Travel the Same Path: A Novel TSP solving strategy

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Abstract

Graph neural network is a rising concept that has demonstrated significant potential in many areas. This paper aims to further explore this potential by applying it to the **Traveling Salesman Problem**. We explore a novel type of reinforcement learning called **imitation learning**. Our research focuses on the ability of models trained with imitation learning on small instances to generalize to larger instances.

Keywords: Travelling salesman problem, Graph Neural Network, Imitation Training, Reinforcement Learning, Integer Programming, Embedding learning, Combinatorial Optimization, Exact solver.

1 Introduction

The travelling salesman problem (TSP) can be described as follows: given a list of cities and the distances between each pair of cities, find the shortest route possible that visits each city *exactly once* then returns to the origin city. Specifically, given an **undirected weighted graph** $\mathcal{G} = (\mathcal{E}, \mathcal{V})$, with an ordered pair of nodes set $\mathcal{E}$ and an edge set $\mathcal{V} \subseteq \mathcal{E} \times \mathcal{E}$ where $\mathcal{G}$ is equipped with **spatial structure**. This means that each edge between nodes will have different weights and each node will have its coordinates, we want to find a simple cycle that visits every node exactly once while having the smallest cost.

We will utilize GCNN (Graph Convolutional Neural Network), a particular kind of GNN, together with imitation learning to solve TSP in an interesting and inspiring way. In particular, we focus on the generalization ability of models trained on small-sized problem instances.[1]

2 Related Works

There has already been extensive work done to optimize TSP solvers both theoretically and practically. We have done extensive research into other solvers; the papers most relevant to our project are summarized below.

Transformer Network for TSP[6]. The main focus of this paper is to detail the application of deep reinforcement learning reapplied to a Transformer architecture originally created for Natural Language Processing (NLP). Unlike our proposed model, this solver does not solve TSP exactly, but

[1]The code is available at https://github.com/sleepymalc/Travel-the-Same-Path.

instead learns heuristics that have very low error rates (0.004% for TSP50 and 0.39% for TSP100). These heuristics can run over a TSP problem much faster than a traditional solver while still achieving similar results.

Exact Combinatorial Optimization with GCNNs[11]. This paper serves as the one of the backbones of our research; its main focus is to detail how MIPS can potentially be solved much quicker than a traditional solver by using GNNs (specifically GCNNs). It did this by training its model using imitation learning (using the strong branching expert rule) and was able to effectively produce outputs for problem instances much greater than what they were trained on.

State of the Art Exact Solver. There has been a lot of progress on the symmetric TSP in the last century. With the increase in the number of nodes, there is a super-polynomial (at least exponential) explosion in the number of potential solutions. This makes the TSP problem difficult to solve on two parameters, the first being finding a global shortest route as well as reducing the computation complexity in finding this route. `Concorde`[9], written in the ANSI C programming language, is widely recognized as the fastest state-of-the-art (SOTA) exact TSP solution for large instances.

3 Preliminary

3.1 Integer Linear Programming Formulation of TSP

We first formulate TSP in terms of **Integer Linear Programming**. Given an undirected weighted group $\mathcal{G} = (\mathcal{E}, \mathcal{V})$, we label the nodes with numbers $1, \ldots, n$ and define

$$x_{ij} := \begin{cases} 1, & \text{if } (i,j) \in \mathcal{E}' \\ 0, & \text{if } (i,j) \in \mathcal{E} \setminus \mathcal{E}', \end{cases}$$

where $\mathcal{E}' \subset \mathcal{E}$ is a variable which can be viewed as a compact representation of all variables $x_{ij}, \forall i, j$. Furthermore, we denote the weight on edge (i,j) by c_{ij}, then for a particular TSP problem instance, we can formulate the problem as follows.

$$\begin{aligned}
\min \sum_{i=1}^{n} \sum_{j\neq i, j=1}^{n} & c_{ij} x_{ij} \\
& \sum_{i=1, i\neq j}^{n} x_{ij} = 1 && j = 1, \ldots, n; \\
& \sum_{j=1, j\neq i}^{n} x_{ij} = 1 && i = 1, \ldots, n; \\
& u_i - u_j + n x_{ij} \leq n - 1 && 2 \leq i \neq j \leq n; \\
& 1 \leq u_i \leq n - 1 && 2 \leq i \leq n; \\
& x_{ij} \in \{0, 1\} && i, j = 1, \ldots, n; \\
& u_i \in \mathbb{Z} && i = 2, \ldots, n.
\end{aligned} \tag{1}$$

This is the Miller-Tucker-Zemlin formulation[20]. Note that in our case, since we are solving TSP exactly, all variables are integers. This type of integer linear programming is sometimes known as **pure integer programming**.

3.2 Solving the Integer Linear Program

Since integer programming is an NP-Hard problem, there is no known polynomial algorithm that can solve this explicitly. Hence, the modern approach to such a problem is to **relax** the integrality constraint, which makes Equation 1 becomes continuous linear programming (LP), whose solution provides a lower bound to Equation 1 since it is a relaxation, and we are trying to find the minimum.

Since an LP is a convex optimization problem, we have many polynomial-time algorithms to solve the relaxed version. After obtaining a relaxed solution, if such LP relaxed solution respects the integrality constraint, we see that it's indeed a solution to Equation 1. But if not, we can simply divide the original relaxed LP into two sub-problems by **splitting the feasible region** according to a variable that does not respect integrality in the current relaxed LP solution $\boldsymbol{x}^*$,

$$x_i \leq \lfloor x_i^* \rfloor \vee x_i \geq \lceil x_i^* \rceil, \qquad \exists i \leq p \mid x_i^* \notin \mathbb{Z}. \tag{2}$$

We see that by adding such additional constraints in two sub-problems respectively, we get a recursive algorithm called **Branch-and-Bound** [26]. The branch-and-bound algorithm is widely used to solve integer programming problems. We see that the key step in the branch-and-bound algorithm is selecting a non-integer variable to branch on in Equation 2. And as one can expect, some choices may reduce the recursive searching tree significantly [2], hence the *branching rules* are the core of modern combinatorial optimization solvers, and it has been the focus of extensive research [18, 22, 10, 1].

3.3 Branching Strategy

There are several popular strategies [3] used in modern solvers.

Strong branching. Strong branching is guaranteed to result in the smallest recursive tree by computing the expected bound improvement for **each** candidate variable before branching by finding solutions of two LPs for every candidate. However, this is extremely computationally expensive. [4]

Hybrid branching. Hybrid branching computes a strong branching score at the beginning of the solving process, but gradually switches to other methods like Conflict score, Most Infeasible branching, or some other, hand-crafted, combinations of the above. [3, 1].

Pseudocost branching. This is the default branching strategy used in SCIP. By keeping track of each variable x_i the change in the objective function when this variable was previously chosen as the variable to branch on, the strategy then chooses the variable that is predicted to have the most change on the objective function based on past changes when it was chosen as the branching variable[22].

4 Problem Formulation

In order to solve TSP with ILP efficiently, we use the branch-and-bound algorithm. Specifically, we want to take advantage of the fast inference time and the learning ability of the model, hence we choose to learn the most powerful branching strategy known: strong branching. Our objective is then to learn branching strategy without expensive evaluation. Since this is a discrete-time control process, we model the problem by Markov Decision Process (MDP) [15].

4.1 Markov Decision Process (MDP)

Given a regular Markov decision process $\mathcal{M} := (\mathcal{S}, \mathcal{A}, p_{\text{init}}, p_{\text{trans}}, R)$, we have the state space $\mathcal{S}$, action space $\mathcal{A}$, initial state distribution $p_{\text{init}} : \mathcal{S} \to \mathbb{R}_{\geq 0}$, state transition distribution $p_{\text{trans}} : \mathcal{S} \times \mathcal{A} \times \mathcal{S} \to \mathbb{R}_{\geq 0}$ and the reward function $R \colon \mathcal{S} \to \mathbb{R}$. One thing to note is that the reward function R need not be deterministic. In other words, we can define R as a random function which will take a value based on a particular state in $\mathcal{S}$ with some randomness. Note that if R in $\mathcal{M}$ is equipped with any kind of randomness, we can write the reward r_t at time t as $r_t \sim p_{\text{reward}}(r_t \mid s_{t-1}, a_{t-1}, s_t)$. This can be converted into an equivalent Markov Decision Process $\mathcal{M}'$ with a deterministic reward function R', where the randomness is integrated into parts of the states. With an action policy $\pi \colon \mathcal{A} \times \mathcal{S} \to \mathbb{R}_{\geq 0}$ such that the action a_t taken at time t is determined by $a_t \sim \pi(a_t \mid s_t)$, we see that an MDP can be unrolled to produce a *trajectory* composed by state-action pairs as $\tau = (s_0, a_0, s_1, a_1, \ldots)$ which obeys the joint distribution

$$\tau \sim \underbrace{p_{\text{init}}(s_0)}_{\text{initial state}} \prod_{t=0}^{\infty} \underbrace{\pi(a_t \mid s_t)}_{\text{next action}} \underbrace{p_{\text{trans}}(s_{t+1} \mid a_t, s_t)}_{\text{next state}}$$

4.2 Partially Observable Markov Decision Process (PO-MDP)

Following from the same idea as MDP, the PO-MDP setting deals with the case that when the **complete** information about the current MDP state $\mathcal{S}$ is unavailable or not necessarily for decision-making [27]. Instead, in our case, only a partial **observation** $o \in \Omega$ is available, where Ω is called the **partial state space**. We can use an active perspective to view the above model; namely, we are merely applying an observation function $O\colon \mathcal{S} \to \Omega$ to the current state s_t at each time step t. Hence, we define a PO-MDP $\widetilde{\mathcal{M}}$ as a tuple $\widetilde{\mathcal{M}} \coloneqq (\mathcal{S}, \mathcal{A}, p_{\text{init}}, p_{\text{trans}}, R, O)$. Within this setup, a trajectory of PO-MDP takes form as $\tau = (o_0, r_0, a_0, o_1, r_1, a_1, \ldots)$, where $o_t \coloneqq O(s_t)$ and $r_t \coloneqq R(s_t)$. It is important to note that here r_t still depends on the state of the OP-MDP, **not** the observation. We introduce a convenience variable $h_t\colon (o_0, r_0, a_0, \ldots, o_t, r_t) \in \mathcal{H}$, which represents the PO-MDP history at time step t **without the action** a_t. Due to the non-Markovian nature of the trajectories, $o_{t+1}, r_{t+1} \not\perp h_{t-1} \mid o_t, r_t, a_t$, the decision-maker must take the whole history of observations, rewards and actions into account to decide on an optimal action at the current time step t. We then see that action policy for PO-MDP takes the form $\widetilde{\pi}\colon \mathcal{A} \times \mathcal{H} \to \mathbb{R}_{\geq 0}$ such that $a_t \sim \pi(a_t \mid h_t)$.

4.3 Markov Control Problem

We define the MDP control problem as that of finding a policy $\pi^*\colon \mathcal{A} \times \mathcal{S} \to \mathbb{R}_{\geq 0}$ which is optimal with respect to the expected total reward. That is,

$$\pi^* = \arg\max_{\pi} \lim_{T\to\infty} \mathbb{E}_{\tau}\left[\sum_{t=0}^{T} r_t\right]$$

where $r_t \coloneqq R(s_t)$. To generalize this into a PO-MDP control problem, similar to the MDP control problem, the objective is to find a policy $\widetilde{\pi}^*\colon \mathcal{A} \times \mathcal{H} \to \mathbb{R}_{\geq 0}$ such that it maximizes the expected total rewards. By slightly abusing the notation, we simply denote this learned policy by $\widetilde{\pi}^*$ where the objective function is completely the same as in the MDP case.

5 Methodology

Since the branch-and-bound variable selection problem can be naturally formulated as a Markov decision process, a natural machine learning algorithm to use is reinforcement learning [25]. Specifically, since there are some SOTA integers programming solvers out there, `Gurobi`[14], `SCIP`[5], etc., we decided to try imitation learning[16] by learning directly from an expert branching rule. There are some related works in this approach [11] aiming to tackle **mixed integer linear programming** (MILP) where only a portion of variables have integral constraints, while other variables can be real numbers. Our approach extends this further. We are focusing on TSP, which not only is pure integer programming, but also the variables can only take values from $\{0, 1\}$.

5.1 Learning Pipeline

Our learning pipeline is as follows: we first create some random TSP instances and turn them into ILP. Then, we use imitation learning to learn how to choose the **branching target** at each branching. Our GNN model produces a set of actions with the probability corresponding to each possible action (in our case, which variable to branch). We then use **Cross-Entropy Loss** to compare our prediction to the result produced by `SCIP` and complete one iteration.

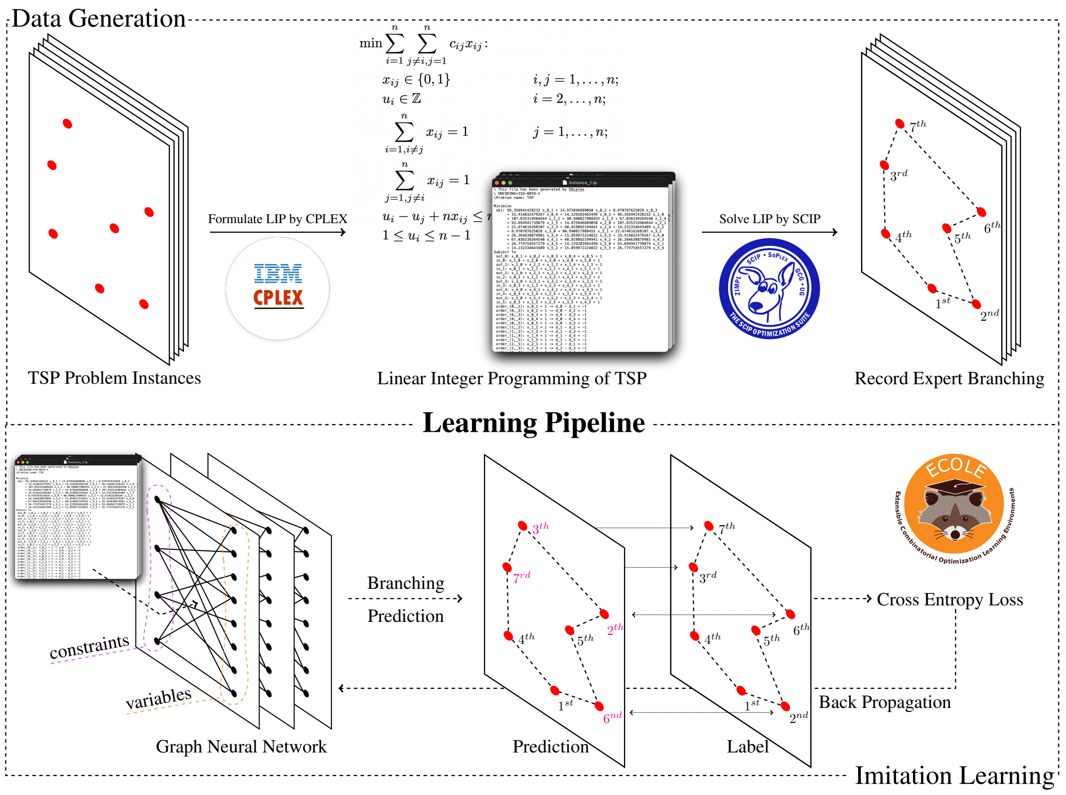
Instances Generation. For each TSP instance, we randomly generate the coordinates for every node and formulate it by using Miller-Tucker-Zemlin formulation[20] and record it in the linear programming format called `instances_*.lp` via `CPlex`[8].

Samples Generation. By passing every `instances_*.lp` to `SCIP`, we can record the branching decision solver made when solving it. The modern solver usually uses a mixed branching strategy to balance the running time, but since we want to learn the best branching strategy, we ask `SCIP` to use strong branch with some probability when branching, and only record the state and branching decision (state-action pairs) $\mathcal{D} = \{(s_i, \boldsymbol{a}_i^*)\}_{i=1}^{N}$ when `SCIP` uses strong branch.

Imitating Learning. We learn our policy $\widetilde{\pi}^*$ by minimizing the cross-entropy loss

$$\mathcal{L}(\theta) = -\frac{1}{N} \sum_{(\boldsymbol{s}, \boldsymbol{a}^*) \in \mathcal{D}} \log \widetilde{\pi}_\theta(\boldsymbol{a}^* \mid \boldsymbol{s})$$

to train by behavioral cloning[23] from the state-action pairs we recorded.


Data Generation
$\min \sum_{i=1}^{n} \sum_{j\neq i, j=1}^{n} c_{ij}x_{ij}:$
$x_{ij} \in \{0,1\}$ $i,j = 1,\ldots,n;$
$u_i \in \mathbb{Z}$ $i = 2,\ldots,n;$
$\sum_{i=1, i\neq j}^{n} x_{ij} = 1$ $j = 1,\ldots,n;$
$\sum_{j=1, j\neq i}^{n} x_{ij} = 1$
$u_i - u_j + nx_{ij} \leq$
$1 \leq u_i \leq n-1$
Formulate LIP by CPLEX
Solve LIP by SCIP
TSP Problem Instances
Linear Integer Programming of TSP
Record Expert Branching
Learning Pipeline
constraints
variables
Graph Neural Network
Branching
Prediction
Prediction
Label
Cross Entropy Loss
Back Propagation
Imitation Learning

Evaluation. We evaluate our model on TSP instances with various sizes to see the generalization ability. To compare the result of default `SCIP` performance to our learned branching strategy, we look at the wall-time needed for solving. Also, we look at the performance of the SOTA TSP solver to see the performance between our naive formulation and solving strategy and the SOTA solver which fully exploits the problem structure of TSP.

5.2 Policy Parametrization by GCNN

We use GCNN[13, 7, 21] to parametrize the variable selection policy. This specific choice is due to the natural problem structure of branch and bound decision process since we equipped our input with a *bipartite graph*[11], and utilize the message passing mechanism inherited by GCNN. Other models are compared in the Gasse et al.'[11], and GCNN outperforms all other models like LMART, SVMRANK, TREES, etc.

6 Experiments

Our implementation of the imitating learning model generally follows the work by Gasse et al[11] and depends on several packages[14, 5, 8, 24]. We test the generalization ability of our model trained with TSP10 and TSP15 on TSP instances with various sizes using GreatLakes with one A100 GPU and 8GB, 16 cores CPU. The figures below plot the wall-time needed for our model to solve a particular TSP instance as a direct comparison to our baseline `SCIP`, the solver we're imitating during the training phase, and also compare to the SOTA TSP solver `Concorde`.

Figure 1 and Figure 3 show the testing result of the models trained on TSP10 and TSP15, respectively. The analytical result is also shown in Table 1 and Table 2. Note that since some instances are much harder than others, we divide the data by the wall-time needed for `SCIP` and do a detailed comparison. Also, we compare the performance between `Concorde` and the TSP solving API provided by `Gurobi` in Figure 15 and Figure 16. The result is similar when the TSP size is small, so we didn't include the `Gurobi` result in the following plots.

Test Size	Avg. Walltime(s)		Avg. Improvement(s)			Avg. Improvement(%)		
	SCIP	GCNN	All	First 80	Last 20	All	First 80	Last 20
TSP10	0.507s	0.484s	0.022s	0.012s	0.063s	4.40%	3.41%	5.68%
TSP15	2.932s	2.764s	0.168s	0.090s	0.481s	5.73%	5.77%	5.71%
TSP20	50.794s	44.972s	5.822s	0.985s	25.174s	11.46%	7.14%	12.66%
TSP25	238.699s	231.872s	6.827s	3.527s	20.028s	2.86%	6.52%	2.05%

Table 1: Model Trained on TSP10

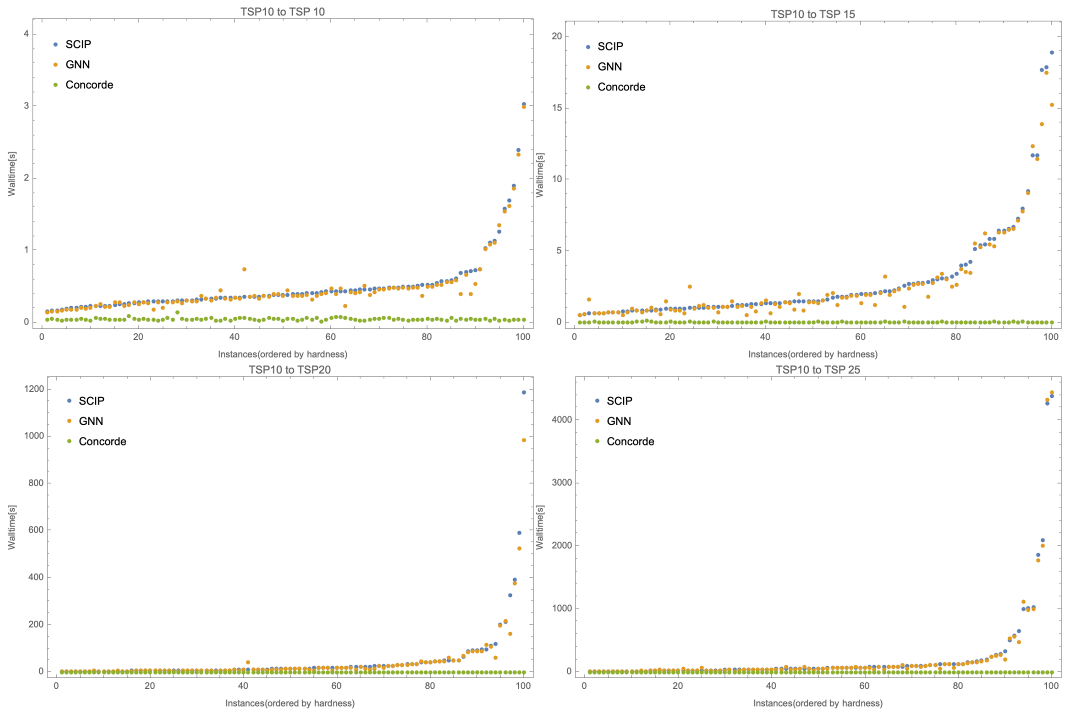


Figure 1: Result of model trained on TSP10 generalizes to TSP with various sizes.

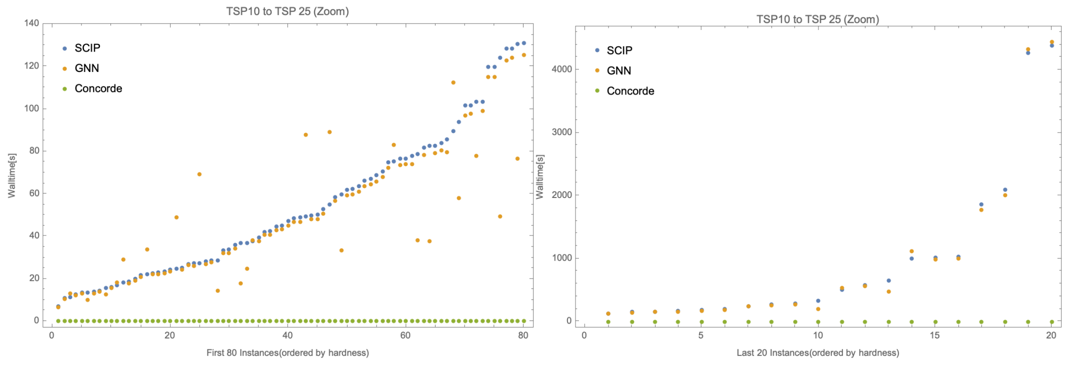


Figure 2: Result of model trained on TSP10 generalizes to TSP25 with zoomed-in.

Test Size	Avg. Walltime(s)		Avg. Improvement(s)			Avg. Improvement(%)		
	SCIP	GCNN	All	First 80	Last 20	All	First 80	Last 20
TSP10	0.490s	0.461s	0.028s	0.020s	0.063s	5.80%	5.60%	6.07%
TSP15	2.822s	2.661s	0.161s	0.050s	0.605s	5.70%	3.31%	7.48%
TSP20	49.020s	47.181s	1.8389s	0.878s	5.683s	3.75%	6.58%	2.96%
TSP25	256.253s	239.864s	16.389s	3.515s	67.886s	6.40%	6.56%	6.36%

Table 2: Model Trained on TSP15

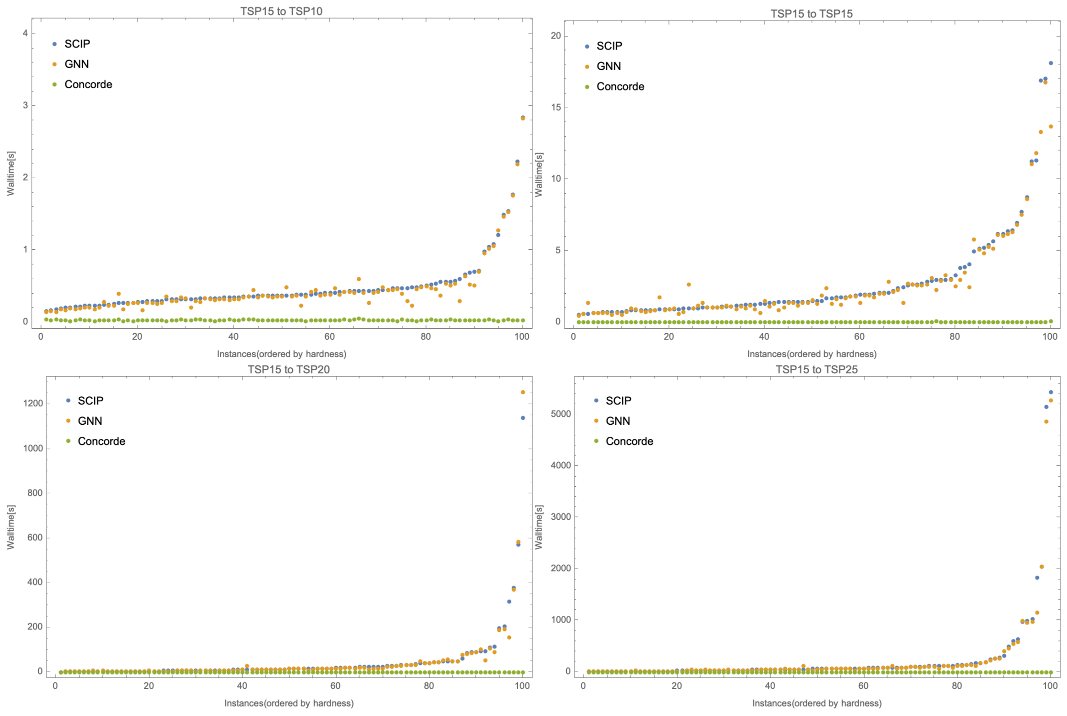


Figure 3: Result of model trained on TSP15 generalizes to TSP with various sizes.

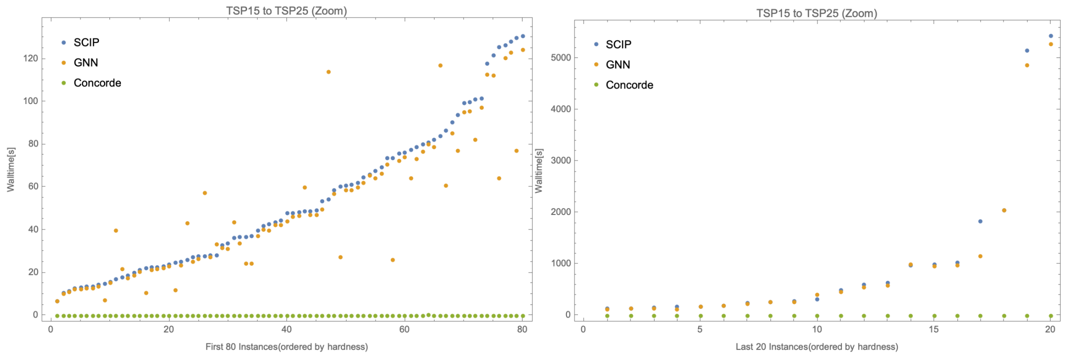


Figure 4: Result of model trained on TSP15 generalizes to TSP25 with zoomed-in.

The zoomed-in plots for other cases can be found in Appendix A.1 and Appendix A.2.

7 Discussion

7.1 Generalization Ability

We observe that our TSP10 and TSP15 imitation models outperform the `SCIP` solver on baseline test instances, and **successfully generalizes to TSP15, TSP20, and TSP25**. They perform significantly better on average than `SCIP` in difficult-to-solve TSPs as compared to easier instances. They also perform better in cases of larger test instances like TSP20 and TSP25 as compared to TSP10 and TSP15. This might be due to an inherent subset structure between TSP10 and TSP20 instances, and similarly TSP15 and TSP25 instances which might not be the case for smaller test sizes. Unlike other problems, when we formulate TSP as an ILP, the problem size is growing quadratically.[2] In other words, when we look at the model performance, the generalization ability from TSP10 to TSP25 is not a $2.5\times$, but rather a $6\times$ generalization in our formulation. By adapting this methodology on a more sophisticated algorithm which formulates TSP linearly, the generalization ability should remain and the performance will be even better in terms of TSP sizes.

Recent works on finding sub-optimal solutions of TSPs, have not been able to generalize well to large test instances[17]. Generalization ability is one of the most significant properties of Combinatorial Optimization algorithms due to the increasing computational complexity when the problem size scales up. Finding a sub-optimal solution maybe undesirable in a lot of real world applications since there is no guarantee on the approximation ratio of all machine learning approaches. Hence, our work is a vital step in this direction.

7.2 Bottlenecks and Future Work

There is a huge performance difference between our proposed model (also `SCIP`) and the SOTA TSP solver, `Concorde`. Since the proposed model's backbone is branch and bound algorithm, by formulating TSP into an ILP, we lost some useful problem structures which can be further exploited by algorithms used in `Concorde`. But the existence of a similar pattern of growth in solving time for more difficult instances of larger TSP sizes even for `Gurobi` and `Concorde` is promising (see Appendix A.3), as our imitation model applied to these solvers should lead to similar time improvements. A major bottleneck is that SOTA solvers like `Gurobi`, or `Concorde`, are often licensed, hence not open-sourced[14, 9]. This results in the difficulty of utilizing a stronger baseline and learn from which to get a further improvement.

On the other hand, the imitation method can be readily adapted to other algorithms where sequential decision-making is part of the optimization process. One promising avenue would be a direct adaption to cutting plane methods.[3] However, this might be difficult as modern solvers usually utilize different techniques **interchangeably**, which makes a direct adaption non-trivial.

Another concern is that the hyperparameters are not being cross-validated. This is essentially due to the computational and hardware limitations. We can increase the **entropy reward** when calculating cross-entropy for instances, which will motivate the model to be more active when searching for the optimum on the loss surface. We can also let `SCIP` use strong branch with different probabilities, the converging rate may change and can effect the performance as well.

8 Conclusion

Finding exact solutions of combinatorial optimization problems as fast as possible is a challenging avenue in modern theoretical CS. Our proposed method is a step toward this goal via machine learning. For nearly all exact optimization solving algorithms, there is some kind of *exhaustion* going on which usually involves decisions-making when executing the algorithm. For example, the cutting plane algorithm[12, 19] also involves decisions-making on variables when it needs to choose a variable to cut. We see that by using our model to replace several such algorithms, we can speed up the inference time while still retaining a high-quality decision strategy. Furthermore, our experimental results show that the model can effectively learn such strategies while using less time when inference, which is a promising strategy when applied to other such algorithms.

[2]This due to the growth rate of edges is quadratic and the number of variables (also constraints) depends on the number of edges directly.

[3]Specifically, Ecole[24] is working on this. See `https://github.com/ds4dm/ecole/issues/319`.

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Appendix

A Additional Experimental Results

A.1 Model Trained on TSP10

A.1.1 Full Size Plots

We include the full-size plots for the testing result on the model trained with TSP10.

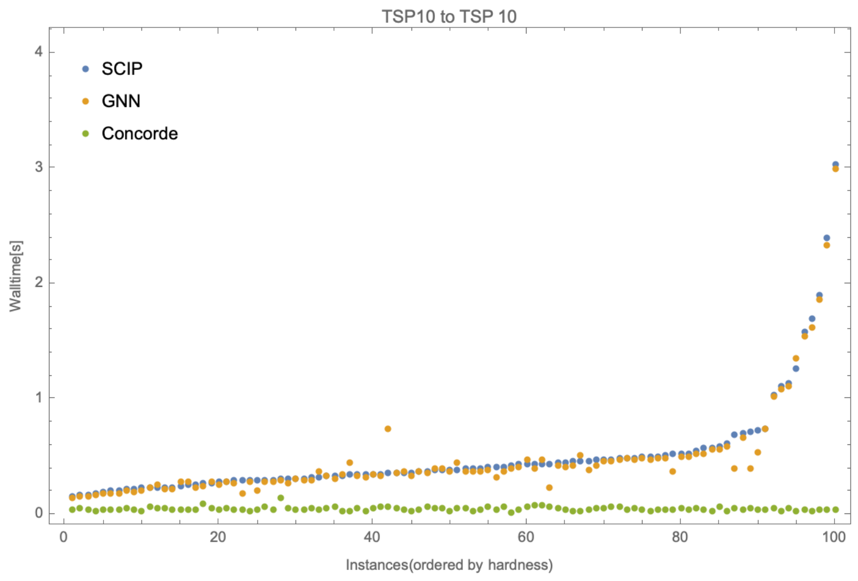

Figure 5: Test on TSP10

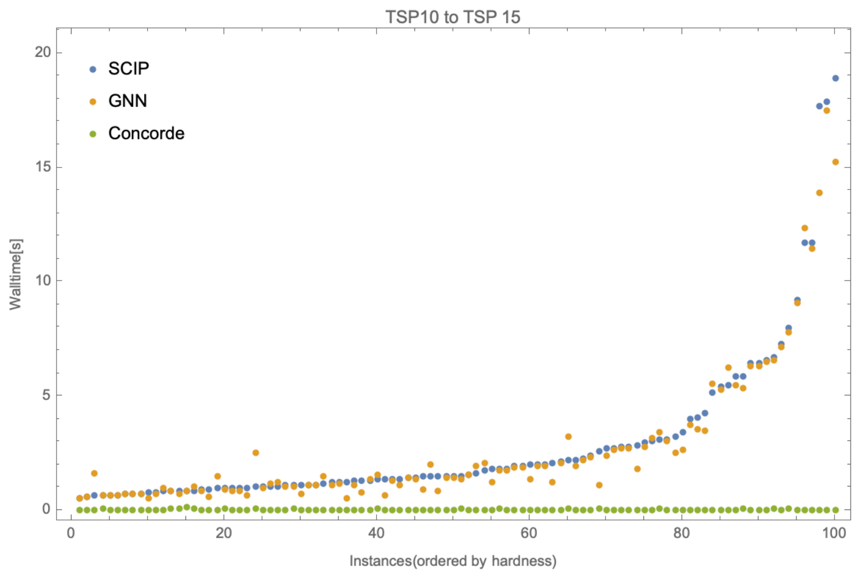

Figure 6: Test on TSP15

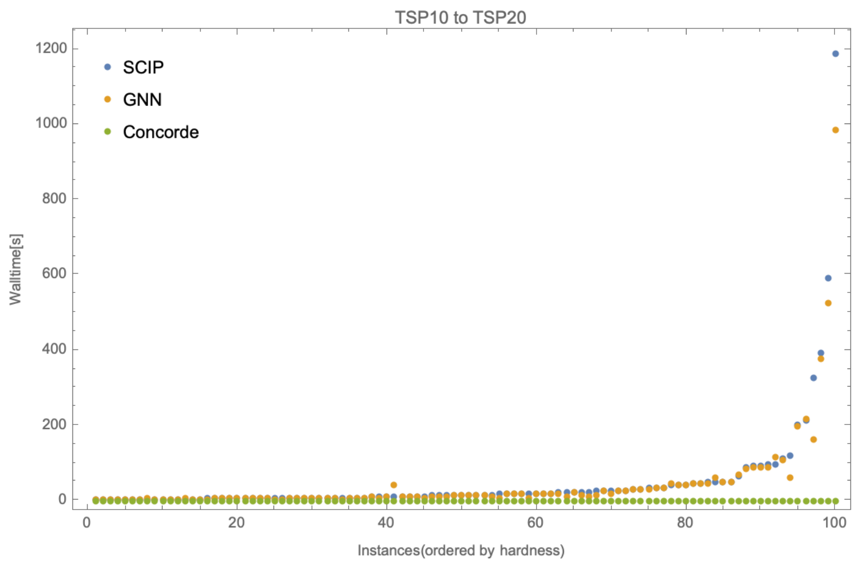

Figure 7: Test on TSP20

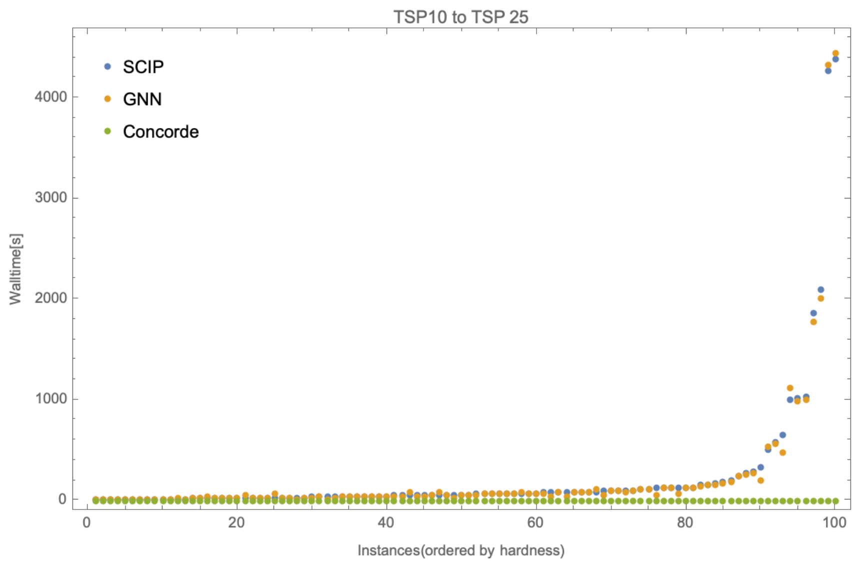

Figure 8: Test on TSP25

A.1.2 Zoom In Plots

We include the zoom-in plots for the testing result on the model trained with TSP10.

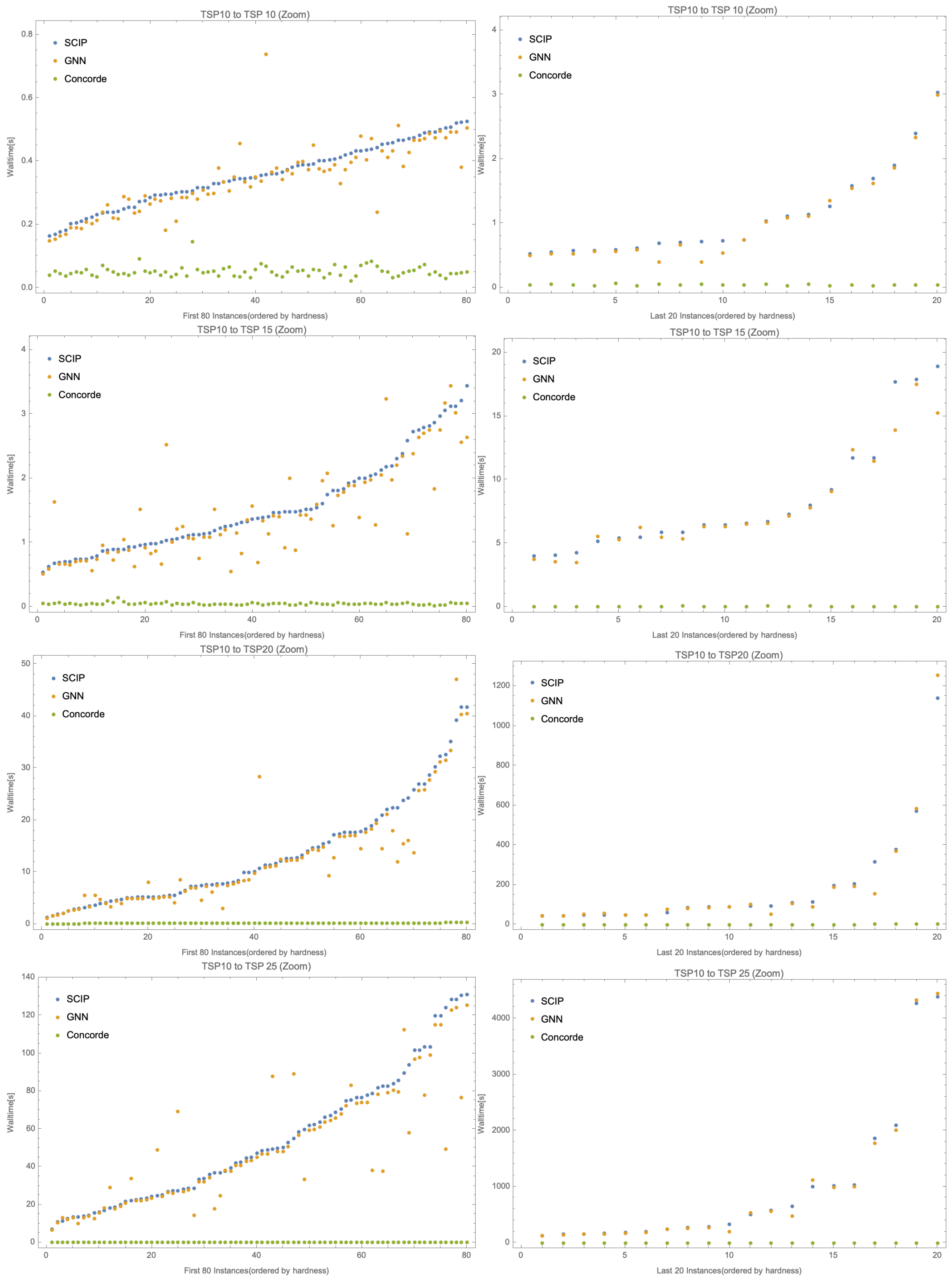

Figure 9: Result of model trained on TSP10 generalizes to TSP with various sizes with zoomed-in.

A.2 Model Trained on TSP15

A.2.1 Full Size Plots

We include the full-size plots for the testing result on the model trained with TSP15.

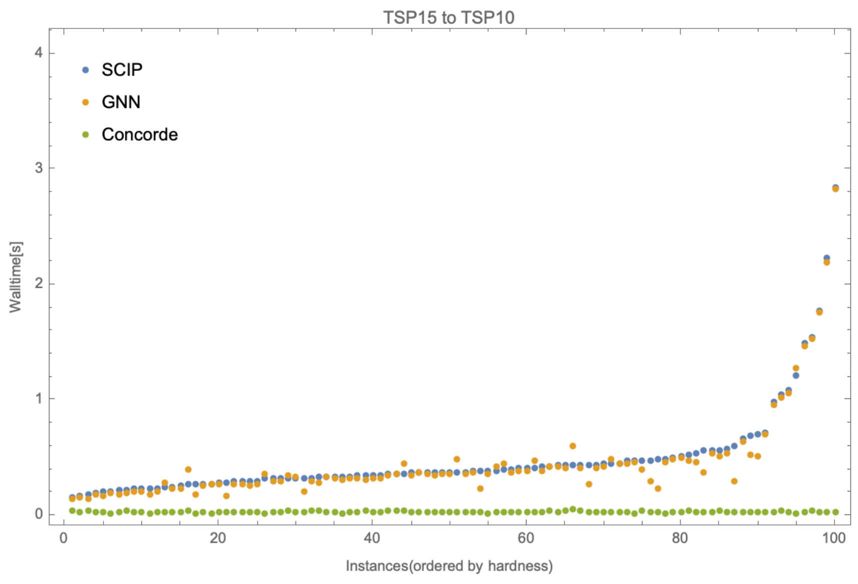

Figure 10: Test on TSP10

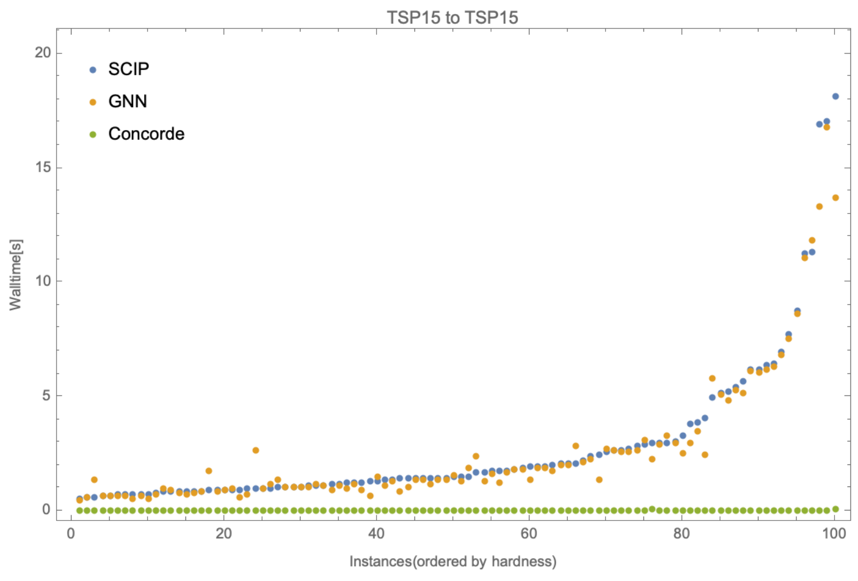

Figure 11: Test on TSP15

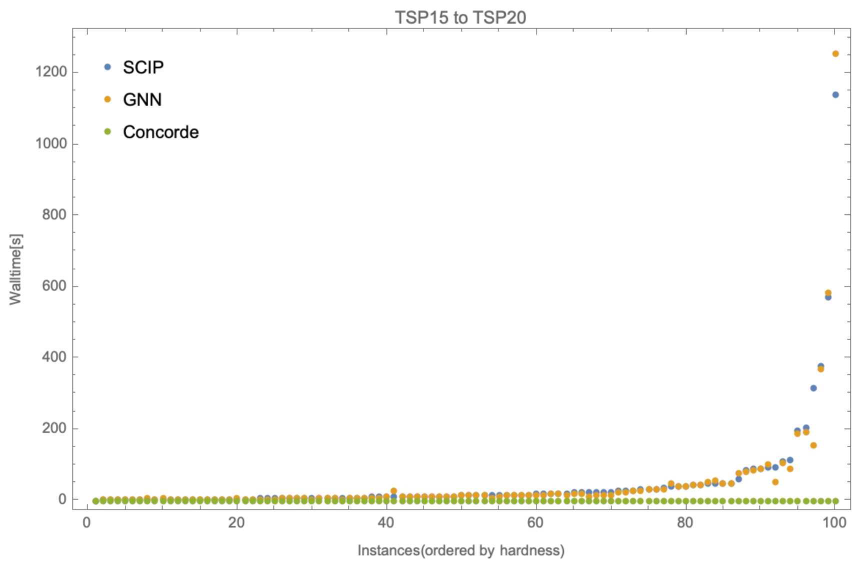

Figure 12: Test on TSP20

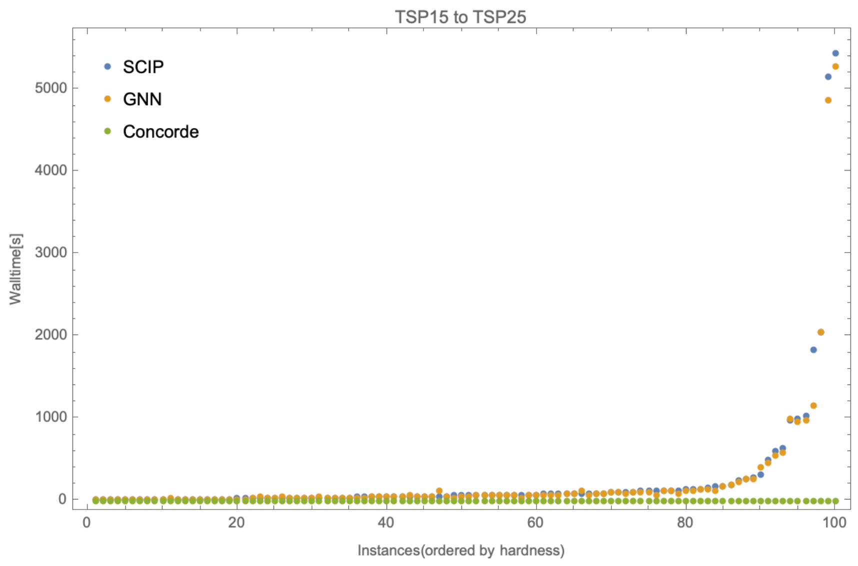

Figure 13: Test on TSP25

A.2.2 Zoom In Plots

We include the zoom-in plots for the testing result on the model trained with TSP15.

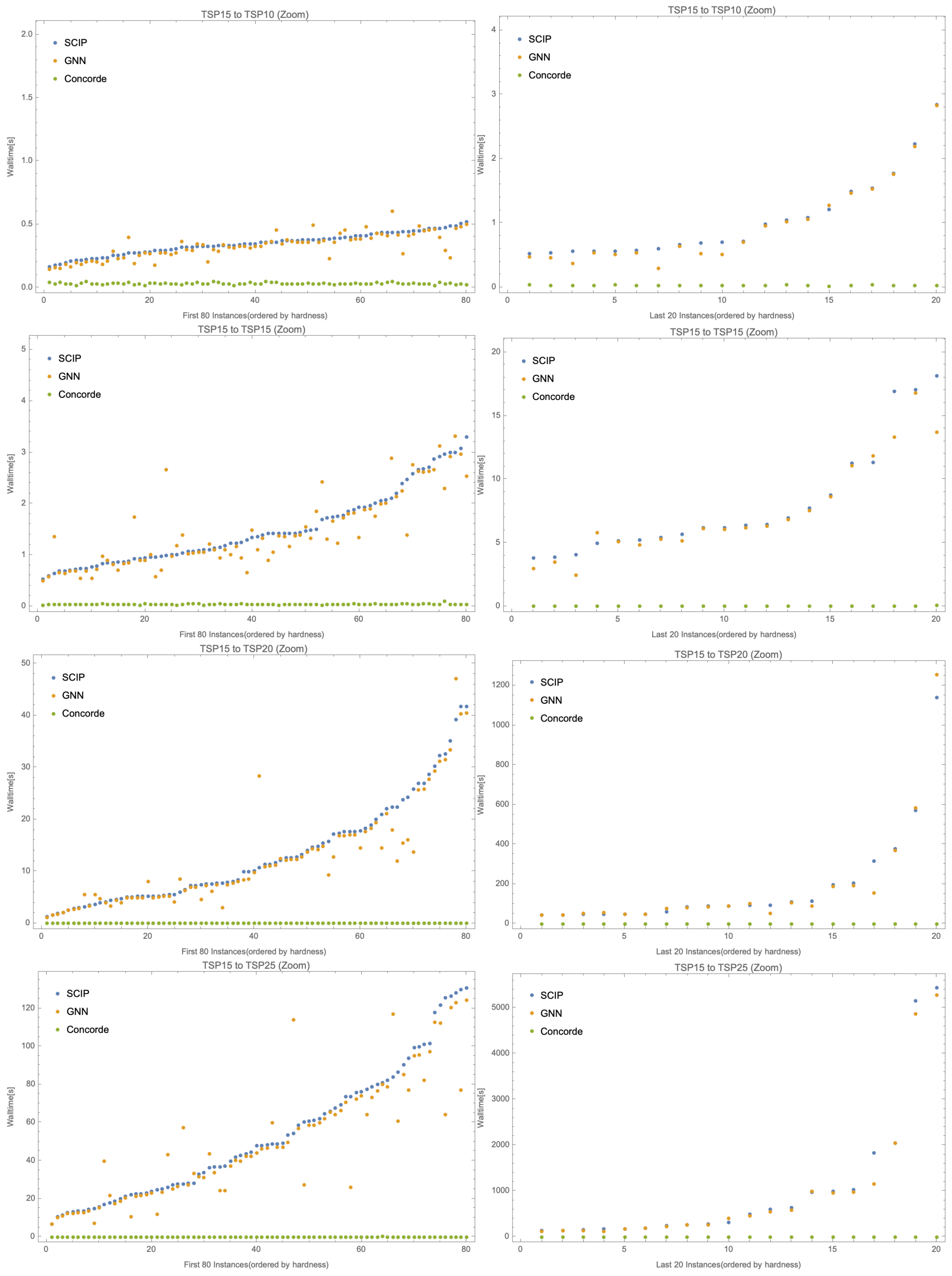

Figure 14: Result of model trained on TSP15 generalizes to TSP with various sizes with zoomed-in.

A.3 Comparison between `Gurobi` and `Concorde`

As a sanity check, we compare the performance between `Concorde` and the TSP API provided by `Gurobi`.

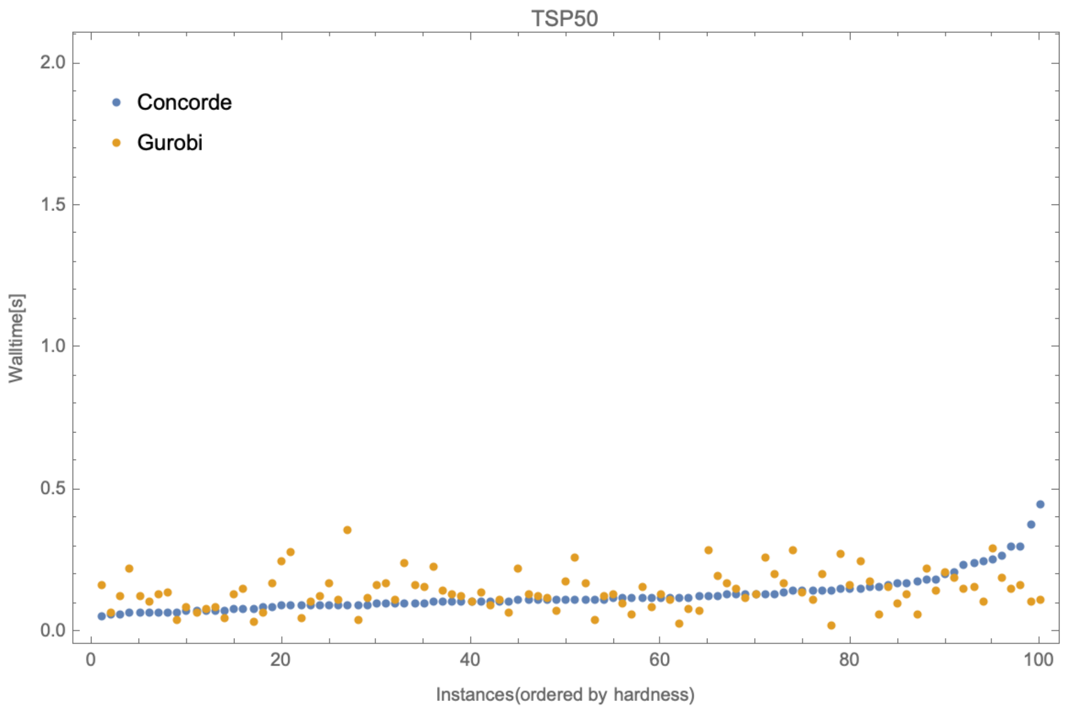

Figure 15: `Concorde` v.s. `Gurobi` on TSP50

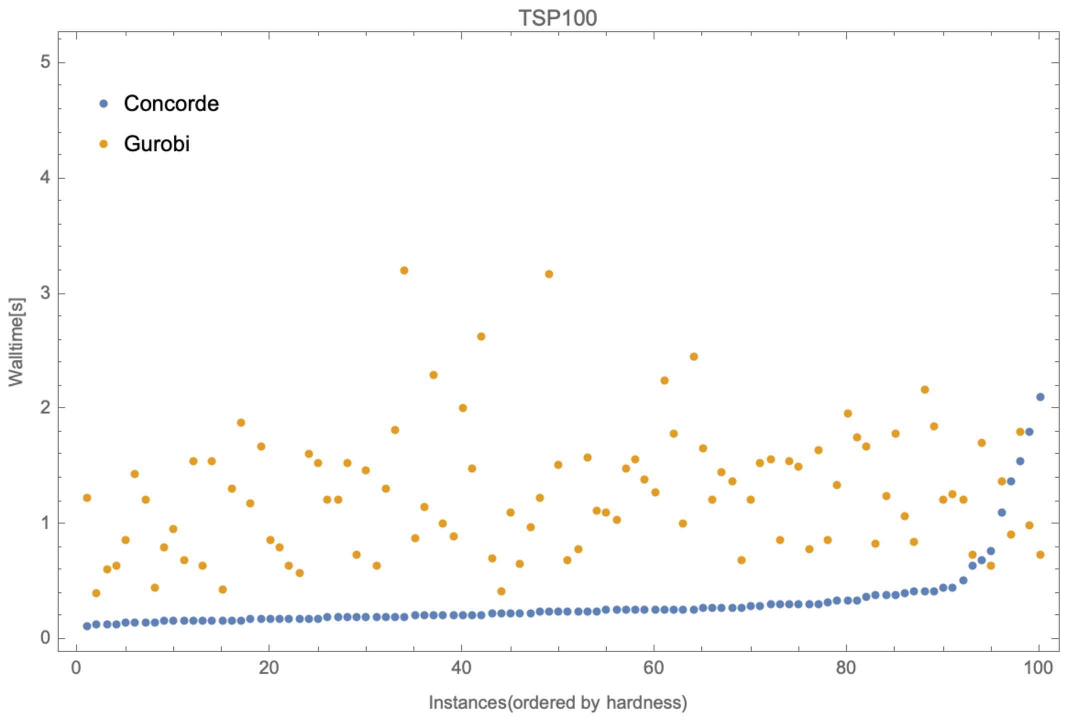

Figure 16: `Concorde` v.s. `Gurobi` on TSP100

B Author Contributions

All co-authors contributed equally to this project. All co-authors attended the meetings regularly for brainstorming ideas and reading relevant related-work. All co-authors worked on instance, sample generation and debugging. Yi and Jonathan summarized the literature on the current developments and drafted the abstract, introduction and related work. Yi, Pingbang, and Shubham worked on coming up with a learning pipeline framework. Yi, Pingbang, Anuraag, and Shubham worked on implementing the pipeline and running experiments. Pingbang was responsible for maintaining the github repository. Jonathan proofread and finalized the paper.