A Supervised Machine Learning Approach for the Vehicle Routing Problem

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Abstract: This paper expands on previous machine learning techniques applied to combinatorial optimisation problems, to approximately solve the capacitated vehicle routing problem (VRP). We leverage the versatility of graph neural networks (GNNs) and extend the application of graph convolutional neural networks, previously used for the Travelling Salesman Problem, to address the VRP. Our model employs a supervised learning technique, utilising solved instances from the OR-Tools solver for training. It learns to provide probabilistic representations of the VRP, generating final VRP tours via non-autoregressive decoding with beam search. This work shows that despite that reinforcement learning based autoregressive approaches have better performance, GNNs show great promise to solve complex optimisation problems, providing a valuable foundation for further refinement and study.

1 INTRODUCTION

The vehicle routing problem (VRP) is a classical and complex combinatorial optimisation problem in the field of operations research (OR). At its core, the problem involves finding the most efficient routes for a fleet of vehicles to visit a set of locations, while satisfying operational constraints. It is the generalised variant of the travelling salesman problem (TSP), for which there is only one vehicle (travelling salesman). The VRPs complexity and relevance across various sectors such as transportation, logistics, and supply chain management make it a significant subject. For example, the problem has practical applications in last-mile package delivery, the operations carried out by companies such as DPD, UPS and FedEx among others. With demand for last-mile delivery expected to grow by 78% by 2030, the world's top 100 cities (Hillyer, 2020) are expected to see an increase in delivery vehicles and therefore carbon emissions. Thus, improvements in route optimisation can have a positive impact on the global carbon footprint. This makes it important to study different views and approaches to realise these improvement in the near future.

To solve VRPs optimally, an approach like linear programming can be used to solve small-sized problem instances. However obtaining optimal solutions is challenging when the problem size increases due to the NP-hard nature (Archetti et al., 2011). To mitigate this issue, heuristic methods such as the Clarke & Wright's savings algorithm (Clarke and Wright, 1964) trade solution quality for reduced computation time, see (Konstantakopoulos et al., 2020) for a survey of these methods. Developing such heuristic methods is not trivial and often require experts domain knowledge, problem-specific assumptions and constraints. Furthermore, these heuristics fail to generalise to small changes in the inputs and need to be solved from scratch (Bogyrbayeva et al., 2022).

In recent years, machine learning (ML), with its ability to learn from and make decisions based on data, has emerged as a promising tool for solving complex problems. The strength of using ML is its ability to "learn" approximations of functions, without the need to explicitly formulate these functions (Bogyrbayeva et al., 2022). While combinatorial optimisation problems have traditionally been part of the OR community, this incredible versatility of ML has led to an increased interest in the ML community to tackle combinatorial optimisation problems without explicitly exploiting the structures of the mathematical models (Bai et al., 2023).

This paper aims to advance the ML and OR

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communities' intersection by using graph neural networks (GNNs) to address the challenging capacitated VRP. In the literature, two main methods are prevalent: supervised and reinforcement learning. Supervised learning (SL) approximates VRP solutions using training data, while reinforcement learning is employed when such solutions are unavailable. We investigate the effectiveness of a supervised ML approach in solving the capacitated VRP, which is an underexplored area, as discussed in the following section. To accomplish this, we extend the work of (Joshi et al., 2019), who applied a graph convolutional neural network (GCNN) to the TSP.

2 RELATED WORK

In 1985, Hopfield and Tank were the first to demonstrate the use of a neural network to solve the TSP (Hopfield and Tank, 1985), which is related to VRP. They used the Hopfield neural network converting the objective function of the problem into the energy function of the neural network. This allowed the network to find locally optimal solutions to the TSP with up to 30 nodes (cities). Most of the early literature in this area focused on tackling the TSP through Hopfield networks and self-organising feature maps (Smith, 1999).

Over the last two decades, there has been increasing interest in using neural networks to solve combinatorial optimisation problems, including a wide range of routing problems and their variants. A notable contribution is the introduction of the pointer network by (Vinyals et al., 2015), which consists of an encoder and decoder implemented as recurrent neural networks (RNNs). Using SL, the model is able to generate a probability distribution (heat-map) over the cities to be visited. During the inference stage, beams search is used to generate valid tours for the TSP. Although this approach gave promising results for the TSP instance with up to 30 nodes, it faced challenges when handling larger instances of up to 40 or 50 nodes. To address this limitation, (Bello et al., 2017) extended the approach by incorporating reinforcement learning with an actor-critic scheme, which led to improved performance for TSP instances with up to 100 nodes. This work was further extended by (Deudon et al., 2018) and (Kool et al., 2019). Their models performs comparable to methods such as Concorde, LKH3 and Gurobi, and outperforms approaches by (Vinyals et al., 2015), (Bello et al., 2017), (Khalil et al., 2017) and (Nowak et al., 2017) for the TSP. To address the dynamic nature of the VRP, (Peng et al., 2020) extend (Kool et al., 2019) with a dynamic attention model consisting of a dynamic encoder-decoder architecture. Another notable contribution for solving VRPs with neural networks is the work done by (Nazari et al., 2018). This allowed them to solve the capacitated VRP and its variants; split-delivery and stochastic VRPs. The model was trained with an actor-critic scheme, and the solution was obtained by beam search.

Several approaches exist that employ SL instead of reinforcement learning. For instance, (Prates et al., 2019) trains a GNN to determine if a TSP tour with a cost below a given threshold exists. (Nowak et al., 2017) and (Joshi et al., 2019) take an end-to-end approach, training GNN and GCNN models to output probable edge connections between nodes non-autoregressively, converting these connections into valid TSP tours using beam search. While Joshi's approach outperforms autoregressive methods (Vinyals et al., 2015; Bello et al., 2017; Khalil et al., 2017; Kool et al., 2019), it faces limitations as instance sizes increase. The work in (Fu et al., 2021) addresses large-scale TSPs by dividing the graph into subgraphs, training a model to produce probability matrices for each subgraph, and using Monte Carlo tree search (MCTS) to find solutions. Duan (Duan et al., 2020) combines reinforcement and SL, using a GCNN encoder and two decoders to effectively solve VRPs based on real-world data.

There are hybrid methods that combine ML with non-learning techniques. (Kool et al., 2022) replaces beam search with dynamic programming to solve TSP and VRP, tackles (Li et al., 2021) large-scale VRP by iteratively improving solutions with SL and a mixed integer linear solver and (Hottung and Tierney, 2020) uses a deep neural network trained by policy gradient reinforcement learning to enhance large neighbourhood search (LNS) operators, outperforming other LNS algorithms and previous ML-based methods.

In this work, we propose to extend the work by (Joshi et al., 2019) to address the capacitated VRP.

3 METHODOLOGY

3.1 General Overview

Given a VRP graph with n nodes as input, our approach is to train a GNN through SL to output an adjacency matrix $P = \{p_{ij}\}_{i,j=0}^{n}$ corresponding to the tours of the VRP. Each entry $p_{ij} \in [0,1]$ represents the probability that nodes i and j are connected in the VRP solution. We use beam search to decode the probabilistic matrix P and output the final sequence of nodes of the VRP tours.

Our proposed model[1] uses the GCNN presented by (Joshi et al., 2019) for the TSP, but we adapt the network architecture to support the VRP. The model takes node and edge features as input and learns an initial representation (embedding) vector for each node and edge. The embedding vectors are updated by passing through a series of graph convolution layers and exchanging information between adjacent nodes and edges. This is known as the *message-passing* framework, where at each layer (iteration) nodes and edges aggregate information (the messages) from their local neighbourhood (Hamilton, 2020). This is the main idea that distinguishes standard neural networks from GNNs. This is a powerful mechanism because after passing through L layers, node i and edge (ij) will have aggregated feature information from their L-hop neighbours into their own feature vectors. This allows the GNN to incorporate the structural (graph-like) nature of the problem.

The edge embedding vector from the last graph convolution layer is passed through a multilayer perceptron (MLP) to independently predict for each edge whether it is part of the VRP solution or not. Finally, we use a decoding strategy known as beam search to take the edge predictions and generate a final VRP solution.

3.2 Graph Convolutional Network for Vehicle Routing Problem

3.2.1 Input Layer

The model receives node and edge features as input. The input layer is responsible for projecting the initial feature vectors into a h-dimensional latent space. We extend the approach of (Joshi et al., 2019) to support VRP by adding two additional node features and removing one of the edge features, the edge type indicator matrix. Each node i has an input feature vector $z_i = [x_i \; q_i \; t_i]$, where x_i is the two-dimensional location, q_i is the demand, and t_i is a node token. For the depot node $t_0 = 1$ and for all other nodes $t_i = 0$. Without loss of generality, we normalise the demand with respect to the vehicle capacity per dataset. The node feature vector is embedded in h dimensional space:

$$\alpha_i = A_1 z_i + b_1 \tag{1}$$

where $A_1 \in \mathbb{R}^{h\times 4}$ and and b_1 are a trainable parameter matrix and bias term, respectively. The Euclidean distance d_{ij} is embedded as a h-dimensional edge feature vector β_{ij} defined as

$$\beta_{ij} = A_2 d_{ij} + b_2 \tag{2}$$

[1]Code and data are available at https://github.com/sebammon/vrp-thesis

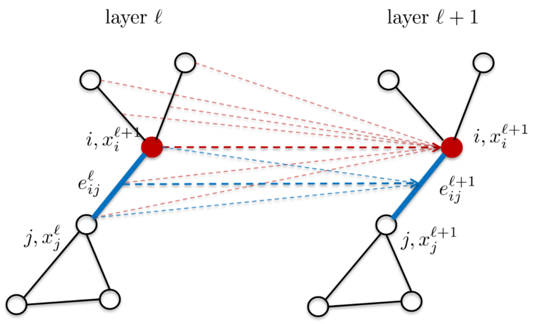


Figure 1: Illustration of how feature vectors at the next layer $\ell+1$ aggregate information from their neighbours at the previous layer ℓ. The dashed red and blue lines show the information flow for the node and edge features, respectively. Adapted from (Joshi et al., 2019).

where $A_2 \in \mathbb{R}^{h\times 1}$ and b_2 are a trainable parameter matrix and bias term, respectively. (Joshi et al., 2019) also define an edge type indicator matrix to signal k-nearest neighbours, self-connections and normal edge connection types. They argue that this speeds up learning since connected nodes in the TSP solution are often in close proximity. We experimented with this matrix but did not find that its presence improved the learning process or the quality of the solution.

3.2.2 Graph Convolution Layer

The graph convolution layer is responsible for updating the node and edge feature vectors by aggregating information from their local neighbourhoods. Let x_i^{ℓ} and e_{ij}^{ℓ} denote the node and edge feature vectors at layer ℓ, for $\ell = 0,\ldots,L$, associated with node i and edge (ij) respectively. In the input layer, $x_i^{\ell=0} = \alpha_i$ and $e_{ij}^{\ell=0} = \beta_{ij}$. The information aggregation for x_i^{ℓ} and e_{ij}^{ℓ}, at the next layer $\ell+1$ is:

$$x_i^{\ell+1} = \mathrm{UPD}^{\ell}\left(x_i^{\ell},\ \mathrm{AGG}^{\ell}\left(\{(x_j^{\ell},\ \eta_{ij}^{\ell}), \forall j \in \mathcal{N}(i)\}\right)\right)$$
$$e_{ij}^{\ell+1} = \mathrm{UPD}^{\ell}\left(e_{ij}^{\ell},\ \mathrm{AGG}^{\ell}\left(x_i^{\ell},\ x_j^{\ell}\right)\right)$$

where UPDATE (UPD) and AGGREGATE (AGG) are arbitrary differentiable functions (Hamilton, 2020), $\mathcal{N}(i)$ is the set of neighbours for node i (which are all nodes, since we use a fully connected input graph), and η_{ij}^{ℓ} are learnable edge gates. The edge gates allow the model to learn the relative importance of each neighbour of node i when aggregating their information. Figure 1 shows the flow of information between nodes and edges from one layer to the next.

More concretely, (Joshi et al., 2019) define the node and edge feature vectors as:

$$x_i^{\ell+1} = x_i^\ell + \text{ReLU}\left(\text{BN}\left(W_1^\ell x_i^\ell + \sum_{j\in\mathcal{N}(i)} \eta_{ij}^\ell \odot W_2^\ell x_j^\ell\right)\right)$$
$$\eta_{ij}^\ell = \frac{\sigma(e_{ij}^\ell)}{\sum_{j'\in\mathcal{N}(i)}\sigma(e_{ij'}^\ell)+\varepsilon},$$
$$e_{ij}^{\ell+1} = e_{ij}^\ell + \text{ReLU}\left(\text{BN}\left(W_3^\ell e_{ij}^\ell + W_4^\ell x_i^\ell + W_5^\ell x_j^\ell\right)\right),$$

where $W_1^\ell, W_2^\ell, W_3^\ell, W_4^\ell, W_5^\ell \in \mathbb{R}^{h\times h}$ are trainable parameter matrices, σ is the sigmoid activation function, $\odot$ is the Hadamard element-wise product, ε is a small value, ReLU is the rectified linear unit function and BN applies the batch normalisation (Ioffe and Szegedy, 2015). Due to the symmetric nature of the VRP, $W_4^\ell = W_5^\ell$.

3.2.3 Multilayer Perceptron Classifier

An MLP is a fully connected feedforward artificial neural network consisting of an input layer, hidden layers and an output layer. The MLP is used to independently compute the edge probability p_{ij}, i.e., the probability that edge (ij) is active in the final VRP solution, from the final edge feature vector e_{ij}^ℓ:

$$p_{ij} = \text{MLP}(e_{ij}^\ell) \tag{3}$$

The h dimensional hidden layers of the MLP are connected via the ReLU activation function. We apply a softmax activation function to the last layer to translate it to the range $[0,1]$.

3.2.4 Loss Function

The model is trained in a supervised fashion by minimising the weighted cross-entropy loss between the edges $P = \{p_{ij}\}_{i,j=0}^n$ predicted by the model and the ground truth edges $T = \{t_{ij}\}_{i,j=0}^n$ from the solver, where n is the number of nodes. Cross-entropy is a loss function commonly used for binary classification tasks, which is essentially what this problem is – an edge can be either active or inactive – defined as:

$$\text{Loss}_{ij} = \sum_{c=0}^{1} w_c \log(p_{ij}) I_{ij,c}, \tag{4}$$

where $I_{ij,c}$ is defined as the indicator function that takes the value of 1 if class is c, and 0 otherwise.

Since the adjacency matrix of VRP is usually sparse, i.e., there are many more inactive edges than active ones, (Joshi et al., 2019) provide the cross-entropy with the weights for each class. They state that the classification becomes highly unbalanced towards the negative class as the problem size increases and appropriate class weights are needed to mitigate this issue. The class weights for each class c, active or inactive, are calculated per dataset by:

$$w_c = \frac{n^2 \cdot \sum_{c=0}^{1} I_c}{2\cdot I_c}$$

where $I_c = \sum_{i,j=0}^{n} I_{ij,c}$ is the number of occurrences of class c, $\sum_{c=0}^{1} I_c$ is the number of instances in the dataset. The loss per training epoch is calculated as the average loss over all mini-batches.

3.3 Beam Search Decoding

The model outputs a probabilistic adjacency matrix of edges, where each entry p_{ij} indicates the probability that the edge (ij) is part of the VRP solution. This matrix cannot be converted directly into VRP routes, e.g., using the *argmax* function, as this may result in invalid tours with missing or redundant edges. A decoder is required to deal with this.

Beam search is a limited-width breadth-first search algorithm commonly used to generate highly probable output sequences for natural language processing tasks (Medress et al., 1977). It iteratively expands the next most likely nodes, keeping only the b most likely sequences found so far, where b refers to the beam width. This is a greedy algorithm as it only keeps a limited number of possible solutions.

Beam search decoding can be used to generate tours (a sequence of nodes) by expanding the most probable edges between nodes to form a tour. According to (Joshi et al., 2019), the probability of a partial tour π' is based on the chain rule of probability as:

$$p(\pi') = \prod_{j'\sim i'\in\pi'} p_{i'j'} \tag{5}$$

where each node j' follows node i' in the partial tour π'. Starting from the first node i, the beam search expands the b most probable edges from the probability adjacency matrix by exploring the neighbours of the node. At each iteration, the next b most probable partial tours are expanded until all nodes have been visited. To ensure that nodes are not visited more than once, (Joshi et al., 2019) use a masking strategy to hide previously visited nodes.

While the approach of (Joshi et al., 2019) works well for a single TSP tour, it is not directly applicable to VRP because it does not consider two points. First, the fact that each vehicle requires a tour; second, the capacity constraint of the vehicles. To address the first point, we adapt the masking strategy to hide the depot node only when it has been visited K many times, where K is the number of vehicles. The other nodes are masked as soon as they have been visited.

This translates into a tour per vehicle as follows: assuming a partial tour $\pi' = \{0,3,2,4,0,1,6,5\}$, where $K = 2$ and all $n = 6$ nodes have been visited, then the tours for the two vehicles can be extracted as $R_1 = \{0,3,2,4,0\}$ and $R_2 = \{0,1,6,5,0\}$.

To take into account the second point, namely the capacity constraints of the vehicles, we keep track of the remaining capacity of the vehicle after visiting the nodes of the partial tour. When expanding the next b-most probable partial tours, we hide nodes where the demand exceeds the remaining capacity of the vehicle (current tour), which is reset when the depot node is visited. We follow two beam search approaches to construct the final tours.

3.3.1 Standard Beam Search

Following the description above, we generate b most probable tours by specifying the beam width parameter. From these tours we select the one with the highest probability in Equation 5. However, the most probable tour is not guaranteed to be the shortest. For this reason, we only use this approach during the validation phase when training the model. Intuitively, the model improves its predictions as the probability of promising edges should increase while the probability of less promising edges should decrease. Using the most promising tour during training gives an indication for model improvement.

3.3.2 Shortest Tour Heuristic

In this approach, instead of selecting the most probable tour among the candidates, we select the shortest tour by evaluating and comparing the distance of each tour. This algorithm takes considerably more time to execute, so we only use it after training as a final evaluation of the model's performance.

4 EXPERIMENTAL DESIGN

4.1 Data Setup

The data is based on the VRP in the two-dimensional Euclidean plane. Given an input graph, we define a VRP instance with n customers (nodes) as a sequence of tuples $S = \{(x_i, q_i)\}_{i=0}^{n}$, where $x_i \in [0,1]^2$ is the location in the unit square and $q_i \in \{1,...,9\}$ is the demand. We add a special node at index 0, called the depot, with location x_0 and demand $q_0 = 0$. Additionally we define the cost of each edge between nodes i and j, to be the Euclidean distance $d_{ij} = \|x_i - x_j\|_2$.

The goal is to find a set of routes (vehicles) that start and stop at the depot, visiting each customer only once (across all routes), while minimising the total distance travelled. All vehicles are homogeneous and each vehicle has a (positive) capacity (κ) that may not be exceeded, so $\sum_{i \in R_k} q_i \leq \kappa$, where R_k is the set of nodes visited by vehicle $k \in \{1,...,K\}$.

To solve an instance to create training and validation instances, we use the VRP solver from the open source software suite OR-Tools (Perron and Furnon, 2023). The solutions it finds are not guaranteed to be optimal, as the solver uses heuristics along with metaheuristics to find approximate solutions. As input to the solver we give it a $n \times n$ distance matrix $D = \{d_{ij}\}_{i,j=0}^{n}$, the customer demand q_i, the depot node index $i = 0$, the vehicle capacity κ and the total number of available vehicles K. Additionally, we need to specify the heuristic and metaheuristic to be used by the solver. Here we used the *path cheapest arc* heuristic, as it is a constructive heuristic that incrementally builds the routes from the depot by adding the next node that produces the cheapest route segment (Perron and Furnon, 2023). For the metaheuristic, we opt for *Guided Local Search* (Voudouris et al., 2010), which guides the solver to escape local minima. The stopping criterion used for this approach is a time limit (in seconds). In order for the solver to consistently find good solutions for different problem sizes (number of nodes), we adjust the time limit for each generated dataset.

The obtained set of routes $\{R_k\}_{k=1}^{K}$ are then converted into an adjacency matrix $T^k = \{t_{ij}^k\}_{i,j=0}^{n}$, which constitutes target matrix for model training. For each entry in the target matrix, $t_{ij}^k = 1$ if nodes i and j are connected in route R_k, and 0 otherwise. Due to the symmetric nature of VRP, if nodes i and j are connected, then the reverse is also true, hence $t_{ij}^k = t_{ji}^k$.

4.2 Training Procedure

To train the ML model, we generate training and validation data. To explore the ability of the model to generalise to different problem sizes, we generate three different datasets, VRP10, VRP20 and VRP50 with 10, 20 and 50 customer nodes respectively. Following the approach of (Nazari et al., 2018), for each dataset we set the vehicle capacity to 20, 30 and 40 respectively and the number of available vehicles to 4, 5 and 10. For the datasets VRP10 and VRP20, we generate and solve 20,000 instances, of which 1,000 instances are kept as a validation set. We set the time limit for the metaheuristic to 1 and 3 seconds for each dataset. For the VRP50 dataset, with the larger 50 node instances, we increase the solver time limit to 8 seconds in order to obtain better solutions. This marginal increase has a significant impact on the running time for data generation. Thus, we only generate 10,000 instances, of which 500 are kept for validation. The model is trained separately on each dataset.

Different models are trained, each dedicated to one of the following datasets: VRP10, VRP20 and VRP50. The same hyperparameters are adopted for all models, allowing a comparative analysis. We use 32 hidden units, 12 GCN layers, 3 MLP layers. The model is trained by minimising the weighted cross-entropy loss between the predicted edges and the ground truth edges for each mini-batch. The loss minimisation task is performed using the stochastic gradient descent technique and Adam optimiser (Kingma and Ba, 2015), with a learning rate of 0.001, 50 epochs and a batch size of 64. Each training and validation dataset is divided into mini-batches of 64 instances. For each epoch of the training phase, the model makes one pass through the entire training dataset. Models are trained for 50 epochs. All computations are performed on the Nvidia T4 GPU provided by the Google Colab platform.

4.3 Evaluation Procedure

At the end of each epoch of the training process, we evaluate the performance of the model on the entire validation set. The predicted edge adjacency matrix is converted into a valid VRP tour using the *standard beam search* strategy described in Section 3.3.1, with a beam width of $b = 10$. The most likely of the candidate tours is selected. This approach encourages fast evaluation while still allowing exploration among the candidate tours to find the most likely tour.

To compare the quality of the tours found by the model with those obtained by the OR-Tools solver, we use the average optimality gap. Given the length l of the predicted tour and the length $\hat{l}$ of the solver tour, average optimality gap over m instances is:

$$\frac{1}{m}\sum_{i=1}^{m}\left(\frac{l_m}{\hat{l}_m}-1\right) \tag{6}$$

For the final evaluation of the model, we use the *shortest tour heuristic* (see Section 3.3.2) to convert the edge adjacency matrix into valid VRP tour candidates, from which we select the shortest. This allows us to sample routes from the b most likely candidates and select the best (shortest) ones. The size of the beam width b creates a trade-off between execution time and solution quality. A larger beam width explores more candidates at the expense of execution time, while a smaller beam width does the opposite. Figure 2 shows the trade-off between beam width and solution quality. For the beam width we choose $b = 1280$, similar to the choice made by (Joshi et al., 2019).

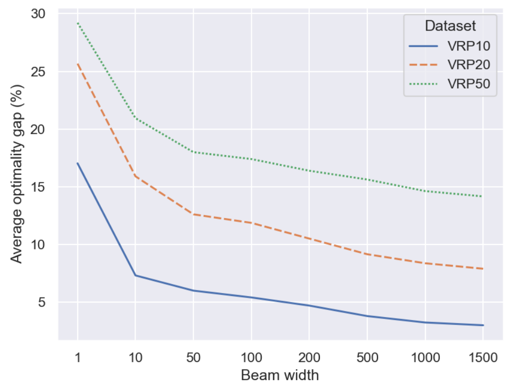


Figure 2: Trade-off between the beam width and the quality of the solution (average optimality gap) for different datasets.

Table 1: Average optimality gap with respect to OR-Tools for our model (GCN), the random baseline and the models of Kool (Kool et al., 2019) and Duan (Duan et al., 2020).

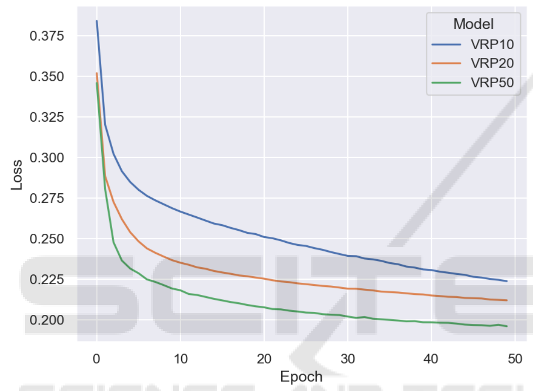
Model	Validation set		
	VRP10	VRP20	VRP50
OR-Tools	0.00%	0.00%	0.00%
Beam search:			
GCN	6.08%	16.06%	20.97%
Duan	-	-0.41%	-2.42%
Kool (greedy)	-	-0.47%	-2.90%
Random baseline	50.99%	105.38%	176.88%
Shortest tour:			
GCN	3.28%	8.69%	16.12%
Duan	-	-0.46%	-2.42%
Kool	-	-2.80%	-6.10%

5 RESULTS

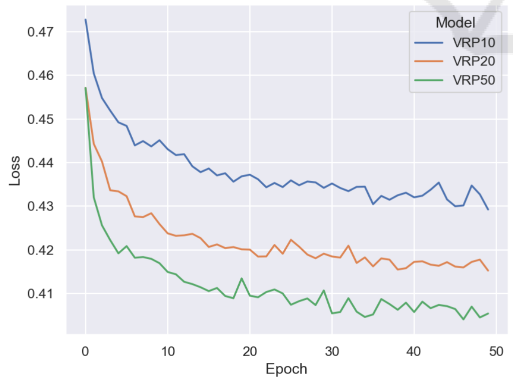
5.1 Average Optimality Gap Analysis

Table 1 shows the average optimality gap between the model (GCN) and the OR-Tools solver evaluated on all instances of the validation set. For comparison, we include the average optimality gap obtained using the *standard beam search* and *shortest tour heuristic* decoding strategies. We also include the random baseline results, where we apply the standard beam search to randomly generated edge probabilities. This comparison indicates of whether the model learns meaningful representations for solving VRP instances.

Next, we include results reported by (Kool et al., 2019) for the attention model and (Duan et al., 2020) for the GCN node model. They test their models on VRP20 and VRP50 datasets with instances generated in a similar way. They do not report their optimality gap with respect to OR tools.Also, their model does not have a decoding approach similar to our standard beam search strategy, so we present their greedy strategy, which is similar to setting $b = 1$. Our model clearly outperforms the random baseline by a factor of about 10, indicating that the model has learned representations that are useful for the decoding process. Across all datasets, the shortest tour heuristic model outperforms the standard beam search approach. This is to be expected when sampling more solutions and selecting the best among them. Second, our model falls short when compared to the reinforcement learning approaches of (Kool et al., 2019) and (Duan et al., 2020). These reinforcement learning models have the advantage of generating VRP tours in an autoregressive manner, making informed predictions about edge connections at each decoding step. In contrast, the non-autoregressive approach of the model generates edge predictions one-shot, which may not account for the capacity of the current partial tour.



(a) Training loss.



(b) Validation loss.

Figure 3: Training and validation loss for each model over 50 epochs.

5.2 Training Progress and Loss Curves

Figure 3 shows the training progress of the models over 50 epochs. The training and validation loss curves follow a similar trajectory, with a sharp decrease initially and a steady decrease afterwards. While the training loss follows a smoother path, the validation loss becomes more irregular, but there's no evidence of overfitting. The relationship between validation loss and average optimality gap is not straightforward, which is challenging for model evaluation and interpretation.

Table 2: Average optimality gap per model trained and evaluated on different problem sizes.

Model	Validation set		
	VRP10	VRP20	VRP50
GCN (VRP10)	*3.28%*	18.97%	52.86%
GCN (VRP20)	6.57%	*8.69%*	28.70%
GCN (VRP50)	5.79%	16.00%	*16.12%*

5.3 Generalization of the Model

Table 2 explores the generalisation of the model to different input sizes. Models trained on their respective datasets tend to outperform models generalizing to different datasets. Models trained on more complex problems seem to learn representations that are beneficial when solving less complex problems. The results suggest that models trained on less complex problems may not scale well.

6 CONCLUSIONS

In this paper, we introduced a supervised ML approach for solving VRP, harnessing the power of GCN. Our model effectively tackles VRP instances with 10, 20, and 50 customer nodes, delivering results that significantly surpass random baselines. This success underscores our model's capacity to acquire the essential knowledge needed for problem-solving. Nonetheless, reinforcement learning-based autoregressive methods still outperform our approach. Our model faces limitations when it comes to leveraging prior information for making informed predictions, especially regarding the edges. This becomes particularly critical in the context of VRP, where considering vehicle capacity is essential for valid routes.

While SL methods hold promising results, practical challenges arise. Large amounts of training data are required, especially for larger and more complex VRP problem instances. Generating such data demands significant time and resources, which increases with problem complexity increases. Finally, we indirectly demonstrated the expressive power of GNNs by extending the model architecture for TSP to support VRP. This shows that there is much potential for using GNNs to solve combinatorial optimisation problems. In order to improve model performance, future work can focus on different decoding strategies which are more appropriate the VRP problem complexity by using an autoregressive decoder.

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