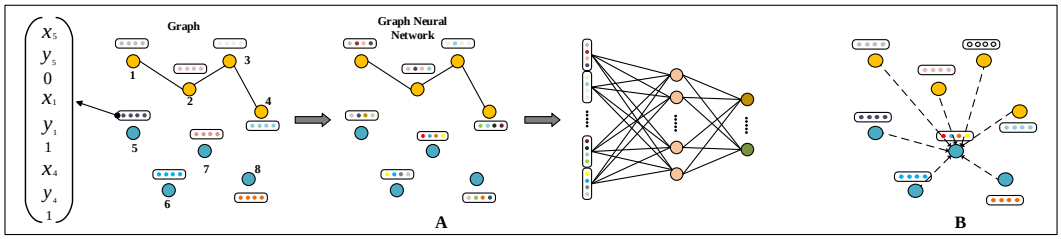

Figure 2: Neural network architecture. The architecture on the left (A) is used to compute the prior probability map that indicates how likely each vertex being in the tour sequence. Firstly, the "tagged" graph is fed into the SE-GNN to generate new feature expressions for each vertex. Then all new node feature is concentrated into a long vector that denotes the context of the "tagged" graph. Lastly, the vector is fed into a multilayer perceptron to output the prior probability. The picture on the right (B) depicts the mechanism of computing a new feature of the vertex in one update-layer.

- ***Policy***: based on the improved probability $\hat{P}$ of selecting the next vertex, a deterministic greedy policy $\pi(v|S) := \arg\max_{v' \in \bar{S}} \hat{P}(S, v')$ is used.

4.2 Deep neural network architecture

To compute a good policy, information about the global structure of the graph and the current constructed tour sequence $S = \{v_1, ..., v_i\}$ is required. We tag the nodes which have been visited as $x_v = 1$. Intuitively, $f(G|S)$ should summarize the state of such a "tagged" graph and generate the prior probability that indicates how likely each vertex is to belong to S. It is challenging to design a neural network $f(G|S)$ to capture local and global graph structure. In order to represent such a complicated context, we propose a new deep learning architecture based on graph neural networks (GNN) to parameterize $f(G|S)$.

Static edge graph neural networks

Similar to the basic GNN, we design the neural network $f(G|S; \Theta)$ to compute a l-dimensional feature H_v for each vertex of a "tagged" graph. We use H_v^t to denote the real-valued feature vector associated with v after the computation by the layer t. A GNN model consists of a stack of T neural network layers, where each layer aggregates local neighborhood information, i.e., features of neighbors around each node, and then passes this aggregated information on to the next layer. Specifically, the basic GNN model (Hamilton et al., 2017) can be implemented as follows. In each layer $t \in [0, T]$, a new feature is computed as:

$$H_v^{t+1} = \sigma(H_v^t W_1^t + \sum_{u \in \mathcal{N}(v)} H_u^t W_2^t) \tag{1}$$

where $\mathcal{N}(v)$ is the set of neighbors of vertex v, W_1^t and W_2^t are parameter matrices for the layer t, and σ denotes a component-wise non-linear function, e.g., a sigmoid or a ReLU. For $t = 0$, H_v^0 denotes the feature initialization at the input layer.

The above GNN architecture has been demonstrated to perform well on combinatorial optimizations problems such as Maximal Independent Set (MIS), Minimum Vector Cover (MVC), etc. (Li et al., 2018). As observed from the Equation 1 , the edge information is not taken into account for MIS, MVC, but, for TSP, edge information cannot be ignored, because the object of TSP is computed based on the edge cost, i.e., the distance between the two vertices. We propose a static edge graph neural network (SE-GNN) that integrates edge information into the new node feature H as follows,

$$H_v^{t+1} = \sigma(H_v^t W_1^t + \sum_{u \in \mathcal{N}(v)} H_u^t W_2^t + \frac{1}{|\mathcal{N}(v)|} \sum_{u \in \mathcal{N}(v)} e_{v,u} W_3^t) \tag{2}$$

where $e(v,u)$ is the distance[1] between two vertices and W_3^t are parameter matrices for the layer t.

Dai et al.(Dai et al., 2017) proposed a graph embedding network (GEN) based on structure2vec to compute new node feature μ as follows,

$$\mu_v^{t+1} = \text{relu}(\theta_1 x_v + \theta_2 \sum_{u \in \mathcal{N}(v)} \mu_u^t + \theta_3 \sum_{u \in \mathcal{N}(v)} \text{relu}(\theta_4 w(v,u))) \tag{3}$$

where $\theta_1 \in \mathbb{R}^l$, $\theta_2, \theta_3 \in \mathbb{R}^{l \times l}$ and $\theta_4 \in \mathbb{R}^l$ are model parameters.

Compared with GEN, the key improvements are: 1) The SE-GNN replaces x_v in Equation 3 with H_v so that the SE-GNN could integrate the latest feature of the node itself directly in each update procedure. 2) One can regard each update process in the GEN as one update layer of the SE-GNN, i.e., each calculation is equivalent to going one layer forward, and counting T times is the T layers. Parameters of each layer in SE-GNN are independent, while parameters are shared between different update processes in GEN which limits the ability of the neural network. 3) Instead of aggregating edge weight by "sum" operation, we use "average" operation to balance the weight of node and edge feature. Experimental results show that the above improvements enhance the performance of the neural network.

We initialize the node feature H^0 as follows. Each vertex has a feature tag which is a 3-dimensional vector. The first element is binary and equal to 1 if the tour sequence S contains the vertex. The second and third elements of the feature tag are the coordinates of the vertex. When a partial tour has been constructed, it can not be changed, and the remaining problem is to find a path from the last vertex, through all unvisited vertices, to the first vertex. To know the first and the last vertex in partial tour sequence S, besides basic feature tags described above, we extend the node feature H^0 by adding feature tags of the first and last vertex in tour sequence S (see in Figure 2).

PARAMETERIZING $f(G|S;\Theta)$

Once feature for each vertex is computed after T iterations, and we use the new feature of vertices to define the $f(G|S;\Theta)$, which outputs the prior probability indicating how likely each vertex is to belong to tour sequence S. More specifically, we fuse all vertex feature H_v^T as the current state representation of the graph and parameterize $f(G|S;\Theta)$ as follows ,

$$f(G|S;\Theta) = \text{softmax}(W_5 \sigma(W_4[H_1, ..., H_n])) \tag{4}$$

where $W_4 \in \mathbb{R}^{l \times nl}$, $W_5 \in \mathbb{R}^{n \times l}$ are parameter matrices, σ denotes a component-wise non-linear function, e.g., a sigmoid or a ReLu, and $[\cdot,\cdot]$ denotes horizontal concatenation operator.

During training, we minimize the cross-entropy loss for each training sample (G_i, S_i):

$$\ell(S_i, f(G_i|S_i;\Theta)) = -\sum_{j=1}^{N} y_j \log f(G_i|S_i(1:j-1);\Theta) \tag{5}$$

where S_i is a tour sequence which is a permutation of the vertices over graph G_i and y_j is a one-hot vector whose length is N and $S(j)$-th position is 1.

The architecture of the deep neural network is illustrated in Figure 2.

4.3 GRAPH NEURAL NETWORK ASSISTED MONTE CARLO TREE SEARCH

Similar to the implement in (Silver et al., 2016), the GNN-MCTS uses deep neural network as a guide. Each node s in the search tree contains edges (s,a) for all legal actions $a \in A(s)$. Each edge stores a set of statistics,

$$\{N(s,a), Q(s,a), P(s,a)\}$$

where $N(s,a)$ is the visit count, $Q(s,a)$ is the action value and $P(s,a)$ is the prior probability of selecting that edge.

To be mentioned, three biggest differences between GNN-MCTS and AlphaGo are:

[1]Euclidean distance: given two points (x_1, y_1) and (y_1, y_2) in two-dimensional plane, $D = \sqrt{(x_2 - x_1)^2 + (y_2 - y_1)^2}$

- When playing the game of Go, the branch with a high average rate of winning indicates that the route is strong. While TSP is interested in finding the extreme, the average value makes no sense if several suboptimal routes surround the extreme route. Instead of recording the average action value, we propose to track the best action value found under each node's subtree for determining its exploitation value.
- In the game of Go, it is common to use $\{0, 0.5, 1\}$ to denote the result of a game composed of $loss$, $draw$, and win. Not only is this convenient, but it also meets the requirements of UCT (Kocsis & Szepesvári, 2006) for rewards to lie in the $[0, 1]$ range. In TSP, an arbitrary tour length can be achieve that does not fall into the predefined interval. One can solve this issue by adjusting the parameter c_{puct} of UCT in such a way that it is feasible for a specified interval. It requires substantial trial-and-error on adjusting c_{puct} due to the change in the number of cities. Instead, we address this problem by normalizing the action value of each node n whose parent is node p to $[0, 1]$ as follows,

$$Q_n = \frac{Q_n - w_p}{b_p - w_p} \tag{6}$$

  where b_p and w_p are, respectively, the best (maximum) and the worst (minimum) action value under p, and Q_n is the action value of n. The best action value under p is normalized to the value of 1, the worst action value is normalized to 0, and all other results are normalized to $[0, 1]$.
- AlphaGo used a learned value function (critic) $v(s, \theta)$ to estimate the probability of the current player winning from position s, where the parameters θ are learned from the observations (s, π). However, getting such algorithms to work is non-trivial. Instead, we design a value function $h(s)$ that combines the SE-GNN and beam search to evaluate the possible tour length from the current state to the end state. Guided by the output of SE-GNN, the value function executes beam search from the state corresponding to the leaf node l until reaching an end state. We compute the value of leaf node V_l according to the tour sequence S corresponding to the end state as follows,

$$V_l = -(\sum_{i=1}^{|S|-1} w\left(S(i), S(i+1)\right) + w\left(S(|S|), S(1)\right)) \tag{7}$$

  The value function is described in A.1.

The GNN-MCTS proceeds by iterating over the four phases and then selects a move to play.

Selection Strategy. The first in-tree phase of each playouts begins at the root of node s_0 of the search tree and finishes when the playouts reaches a leaf node s_l at time step l. At each of these time steps, $t<l$, we use a variant of PUCT (Rosin, 2011) to balance exploration(i.e., visiting states suggested by the prior policy) and exploitation(i.e., visiting states that have the best value) according to the statistics in the search tree.

$$a_t = \arg\max_a \left(Q(s_t, a) + U(s_t, a)\right) \tag{8}$$

$$U(s, a) = c_{puct} P(s, a) \frac{\sqrt{\sum_b N(s, b)}}{1 + N(s, a)} \tag{9}$$

where c_{puct} is a constant to trading off between exploration and exploitation.

Expansion Strategy. When a leaf node l is reached, the corresponding state s_l is evaluated by the deep neural network to obtain the prior probability p of its child nodes. The leaf node is expanded and the statistic of each edge (s_l, a) is initialized to $\{N(s_l, a) = 0, Q(s_l, a) = \infty, P(s_l, a) = p_a\}$.

Simulation Strategy. Rather than using a random strategy, we use value function $h(s)$ to evaluate the length of the tour that may be generated from the leaf node s_l.

Back-Propagation Strategy. For each step $t < L$, the edge statistics are updated in a backward process. The visit counts are increased, $N(s_t, a_t) = N(s_t, a_t) + 1$, and the action value is updated to best value, $Q(s_t, a_t) = \max(Q(s_t, a_t), V_l)$.

Play. At the end of several playouts, we select node with the biggest $\hat{P}(a|s_0) = 1 - \frac{Q(s_0,a)}{\sum_b Q(s_0,b)}$ as the next move a in the root position s_0. The search tree will be reused at subsequent time steps: the child node relating to the selected node becomes the new root node, and all the statistics of sub-tree below this child node is retained.

Table 1: Our method vs baselines. The gap % is w.r.t. the best value across all methods

Method	Rondom						Clustered					
	n=20		n=50		n=100		n=20		n=50		n=100	
	Obj.	Gap	Obj.	Gap	Obj.	Gap	Obj.	Gap	Obj.	Gap	Obj.	Gap
Concorde	3.92	0.0%	5.68	0.0%	7.73	0.0%	3.30	0.0%	3.38	0.0%	3.39	0.0%
Gurobi	3.92	0.0%	5.68	0.0%	7.73	0.0%	3.30	0.0%	3.38	0.0%	3.39	0.0%
Nearest Neighbor	4.57	16.50%	7.02	23.44%	9.63	24.58%	3.95	19.48%	4.18	23.76%	4.23	25.02%
Nearest Insertion	4.40	12.24%	6.77	19.08%	9.48	22.64%	3.66	10.62%	3.97	17.36%	4.08	20.46%
Random Insertion	4.08	4.12%	6.09	7.12%	8.45	9.24%	3.46	4.67%	3.65	7.93%	3.72	9.70%
Farthest Insertion	4.03	2.73%	5.98	5.29%	8.33	7.78%	3.40	2.87%	3.58	5.91%	3.64	7.55%
Vinyals et al. (gr.)	3.97	1.30%	6.41	18.58%	-		-		-		-	
Bello et al. (gr.)	3.99	1.83%	5.95	4.75%	8.26	6.82%	-		-		-	
Kool et al. (gr.)	3.93	0.36%	5.78	1.75%	8.08	4.57%	-		-		-	
Dai et al.	4.03	2.76%	5.98	5.26%	8.33	7.76%	3.37	2.07%	3.58	6.01%	3.66	8.17%
Our	**3.92**	**0.03%**	**5.70**	**0.32%**	**7.85**	**1.53%**	**3.30**	**0.00%**	**3.39**	**0.34%**	**3.44**	**1.61%**

5 EXPERIMENTS

5.1 EXPERIMENTAL SETUP

INSTANCE GENERATION

To evaluate our method against other approximation algorithms and deep learning-based approaches, we use an instance generator from the DIMACS TSP Challenge (Johnson et al., 2001) to generate two types of Euclidean instances: "random" instances consist of n points scattered uniformly at random in the $[10^6, 10^6]$ square; "clustered" instances include n points that are clustered into $n/100$ clusters. We consider three benchmark tasks, Euclidean TSP20, 50 and 100, for which we generate a train set of 50,000 instances and a test set of 1,000 instances.

BASELINES

To compute optimal solutions for both TSP, we use two state-of-the-art solvers, Concorde [2] (Applegate et al., 2006a) and Gurobi [3] (Optimization, 2013). We compare against Nearest, Random and Farthest Insertion, as well as Nearest Neighbor, which are non-learned baseline algorithms that also derive a tour by adding vertices successively. Additionally, we compare against excellent deep learning-based methods based on the greedy framework as mentioned in Section 2, most importantly Vinyals *et al.* (Vinyals et al., 2015), Bello *et al.* (Bello et al., 2016), Kool *et al.* (Kool et al., 2019), and Dai *et al.* (Dai et al., 2017).

GRAPH NEURAL NETWORK SETTINGS

Our SE-GNN has $T = 3$ node-update layers, which is deep enough for nodes to aggregate information associated with their neighbor vertices. Since the input is a "tagged" graph with 9-dimensional feature on vertices, the input contains vectors of size $H^0 = 9$. The width of other layers are identical: $H^t = 64$ for $t = 1, 2$. For parameterizing $f(G|S; \Theta)$, we use a two-layer perceptron. Except that the number of hidden units in the last layer is equal to the number of vertices in the graph, the other layers have 64 hidden units respectively. Different settings of the SE-GNN are discussed in Appendix B.

TRAINING AND TESTING

We generate 50,000 instances for TSP20, TSP50, and TSP100, respectively, to train the deep neural network. We use state-of-art solvers (Gurobi and Concorde) to obtain the optimal tour sequence for each instance. Then we generate N samples for each instance according to the optimal tour sequence. We divide the dataset into a training set, a validation set, and

Table 2: Parameter setting of GNN-MCTS

	$playouts$	c_{puct}	$beam\ width$
TSP20	800	1.3	1
TSP50	800	1.3	1
TSP100	1200	1.3	1

[2] http://www.math.uwaterloo.ca/tsp/concorde/

[3] http://www.gurobi.com/

Table 3: Confidence interval on different confidence intervals

Confidence level		90%	95%	99%
Random	n=20	3.922±0.046	3.922±0.054	3.922±0.071
	n=50	5.701±0.041	5.701±0.048	5.701±0.064
	n=100	7.850±0.039	7.850±0.047	7.850±0.062
Clustered	n=20	3.305±0.078	3.305±0.093	3.305±0.122
	n=50	3.391±0.051	3.391±0.061	3.391±0.080
	n=100	3.442±0.036	3.442±0.043	3.442±0.056

a test set according to the ratio of 8: 1: 1. We
use Adam (Kingma & Ba, 2014) with 128 mini-batches and learning rate 10^{-3}. Training proceeds for 30 epochs on a machine with 2080ti GPU. After training models for TSP20, 50, and 100, respectively, we use pre-trained deep neural networks to guide MCTS. During testing, we randomly generate 1000 instances for the above three problems. The parameter setting of the GNN-MCTS used in our experiments is shown in Table 2.

5.2 RESULTS

Besides non-learned algorithms, we mainly compare our method with excellent deep learning-based works that derive tours on the greedy mechanism. We implement and train a Pointer network with supervised learning, but we find that our supervised learning results are not as good as those reported by (Vinyals et al., 2015). Results of Pointer network on the random instances are from the $optimality\ gaps$ they report on 20, 50 vertex graphs. For other deep learning-based methods, we use experimental settings suggested by authors to train and get the same performance as reported.

Rather than reporting the approximation ration $\frac{c}{c^*}$, where c is the objective solution value of tour S and c^* is the best-known solution value of instance G, we use the average optimality gap $\frac{c-c^*}{c^*} = \frac{c}{c^*} - 1$ mentioned in (Kool et al., 2019). Table 1 reports the gap between the solution of each approach and the best-known solution for TSP20, 50, and 100. Our approach performs favorably against other methods up to 100 nodes on the "random" and "clustered" instances. Table 3 reports the confidence interval on different confidence levels.

5.3 ABLATION STUDY

We analyze the effect of different strategies used in the GNN-MCTS procedure. The comparison of different strategies are: 1) **best.** Different from AlphaGo, we track the best action value found under each node's subtree for determining its exploitation value. At the end of several playouts, we select the node with the best (biggest) action value as the next move in the root position. 2) **average.** As with the strategy used in AlphaGo, which is common in a two-player game, we track the average action value found under each node's subtree as exploitation value. Rather than selecting the node with the best (biggest) action value, we select the most visited node as the next move in the root position.

Table 4 shows the gap between solutions of our approach with two strategies and the best-known solution for TSP20, 50, and 100. (Up) "random" instances and (Down) "clustered" instances. The experimental results show that using the "best" strategy is far better than using the "average" strategy for TSP.

We also conduct a controlled experiment on the TSP test set to analyze how each component contributes to the presented approach. First, we use the SE-GNN to generate solutions in a greedy way, i.e., selecting the vertex with the biggest prior probability at each step; we refer to this version as SE-GNN. Then we use a graph neural network assisted MCTS which replaces the value function $h(s)$ (see in A.1) with random rollout to evaluate leaf nodes; we refer to this version as SEGNN+Tree$_{\text{-v}}$. Our full method (SE-GNN+Tree) is listed for comparison.

Table 5 shows the gap between the solution of each approach and the best-known solution for different TSP problems. (Up) "random" instances and (Down) "clustered" instances. The results from SEGNN+Tree$_{\text{-v}}$ and SE-GNN+Tree show that value function $h(s)$ can well estimate the path length from the leaf node and the MCTS, which uses a suitable value function, can perform better than one

using a random rollout. Furthermore, the gap of performance between SE-GNN and SE-GNN+Tree shows that the developed MCTS can efficiently avoid algorithm falling into local optimal and plays an important role in enhancing the performance of our method.

Table 4: Effect of strategies used in the MCTS

	n=20	n=50	n=100
average	1.62%	7.21%	14.23%
best	**0.03%**	**0.32%**	**1.53%**
average	1.25%	7.27%	14.11%
best	**0.00%**	**0.34%**	**1.61%**

Table 5: Controlled experiment on TSP test set

	n=20	n=50	n=100
SE-GNN	2.21%	5.26%	11.34%
SEGNN+Tree$_{-v}$	0.08%	1.64%	4.24%
SE-GNN+Tree	**0.03%**	**0.32%**	**1.53%**
SE-GNN	2.19%	5.61%	10.22%
SEGNN+Tree$_{-v}$	0.04%	1.13%	5.67%
SE-GNN+Tree	**0.00%**	**0.34%**	**1.61%**

5.4 Comparison with other deep neural network

Compared with the basic GNN, SE-GNN integrates static edge information for computing new node feature, and it should extract more information and perform well than basic GNN for TSP. To support this statement, we compare the performance of GNN and SE-GNN on random instances, including TSP20, 50, and 100. We generate tour sequences by using the neural network in a greedy way, i.e., selecting vertex with the biggest prior probability at each step. The performance of two GNN is reported in Table 6.

To support the key improvements made by SE-GNN, we compare the performance of GEN and SE-GNN on the random instances including TSP20, 50 and 100. Similar to the comparison experiment above, we generate tour sequences by using neural network in a greedy way. The performance of GEN and SE-GNN is reported in Table 6. Furthermore, we use GEN and SE-GNN to guide MCTS separately on "random" and "clustered" instances, including TSP20, 50 and 100. Table 7 reports the quality of solutions and the MCTS can get shorter tours when guided by SE-GNN.

Table 6: Performance of different neural networks on random instances

	n=20		n=50		n=100	
	Acc.*	Gap	Acc.	Gap	Acc.	Gap
GNN	89.8%	4.8%	80.8%	21.1%	63.8%	58.9%
GEN	89.7%	4.1%	84.2%	12.5%	78.9%	21.9%
SE-GNN	**94.2%**	**2.2%**	**91.5%**	**5.3%**	**88.7%**	**11.3%**

* The highest accuracy of the neural network can be achieved on the test-set when we train the neural network.

Table 7: The gap of objective solution between the best-known solution

	Rondom			Clustered		
	n=20	n=50	n=100	n=20	n=50	n=100
MCTS+GEN	0.1%	1.3%	4.5%	0.2%	1.0%	4.7%
MCTS+SE-GNN	**0.0%**	**0.3%**	**1.5%**	**0.0%**	**0.3%**	**1.6%**

6 Conclusion

We proposed a graph neural network assisted Monte Carlo Tree Search (GNN-MCTS) for the classical traveling salesman problem. The core idea of our approach lies in converting the TSP into a tree search problem. To capture the local and global graph structure, we train a static graph neural network (SE-GNN) which integrates node feature and edge weight into the feature update process. Instead of using the prior probability output by SE-GNN in a greedy way, we designed a GNN-MCTS to provide scouting simulation so that the algorithm could avoid being stuck into the local optimum. Our approach is, to our best of knowledge, the first MCTS combined with the deep neural network for TSP. The experimental results show that the proposed approach can obtain shorter tours than other learning-based methods. We will release code to support future progress in this direction.

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A ALGORITHMS

A.1 VALUE FUNCTION

The evaluation function is summarized in A.1. Let $start$ denotes the state of leaf node l, B denotes the beam width.

Algorithm 1 Heuristic Function

Initialize BEAM = $\{start\}$
while BEAM $\neq \varnothing$ **do**
    SET = $\varnothing$
    for state in BEAM **do**
        for successor of state **do**
            Compute value[4] of the successor
            SET = SET $\cup$ { successor }
    BEAM = $\varnothing$
    while SET $\neq \varnothing$ and $B <$ |SET | **do**
        state = successor in SET with smallest value
        SET $\setminus$ { state }
    for state in SET **do**
        if state is end **then**
            return state in SET with biggest value
        else
            BEAM = BEAM $\cup$ { state }

B STATIC EDGE GRAPH NEURAL NETWORKS

The proposed SE-GNN has a deep architecture that consists of several node-update layers. Therefore, as the model gets deeper with more layers, the more information can be aggregated by nodes. We train SE-GNN with the different number of layers on random instance from TSP20. We greedily use the prior probability, i.e., selecting the vertex with the biggest prior probability, to derive tour sequence. Table 8 reports the results. Acc. means the highest accuracy of the neural network can be achieved on the test-set when we train the neural network. As the number of SE-GNN layers increases, the performance gets better.

Table 8: Effect of the number of layers on random instances

Layers	n=1	n=2	n=3
Acc.	88.2%	91.3%	94.2%
Gap	5.1%	3.2%	2.2%

[4] value = $\prod_{j=1}^{|S|} f(G|S(1:j-1)$, where S is the partial tour sequence corresponding to the state.