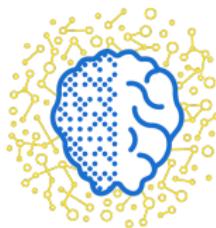


Dynamic Attention Model for Vehicle Routing Problems

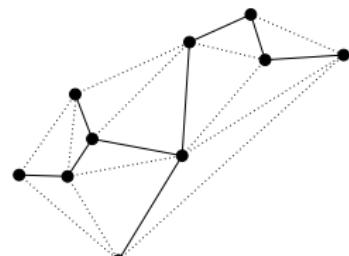
Dmitry Eremeev, Alexey Pustynnikov

Advanced Topics in Deep Reinforcement learning

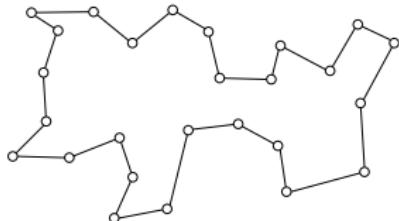
DeepPavlov.ai



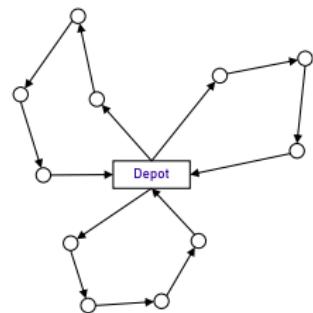
- Minimum spanning tree



- Travelling Salesman Problem

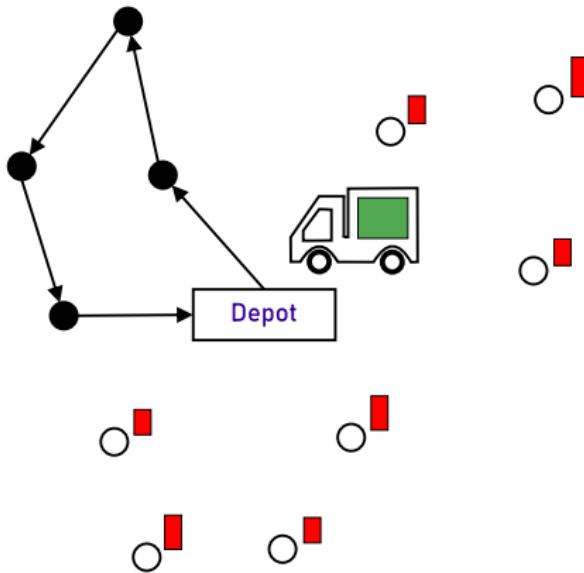


- Vehicle Routing Problem



Capacitated Vehicle Routing Problem

Particular case of VRP: 1 vehicle with a limited carrying capacity.



- Complete graph

$$X = (V, E),$$

with set of nodes

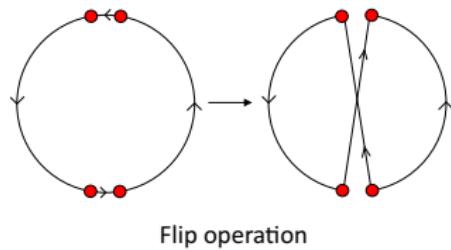
$$V = \{x_0 \equiv D, x_1, x_2, \dots, x_n\}.$$

- Each node is associated with a demand d_i , $d_i < C$, $d_D = 0$.
- Each edge is associated with a cost c_{ij} (L^2 -norm).
- A vehicle with capacity C is moving along graph starting from depot node D . Every non-depot node x_k can be visited only once. It is allowed to return to D arbitrary many times.
- Goal: find a path $\pi = \{\pi_1, \dots, \pi_T\}$, $\pi_t \in V$ that minimizes **total cost**.

- VRP is an **NP-hard** problem (Lenstra and Rinnooy Kan, 1981). Exact algorithms are only efficient for small problem instances.
- The number of near-optimal algorithms are introduced in academic literature. There are multiple professional tools for solving various VRP problems (ex. Google OR-Tools).

LKH algorithm: highly effective

- implementation (Helsgaun-2000, ...) of Lin-Kernighan (1973) heuristic.



- 1) Generate random initial solution.
- 2) Construct the alternating path by a sequence of flip operations.
- 3) These flips replace k edges x_i in current tour (circle) by edges y_i which are NOT in current tour. Keep increasing k as long as cost decreasing.

Deep Learning for VRP

ATTENTION, LEARN TO SOLVE ROUTING PROBLEMS!

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A Deep Reinforcement Learning Algorithm
Using Dynamic Attention Model for Vehicle
Routing Problems

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Department of Computer Science, Sun Yat-sen University, Guangzhou, China

[arXiv:1803.08475 \[stat.ML\]](https://arxiv.org/abs/1803.08475)

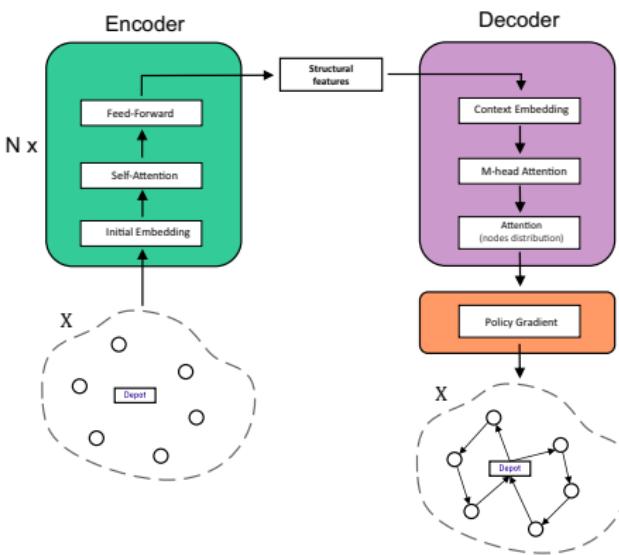
[arXiv:2002.03282 \[cs.LG\]](https://arxiv.org/abs/2002.03282)

Share common idea: utilize Reinforcement Learning (RL) to generate solutions

- Make use of Graph Attention Networks (GAT) to obtain graph embeddings.
- Train RL agent that can learn heuristics and provide suboptimal solutions.

Differ in their approaches to generating embeddings

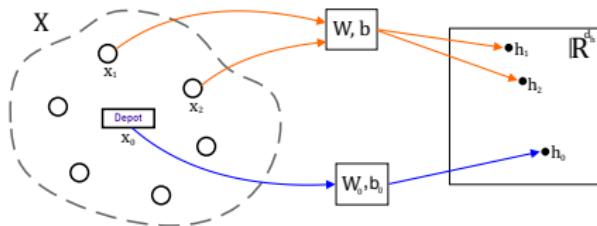
VRP problem as a sequential decision making problem



- At each decoding construction step, one node is selected and appended to the current solution.
- Probability of solution for path $\pi = \{\pi_1, \dots, \pi_T\}$ and graph instance X :

$$p_{\theta}(\pi|X) = \prod_{t=1}^T p_{\theta}(\pi_t|X, \pi_{1:t-1})$$

Encoder in detail: Initial Embedding

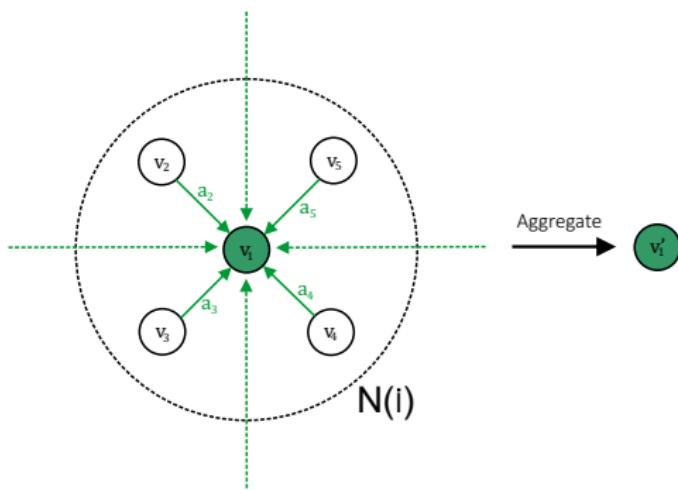


$$h^{(0)} : \mathbb{R}^3 \hookrightarrow \mathbb{R}^{d_h}, d_h = 128$$

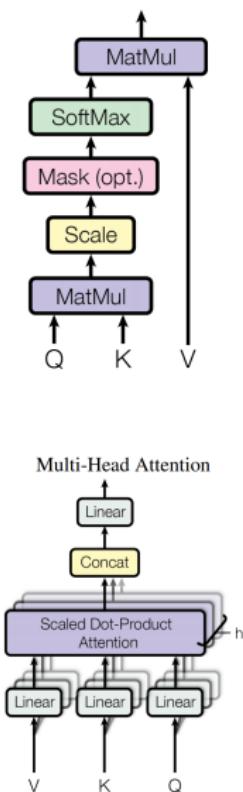
- For each node linearly project $x_i = (s_{1i}, s_{2i}, \text{demand}_i) \in \mathbb{R}^3$ to \mathbb{R}^{128}
- Learnable parameters $W \in \mathbb{R}^{3 \times d_h}$, $b \in \mathbb{R}^{d_h}$. Also separate parameters W_0 , b_0 are used for the depot:

$$h_i^{(0)} = \begin{cases} W \cdot x_i + b & i \neq 0 \\ W_0 \cdot x_i + b_0 & i = 0 \end{cases}$$

- Use neural message passing via **self-attention** (Velickovic et. al., 2018)
- Embedding (hidden state) for each node v_i is obtained by a weighted sum of features of all nodes $v_{j \in N(i)}$ in some neighbourhood $N(i)$.
- Weights a_j are calculated by attention mechanism, representing the importance (similarity) of each neighbour for a specific node.



Encoder in detail: Multi-Head Attention (Vaswani et al., 2017)



- Linearly project initial node embeddings $H \in \mathbb{R}^{batch \times n \times d_h}$ (query, key, value):

$$Q = HW^Q, K = HW^K, V = HW^V,$$

$$W^Q, W^K, W^V \in \mathbb{R}^{d_h \times d}.$$

- Split into M heads and compute compatibility matrix $A \in \mathbb{R}^{batch \times M \times n \times n}$ for graph nodes:

$$A = \text{softmax} \left(\frac{U}{\sqrt{d/M}} \right) = \text{softmax} \left(\frac{QK^T}{\sqrt{d/M}} \right).$$

- Compute attention messages for each head:

$$H' = AV \in \mathbb{R}^{batch \times M \times n \times d/M}.$$

- Concatenate heads and project out with $W^O \in \mathbb{R}^{d_h \times d}$:

$$MHA = \text{Concat}(H'_1, \dots, H'_M) W^O \in \mathbb{R}^{batch \times n \times d}.$$

For each node i apply fully connected feed-forward (FF) network with skip-connections, $\ell \in \{1, \dots, N\}$:

$$\hat{h}_i^{(\ell)} = \tanh \left(h_i^{(\ell-1)} + \text{MHA}_i^{(\ell)} \left(h_0^{(\ell-1)}, \dots, h_n^{(\ell-1)} \right) \right),$$

$$\text{FF}(\hat{h}_i^{(\ell)}) = W_1^F \text{ReLU}(W_0^F \hat{h}_i^{(\ell)} + b_0^F) + b_1^F,$$

$$h_i^{(\ell)} = \tanh(\hat{h}_i^{(\ell)} + \text{FF}(\hat{h}_i^{(\ell)})).$$

Finally, after N layers we get final node embeddings:

$$h_i^N = \text{ENCODE}_i^N(h_0^0, \dots, h_n^0).$$

At each construction step $t \in 1, \dots, T$ concatenate mean graph embedding over all nodes, embedding of the previously selected node and remaining capacity of the vehicle:

$$\hat{\mathbf{h}}_c = \begin{cases} [\bar{h}_t; h_0^N; D_t] & t = 1 \\ [\bar{h}_t; h_{\pi_{t-1}}^N; D_t] & t > 1 \end{cases}$$

Policy is governed by two sequential attention layers in decoder.

- Query vector from context vector: $\mathbf{q} = W^Q \hat{\mathbf{h}}_c$. Keys and Values from embeddings of nodes.
- Add mask to attention: mask nodes that have already been visited or have too much demand.
- ① M-head attention layer**

$$\mathbf{q} = W^Q \hat{\mathbf{h}}_c, \mathbf{k}_i = W^K \mathbf{h}_i, \mathbf{v}_i = W^V \mathbf{h}_i,$$

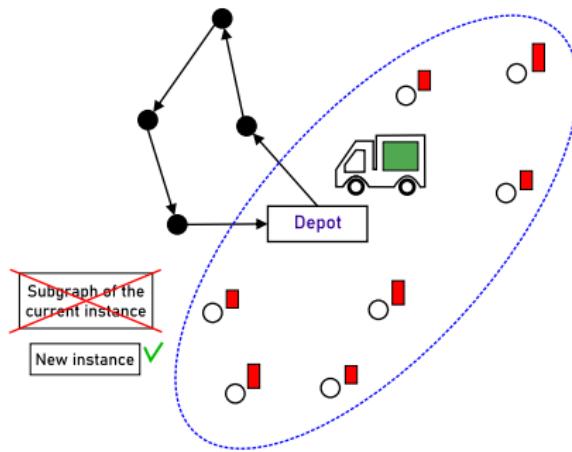
$$u_j = \begin{cases} \mathbf{q} \cdot \mathbf{k}_j^T & d_j \leq D_t, x_j \notin \pi_{1:t-1} \\ -\infty & \text{otherwise} \end{cases}$$

- ② Single-head attention layer** (only compatibility) for probabilities:

$$\mathbf{k}_{\tanh i} = W^{K_{\tanh}} \mathbf{h}_i,$$

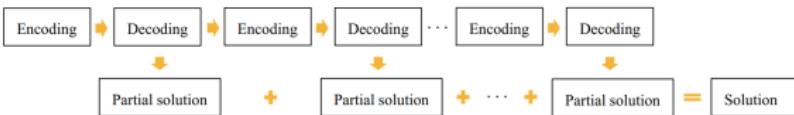
$$u_j = \begin{cases} C \cdot \tanh(\mathbf{q} \cdot \mathbf{k}_{\tanh j}^T) & d_j \leq D_t, x_j \notin \pi_{1:t-1} \\ -\infty & \text{otherwise} \end{cases}$$

$$p_\theta(\pi_t | X, \pi_{1:t-1}) = \frac{e^{u_j}}{\sum_{j'} e^{u_{j'}}}$$



- After vehicle returns to depot, the remaining nodes could be considered as a new (smaller) instance (graph) to be solved.
- Idea: **update embedding** of the remaining nodes using encoder when agent arrives back to depot.

$$h_i^t = \begin{cases} \text{ENCODE}_i^N(h_0^0, \dots, h_N^0) & \pi_{t-1} = x_0 \\ h_i^{t-1} & \text{otherwise} \end{cases}$$



Implementation:

- Force RL agent to wait for others once it arrives to x_0 .
- When all are in depots, apply encoder with **mask** to the whole batch.
- Typical solution will be of the form

```
[17., 3., 4., 7., 2., 16., 0., 0., 0., 0., 15., 20., 5.,
 0., 0., 0., 0., 11., 12., 13., 10., 9., 0., 0., 0., 19.,
 6., 8., 14., 1., 18., 0.],
```

We train model using policy gradient:

Theorem (Policy Gradient)

Gradient of expected cost for episode:

$$\nabla_{\theta} J(\theta) \sim \mathbb{E}_p [(L^p(X, \pi) - b(X)) \nabla_{\theta} \log(p_{\theta}(\pi|X))],$$

where conditional probability of solution is:

$$p_{\theta}(\pi|X) = \prod_{t=1}^T p_{\theta}(\pi_t|X, \pi_{1:t-1}),$$

and b is baseline.

- Baseline is a **copy of a model** with fixed weights from one of the preceding epochs.
- Use warm-up for early epochs: mix exponential moving average (controlled by $\beta = \text{const}$) of model cost over past epochs with baseline model.
Warm-up is controlled by $\alpha \in [0; 1]$.
- **Update baseline** at the end of epoch if the difference in costs for candidate model and baseline is statistically-significant (t-test).
- Baseline uses separate dataset for this comparison. This dataset is updated after each baseline renewal.

- Estimate model cost by **Monte Carlo**: generate an episode $S_1, A_1, \dots, S_T, A_T$, following $p_\theta(\cdot|\cdot)$ in **sampling** mode (stochastic policy). Then loop through all steps to get cost of the whole episode.
- Evaluate baseline in **greedy** mode (select the node with maximum probability - deterministic policy).
- Estimate gradient according to policy-gradient formula and update weights of the neural network.

Input: number of epochs E , steps per epoch F , batch size B
Initialize parameters θ

```

1: for epoch = 1 to  $E$  do
2:   for step = 1 to  $F$  do
3:      $X_i = \text{RandomInstance}()$  for  $i \in 1, \dots, B$ 
4:      $\pi_i^s = \text{SampleRollout}(p_\theta(\cdot|X_i))$  for  $i \in 1, \dots, B$ 
5:      $\pi_i^g = \text{GreedyRollout}(p_\theta(\cdot|X_i))$  for  $i \in 1, \dots, B$ 
6:      $\nabla \mathcal{L} = \frac{1}{B} \sum_{i=1}^B (L(\pi_i^s) - L(\pi_i^g)) \nabla_\theta \log p_\theta(\pi_i^s | X_i)$ 
7:      $\theta = \text{Adam}(\theta, \nabla \mathcal{L})$ 
8:   end for
9: end for

```

- Generate **new training dataset** (1 280 000 random graph instances) at the beginning of each epoch.
- Create and save validation dataset (10 000 graph instances) with fixed seed before first epoch. At the end of each epoch validate model in **greedy** mode.

Common Parameters

Parameter	Value
Embedding dimension	128
Rollout Samples	10000
Number of warmup epochs	1
Gradient norm clipping	1.0
Validation batch size	1000
Validation set size	10000
Number of heads in MHA	8
Tanh Clipping (C)	10
FF Hidden Layer neurons	512
Warmup Exponential Beta	0.8

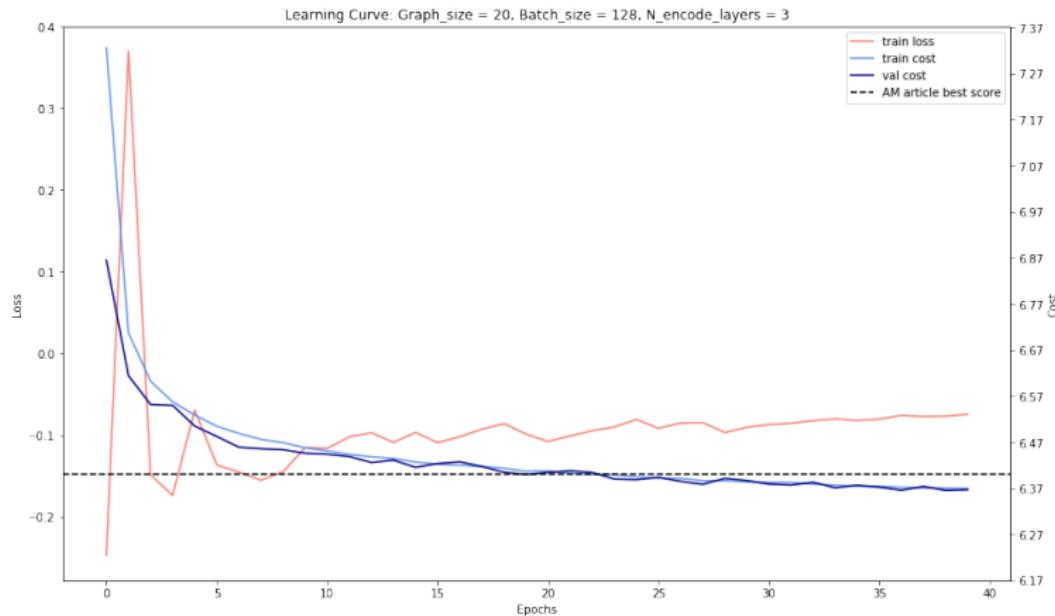
- Our implementation is based on TensorFlow 2.1  TensorFlow
- <https://github.com/>
- We looked at model behaviour for graph sizes (number of nodes) of 20/50, varying batch size and learning rate.
- For graph size 20 we tested different number of encoding layers: 2, 3.
- To compare our result with Lin–Kernighan heuristic, we used LKH-3 binaries from <http://akira.ruc.dk/~keld/research/LKH-3/>. We evaluated it on the same validation sets as for AM-D. Quality and inference time differ drastically.

Experiments

Experiment ID	Number of nodes	Batch size	Number of epochs	Number of MHA-layers	Learning Rate	Test cost (article AM)	Test cost (article D-AM)	Test cost (LKH-3)	Test cost baseline	Mean Inference time (s)	Mean Inference time (s) (LKH-3)
1	20	1024	100	2	0.0001	6.35	6.40	6.28	6.13	0.19	4.98
2	20	128	40	2	0.0001	6.38	6.40	6.28	6.13	0.2	4.98
3	20	128	40	3	0.0001	6.36	6.40	6.28	6.13	0.2	4.98
4	50	256	55	2	0.0003	10.91	10.98	10.78	10.08	0.44	18.78

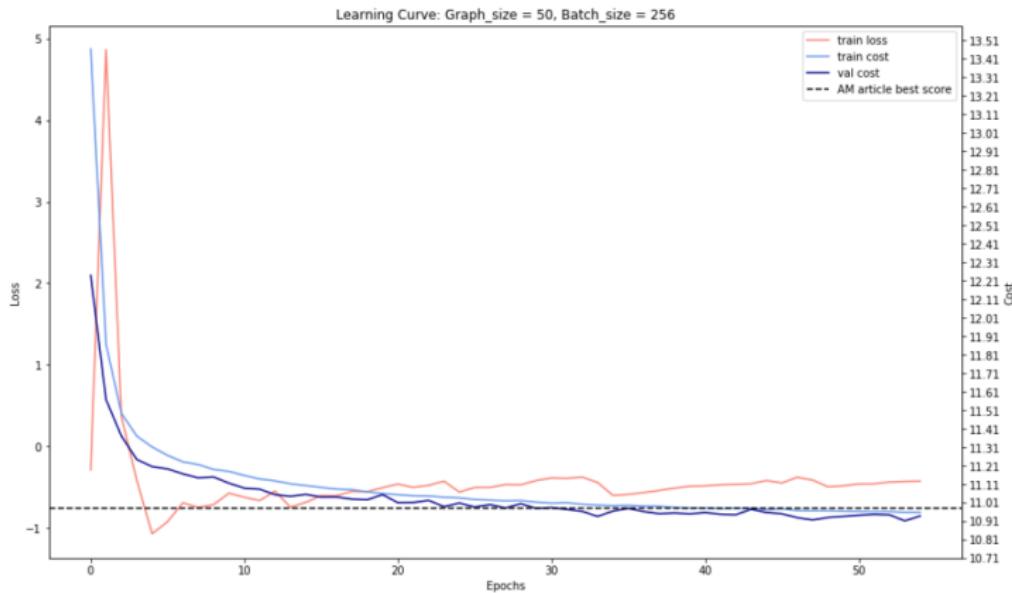
Results and Experiments: Learning Curve

Learning Curve: VRP 20



Results and Experiments: Learning Curve

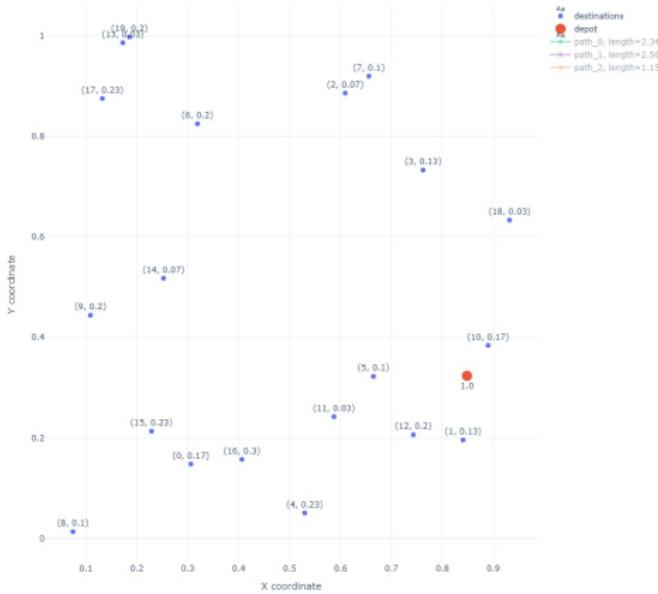
Learning Curve: VRP 50



Example

Solving VRP20

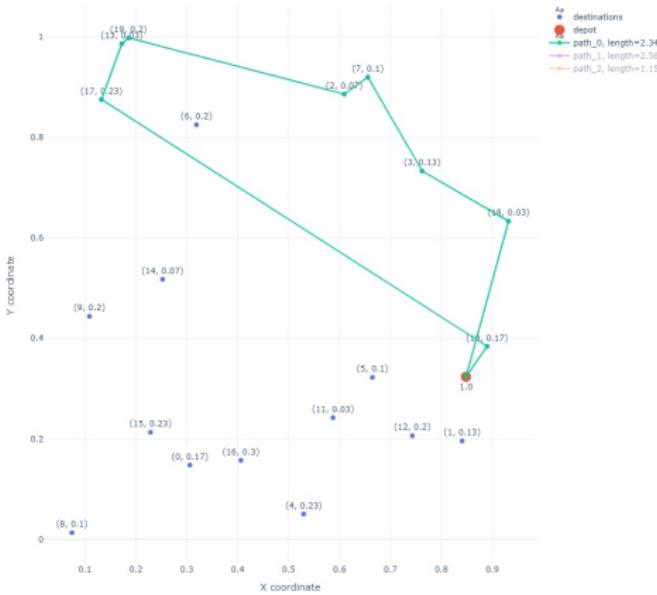
Example: Graph_size = 20, Batch_size = 1024



Example

Solving VRP20

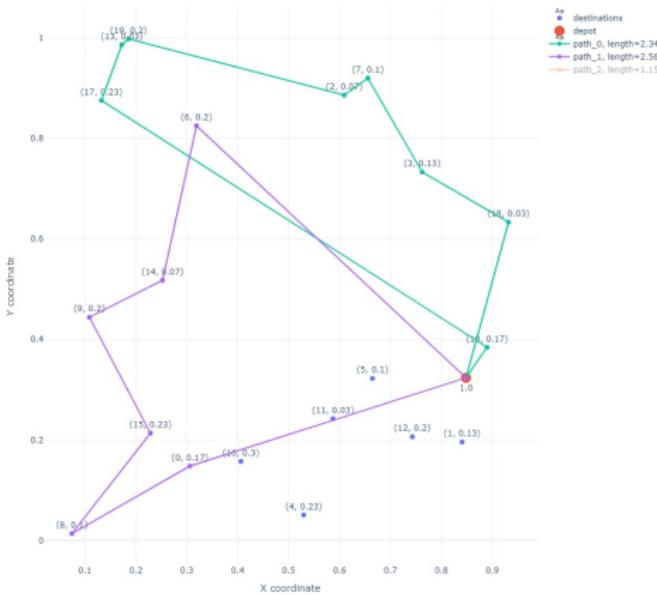
Example: Graph_size = 20, Batch_size = 1024



Example

Solving VRP20

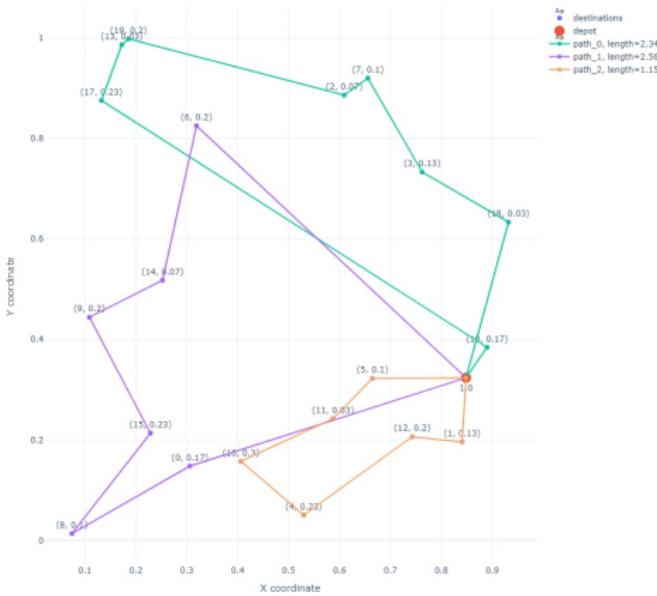
Example: Graph_size = 20, Batch_size = 1024



Example

Solving VRP20

Example: Graph_size = 20, Batch_size = 1024

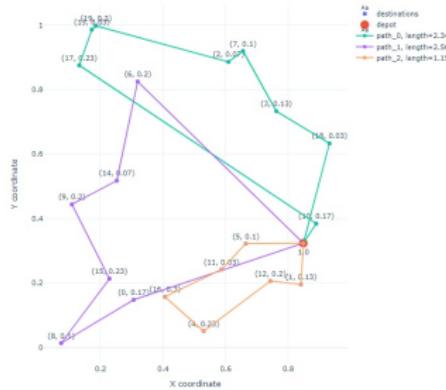


Example

Different models solving common instance:

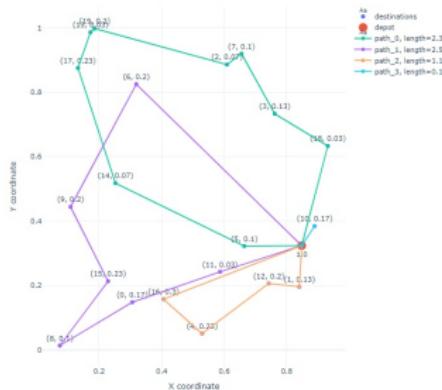
Current cost: 0.84
Current path: [0,0, 19,0, 4,0, 8,0, 5,0, 20,0, 14,0, 18,0, 11,0, 0,0, 7,0, 15,0, 10,0, 18,0, 9,0, 1,0, 0,0, 5,0, 12,0, 17,0, 5,0, 13,0, 2,0, 0,0]

Example: Graph_size = 20, Batch_size = 1024



Current cost: 0.17
Current path: [0,0, 19,0, 4,0, 8,0, 5,0, 20,0, 14,0, 18,0, 15,0, 6,0, 9,0, 7,0, 10,0, 16,0, 9,0, 1,0, 12,0, 0,0, 2,0, 13,0, 5,0, 17,0, 0,0, 11,0, 0,0]

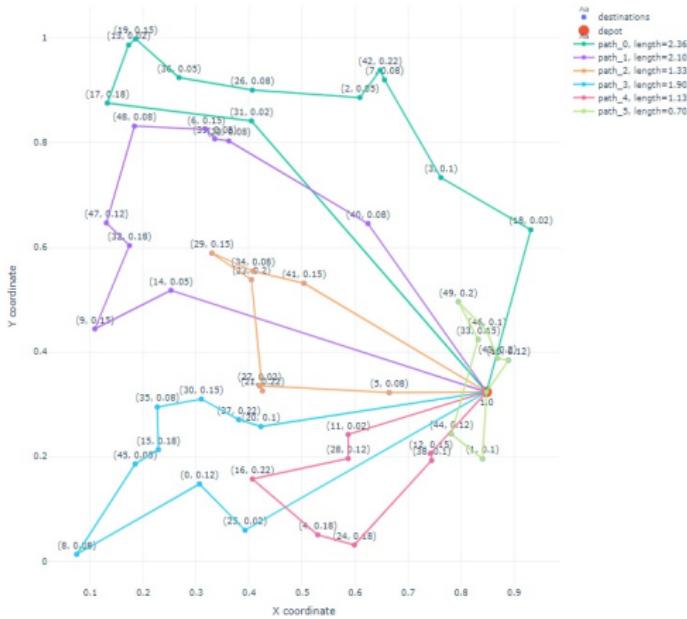
Example: Graph_size = 20, Batch_size = 128



Example

Solving VRP50

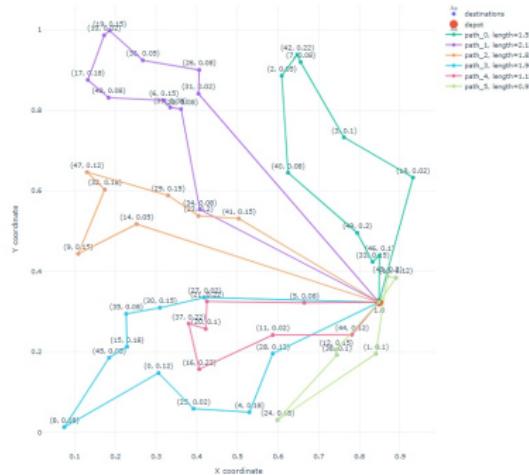
Example: Graph_size = 50, Batch_size = 256



Example

Solving VRP50: notable changes from epoch = 33 to epoch = 53:

Example: Graph_size = 50, Batch_size = 256



Example: Graph_size = 50, Batch_size = 256

