Reinforcement Learning for Multi-Truck Vehicle Routing Problems

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Vehicle routing problems and other combinatorial optimization problems have been approximately solved by reinforcement learning agents with policies based on encoder-decoder models with attention mechanisms. These techniques are of substantial interest but still cannot solve the complex routing problems that arise in a realistic setting which can have many trucks and complex requirements. With the aim of making reinforcement learning a viable technique for supply chain optimization using classical computing today and quantum computing in the future, we develop new extensions to encoder-decoder models for vehicle routing that allow for complex supply chains. We make two major generalizations. First, our model allows for routing problems with multiple trucks. Second, we move away from the simple requirement of having a truck deliver items from nodes to one special depot node, and instead allow for a complex tensor demand structure. We show how our model, even if trained only for a small number of trucks, can be embedded into a large supply chain to yield viable solutions.

I. INTRODUCTION

In the setting of commercial operations, computational problems of substantial theoretical and practical difficulty regularly arise. Even a small improvement on the quality of solutions to such problems can translate to a very substantial benefit. One such problem, heavily studied in operations research, is the vehicle routing problem [1][2].

Vehicle routing problems are NP-hard combinatorial optimization problems for which there are numerous heuristic algorithms which yield approximate solutions. Relatively recently, there has been interest in solving such routing problems using reinforcement learning (RL) [3]. In this context, a truck driving between nodes can be thought of as an agent performing actions (selecting its next node to drive to) in the environment of the supply chain. This approach has been successful for a wide range of combinatorial optimization problems, especially when using models with an encoder-decoder attention mechanisms [4].

In a sense, the use of reinforcement learning for such problems is very natural. RL is appropriate in contexts where decisions must be made with complex consequences can only be learned through experience. Games like Go naturally fit that description, and indeed they have been well-addressed with RL methodology [5]. More easily overlooked is that the routing of a truck through a supply chain is in many ways similar to a game like Chess or Go. The “moves” in this game are the selections of where to drive, what to pick up, and what to drop off. The consequences of these moves are complicated and can have long-term effects that are best learned through experience.

Unfortunately, reinforcement learning approaches for combinatorial optimization are not readily deployed in a commercial setting because of simplifications that they make. For the vehicle routing problem in particular, past work has largely focused on the case of a single truck with a simple task: bring “demand” from nodes to a depot. In reality, supply chains involve numerous trucks, and requirements are more complex than simply bringing material to one depot node, and the current machine learning models are not equipped to handle such complex situations.

In this work, we take steps toward developing RL agents that can obtain good solutions in complex supply chains. We use as our model a real commercial supply chain of Aisin Corporation, a Japanese automotive manufacturing company. We build on the work of [4] by adding new techniques allowing for multiple trucks and for far more general requirements for trucks. While our model is specially designed with Aisin Corporation’s vehicle routing problems in mind, our techniques for applying RL to a very general class of routing problems apply widely.

II. VEHICLE ROUTING PROBLEMS

This section describes the particular vehicle routing problem that we apply a reinforcement learning method to solve as well as the full-scale logistical problem that it is based on.

Broadly speaking, vehicle routing problems (VRPs) [1][2] are combinatorial optimization problems where one or more trucks must carry material between locations to accomplish certain requirements subject to constraints like capacity and time limitations. There are numerous variants of VRPs so “vehicle routing problem” is an umbrella term rather than a specific computational problem.

The three subsections below describe VRPs of gradually increasing complexity. Section [1A] reviews standard vehicle routing problems for which there are already many solution methods including reinforcement learning. Section [1B] describes a more general form of VRP that we use as the environment for our reinforcement learning agent. Unlike the basic VRP, the general VRP allows for multiple trucks and all-to-all connectivity for demand structure. Finally, section [1C] describes a real routing problem encountered by
Aisin Corporation. This real routing problem is quite similar to the general VRP of section\[14\] but includes additional constraints that are difficult to model on a GPU.

\subsection{Basic Vehicle Routing Problems}

In this section, we review the the capitated vehicle routing problem with split-deliveries (SDVRP). We use the term “basic VRP” to refer to this problem because it can be thought of as the base-model from which we generalize.

For the SDVRP, we are given a graph where nodes $z_0, z_1, \ldots, z_n$ are locations and weighted directed edges are the times needed to drive between the locations. One of the nodes $z_0$, is special and is called the depot. To every non-depot node $i$, there is a certain nonnegative real number $d_i$ called the demand for node $i$. A truck, which starts at the depot, must drive between the nodes, pick up demand, and return it to the depot. The truck has limited capacity $1$ so it may need to make multiple trips to the depot.

To be precise, an instance of the basic VRP is specified by:

1. A graph $G$ with $n + 1$ nodes $z_0, z_1, \ldots, z_n$.
2. An $n + 1 \times n + 1$ matrix $T$ with non-negative entries and $T_{ii} = 0$ for all $i \in \{0, 1, \ldots, n\}$ called the time matrix.
3. A non-negative number $d_i$ assigned to each node $z_i$ except for the depot ($i \neq 0$). These numbers are called initial demands.

The nodes of the graph can be abstract, but in many cases they are explicitly given as coordinates for locations that trucks might drive to. The time matrix entry $T_{ij}$ is supposed to be the time it take a truck to drive from node $i$ to node $j$. That is why we require $T_{ii} = 0$. The initial demand $d_i$ is supposed to be the amount of material that must be carried by a truck from the node $z_i$ to the depot node $z_0$.

A candidate solution to this VRP is given by a route: a list of integers $\xi = \xi_1, \xi_2, \ldots, \xi_k$ where $k$ is some positive integer (called the route length) and each $\xi_i$ is an element of $\{0, 1, \ldots, n\}$. We require that $\xi_1 = 0$ and $\xi_k = 0$ so that the truck starts and ends at the depot. Given such a sequence, there are two questions:

- What is the total driving time for $\xi$?
- Is $\xi$ a demand-satisfying route?

Here, the driving time for the route $\xi$ is defined as

$$\text{time}(\xi) = \sum_{t=1}^{k-1} T_{\xi_t \xi_{t+1}}.$$  \hspace{1cm} (1)

Meanwhile, the question of whether or not the route is demand-satisfying is intuitive but not mathematically elegant to describe. In short, a route is demand satisfying if it will result in a truck carrying all of the initial demand to the depot. The truck which starts at $\xi_1$ and follows the route has a capacity which we always take to be 1. This is the amount of demand that the truck can store. The amount of demand the truck is carrying at a given time is called on-board demand to distinguish it from off-board demand which is the dynamical demand waiting to be picked up at each node. As the truck navigates its route, it picks up as much demand as possible\[2\] at each stop, converting off-board demand to on-board demand. The on-board demand is never allowed to exceed 1. When the truck returns to the depot, the on-board demand is reset to 0, and the route can continue until all off-board demand is zero and the truck as at the depot.

The optimization goal of this basic vehicle routing problem is to find, among all demand-satisfying routes, the one with minimal driving time.

The usage of reinforcement learning for this split-delivery vehicle routing problem is well-established in the literature [4]. In fact, the model we use is a generalization of that of Kool et al. our

\subsection{Generalized Vehicle Routing Problems}

We now turn to a generalization of the basic vehicle routing problem which is inspired by the realistic supply chain optimization problem of Aisin Corporation that we explain in detail in section\[14\]. The purpose of the “general VRP” is to find a middle ground between the overly simple basic VRP and the enormously complex Aisin Corporation VRP. This middle ground has major features of the full-scaled supply chain logistics problem, but does not include some messy constraints that are difficult to simulate efficiently for training.

There are two ways that the general VRP is more complex than the basic variant:

1. There are multiple trucks.
2. There is no special depot. Instead, demand is required to be moved between specific nodes with various constraints. We refer to this as a tensor demand structure and explain it in detail below.

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1 “Amount of material” is intentionally vague. In a practical application, demand can be quantified by geometrical volume, by weight, or even by monetary value. For our purposes, we will use geometrical volume as the standard meaning for “amount of material” which makes it sensible that trucks have a limited carrying capacity.

2 Actually, we might decide to not pick up the full demand at a given node by optimizing a pickup-selection algorithm, but we don’t consider this case here.
The use of multiple trucks is an obvious challenge for any routing algorithm as optimal routes can involve subtle collaboration between trucks. Less obvious is the surprisingly complex issue of tensor demand structure, where any node can be a depot. For both these new ingredients, we have made modifications to the encoder and decoder models of [4].

Tensor Demand Structure

The basic VRP discussed in section [1A] has the property that all demand must be taken to the same destination node (the depot). This is built into the mathematical description of the problem because the off-board demand has a vector demand structure. This means that the demand at a given time step $t$ is given by a vector

$$d^t = (d^t_1, d^t_2, \ldots, d^t_n).$$

In a realistic supply chain, we do not have the luxury of a single delivery destination. Goods from a given node may be split into groups which need to be taken to various delivery destination nodes. To accommodate such a situation, we introduce the concept of a tensor demand structure. We begin with a rank-2 tensor.

Rank-2 Demand

Assume that there is only one truck and consider a graph with $n$ nodes $z_1, \ldots, z_n$. (There is no longer any need for a special $z_0$ node). We introduce an $n \times n$ matrix $D^{i=0}$ with non-negative entries. The meaning of the entry $D^{i,j}_{k}$ is, intuitively, the initial amount of demand that is located at node $i$ and must be shipped to node $j$. $D$ is referred to as rank-2 off-board demand or as a matrix demand structure.

When the truck arrives at node $i$ at time $t$ with this sort of demand structure, an issue arises: a pickup selection decision must be made. There are $n$ different types of demand that can be picked up from node $i$: $(D^{i-1}_{i1}, D^{i-1}_{i2}, \ldots, D^{i-1}_{im})$. There is not an obvious way to perform pickup selection. In principle, a reinforcement learning agent could learn optimal pickup selection, but this is beyond the scope of our work. We assume that some reasonable selection algorithm is used.

After pickup selection, we obtain a new matrix $D^t$ by reducing $D^{t-1}$ by the amount of demand picked up by the truck from node $i$. Another issue now appears: with demand on the truck, we have to remember which parts of the on-board demand must go to which destination nodes. This can be dealt with by promoting on-board demand at time $t$ to a vector $E^t = (E^t_1, E^t_2, \ldots, E^t_n)$. The meaning of $E^t_i$ is that, after the operations at time step $t$ (including pickup), $E^t_i$ is the amount of demand on the truck which must be delivered to node $i$.

Now that there is on-board demand in the truck, we need to revisit what happens when the truck first arrives at a given node $i$. Before pickup selection or any other operation, the first step is now to completely drop off demand $E^t_i$. Mathematically, this simply means setting $E^t_i = 0$. If we wish, we can also keep track of the overall total demand satisfied after each time step, in which case we would iteratively defined a sequence $S$ by

$$S^0 = 0,$$

$$S^t = S^{t-1} + E^t,$$

where $E_i$ refers to the node visited at time step $t$.

Arbitrary Rank Demand

The ideas of a demand matrix $D^{i,j}$ can readily be generalized to higher-rank tensors. The reason for doing this is that in a practical supply chain (including the one our study is based on), there are delivery requirements along the lines of “move this box from node 3 to node 7, and then from node 7 to node 5.” Such multi-leg requirements may sound odd, but they can arise for numerous practical reasons. There may be capacity limitations at node 5, and node 7 may be a storage warehouse. Or perhaps the box needs to have an operation performed on it before its final delivery. Another important reason for multi-leg delivery requirements is that a cargo container may need to be sent somewhere else after delivery.

Whatever the reason, there promoting the matrix and vector structure of $D$ and $E$ to higher rank tensors allows us to encode the data that we need for this new situation. An initial demand tensor $D^{i,j,k}_{t}$ can be interpreted as “there is initially demand $D^{i,j,k}_{0}$ at node $i$ which needs to first travel to node $j$ and then travel to node $k$.”

Unfortunately, with higher-rank tensor structure like this, the operations that are performed when a truck arrives at a node become even more complicated. Consider first an empty truck arriving at node $i$ at time $t$. It starts by performing pickup selection to decide what off-board to pick up: any part of $D^{i,j,k}_{t}$ is fine as long as the first index is $i$. After the pickup, the off-board demand is correspondingly reduced. However, the loaded demand is now material with instructions like “go to node $j$, then go to node $k$” so we must introduce a matrix on-board demand $E^{i,j}_{t}$ to track this. However, now that the truck has this on-board demand, when it later drives to node $j$, the on-board $E^{i,j}_{t}$ will be dropped off. This demand is not satisfied because it hasn’t reached its final destination of node $k$. We are therefore forced to introduce a rank-2 matrix off-board demand structure when this demand is dropped off! When that matrix off-board demand is later picked up, it is converted to rank-1 vector on-board demand.

In conclusion, rank-r off-board demand will automatically require tracking off-board demands with
ranks 2 through \(r\) as well as on-board demands with ranks 1 through \(r - 1\). These can be separately tracked by a collection of tensors like
\[
D^r_t \\
D^{r-1}_t \\
\vdots \\
D^2_t \\
E^2_t \\
E^1_t
\]
or, alternatively, we can use “diagonal entries” like \(D_{ij}\) instead of \(D_{ij}^r\). Regardless of the organizational approach, there is no question that bookkeeping is one of the major issues that arise when dealing with this more realistic version of a vehicle routing problem.

As with the cases above, we can introduce a “total demand satisfied” sequence \(S^t\) which accumulates only when demand is sent to its final destination. We do not accumulate \(S\) when rank-2 on-board demand arrives at a node, but we do accumulate it when rank-1 on-board demand arrives because that node is the final destination for that material.

**Multiple Trucks**

The next complexity to consider is the involvement of multiple trucks. This is intuitive and easy to describe mathematically, but it adds immense difficulty for optimization.

The main observation to make about the mathematical structure is that there is an on-board demand for every truck, but there is only one off-board demand. Thus, we need a new index \(m\), which ranges from 1 to the number of trucks \(N\), added to on-board demand. For instance:

\[
E_{ij}^{t,m}
\]

for rank-2 on-board demand. In this notation, we are dropping the \(r = 2\) symbol as it is implied by the fact that there are two lower indices \((i\) and \(j)\). In fact, because the notation involves so many indices, we will occasionally also drop the reference to time as well. To help clarify, we use notation like

\[
E^{m=2}_{ij}
\]
to refer to rank 2 on-board demand for truck 2 in cases where we leave time \(t\) implicit. In other words, we explicitly write “\(m = 2\)” to indicate that we are referring to truck number which ranges from 1 to \(N\).

In general, different trucks to have different capacities \(C_1, \ldots, C_N\), but throughout our work we assume that all trucks have capacity 1. There is very little difficulty in adding varying capacities to our models if needed.

The introduction of multiple trucks adds great subtleties to the problem. The optimal solution to an instance with many trucks may involve highly collaborative relationships between trucks.

**Cyclic Demand Structure**

The mathematical structure above is sufficient to describe another closely related scenario with very little modification. In some commercial logistics problems, trucks are required not only to deliver material but to then return empty containers back to the origin location. This constraint is particularly common for operations that occur in a repeating manner: trucks may need to make regular (e.g. daily or weekly) shipments of identical items, and the same specialized containers may need to be used. We allow for this constraint in our general VRP.

Mathematically, we regard an empty box as no different from a full box as it occupies the same amount
of space in a truck. The most straightforward way to enforce a box return constraint is to simply increase the rank of tensor demand by one. However, there is a more memory-efficient approach: we introduce a concept of cyclic off-board demand. Meanwhile, we use the term direct off-board demand to refer to the sort of demand described earlier.

As an example of cyclic off-board demand, consider figure 1 in which material initially at node 2 must be brought to node 5 before being returned to node 2. We encode this demand as a term in a rank-2 tensor: \( D_{25}^{cyclic} \). When a truck stops at node 2 to pick up this cyclic demand, something different happens from the case of picking up direct demand: the demand is converted to rank-2 on-board demand rather than rank 1. Specifically, such a pickup of \( D_{25}^{cyclic} \) contributes to \( E_{52} \) because the demand must be brought to node 5 and then it must later be brought to node 2. It’s important to understand that once this demand is dropped off at node 5, it contributes to direct off-board demand \( D_{52}^{direct} \) as discussed above.

To summarize the flow of demand in this example, we can write the following table which shows how relevant components of demands are nonzero at various moments of time:

| Component   | Description of most recent event. |
|-------------|-----------------------------------|
| \( D_{25}^{cyclic} \) | Initial material is at node 2; must be brought to node 5, then node 2 |
| \( E_{52}^{m=1} \) | Box picked up from node 2 by truck 1; must go to node 5, then node 2 |
| \( D_{52}^{direct} \) | Box dropped off and emptied at node 5 by truck 1, must be returned to node 2 |

At this point, the situation can continue. Suppose that truck 3 now picks up the empty box. Then, then route for the box would end as follows:

| Component   | Description of most recent event. |
|-------------|-----------------------------------|
| \( E_{3}^{m=3} \) | Empty box picked up from node 5 by truck 3; next stop: node 2 |
| 0 | Empty box returned to node 2 by truck 3, requirements fulfilled |

Note that our notation may cause confusion initially. When truck #3 picks up the empty box from node 5, the demand tensor component that gets a contribution is \( E_{2}^{m=3} \) which makes no reference to node 5. This is because node 5 is no longer relevant. The fact that the node is currently located at node 5 is handled by tracking truck locations, which is a separate matter from tracking demand flow.

The general behavior of cyclic and direct demand, at rank 3 and beyond, is intuitive but even more confusing. The following table shows a sequence of events for cyclic initial demand starting at node 3 that must go to node 7 and then node 4 before returning to node 3.

| Component   | Description of most recent event. |
|-------------|-----------------------------------|
| \( D_{374}^{cyclic} \) | Initial material is at node 3; must be brought to node 7, then node 4, then node 3 |
| \( E_{743}^{m=2} \) | Picked up from node 3 by truck 2, next stop node 7 |
| \( D_{743}^{direct} \) | Dropped off at node 7 by truck 2; must be brought to node 4, then node 3 |
| \( E_{743}^{m=1} \) | Picked up from node 7 by truck 1, next stop node 4 |
| \( D_{43}^{direct} \) | Dropped off at node 4 by truck 1; must be brought to node 3 |
| \( E_{43}^{m=3} \) | Picked up from node 4 by truck 3, next stop node 3 |
| 0 | Dropped off at node 3 by truck 3, requirements fulfilled |

Restricted Driving Windows

Typical VRPs involve minimizing driving time to accomplish the goal of fulfilling all deliveries. How-

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3 Here, we are using volume as the metric limited by truck capacity. We do not consider models constrained by both weight and volume.
In a commercial setting, there is a limitation on the time in which trucks can drive. As a result, we may need to consider routes that fail to satisfy all demand.

Suppose that all trucks are only allowed to drive during an overall period of time $T_{\text{max}} > 0$. The trucks drive simultaneously during this time. We are not necessarily guaranteed that it is possible to fully satisfy demand within that constraint, and the optimization goal is no longer obvious because we need to make some decision about the relative importance of maximizing demand satisfied and minimizing driving time.

### C. Aisin Corporation Vehicle Routing Problem

The goal of this work is to develop a new technique for solving a supply chain logistics problem that arises in the operations of Aisin Corporation. In this section, we explain the remaining complexities of that Aisin Corporation VRP which we refer to as the AVRP for brevity. Note, however, that we do not consider AVRP to be a well-defined computational problem; it is better thought of as a problem instance. In fact, when we discuss the AVRP below, we always mean a specific instance which has 21 nodes and a specific demand structure that we now explain.

The general VRP from section II B is carefully designed to already accommodate most of the key details of the AVRP already. As a result, an instance of the general VRP can be found to model the AVRP. Our approach is therefore to train a machine learning model (see section III) that can solve the general VRP and to then apply it to instances that approximate the AVRP.

Perhaps the most substantial AVRP complexity is the presence of individual boxes. Demand is not an ambiguous real number but is composed of discrete boxes that occupy a certain volume and have certain routing requirements. We can use an index $a$ which we call box number:

$$ a \in \{1, \ldots, \text{number of boxes}\} $$

to list all of the boxes. Given a box number $a$, there is a specific routing requirements

$$ R_a = (R^1_a, R^2_a, \ldots, R^r_a) $$

where each $R^k_a$ is a node. The meaning of this is that box $a$ must start at the node $R^1_a$ and then it must visit the node $R^2_a$ and so on. Moreover, for the AVRP, after visiting the final node $R^r_a$, all boxes must then be returned to the starting node.

The difficulty of the AVRP somewhat reduced by the following facts:

- All boxes either have $r_a = 2$ or $r_a = 3$.
- Although there $\sim 330,000$ boxes for the AVRP, there are actually “only” 107 unique paths for boxes.

Given these observations, a general VRP instance that models the AVRP must have initial off-board rank-2 and rank-3 cyclic demand and no initial direct demand. We sometimes refer to the simplification of using continuous quantities for demand, rather than discrete boxes, as the box soup simplification.

The AVRP has 21 nodes and it has driving time windows: $T_{\text{max}}$ is equal to 16 hours, providing a pair of 8 hour shifts for each truck. Driving times between nodes are illustrated in figure 2. The scale of the initial demand is substantial: Aisin Corporation logistics experts currently use 142 trucks to delivery parts following routes illustrated in figure 3.
III. POLICY NEURAL NETWORKS

There are a variety of ways to solve routing optimization with reinforcement learning [6], [7]. Our specific model is an encoder and decoder directly inspired by that of Kool et al. [4]. Their model is quite general: after training with REINFORCE [5], it performs well for numerous routing problems including the traveling salesman problem, basic vehicle routing problems, and the orienteering problem. However, it does not account for multiple trucks. Moreover, there is no obvious way to incorporate a tensor demand structure into their model without a substantially new approach.

A. RL Structure for Routing Problems

Before describing our neural networks, we first explain how a routing problem like the general VRP fits into the framework of reinforcement learning and also how and encoder and decoder furnish a policy.

Reinforcement learning concerns a Markov decision process (MDP) where an agent, presented with state of the environment, performs an action of its choice which results in a new environment state and gives the agent some reward. The new state as well as the reward are both stochastic: there is a probability of a given new state and reward value given the original state and the agent’s action. The goal of the agent is not to maximize the reward for a given action but to maximize the long term reward (a concept known as the return).

The agent does not know the probability of getting a certain new state and action, but can learn through experience the best actions to take in given states. The agent learns a policy which is a probability distribution over possible actions to take in a given state. In other words, given a state s and a potential action a, the agent computes a quantity \( \pi(a | s) \in [0, 1] \) such that \( \sum_a \pi(a' | s) = 1 \). \( \pi \), interpreted as a conditional probability distribution, is known as a policy, and the agent samples from \( \pi \) to select an action. Finding the optimal policy (the one that maximizes the expected value of return) is the goal of the agent’s learning process.

Consider the case of a basic vehicle routing problem with one truck. When the truck is at a given node \( \xi_{t-1} \) at time \( t-1 \), we want to use an RL agent to determine the next node \( \xi_t \) for the truck to drive to.

The most obvious approach is to make the state include the following information:

- The route so far up to a given moment: \( (\xi_0,\xi_1,\ldots,\xi_{t-1}) \),
- The current remaining truck capacity,
- The remaining demand to be picked up at each node,
- The time matrix \[1\]

Given this, the probability of going to node \( z \) in a given state can be written as

\[
\pi(z | (\xi_0,\ldots,\xi_{t-1}), D_{t-1}).
\]

where \( D_{t-1} \) is meant to include all of the demand information at time \( t-1 \).

Assuming that we use the same policy \( \pi \) for every step of the route, the probability for selecting an entire route \( x_0,\ldots,\xi_k \) is

\[
\pi(x | D_0) = \prod_{t=1}^{k} \pi(\xi_t | (\xi_0,\ldots,\xi_{t-1}), D_{t-1}).
\]

This formula leads to an important observation that we will make use of when discussing the learning algorithm below. Rather than thinking of the route as consisting of \( k \) actions, we can alternatively think of it as one single action which has probability given by equation \[2\]. Although this may seem unnecessarily complicated, it’s convenient for the REINFORCE algorithm which involves the logarithm of the probability which conveniently converts to product in equation \[2\] to a summation.

**RL Structure With Multiple Trucks**

How does the discussion above need to change when we consider a vehicle routing problem (or another routing problem) with multiple trucks? There are two natural approaches:

- Use a different policy for each truck, and have multiple agents interact simultaneously with the environment, learning to work together.
- Use the same shared policy for each truck.

The first approach is arguably a more powerful technique, allowing different trucks to use different strategies in the same situation. However, the second approach is simpler to implement and still has the potential to approach optimality for vehicle routing problems. We use the second approach throughout this work.

The concept is that every truck has the same policy and views every other truck as a part of the environment. At the start of an episode, all trucks are at initial nodes and we start with the first truck (\( m = 1 \)). That truck is presented with the environment which can include, in principle, all of the information about the locations of the other trucks as well as all of the initial demand. The \( m = 1 \) truck uses the (shared)

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\[1\] The time matrix is static throughout the episode, but is conveniently included in the state data as we may want to train over states with various time matrices.
policy to select its next node. We then go to the next truck \( m = 2 \) and do the same.

After all \( N \) trucks have assignments, the next step has an important difference. All trucks now drive to their selected nodes, but they may not all arrive at the next node at the same time. This is controlled by a time matrix \( T_{ij} \) giving driving times between nodes. Suppose that truck \( m = 3 \) happens to arrive at its node first. In that case, we proceed by using the policy for truck 3 to give it a new node. When we do this, every truck other than truck 3 is treated as a passive truck while the other trucks with \( m \neq 3 \) are called active trucks. One point of potential confusion here is that there are two usages of “time”. The first, which we will sometimes refer to as physical time, is the time measured by the time matrix. The order in which active trucks are selected is determined by the order of the physical times for arrivals. The other “time” is a discrete index which enumerates arrival nodes for trucks. It’s important to understand that if we say that an episode has a “route” \( (\xi_0, \ldots, \xi_k) \), then the nodes \( \xi \) are all not for the same trucks. We thus need to separately keep track of the active trucks at each time step \( (m_0, \ldots, m_k) \).

### B. Encoder Without Tensor Demand

We begin by discussing a modification of the model of Kool et al. which accounts for multiple trucks. This model accounts for many of the complexities in the problem, but does not have any way to deal with tensor demand structure described in section II.B. Tensor demand structure requires a modification to the attention mechanism, and we describe two approaches to this later.

The encoder-decoder model we use follows the basic idea of the transformer network [9]. A sequence of input data is converted to a sequence of vectors \( \mathbf{x}_i \) with dimension \( d \) by an encoder. Then, a decoder acts on the encoded sequence and some additional information (called context) to determine a probability distribution over the inputs. We can then select one of the inputs by sampling from that distribution.

#### Encoder Overview

The encoder is essentially identical to the encoder of Kool et al., so we do not cover it in great detail here. The input data is a sequence of node coordinates \( \mathbf{x}_1, \ldots, \mathbf{x}_n \) with each \( \mathbf{x}_i \) a two-dimensional point.\(^5\)

The input sequence should contain information not only about the locations of the points but also about the initial demand structure. Initially, even if there is high-rank tensor demand, we can compute a myopic rank-2 demand \( D_{ij} \) giving the material that is located at node \( i \) and needs to go to node \( j \) as its first stop. For example, if we have cyclic rank-3 initial demand \( D_{ijk}^{\text{cyclic}} \), then we can sum over the third index to obtain a contribution to \( D_{ij} \). At this point, define

\[
\delta^{\text{out,init}}_i = \sum_j D_{ij}, \quad (4)
\]
\[
\delta^{\text{in,init}}_i = \sum_j D_{ji}. \quad (5)
\]

These quantities are “myopic outgoing and ingoing demands” for every node. We can concatenate the initial coordinates with these demands:

\[
\mathbf{x}_i = \mathbf{x}_i \oplus (\delta^{\text{in,init}}_i, \delta^{\text{out,init}}_i) \quad (6)
\]

where \( \oplus \) denotes direct sum (which is equivalent to concatenation in this context). We use these extended vectors \( (\mathbf{x}_1, \ldots, \mathbf{x}_n) \) as the sequence of inputs for the encoder.

The first encoding step is a learned linear map with bias from the initial input space \( \mathbb{R}^d \) to an encoding space \( \mathbb{R}^4 \). (In our experiments, we typically take \( d = 128 \).) We denote this by

\[
\mathbf{h}_i^0 = W^{\text{init}} \mathbf{x}_i + b^{\text{init}} \quad (7)
\]

where \( W^{\text{init}} \) is a \((d, 4)\) matrix and \( b^{\text{init}} \) is a \( d \)-dimensional vector. We emphasize that the same mapping is applied to every input entry in the sequence: \( W^{\text{init}} \) and \( b^{\text{init}} \) do not depend on \( i \).

After this initial encoding, we proceed with a sequence of three encoder layers. Each encoder layer can be thought of as a two step process: an attention layer (equation \((8)\)) followed by a feedforward layer (equation \((9)\)).

\[
\tilde{\mathbf{h}}_{i-1} = \text{BN}(\mathbf{h}_{i-1} + \text{MHA}(\mathbf{h}_{i-1})), \quad (8)
\]

\[
\mathbf{h}_i = \text{BN}(\tilde{\mathbf{h}}_{i-1} + \text{FF}(\tilde{\mathbf{h}}_{i-1})). \quad (9)
\]

In these equations, BN is a batch normalization layer [10], FF is a feedforward network, and MHA is a multi-head attention layer which we describe in detail below. The feedforward layers have a single hidden dimension \( d_{ff} \) and consist of a linear layer with bias mapping \( \mathbb{R}^d \to \mathbb{R}^{d_{ff}} \) followed by a ReLU activation function, a dropout layer, and finally a linear map with bias back to \( \mathbb{R}^d \).

---

\(^5\) We use two dimensions in our analysis, making nodes points on a plane. However, any dimension can be used as an input dimension.
Multi-Head Attention

The function MHA is a multi-head attention mechanism identical to that of [3]. Below we consider two major generalizations of this attention mechanism to deal with tensor demand structure, and this subsection establishes the groundwork needed for those generalizations.

We begin by using prior embedded nodes \( h_1, \ldots, h_n \in \mathbb{R}^d \) to compute vectors known as queries, keys, and values. In a single-head attention mechanism, we compute a single query, key, and value vector for each encoded node \( h_i \):

\[
q_i = M_\text{query} h_i \in \mathbb{R}^\alpha, \quad k_i = M_\text{key} h_i \in \mathbb{R}^\alpha, \quad v_i = M_\text{value} h_i \in \mathbb{R}^d.
\]

Here, each \( M \) is a matrix mapping \( \mathbb{R}^d \) to either \( \mathbb{R}^d \) or \( \mathbb{R}^\alpha \) where \( \alpha \) is some a new hyper-parameter.

For the multi-head attention mechanism, we have a positive integer \( n_{\text{heads}} \), which we typically take to be 6. For each \( s \in \{1, \ldots, n_{\text{heads}}\} \), we have a different query, key, and value map and thus different queries, keys, and values computed:

\[
q_{s,i} = M_s^\text{query} h_i \in \mathbb{R}^\alpha, \quad k_{s,i} = M_s^\text{key} h_i \in \mathbb{R}^\alpha, \quad v_{s,i} = M_s^\text{value} h_i \in \mathbb{R}^d.
\]

The linear maps \( M \) are learned during training. Note that like other aspects of the encoder that we have discussed, \( i \) behaves as batch index, allowing sequences to have arbitrary length.

The next step is to compute a compatibility for every query-key pair (for each head). We define

\[
\rho_{s,i,a} = \frac{1}{\sqrt{\alpha}} q_{s,i} \cdot k_{s,a}
\]

with \( \cdot \) denoting a standard dot product. After this, a softmax version of compatibility is computed

\[
\rho_{s,i} = \frac{\exp(\rho_{s,i,a})}{\sum_a \exp(\rho_{s,i,b})} \in \mathbb{R}
\]

which is used to weight a sum over values:

\[
h'_i = \sum_a \rho_{s,i,a} v_{s,a}.
\]

The only remaining step to to merge the data from the \( n_{\text{heads}} \) attention heads. To do this, we simply concatenate the output from each head,

\[
h'_1 \oplus \ldots \oplus h'_{n_{\text{heads}}},
\]

and use a learned linear map with bias on this vector, from dimension \( n_{\text{heads}} \times \beta \) to dimension \( d \) to recover a vector \( h'_i \in \mathbb{R}^d \).

We use the symbol MHA to denote the function which starts with encoded vectors \( h_i \in \mathbb{R}^d \), and returns the output sequence \( h'_i \in \mathbb{R}^d \). MHA computes queries, keys, and values following equations (13)-(28), then computes compatibility and new encoded vectors for each head, and finally maps to the original encoding dimension.

C. Decoder Without Tensor Demand

Unlike our discussion of the encoder, this section deviates meaningfully from the model of [3] because we include new techniques for using multiple trucks.

After encoding, through \( l \) layers, we obtain a tuple of \( n \) vectors \( \{h_i^n\}_{i=1}^n \) which are interpreted as encoded nodes for the graph. To obtain the probability of selecting a given node as a next action, we “decode” the nodes along with some additional information called context.

At the moment of decoding, we are given

- The encoded nodes \( \{h_i^n\}_{i=1}^n \) which were encoded once at the start of the episode,
- the active truck \( m_{\text{t-1}} \),
- the current on-board demands \( E_{i_1, \ldots, i_r}^m \),
- the current off-board demands \( Di_1, \ldots, i_r, D_{\text{cycle}} i_1, \ldots, i_r \),
- the next expected nodes for each passive truck and the time until those trucks arrive, and
- the remaining capacities for all of the trucks.

This is an enormous amount of information, and we do not attempt to convey all of it without loss to our agent.

Information Added to Nodes

As a first step, we consider a myopic form of off-board and on-board demand. We define

\[
i_i^m = \sum_{i_2, \ldots, i_r} E_{i,i_2, \ldots, i_r}^m
\]

and

\[
\delta_i^\text{out} = \sum_{i_2, \ldots, i_r} D_{\text{total}}^i_{i,i_2, \ldots, i_r},
\]

where \( D_{\text{total}}^i \) is the sum of cyclic and direct demand. In words, \( i_i^m \) is the total material on truck \( m \) which needs to be dropped off at node \( i \) for its next stop, and \( \delta_i^\text{out} \) is the total material at node \( i \) that is waiting to
be picked up. We will also define an ingoing myopic off-board demand
\[ \delta_i^m = \sum_{i_1, i_2, \ldots, i_r} D_i^\text{total}_{i_1, i_2, \ldots, i_r}, \]
but we won’t need it for the time being.

The quantities \( \epsilon \) and \( \delta \) do not fully encode on-board and off-board demand but instead only give the most immediately relevant aspects of the demand structure. Below we will give a technique than can encode the full tensor structure at the cost of substantial memory consumption.

Now, let \( m_\ast \) be the active truck index. We then modify the encoded nodes as follows
\[ \mathbf{h}_i = h_i \oplus (\delta_i, \epsilon_i^{m_\ast}, \epsilon_i^1, \ldots, \epsilon_i^{m_\ast-1}, \epsilon_i^{m_\ast+1}, \ldots, \epsilon_i^N) \]
\[ \text{(22)} \]
where \( \oplus \) is concatenation.

It’s worth stopping to observe some key principles for these new encoded nodes. First, note that everything on the right hand side of equation (22) strictly corresponds to the appropriate node: the index \( i \) consistently appears on both sides. This is one of the main reasons that it is difficult to convey a tensor demand structure with attention models: we tensor demand involves more than one node at a time. Our usage of myopic demands avoids the difficulty at the cost of presenting the agent with incomplete environment information.

Another important principle of equation (22) is the ordering of components. The original encoded vectors have dimension \( d \). After the \( \delta^\text{th} \) component, we have a slot for the off-board demand. Then we have a slot for the on-board \textit{active truck}’s demand. Finally we have \( N-1 \) slots for the on-board demands of \textit{passive trucks}. Note that very little care is taken with regard to the order of the passive trucks; this is intentional as all passive trucks should be treated on equal footing.

### Additional Contextual Information

There is still additional information that we need to convey: the remaining truck capacities and the locations of trucks. To do so, we follow the spirit of \[ \text{(1)} \] and introduce one special \textit{context node}. To define it, let \( m_\ast \) be the active truck index and put
\[ \mathbf{C} = (C_{m_\ast}, C_1, C_2, \ldots, C_{m_\ast-1}, C_{m_\ast+1}, \ldots, C_N) \]
\[ \text{(23)} \]
where \( C_k \) is the capacity remaining for truck \( k \). We will use \( \mathbf{C} \) as a part of the context vector, but we need to include also information about truck locations. Let \( z_1, \ldots, z_N \) denote the nodes of all trucks in the sense that \( z_m \) is the current node of the active truck from which it is about to depart and, for the passive trucks, \( z_1, \ldots, z_{m_\ast-1}, z_{m_\ast+1}, \ldots, z_N \) are the next scheduled that the passive trucks are \textit{currently heading toward}. Ideally, we would like to append to the context node
\[ (h_{m_\ast}, h_{z_1}, h_{z_2}, \ldots, h_{z_{m_\ast-1}}, h_{z_{m_\ast+1}}, \ldots, h_{z_N}) \]
but this would be extremely expensive: the context vector would have \( dN \) dimensions just from these components. To avoid this, we take the view that the passive truck is less important than the active truck, and use a single-layer feedforward neural network \( f \) consisting of a linear layer, ReLU nonlinearity, and then one more linear layer, to reduce the dimension of the passive trucks. From this we can define
\[ \mathbf{H} = (h_{z_{m_\ast}}, f(h_{z_1}), f(h_{z_2}), \ldots, f(h_{z_N})). \]
\[ \text{(24)} \]

There is one more ingredient for the context node. An important piece of information is the time until each passive node will arrive at its next scheduled destination. Let \( t_m \) denote the time until truck \( m \) will arrive at its next stop. We emphasize that \( t_m \) measures the remaining physical time (see section \[ \text{III A} \]) until the truck arrives. It is not the absolute physical arrival time of the scheduled event for truck \( m \) but rather the difference between that absolute time and the physical time of the current event for the current active truck. In particular, note that we can have \( t_m = 0 \) if \( m = m_\ast \) or in the event where truck \( m \) has the same arrival time as the active truck.

Now we define
\[ \mathbf{T} = (t_1, \ldots, t_{m_\ast-1}, t_{m_\ast+1}, \ldots, t_N). \]
\[ \text{(25)} \]
Note that the last \( N-1 \) components of \( \mathbf{H} \) (equation (24)) correspond to the same trucks with the same order as the components of \( \mathbf{T} \). This consistency is what matters. With different events, the same components may correspond to different trucks, but for any given event, the components of \( \mathbf{C}, \mathbf{H}, \) and \( \mathbf{T} \) line up in the same way.

We finally define the \textit{context node}:
\[ \mathbf{h}_\text{ctx} = \mathbf{H} \oplus \mathbf{T} \oplus \mathbf{C}. \]
\[ \text{(26)} \]

### Decoder Structure

We now take the modified nodes of equation (22) and put them through a single layer with a structure identical to the encoder layers of equation (8) and (9) except that the nodes have a greater dimension due to the modifications in equation (22) and one additional modification explained momentarily. We denote the output as
\[ \mathbf{h}_i^\text{h} = \mathbf{h}_i^{(1)} \]
\[ \text{(26)} \]
The additional modification is that, following \[ \text{(4)} \], we adjust the computation of keys and values in equations (14) and (15) by adding \textit{source terms}:
\[ k_{si} = M_s^{\text{key}} \mathbf{h}_i + u_s^{\text{key, out}} \delta_i^s + u_s^{\text{key, in}} \delta_i^s, \]
\[ \text{(27)} \]
\[ v_{si} = M_s^{\text{value}} \mathbf{h}_i + u_s^{\text{val, out}} \delta_i^s + u_s^{\text{val, in}} \delta_i^s. \]
\[ \text{(28)} \]
Here, \( s \) is an index for attention heads, and various \( u_s \) are learned vectors with the same dimension as
the left hand side of the equations they appear in; for example, $u_{i,\text{key},\text{out}}$ is a vector with the same dimension as keys which is $\alpha$ as specified in equation (14). Note $\delta_{\text{out}}^i$, defined in equation (20), is a real number that re-scales the vector $u_{i,\text{key},\text{out}}$. This modification of keys and values helps to convey the current demand situation to the attention mechanism directly.

We now proceed with a second attention layer, this one with the same number of heads $n_{\text{heads}}$ but defined on $n + 1$ nodes: the $n$ nodes $\{h_j\}_{j=1}^n$ from the first decoder layer, and the one context node $h_{\text{ctx}}$. However, for this attention layer, following [4], we only make a single query from the context node and have keys for all of the other nodes. In other words, for each head we compute one query (for the context node), $n$ keys, and $n$ values (for the other nodes). In equations (16)-(18), the index $i$ only take on a single value. We use sources $\delta_{\text{out}}^i, \delta_{\text{in}}^i$ just as in equations (27) and (28). Moreover, for this layer we only compute MHA as described at the end of section III B. This is a pure attention layer (as opposed to and encoder layer which uses equation 5) and (9).

The output of this second layer is one new context vector $k_{\text{ctx}}$ with dimension $d_{\text{ctx}}$. This vector is then used for a final (third) layer much like the second layer although we only use one head. Once again, a query $q_{\text{ctx}}$ is computed only for $k_{\text{ctx}}$ and keys are computed for the encoded nodes $h^1_j$.

For this last layer, we obtain compatibility in the usual way except that we regulate with tanh and we allow for masking:

$$u_i = \begin{cases} A \tanh(q_{\text{ctx}} \cdot k_i) & \text{if node } i \text{ is allowed} \\ -\infty & \text{otherwise} \end{cases}$$ (29)

where $A$ is a hyper parameter that we take to be 10. The idea is that we can block certain nodes for the active truck to drive to if we know, for some reason, that doing so is a poor choice. We describe the specific rules we use for masking in section [FILL].

Finally, the $u_i$ are converted to probabilities with a softmax layer, and these probabilities are interpreted as the values of the policy: the probabilities of selecting node $i$ for the active truck’s next destination:

$$\pi(i) = \frac{e^{u_i}}{\sum_{j=1}^{n} e^{u_j}}.$$ (30)

There is no need for values to be computed in the final attention layer.

D. Incorporating Tensor Demand Structure

In the prior sections, we have not fully incorporated tensor demand structure described in section III B. We have been able to incorporate aspects of the demand structure by reducing to quantities like $\delta_{\text{out},\text{in}}$ and $\epsilon^m$; these quantities fit into the framework of [4] because they can be associated with a single node. Consider for example equation (22) where we append the encoded nodes. The left and right hand sides of equation (22) have the same $i$ index in a consistent manner.

A similar observation can be made for equations (27) and (28).

The fact that a quantity like a demand matrix $D_{ij}$ cannot be conveyed to an encoder or decoder demonstrates a limitation of the attention model of [4]. To be certain, their model is very general and very powerful, providing excellent solutions to a wide range of combinatorial optimization problems. However, the difficulty arises in optimization problems where the problem structure unavoidably involves data related to subsets of nodes.

As an example of a combinatorial optimization problem beyond the scope of [4], we could consider a variant of the traveling salesman problem where we are given a tensor $R_{ijk}$ and the goal is to navigate through the graph such that we collect a reward $R_{ijk}$ when the agent moves from node $i$ to node $j$ and next to node $k$. If the goal is to find the tour that maximizes the sum of these rewards, or perhaps to find the path that does so within a time constraint (given travel times between nodes), then there is no way around the fact that a rank 3 tensor is central to the problem. This is a situation where the attention model of [4] would require a meaningful modification.

In this section, we describe two different modifications of [4] which incorporate tensor demand structure. The first, dynamical masking, is a fairly simple modification that does not result in a substantial computational overhead. However, it only accounts for rank-2 quantities. The second technique, which we refer to as a tensor attention mechanism, is general and powerful but can be extremely memory consuming.

Dynamical Masking

The step of the attention mechanism that involves more than one node is the dot product evaluation between keys and queries. If we want incorporate a demand tensor $D_{ij}$, a natural idea would be to replace the dot product with

$$\frac{1}{\sqrt{\alpha}} G_{ij} q_i \cdot k_i$$ (31)

where $G$ is some tensor determined by $D$. This approach can exaggerate query-key compatibility in cases where $D_{ij}$ is large and suppress compatibility when the demand is small.

There are a few reasonable choices for $G$. The first is $G_{ij} = 1$ which reduces to a basic dot product compatibility. Next is $G_{ij} = M_{ij}$ where $M$ is the mask defined as $M_{ij} = 1$ when $D_{ij} > 0$ and $M_{ij} = -\infty$ otherwise. Both of these are within the methodology of [4]. A third and more novel choice of $G$ is $G_{ij} = \log D_{ij}$. This last form has several virtues: it reduces to a mask in the case in the sense that it...
approaches $-\infty$ as $D_{ij} \to 0^+$. Moreover, it can exag-gerate compatibility when $D_{ij}$ is large. A simple additional adjustment is to use

$$G_{ij} = AD_{ij} + B \log D_{ij}$$

which is more sensitive to changes in $D_{ij}$ for larger values.

Rather than having to pick from these various choices, we can in fact choose all of them by taking advantage of the multiple heads. In other words, for a given head $s \in \{1, \ldots, n_{heads}\}$, we can put

$$G_{ij}^s = A_{\text{basic}}^s + A_{\text{mask}}^s M_{ij} + A_{\log}^s \log D_{ij} + A_{\text{lin}}^s D_{ij}. \quad (32)$$

In principle, even more terms can be used, and a more thorough investigation of various models would be sensible.

Tensor Attention Mechanism

The drawback of dynamical masking is that it specializes to rank 2 tensors. To move to arbitrary rank, we could add terms that sum over certain indices like $\sum_k D_{ijk}$ but this will not access to full structure of the tensor.

There is, however, a way to modify the attention mechanism at a more fundamental level. In equation (14)-(15), we obtain queries, keys, and values by mapping embedded nodes $h_i$ to keys by means of “attention vector maps” $M^\text{query, key, value}$. These maps create a correspondence: for each node there is a query and a key.

As before, a final feedforward layer must be used to get something like

$$k_i = M^\text{key} h_i + u D_{ij}. \quad (33)$$

This equation is intentionally nonsensical, but it does reveal what we need. The indices $ijk$ must match on both sides. Thus, in the rank 3 case, rather than requiring that a single node corresponds to a key, we instead define a key $K_{ijk}$ for each 3-tuple of nodes $(i, j, k)$. We do this as follows:

$$K_{ijk} = M^\text{key} (h_i \oplus h_j \oplus h_k) + u D_{ij}. \quad (34)$$

where $M^\text{key}$ is a learned linear map (without bias) from $\mathbb{R}^{3d}$ to $\mathbb{R}^n$ and $u^\text{key}$ is a learned vector with dimension $n$. As before, $\oplus$ denotes concatenation or, equivalently, direct sum.

Note that $M^\text{key}$ acts on the full vector $h_i \oplus h_j \oplus h_k$. The operation that maps $(h_i)_{i=1}^n$ to the the 3-index object $(h^\text{3D})_{i,j,k=1}^n$ is just a reorganization, but it is, unfortunately, an expensive one. In practice, an implementation of this object would have $b \cdot n^3 \cdot 3d$ components where $n$ and $d$ are, the number of nodes and the encoding dimension, and $b$ is whatever batch size is used in the implementation (for, e.g., parallelization). The problem is the $n^3$ factor, which leads to a substantial memory cost for this technique as the number of nodes grows.

Equation (33) is generalized as follows

$$K_{a_1 \ldots a_r}^s = M^\text{key}_s (h_{a_1} \oplus \ldots h_{a_r}) + u^\text{key}_{s} D_{a_1 \ldots a_r}, \quad (34)$$

$$V_{a_1 \ldots a_r}^s = M^\text{value}_s (h_{a_1} \oplus \ldots h_{a_r}) + u^\text{value}_s D_{a_1 \ldots a_r}. \quad (35)$$

In these equations, we refer to the tensor $D_{a_1 \ldots a_r}$ as a source. We can generalize to multiple sources in the obvious way: replacing $u_i D_{a_1 \ldots a_r}$ by

$$\sum_{k=1}^{n_{sources}} u_{k,s} D^{(k)}_{a_1 \ldots a_r}. \quad (36)$$

Note that we are not constructing a tensor query. Our method is to keep using equation (33) for the construction of queries. The concept is that each node queries a sequence of $r$ other nodes, yielding a compatibility

$$u_{i,a_1 \ldots a_r} = q_i^s \cdot K_{a_1 \ldots a_r}. \quad (37)$$

from which we find attention weights

$$\rho_{i,a_1 \ldots a_r}^s = \frac{\exp(u_{i,a_1 \ldots a_r}^s)}{\sum_{b_1 \ldots b_r} \exp(u_{i,b_1 \ldots b_r}^s)} \quad (38)$$

and finally we obtain new nodes through a value sum:

$$h'_{a_1 \ldots a_r} = \sum_{a_1 \ldots a_r} \rho_{i,a_1 \ldots a_r} V_{a_1 \ldots a_r}. \quad (39)$$

As before, a final feedforward layer must be used to convert the concatenated outputs for each head to a single new output node $h'_i$.

IV. TRAINING METHODOLOGY

In this section, we go into some detail for our training techniques. One aspect of this is our reinforcement learning algorithm which, keeping in line with [4], is a variant of REINFORCE [8]. This section also elaborates on our methodology for environment simulation and generation.

Objective Function

Reinforcement learning requires a reward definition. For our purposes, the entire route can be regarded as a single action, and thus we only need to define a reward $R(\xi)$ for a full route $\xi$. Equivalently, we can define an objective function $F(\xi) = -R(\xi)$. This approach is natural because of our use of REINFORCE.

Typical vehicle routing problems can use total driving time as an objective function to minimize. However, our routing problem has a time constraint $T_{max}$...
and we are not guaranteed that all demand will be fulfilled. To address this, we define demand coverage as the percentage $\eta$ of initial demand that is eventually fulfilled. This quantity requires care to calculate: when a truck arrives at a node $i$, all rank 1 on-board demand with index $i$ is dropped off as a final stop. We can keep track of the accumulated total of such demand as it is dropped off. This total, divided by the sum of all components of initial demand, is the demand coverage $\eta$.

We also use a parameter $T$ to denote the physical time of the last truck when it finishes its route. It’s very important to note that $T$ is not the average time for all trucks.

We then introduce the objective function

$$F(\xi) = -B_{\text{coverage}} \eta + T/T_{\text{max}}$$

(40)

where $B_{\text{coverage}}$ is a hyperparameter. Note that we are writing $\xi$ is the input to $F$ to emphasize that $\eta$ and $T$ are determined by the route (and also initial demand, time matrix, etc.)

$B$ is meant to be greater than 1, and a typical value is 10. The idea is that demand coverage takes first priority, and until coverage approaches its maximum value of 1, we do not try to reduce $T$ below the terminal time limit.

Environment Simulation

Training the model of section III for the general VRP requires a simulation of the environment that is able to take advantage of GPU parallelization. We developed such a simulation using PyTorch. There are several challenges that our simulation overcomes that we highlight in this section.

Consider multiple episodes for vehicle routing problems which run in parallel. The truck routes can be stored as a tensor $\xi_{b,t}$. Here, $b$ is a batch index and $t$ is a time index. The value of $\xi_{b,t}$ is a node providing the departure node at (indexed, not physical) time $t$ for batch entry $b$. However, if there are multiple trucks, then it’s not clear which truck $\xi_{b,t}$ refers to. Thus, we need to track a separate tensor $A_{b,t}$ which specifies which truck is the active truck at time $t$ for batch entry $b$. This approach allows us to perform operations in parallel over a batch with a CUDA implementation.

One of the pitfalls of this organizational approach is that routes are likely to terminate for different batch entries with different $t$. As a result, we must accept that $\xi_{b,t}$ will have a tail of repeating entries for most values of $b$.

Demand structure must be tracked with great care for the general VRP. We use tensors to separately track each rank of on-board demand, cyclic off-board demand, and direct off-board demand. For example, we use a tensor $E_{b,m,ijk}$ to track rank-3 on-board demand. The indices refer to, respectively, the batch entry, the truck number, and the three tensor indices.

Environment Generation

Generating episodes is particularly challenging because of the need to efficiently create examples of demand structures. Episodes start with zero on-board demand and zero direct off-board demand, but have initial cyclic off-board demand with ranks 2 and 3. Not just any tensor $D_{ij}, D_{ijk}$ are acceptable. For example, a component like $D_{232}$ must be excluded.

To create instances, we start with a mask tensor with components which are 1 only for allowed tensor components. We give random values within an allowed range for tensors, mask away components that are not allowed. We then randomly further mask components with some given probability. This is meant to cause instances to be more representative of real data, where we don’t have all-to-all connectivity.

REINFORCE Implementation

Following [4] we implemented a variant of REINFORCE [8].

The REINFORCE algorithm is a policy-gradient reinforcement learning algorithm. While many RL algorithms are based on the idea of first trying to estimate (from experience) the “value” of various actions in a given state, and then taking actions with higher estimated value, policy-gradient algorithms circumvent the intermediate step of estimating values. Instead, we work directly with a parameterized policy, varying parameters to optimize the return from an episode.

The REINFORCE algorithm, following [11], is given as follows
REINFORCE can learn much faster when a baseline is added. This essentially means that some function $b$ of states (but not of actions) is constructed with each episode and the return $G$ in the algorithm is replaced by $G - b(s)$. This algorithm still converges to the optimal policy theoretically and, with a well-chosen baseline, does so much faster. This is easiest to understand when $b(s)$ is taken to be an estimate of the return after state $s$ based on data from previous recent episodes. In this case, $G - b(s)$ being positive indicates that this episode was better than expected and thus it's sensible to increase the probability of following this sequence of actions. Meanwhile, if $G - b(s)$ is negative, the return is less than what is considered a reasonable par, and the gradient ascent would reverse and reduce the probability of taking these actions. The REINFORCE algorithm works regardless of whether or not such a baseline is used, but the learning time is dramatically reduced with a good baseline.

For our purposes we take a variant of REINFORCE adapted to our vehicle routing problem as follows. First, the for purposes of the algorithm we take the entire episode to be defined by a single action. In other words, the episode is just $a_0, r_1$. The action $a_0$ is the entire route specification $a_0 = (\xi_1, \xi_2, \ldots, \xi_k)$ where each $\xi_i$ are nodes. This odd-sounding choice is sensible because with the structure $B$ which makes the logarithm of the policy equal to a sum over logarithms of probabilities of each action in an episode. The reward $r_1$ is simply the negation of the route length (or time) $-L(\xi)$ which is computed by summing the appropriate distances between nodes based on a metric or on known travel times.

The second important aspect of our variant is the baseline methodology. This idea is roughly adapted directly from $\text{H}$. We maintain a “baseline agent” which uses the same parameterized policy but does constantly update its parameter $\theta$. Instead, the baseline agent uses an outdated parameter $\theta_{BL}$ which is occasionally updated to match the primary agent’s $\theta$, but only when the agent substantially and consistently outperforms the baseline.

Our REINFORCE variant is given in algorithm 2. Note that this algorithm is broken up into epochs and batches.

```
Algorithm 1 REINFORCE
Input: Parameterized policy $\pi$
Initial parameter $\theta$
while desired performance not achieved do
   Using $\pi(\theta)$, generate episode $(s_0, a_0, r_1, \ldots, r_T) \leftarrow$ episode
   for $t = 0, 1, 2, \ldots, T - 1$ do
      $G \leftarrow r_{t+1} + \gamma r_{t+2} + \ldots + \gamma^{T-t-1} r_T$
      $\nabla J \leftarrow \gamma G \nabla \log (\pi(a_t | s_t, \theta))$
      $\theta \leftarrow \text{Ascent}(\theta, \nabla J)$
   end for
end while
```

```
Algorithm 2 REINFORCE variant for VRP
Input: Parameterized policy $\pi$
Input: Integers num_epochs, batch_size, batches_per_epoch
Input: Initial parameter $\theta$
$\theta_{BL} \leftarrow \theta$
for $e = 1, \ldots, \text{num_epochs}$ do
   for $b = 1, \ldots, \text{batches_per_epoch}$ do
      $\xi \leftarrow \text{batch_size}$ many episodes from $\pi(\theta)$
      $\xi_{BL} \leftarrow \text{batch_size}$ many episodes from $\pi(\theta_{BL})$
      $\nabla J \leftarrow \text{batch_mean} \left( L(\xi) - L(\xi_{BL}) \nabla \theta \log \left( \sum_{i=1}^{k} \pi(\xi_i, \theta) \right) \right)$
      $\theta \leftarrow \text{descent}(\theta, \nabla J(\theta))$
   end for
   if baseline_test() then
      $\theta_{BL} \leftarrow \theta$
   end if
end for
```

One confusing part of this algorithm may be the summation $\sum_{i=1}^{k} \pi(\xi_i, \theta)$. To clarify, this is a sum over the probabilities computed by the encoder/decoder network at each stage of the route. $k$ refers to the number of steps in the route and the index $i$ runs over steps in the route, not over batch entries. The entire computation is performed for each batch entry and averaged over.

The baseline_test() subroutine returns true when the policy $\pi(\theta)$ substantially outperformed the baseline policy $\pi(\theta_{BL})$ in recent episodes. More specifically, after each epoch we compute percentage of epochs in which the policy outperforms the baseline policy. If this percentage exceeds 50% for 10 consecutive epochs then we update the baseline parameters. Moreover, if the percentage exceeds 70% for any epoch, we update the parameters. There is certainly room for experimentation with different methods here (like the one-sided T Test used in $\text{H}$ but our methods were satisfactory).

V. SUPPLY CHAIN MANAGEMENT WORKFLOW

The ultimate goal of our work is to find a way to apply reinforcement learning techniques for combinatorial optimization problems in a realistic commercially valuable setting. Training an agent through the methods of sections $\text{II}$ and $\text{IV}$ yields approximate solutions to the general VRP described in section $\text{II}$. This section explains how we can use such a trained agent to obtain approximate solutions to the full AVRP of section $\text{II}$.C

There are two difficulties to overcome:

1. The scale of the AVRP is too large, with 21 nodes and with so much demand that $\sim 150$
trucks may be necessary to fulfill requirements in the 16 hour time window.

2. The general VRP lacks the discrete box structure of the full VRP.

To deal with the first difficulty, we decompose the graph into pieces that can be treated by agents trained for a smaller number of trucks and nodes as described in section V A). The second difficulty is handled by processing truck routes obtained through the general VRP into a full-scale simulation of the AVRP (see section VB).

A. Node Subset Search

Consider an instance of the general VRP with $n$ and demand structure $D^{\text{init}}$. Given the demand structure, the time matrix, and the driving window $T_{\text{max}}$, we can estimate the number of trucks $N$ that will be necessary to fulfill all requirements.

Suppose that we have an algorithm to find solutions to general VRPs with a smaller number of nodes and trucks and with smaller demand structure. Our algorithm works for $n' < n$ nodes and $N' < N$ trucks.

This situation arises in our context naturally: we can train, for instance, an agent to solve general VRP instances with 10 nodes and three trucks, a scale smaller than the AVRP with its 21 nodes and over 100 trucks.

We should be able to use our smaller-scale algorithm to solve the larger problem by applying it repeatedly to different subsets to nodes to gradually fulfill all demand requirements. This raises a question of how to find good subsets.

We begin by looking at the demand structure $D^{\text{init}}$. For simplicity, assume that this consists only of rank-3 cyclic demand (other cases are very similar and we describe the necessarily modifications below). From $D^{\text{init}}$ we can identify the nonzero components. These are tuples of nodes

\[ i_1, j_1, k_1 \]
\[ i_2, j_2, k_2 \]
\[ \vdots \]
\[ i_u, j_u, k_u \]

where $u$ is some integer (which happens to be 107 for the AVRP). We can begin our node search by uniformly randomly selecting one of these triples of nodes from the list. (In cases where demand also includes rank 2 or another rank, we include tuples of appropriate length in the list for nonzero demand cases and we allow such tuples to be selected as well.) After drawing a tuple from the list, we remove it from the list. Suppose that we select the tuple $(i_3, j_3, k_3)$. We define a starting subset of nodes as $A = \{ i_3, j_3, k_3 \}$.

If $3 < n'$, we continue to draw nodes. Suppose that we next draw $(i_5, j_5, k_5)$. We now consider the set $A = \{ i_3, j_3, k_3, i_5, j_5, k_5 \}$. If any node repeats (for instance, if $i_3 = j_5$), that entry is only counted once in the set. There will now be between 4 and 6 elements in $A$. If $|A| < n'$, we continue and otherwise we stop. Continuing in this way, we can either eventually run out of tuples or we can reach $|A| \geq n'$. If we reach $|A| = n'$, we stop and use $A$ as our first guess of a node subset. If $|A|$ exceeds $n'$, we remove the most recently added subset. If we run out of tuples, we stop.

After this process, we might have $|A| < n'$. In this case, we simply randomly add additional nodes outside of $|A|$ until reaching $|A| = n'$.

At this point, we have obtained a random node subset $A$. We repeat this process $K$ times to obtain $k_{\text{node draws}}$ different random subsets, and we apply our algorithm $k_{\text{node attempts}}$ times for each of the $k_{\text{node draws}}$ subsets. We compute the mean demand fulfilled for the $k_{\text{node attempts}}$ trials, and we select the node subset with the highest mean demand coverage.

B. Execution Loop

With a technique for selecting node subsets, we are now in a position to describe the execution procedure. This begins with the initial demand structure $D^{\text{init}}$ which is determined by the AVRP’s requirements. Next, a node subset is selected through the node search technique of section V A). We identify the portion of $D^{\text{init}}$ that is supported by the subset and we map it onto a demand structure $D'$ for $n'$ nodes. To regulate the policy input, we clip $D'$ at some maximum value $C$. We then apply the trained agent $k_{\text{execution attempts}}$ times and select the trial with the highest percentage of covered demand. This trial has a specific routing for $N'$ trucks and corresponds to a certain demand fulfillment. The route as well as the on-board and off-board demand at each step is saved and the initial demand $D^{\text{init}}$ is modified: it is reduced by the amount of demand satisfied by the route.

This process is repeated, each time first performing node selection and then finding the best route out of $k_{\text{execution attempts}}$ attempts. We repeat until all demand is satisfied. The total number of iterations of this procedure multiplied by $N'$ will be the total number of trucks needed for our solution.

C. Full Scale Simulation

The result of the execution loop yields approximate solutions to the general VRP. We obtain a collection of routes for various trucks $x_m \tau$ where $m$ ranges over trucks and $\tau$ over time steps for each truck. However, here, we are breaking out earlier convention and using a unified time index $t$ and instead using $\tau$ to range over the time steps for individual trucks.
we still need a way to convert such routes to candidate solutions to the AVRP of section II.C.

Our strategy is to interpret the routes \( x \) as “suggested routes” and to attempt to use them in a full-scale supply chain simulation. We make use of a modified variant of the simulation of [13]. Every box is individually tracked and has rank-2 or rank-3 requirements. Unlike [13], we require that demand is cyclic: boxes must be returned to their origin node. Each box has a specific individual volume. The simulation is designed to be as similar as possible to the actual commercial routing problem of Aisin Corporation.

Trucks follow along the routes \( x_{m, \tau} \) that they are assigned from the execution algorithm and they pick up boxes as is appropriate for their route. Boxes are picked up according to the algorithm described in [13] and we carefully ensure that trucks only drive within the allowed drive time windows (two 8 hour shifts). The result of full-scale simulation is that, rather than having a list of suggested truck routes, we obtain a precise statement about what each truck in the supply chain is doing at all times, including exactly which boxes must be picked up and dropped off at various nodes.

VI. RESULTS

A. Training Parameters

When training the general VRP agent, we used an encoding dimension \( d = 128 \) and three encoder layers and 8 attention heads for all layers except for the final policy output layer. For feedforward layers we used 64 dimensional hidden layers. We used dynamical masking as described in section II.B as we found that the memory limitations were too prohibitive for full tensor demand structure. For dynamical masking in the decoder, we used one source \( D_{ij} \) given by

\[
D_{ij} = \sum_k D^{\text{total}}_{ijk} + D^{\text{total}}_{ij}
\]

where \( D^{\text{total}}_{ij} \) is the sum of cyclic and direct off-board demand. We also used dynamical masking in the first encoding layer with the same \( D_{ij} \) (although for the encoder we are using initial demand while for the decoder we are using the demand at the moment of decoding).

Training was conducted in batches of length 256 with the Adam optimization method. Using an initial learning rate of \( 2^{-23} \), we trained 100 epochs each consisting of 64 batches each. The learning rate was taken to decay by a factor of .965 for each epoch until reaching a final rate of \( 2^{-15} \) at which point it was held constant. An example training curve is shown in figure 4.

B. Execution Performance

The methods described in section VI were used with truck groups of size \( N' = 3 \). The estimated demand satisfied by each truck during this process is shown in figure 5 and the estimated remaining demand as truck groups are iteratively assigned is shown in figure 6. Upon full-scale simulation (section VI.C), we obtain the the routing graph shown in figure 7.

VII. CONCLUSION

While there is much additional work to do in exploring algorithmic and workflow improvements, these first results demonstrate that this general VRP agent can successfully train a model to solve the logistics
FIG. 7. The truck-routing connectivity graph obtained by assigning teams of 3 trucks using the methods of section V. Note that this figure only shows connectivity without regard for the demand flow along each edge, routing orientations, or specific timing details.

This reinforcement learning approach is computationally demanding, especially considering multiple trucks and the tensor demand structure, but the introduction of attention head mechanism and decomposing the agents into sub-teams of truck reduced the computational burden while still achieving solutions. The box return constraint especially added to the computational burden of finding solutions, just as it adds greater complexity to real-life operations. This suggests that the design of future logistics approaches might try to mitigate or replace the box return requirement with a different approach that would increase efficiency and reduce cost.

We were only able to study a few training approaches during the course of this project. Further work in alternative training approaches would likely find more efficient and more effective training approaches. While the model incorporates many key features of Aisin data, the overall workflow was not optimized for Aisin data. So exploring problem structure unique to the Aisin data might yield better training results.

And finally, the use of teams of trucks was necessary to make the problem computationally tractable, and was also successful in yielding solutions, but we have only explored a small sub-space of how teams of trucks can be used iteratively to decompose the actions of the entire fleet of trucks. So more work in this area would likely improve results.

Overall the results are quite promising using classical computing today and amenable to benefit from quantum computing in the future. And given the multiple parts of the training algorithm, exploring how to better implement each part in future studies could yield significant improvement in the overall solution quality for supply chain logistics.

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[13] To appear: Toward supply chain logistics with quantum optimization algorithms.