# Revisit the Algorithm Selection Problem for TSP with Spatial Information Enhanced Graph Neural Networks

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- Keywords: Traveling Salesperson Problem, Algorithm Selection, Instance Hardness, Graph Neural Network, Graph Classification.
- Abstract: Algorithm selection is a well-known problem where researchers investigate how to construct useful features representing the problem instances and then apply feature-based machine learning models to predict the best algorithm for each instance. However, even for simple optimization problems like Euclidean Traveling Salesman Problem (TSP), there lacks a general and effective feature representation for problem instances. The important features of TSP are relatively well understood in the literature, based on extensive domain knowledge and post-analysis of the solutions. In recent years, Convolutional Neural Network (CNN) has gained popularity for TSP algorithm selection. Compared to traditional feature-based models, CNN has an automatic feature-learning ability and demands less domain expertise. However, it is still required to generate intermediate representations, i.e., multiple images to represent TSP instances first. In this paper, we revisit algorithm selection for TSP and propose GINES, a new Graph Neural Network (GNN) that uses city coordinates and distances as input. GINES introduces a novel message-passing mechanism and local feature extractor to learn TSP's spatial information. Evaluation of two benchmarks shows GINES outperforms CNN and GINE models and surpasses traditional feature-based methods on one dataset. Our codes and datasets are available at https://github.com/lurenyi233/GINES\_TSP.

# **1 INTRODUCTION**

The Euclidean Traveling Salesman Problem (TSP) is a widely studied NP-hard combinatorial optimization problem with real-world applications and significant theoretical value. It involves finding the shortest route that visits a list of cities with known positions and returns to the starting point. To solve this, researchers have developed exact, heuristic, and learning-based algorithms (Zhao et al., 2021b). Since algorithm performance varies with problem instance characteristics, selecting the right algorithm for each instance can improve efficiency (Kerschke et al., 2018). Algorithm selection for optimization problems is often treated as a classification task, where problem instances are mapped to algorithms based on their characteristics (Pereira et al., 2024). Typically, domain experts craft features (Bossek, 2017) to capture TSP instance characteristics, which are then used to train a machine learning classifier. However, This

feature-based method has several limitations: it requires extensive domain knowledge, features may lack expressiveness, and a feature selection process is needed (Seiler et al., 2020). Handcrafted features do not transfer well to other optimization problems, and designing effective features for less-studied problems than TSP is challenging.

Deep learning models, notably Convolutional Neural Networks (CNN), are used to select TSP algorithms by converting TSP instances into images, making it a computer vision task. CNNs' feature learning eliminates the need for handcrafted features. In (Seiler et al., 2020), a point image, a Minimum Spanning Tree (MST) image, and a k-Nearest-Neighbor-Graph (kNNG) image are generated for each TSP instance, and an 8-layer CNN predicts the best algorithm. In (Zhao et al., 2021b), TSP instances are converted into density maps for classification using ResNet. A similar gridding method in (Huerta et al., 2022) generates images to predict algorithm performance over time with a 3-layer CNN.

Although CNNs outperform traditional models in selecting algorithms for TSP (Huerta et al., 2022;

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Song, Y., Bliek, L. and Zhang, Y.

Revisit the Algorithm Selection Problem for TSP with Spatial Information Enhanced Graph Neural Networks. DOI: 10.5220/0013153400003890 Paper published under CC license (CC BY-NC-ND 4.0) In Proceedings of the 17th International Conference on Agents and Artificial Intelligence (ICAART 2025) - Volume 3, pages 472-479 ISBN: 978-989-758-737-5; ISSN: 2184-433X Proceedings Copyright © 2025 by SCITEPRESS – Science and Technology Publications, Lda.

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Seiler et al., 2020; Zhao et al., 2021b), they have notable drawbacks: (1) Need to generate intermediate representations. Like feature-based methods, generating image representations for CNN input is tedious. Generating MST and kNNG images involves time-consuming calculations (Seiler et al., 2020), and gridding with up-scaling is required for better resolution (Zhao et al., 2021b). Data augmentation like rotation/flipping is widely used (Huerta et al., 2022), leading to the need for multiple images per instance. (2) Introduce problem-irrelevant parameters. In (Seiler et al., 2020), cities and connections in MST and kNNG images are shown as solid dots and lines, but these do not represent TSP properties. Setting image size or grid number in gridding methods (Zhao et al., 2021b) also adds complexity and needs extra parameter tuning. (3) Potentially lose problem-relevant information. The gridding process divides a TSP instance into grids, with values denoting city counts. This results in the loss of local structure. Additionally, (Huerta et al., 2022) limits grid values, causing further distortion. (4) Hard to generalize to other routing problems. While gridding methods can turn TSP instances into images due to their 2D nature, they struggle with TSP variants like the Asymmetric TSP (ATSP) and Vehicle Routing Problem (VRP). Graphs with node/edge features may be more suitable for these cases.

To address these issues, we introduce GINES, an enhanced Graph Neural Network (GNN) for selecting algorithms for TSP. Our key contributions are:

- We are the first to successfully design a GNN to learn the representation of TSP instances for algorithm selection, outperforming the existing feature-based or CNN-based approaches.
- The proposed model merely takes the coordinates of cities and the distance between them as inputs. We show there is no need to design and generate intermediate representations, such as handcrafted features or images, for TSP instances.
- The adopted graph representation methodology has few parameter settings, and the experimental results show it can retain accurate information about the original TSP instances.
- The proposed model is able to capture local features with multiple scales by aggregating information from the neighborhood nodes. Its robust performance is demonstrated on two public TSP datasets, compared with several existing approaches.
- The proposed model can easily generalize to other complex routing problems by adding node features or modifying distance metrics.

The paper is structured as follows: Section 2 covers background and related works, Section 3 presents GINES, Section 4 details its experimental results, and Section 5 concludes.

## 2 BACKGROUND AND RELATED WORK

## 2.1 Algorithm Selection and Hardness Prediction for Optimization Problems

The No Free Lunch (NFL) theorem states that no algorithm is universally optimal for all optimization problems. Algorithm selection aims to improve overall solving performance by predicting the best algorithm for each instance. Traditional approaches rely on handcrafted features for specific problems like TSP, VRP, and Knapsack Problem (Zhao et al., 2021b). However, these features are often problemspecific and require significant effort to design. Deep learning models eliminate the need for tedious feature engineering by automatically learning instance features. For TSP, CNN-based models have been used to generate intermediate representations such as images (Seiler et al., 2020; Zhao et al., 2021b). In addition to the TSP, CNNs have also been utilized for algorithm selection in various fields like Black-Box Optimization (He and Yuen, 2020), commonly by transforming instances into images or sequences. However, graph-based representations remain underexplored in this context.

Hardness prediction is a research topic closely related to algorithm selection; it involves assessing whether an instance is easy or difficult to solve using a specific algorithm (Jooken et al., 2022). Researchers have identified attributes correlated with instance hardness, such as clustering features, and edge features (Mersmann et al., 2012). These features are often used to evaluate TSP hardness for algorithms like Ant Colony Optimization (ACO) and Lin-Kernighan (LK) (Crişan et al., 2021). However, the relevance of features can vary across algorithms, and traditional feature-based machine learning models remain the primary approach in this field. To our knowledge, deep learning models have not been explored for hardness prediction.

### 2.2 Leveraging GNN for TSP

TSP instances can be effectively represented as graphs, making GNNs a suitable tool for solving re-

lated problems. Current research on GNNs for TSP focuses on three main areas:

GNN for TSP Solving. GNNs have been successfully applied in learning-based TSP solvers using reinforcement or supervised learning (Luo et al., 2023). In reinforcement learning, models like Graph Pointer Networks (Ma et al., 2019) is combined with Deep Q-Learning to optimize policies. Supervised learning approaches often use GNNs as encoders, paired with sequence-to-sequence architectures like Pointer Networks (Vinyals et al., 2015). Hybrid models further enhance efficiency by integrating GNNs with heuristics. For example, Graph Convolutional Network (GCN) predicts edge probabilities for optimal tours (Joshi et al., 2019), while Graph Attention Networks (GAT) guide local search strategies (Hudson et al., 2021). Recent work also highlights the importance of spatial distribution for improving generalization (Jiang et al., 2022).

**GNN for TSP Search Space Reduction.** Search space reduction transforms TSP into an edge classification problem, where GNNs predict edges likely to be part of the optimal solution. For instance, a kNNG represents TSP instances with node coordinates and edge distances (Dwivedi et al., 2023). This approach helps benchmark GNN architectures for tasks like edge classification (Zhang et al., 2022) and improves computational efficiency by narrowing the search space.

**GNN for TSP Algorithm Selection.** Applying GNNs for algorithm selection is still an emerging field. Existing studies show CNNs outperform GCNs for TSP algorithm selection due to GCN's limitations, such as the lack of node-level features and oversmoothing (Zhao et al., 2021b). Current GNN research in TSP solving and search space reduction often overlooks the spatial distribution of cities, which is crucial for instance characterization. To address this, we propose a tailored GNN architecture that incorporates spatial information to enhance algorithm selection for TSP.

# 3 TSP ALGORITHM SELECTION WITH GINES

#### 3.1 Problem Statement

The TSP algorithm selection problem can be defined as follows: given a TSP instance set  $I = \{I_1, I_2, ..., I_l\}$ , a TSP algorithm set  $A = \{A_1, A_2, ..., A_m\}$ , and a certain algorithm performance metric, the goal is to identify a per-instance mapping from *I* to *A* that maximizes its performance on *I* based on the given metric. As discussed in previous sections, the TSP instances can be represented by handcrafted features or images, which are inputs to supervised learning models such as SVM and CNN to learn this mapping.

In this work, we treat a TSP instance  $I_i$  as a graph  $G_i = (V, E)$ , where the node features  $X_v$  for  $v \in V$ is a vector of its  $(x_v, y_v)$  coordinate, the edge feature  $e_{u,v}$  for  $(u,v) \in E$  is the Euclidean distance between two nodes. Here we use kNNG to represent TSP instances. We set the number of nearest nodes k to 10, which is relatively small compared to other papers (Dwivedi et al., 2023) to reduce the computational burden. Let N be the number of cities. The node feature is a [N, 2] matrix, and the matrix size of the edge feature is  $[N \times 10, 1]$ . Given a set of TSP graphs  $\{G_1, G_2, ..., G_l\}$  and their algorithm performance labels  $\{y_1, y_2, ..., y_l\}$ , the task of selecting TSP algorithms can be converted to a graph-level classification task. We develop a GNN model for routing problems, called GINES, which directly takes TSP graphs as inputs for classification. Next, we will describe the architecture of this model in detail.

## 3.2 GINES

Graph Isomorphism Network (GIN) is one of the most expressive GNN architectures for the graphlevel classification task. Researchers have shown that the representational power of GIN is equal to the power of the Weisfeiler Lehman graph isomorphism test, and GIN can obtain state-of-the-art performance on several graph classification benchmark datasets (Xu et al., 2018). GIN uses the following formula for its neighborhood aggregation and messagepassing:

$$\mathbf{x}_{i}^{\prime} = \mathrm{MLP}\left((1+\varepsilon) \cdot \mathbf{x}_{i} + \sum_{j \in \mathcal{N}(i)} \mathbf{x}_{j}\right)$$
(1)

where  $\mathbf{x}_i$  is the target node's features,  $\mathcal{N}(i)$  denotes the neighborhood for node *i*, and  $\mathbf{x}_j$  is the neighborhood nodes' features.  $\varepsilon$  indicates the significance of the target node relative to its neighborhood, with a default value of zero.  $\mathbf{x}'_i$  is the representation of node *i* we get after applying one GIN layer. The function MLP is a Multi-Layer Perceptron, which is used to learn complex transformations of aggregated features. Here, often the SUM aggregator is used to aggregate information from the neighborhood, as it can better distinguish different graph structures than MEAN and MAX aggregators (Xu et al., 2018). A drawback of the original GIN is that the edge features are not taken into account. Thus, the authors of (Hu et al., 2019) proposed GINE that can incorporate edge features in the aggregation procedure:

$$\mathbf{x}_{i}^{\prime} = \mathrm{MLP}\left(\left(1+\varepsilon\right) \cdot \mathbf{x}_{i} + \sum_{j \in \mathcal{N}(i)} \mathrm{ReLU}\left(\mathbf{x}_{j} + \mathbf{e}_{j,i}\right)\right)$$
(2)

where  $\mathbf{e}_{j,i}$  are edge features. In GINE, the neighborhood nodes' features and edge features are added together and make a ReLU transform before the SUM aggregation. With a TSP graph, the dimensions of these two features do not match. Therefore, we perform a linear transform to edge features.

To better tackle the TSP algorithm selection problem, we make several modifications on GINE and propose a GINES (GINE with Spatial information) architecture as follows.

Adopting a Suitable Aggregator. Aggregators in GNNs play a crucial role in incorporating neighborhood information and significantly impact representational capacity (Xu et al., 2018). Common aggregators include MEAN, MAX, and SUM, each suited for specific tasks. For instance, MEAN captures node distribution and works well for distributional tasks (Xu et al., 2018), while MAX highlights representative nodes and is effective in vision tasks like point cloud classification (Qi et al., 2017). SUM, used by GIN, is ideal for learning structural graph properties. With post-analysis, researchers have shown that the standard deviation (SD) or Coefficient of Variation (CV) of the distance matrix is one of the most significant features (Crisan et al., 2021) in algorithm selection or hardness prediction for TSP. Intuitively, when the SD of the TSP distance matrix is very high, it is easy to tell the difference between candidate solutions, and the TSP is easy to solve. At the opposite end of the spectrum, when the SD of the TSP distance matrix is very small, there are many routes with the same minimum cost, and finding one of them is not difficult. So as the SD increases, an easy-hard-easy transition can be observed. Based on the above analysis, we add the SD aggregator, along with the MAX aggregator and SUM aggregator, as the three aggregators in our GINES to aggregate useful information for TSP algorithm selection.

**Extracting Local Spatial Information.** In a TSP instance, cities are distributed in a 2D Euclidean Space. The main characteristic to distinguish TSP instances is the spatial distributions of cities. There

exists a research topic that also focuses on learning the spatial distribution of points, namely, point cloud classification. The point cloud is a type of practical 3D geometric data. Identifying point clouds is an object recognition task with many real-world applications, such as remote sensing, autonomous driving, and robotics (Qi et al., 2017). Unlike image data made up of regular grids, the point cloud is unstructured data as the distance between neighboring points is not fixed. As a result, applying the classic convolutional operations on point clouds is difficult. To tackle this, researchers have designed several GNN architectures, such as PointNet++ (Qi et al., 2017) and Point Transformer (Zhao et al., 2021a). In the message-passing formulation of these GNNs for point clouds, a common component is  $(\mathbf{p}_i - \mathbf{p}_i)$ , here  $\mathbf{p}_i$  and  $\mathbf{p}_i$  indicate the positions of the current point and neighborhood points, respectively. Through this calculation, local neighborhood information, such as distance and angles between points, can be extracted. As the TSP instances can be viewed as 2D point clouds, extracting more local spatial information may help identify the TSP instances' class. We add this component to the message-passing formulation of GINES, as shown follows:

$$\mathbf{x}_{i}^{\prime} = \mathrm{MLP}\left((1+\varepsilon) \cdot \mathbf{x}_{i} + \bigoplus_{j \in \mathcal{N}(i)} \mathrm{ReLU}\left(h_{\Theta}\left(\mathbf{x}_{j} - \mathbf{x}_{i}\right) + \mathbf{e}_{j,i}\right)\right)$$
(3)

where  $\bigoplus$  indicates the selected aggregator, it can be either SD aggregator, MAX aggregator, or SUM aggregator.  $h_{\Theta}$  is a neural network and defaults to be one linear layer to transform the local spatial information. The whole neural network architecture of our GINES is shown in Figure 1. We adopt three GINES layers to extract the salient spatial information from TSP graphs and apply graph-level Sum pooling for each GINES layer to obtain the entire graph's representation in all depths of the model. Then we concatenate these representations together and feed them into the following two linear layers. We make full use of the learned representation in the first two GINES layers as they may have better feature generalization ability (Xu et al., 2018).

## **4 EXPERIMENTS**

#### 4.1 Dataset

We evaluate the proposed GINES on two public TSP algorithm selection datasets. The first dataset is gen-



Figure 1: The GINES neural network architecture for TSP algorithm selection.

erated to assess the Instance Space Analysis (ISA) framework (Smith-Miles and van Hemert, 2011), and the second is for evaluating the proposed CNN-based selector (Seiler et al., 2020). The main difference between the two datasets is the size of the instances. The TSP instances in the first dataset all contain 100 cities, while instances in the second dataset are relatively larger and contain 1000 cities. Applying the proposed model to two different datasets helps us examine its adaptability and compare it with other models. The following part is a detailed description of the two datasets.

**TSP-ISA Dataset.** This dataset contains 1330 instances, each with 100 cities, divided into seven groups based on characteristics: RAN-DOM, CLKeasy, CLKhard, LKCCeasy, LKCChard, easyCLK-hardLKCC, and hardCLK-easyLKCC. The goal is to classify whether Chained Lin-Kernighan (CLK) or Lin-Kernighan with Cluster Compensation (LKCC) performs better. LKCC is the Single-Best-Solver with an accuracy of 71.43% if applied to all instances. To address class imbalance, random oversampling is used for training.

**TSP-CNN Dataset.** This dataset consists of 1000 instances, each with 1000 cities, and focuses on selecting between two algorithms: Edge-Assembly-Crossover (EAX) and Lin-Kernighan Heuristic (LKH). The dataset is balanced, and EAX, as the Single-Best-Solver, achieves 49% accuracy. Instances are specifically designed to favor one algorithm over the other. A 10-fold cross-validation setup,

as used in (Seiler et al., 2020), ensures fair comparisons.

### 4.2 Baseline Model

To evaluate the performance of GINES, we compare it with baseline models, which include traditional feature-based methods and GNNs. For feature-based models, we use Random Forest (RF) as the classifier due to its effectiveness in TSP algorithm selection (Seiler et al., 2020). We evaluate four groups of handcrafted TSP features:

- All140: All 140 TSP features defined by R package named *salesperson* (Bossek, 2017). These features can be divided into 10 groups, including Minimum Spanning Tree (MST) features, kNNG features, Angle features, etc.
- Top15: after the feature selection procedure, (Seiler et al., 2020) propose the best 15 TSP features for the TSP-CNN dataset. Most of those features are statistical values of strong connected components of kNNG, and others are MST features and Angle features.
- MST19: all the 19 MST features defined by *salesperson*, are multiple statistical values of MST distance and depth. Here we study the MST features as MST is strongly related to TSP and can be used to solve TSP approximately. Besides, MST features are essential features for algorithm selection according to the previous studies (Seiler et al., 2020).
- kNNG51: all the 51 kNNG features defined by *salesperson*, including statistical values of kNNG distances, as well as the weak/strong connected components of the kNNG.

For GNN baseline models, we include GCN and GINE. Previous studies have shown that GCN performs worse than CNN for TSP algorithm selection (Zhao et al., 2021b), while GINE offers stronger representation learning capabilities and outperforms GCN on graph-level tasks. This study is the first to apply GINE to algorithm selection. The baseline GNN models share the same architecture and parameters as GINES, except for replacing the three GINES layers with GCN or GINE. Additionally, we test GINES with different aggregators: MAX (GINES-MAX), SUM (GINES-SUM), and SD (GINES-SD). For consistency, datasets are processed following (Seiler et al., 2020), with 10-fold cross-validation on both the TSP-ISA and TSP-CNN datasets. GNN models use a hidden dimension of 32, and an Adam optimizer with a learning rate of 0.01. Models are trained for up to 100 epochs with early stopping (patience = 20).

All experiments were conducted on a laptop with Intel Core i7-9750H, and the code was implemented using PyTorch Geometric.

### 4.3 Result and Analysis

Table 1 shows the average classification accuracy on the TSP-ISA dataset, with the best and second-best results highlighted. Among feature-based approaches, RF with all 140 features achieves the highest accuracy, while using fewer features significantly reduces performance. MST features prove more effective than kNNG features in this task. GNNs outperform traditional feature-based models by automatically extracting valuable features from kNNG. GINE and GINES perform significantly better than GCN, highlighting the importance of tailored GNN architectures for this application. By incorporating a spatial information extractor, GINES achieves higher accuracy than GINE. Tests with different aggregators (MAX, SUM, SD) show comparable results, making GINES a promising approach due to its high accuracy and independence from domain-specific feature design.

Table 1: Algorithm selection performance comparison on the TSP-ISA dataset.

Models	Input data	Accuracy	
SCREN	All140 features	$95.79 \pm 2.26$	
	Top15 features	$87.37 \pm 2.42$	
	MST19 features	$87.82 \pm 2.73$	
	kNNG51 features	$74.36\pm3.60$	
GCN	kNNG	$93.38 \pm 1.71$	
GINE	kNNG	$97.52 \pm 1.17$	
GINES-MAX	kNNG	$\underline{98.87\pm0.91}$	
GINES-SUM	kNNG	$\textbf{98.87} \pm \textbf{0.61}$	
GINES-SD	kNNG	$98.42\pm0.98$	

The experiment results on the TSP-CNN dataset are shown in Table 2. Firstly, We apply the featurebased models and find that RF with MST features can achieve the best performance. Again, we can observe that MST features are more valuable than kNNG features in the TSP algorithm selection task. Then we load the trained CNN model files and test them to get CNNs' performance. It shows that CNN with Points+MST images is better than CNN with other image inputs. At last, we test the proposed GINES and baseline GNN models. GINES can outperform CNN models but is still worse than featurebased models. The main reason may be the handcrafted features fed into RF are heavily engineered, while the GNN models fail to extract some crucial

Table 2: Algorithm selection performance comparison on the TSP-CNN dataset.

Models	Input data	Accuracy
	All140 features	$73.30 \pm 5.10$
RF	Top15 features	$\underline{73.40 \pm 5.66}$
	MST19 features	$\textbf{73.90} \pm \textbf{4.81}$
	kNNG51 features	$72.80\pm5.86$
CNN (Seiler et al., 2020)	Three images	$70.50 \pm 7.55$
	Two images	$72.00 \pm 4.96$
	Points images	$71.80 \pm 6.63$
GCN	kNNG	$62.80\pm5.86$
GINE	kNNG	$66.30 \pm 3.93$
GINES-MAX	kNNG	$70.20\pm5.19$
GINES-SUM	kNNG	$70.00\pm4.47$
GINES-SD	kNNG	$72.60 \pm 4.76$

features, such as MST and clustering features. Besides, there are much more nodes in this dataset, leading to less salient spatial information that can be learned. In GINES, selecting the SD aggregator for message-passing is advantageous as it relates closely to TSP problem hardness. Tests on GINES-MAX and GINES-SUM confirm that using an SD aggregator yields better predictions for the TSP-CNN dataset.

Table 3 summarizes the properties of the featurebased model, CNN, and GINES on the TSP algorithm selection task. Compared to deep learning models such as CNN and the proposed GINES, the traditional feature-based method suffers from the following shortcomings. Firstly, substantial domain expertise is required to design features. Secondly, as shown in Figure 2, the important features of the TSP-ISA dataset and the TSP-CNN dataset are significantly different, indicating that tedious feature engineering is required to choose valuable features. Finally, these selected features are probably inapplicable to other routing problems. The experiment results in Table 2 show that the proposed GINES is a competitive method, and it can slightly outperform CNN in prediction accuracy. GINES has several other advantages compared to CNN. Firstly, CNN takes multiple images as inputs, i.e., Points image, MST image, and kNNG image. Generating these images might be burdensome work, and it is unclear which image can better represent TSP instances. Contrary to CNN, GINES directly takes cities' coordinate and distance matrices as inputs, and we do not need to prepare intermediate representations like images. Secondly, when generating images for CNN, several problemirrelevant parameters must be set, such as image size, dot size, and line width in MST and kNNG images. Tuning these parameters can be a heavy workload,



Figure 2: The Top 10 importance features for TSP-ISA dataset and TSP-CNN dataset.

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Properties	Feature-based	CNN (Seiler et al., 2020)	GINES
Intermediate representations	Handcrafted features	Points/MST/kNNG images	None
Feature Engineering	Yes	No	No
Problem-irrelevant parameters	None	Image size, Dot size, Line width	None
Data Augmentation	None	Random rotation/flipping	None
Problem-relevant information loss	Domain dependent	Resolution dependent	None
Generalize to VRP (Distinguish different points)	Hard	Hard	Easy to add node features
Generalize to ATSP (To Non-Euclidean Metric Space)	Hard	Hard	Easy to add edge features

although theoretically, these parameters should not affect the learned mapping from instances to algorithms. In GINES, on the other hand, the TSP instances are treated as graphs, and there are not many instance representation parameters to be designed or adjusted. Besides, when setting the image resolution in the CNN method, we should consider the city number in the TSP instance. Otherwise, the representation ability of the image is inadequate, and problem instance information is lost. At last, generating images for TSP instances and applying CNN to select algorithms is not very difficult because cities in TSP are homogeneous and distributed in 2D Euclidean space. If we look into some complex routing problems, we will find that applying the CNN-based method is challenging. For VRP algorithm selection, it is hard to differentiate the depot and customer with image representations. While in GINES, we can simply add the point features to tell them apart. Considering the routing problem in Non-Euclidean space such as ATSP, drawing the problem instance on a 2D plane is nearly impossible. While GINES can naturally recognize the neighborhood in ATSP, we can also modify the message-passing formulation in GINES to aggregate more valuable edge features.

# **5** CONCLUSION

In this work, we propose a novel GNN named GINES to select algorithms for TSP. By adopting a suitable aggregator and local neighborhood feature extractor, this model can learn useful spatial information of TSP instances and outperform traditional featurebased models and CNNs on public algorithm selection datasets. GINES handles TSP instances as graphs and only takes cities' coordinates and distances between them as inputs. Thus no intermediate representations for problem instances, such as features or images, need to be designed and generated before model training. In contrast to converting TSP instances to images, the graph representation is more natural and efficient, as it neither introduces problem-irrelevant parameters nor loses problem-relevant information. The proposed GINES is promising as it is easy to generalize to other routing problems. For example, we can distinguish nodes and routes in the problem instances by adding node features and edge features. This work can be a good starting point for selecting algorithms or predicting instance hardness for combinatorial optimization problems defined on graphs. In the future, we will explore GINES architectures for

more complex problems like ATSP, VRP, and real-world problems.

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