Proceedings of the 2024 Winter Simulation Conference
H. Lam, E. Azar, D. Batur, S. Gao, W. Xie, S. R. Hunter, and M. D. Rossetti, eds.

CATALYZING INTELLIGENT LOGISTICS SYSTEM SIMULATION WITH DATA-DRIVEN DECISION STRATEGIES

Shiqi Hao[1], Yang Liu[2], Yu Wang[1], Xiaopeng Huang[1], Muchuan Zhao[1], and Xiaotian Zhuang[1]

[1]Department of OpsAI, JD Logistics, Beijing, CHINA
[2]Department of X, JD Logistics, Beijing, CHINA

ABSTRACT

Machine learning is becoming an important technique in modern simulation systems due to the strong capability on capturing the random, complex, and dynamic features of the physical world. Based on these advantages, it has been employed as a powerful tool that enables the intelligent simulation of large-scale logistics systems in a highly efficient manner. Inspired by these applications, this work presents a new paradigm, where machine learning is utilized to generate data-driven decision strategies to accurately emulate the practical operations in logistics systems, and improve the simulation accuracy. Compared with existing approaches, the proposed method is also characterized by the high flexibility and transparency. Consequently, it can adapt to a large variety of logistics system architectures, and catch adequate details of system dynamics. Experiments have been conducted based on the simulation of large-scale real-world logistics systems, where the proposed method demonstrates superior accuracy on both strategy learning and simulation.

1 INTRODUCTION

Logistics plays a crucial role in modern society by facilitating the connections between suppliers and consumers, thereby supporting business and industrial activities, and contributing to economic growth (Liu et al. 2023; Hao et al. 2022). To meet diverse customer demands for delivery efficiency and transportation volumes, large logistics corporations often maintain extensive hierarchical networks. Within these networks, numerous rapid decisions regarding optimal resource allocation and utilization must be made to ensure the efficient, cost-effective, and reliable movement of goods (Liu et al. 2023; Liu et al. 2023). However, due to the high complexity and dynamic nature of logistics systems and their external environments, predicting the outcomes of these decisions is challenging. Local operations can have global repercussions within the entire logistics system (Liu et al. 2023; Rabe et al. 2018) or even lead to unintended consequences (Rushton et al. 2006; Liu et al. 2020).

To tackle the challenge aforementioned, simulation, particularly discrete event simulation (DES), is employed as a powerful tool to replicate real-world behavior through digital representation (Liebler et al. 2013; Urzua et al. 2019; Pedrielli et al. 2016). It offers timely feedback on the effects of proposed operations, thereby avoiding the need for costly and sometimes impossible on-site experiments (Lang et al. 2022; Tripathy et al. 2021a; van Steenbergen et al. 2021; Gerrits and Schuur 2021; Paul and Doreswamy 2021). Its capability to capture system intricacies at any desired level enables it to effectively model the stochastic nature of physical systems. This makes simulation a robust tool for exploring "what-if" scenarios, especially when compared to pure mathematical formulations that frequently lack sufficient detail and fail to capture the dynamic outcomes of operations (Tripathy et al. 2021b; Herrera et al. 2021; Tordecilla et al. 2020; Ramírez-Villamil et al. 2020; Ghorpade and Corlu 2020; Nag and Pal 2022; Onggo et al. 2022). For this reason, simulation has been widely adopted as a component of optimization frameworks to evaluate the efficacy of optimization strategies in vehicle routing (Peyman et al. 2021; Ramírez-Villamil et al. 2020), facility location selection (Tordecilla et al. 2020; Onggo et al. 2022), replenishment (Nag and Pal 2022), etc., while accommodating the potential uncertainties from multiple sources, such as travel time (Peyman et al. 2021; Onggo et al. 2022; Ramírez-Villamil et al. 2020) and customer demand (Tordecilla et al. 2020; Ghorpade and Corlu 2020; Nag and Pal 2022). In recent years, machine learning has attracted great popularity in the simulation of logistics systems (Liu et al. 2023; Liu et al. 2020), to investigate the correlations between external factors and critical parameters in simulation, thereby facilitating input data modeling (Liu et al. 2020; Barra Montevechi et al. 2021; Reed and Löfstrand 2022; Cen et al. 2020), surrogate modeling (Cen and Haas 2022; Feng et al. 2018; Zhao et al. 2021), and other task-specific applications (Montevechi et al. 2022; Wozniak et al. 2022) in simulation systems, as depicted in Figure 1(a), (b), and (c).

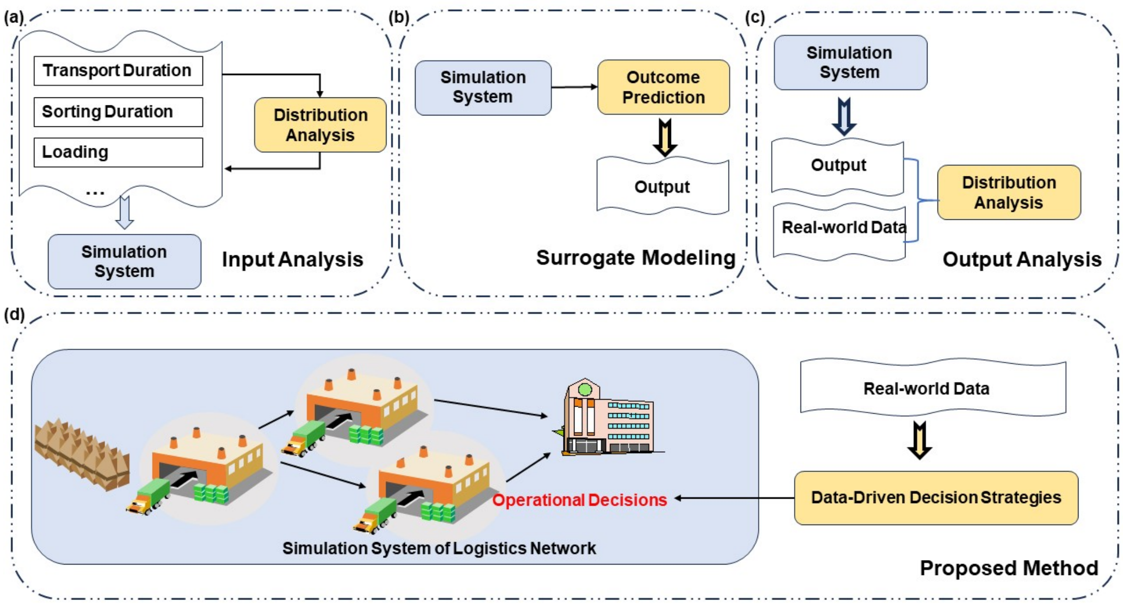

Figure 1: Conventionally, machine learning has been utilized in DES for (a) input parameter modeling, (b) surrogate modeling, and (c) output analysis. In this work, a new paradigm (d) is proposed that utilizes machine learning to emulate the strategies for operational decisions.

In this work, we introduce a novel paradigm of integrating machine learning into logistics simulation. Unlike existing approaches that focus on modeling inputs or outputs of simulation programs, our proposed method is specifically tailored to model internal decision strategies within simulations. This allows for the accurate emulation of practical actions taken at various stages of parcel handling, accounting for complex influencing factors such as resource availability, urgency of delivery requirements, and even operator habits across different shifts, as illustrated in Figure 1(d).

In fact, this is similar to embedding agent-based simulation in a DES framework as each decision maker can be regarded as an agent. In existing literature, this is usually implemented using rule-based strategies (Zhang et al. 2020; Aerts et al. 2018; Kandemir et al. 2022). For instance, when modeling the product picking operations in the warehouse, pickers are programmed to take the shortest path and pick the products in the central point of the pick face only in (Lang et al. 2022). However, the operations in real world can be impacted by multiple factors such as environmental issues and personal preference, while the hard-coded logic can hardly evolve along with them. In order to tackle these challenges, this work intends to model the decision strategies for logistics operations through investigating the underlying philosophies from historical records. To reach this goal, machine learning is utilized to establish data-driven decision strategies, thereby catalyzing the intelligent simulation of logistics systems.

Compared with conventional approaches, the proposed method also features high flexibility and transparency. While the established machine learning models can emulate the behavior of decision makers and generate corresponding operational actions, they can be conveniently organized to adapt to a wide variety of simulation system architectures, regardless the limitation of any specific network topology. Although the surrogate models can also draw data-driven insights from historical records, they are limited by the black-box nature of machine learning models, and cannot reflect the details of decision making. Even though explainable machine learning techniques have been studied to address this issue by interpreting the output of machine learning models (Ribeiro et al. 2016; Lundberg and Lee 2017), there still exists inevitable gaps for matching all necessary entities in the physical world. In contrast, the proposed method can gain both global view on the performance of entire system and the details of how each task is processed. This can also help understand the internal mechanisms that the operational decisions are impacted by external factors.

To validate the proposed method, we utilize a DES simulation model designed to replicate the packing, sorting, transportation, and delivery processes of parcels within real-world logistics systems. While this model has demonstrated high accuracy in evaluating network throughput from a strategic standpoint, it struggles to accurately mimic tactical decisions. To be specific, parcels typically traverse the logistics network from origin to destination in a sequential manner. Precisely modeling each shipment segment, also known as a hop, is crucial for predicting resource utilization and identifying potential bottlenecks. Although hard-coded rules can capture the predominant patterns of parcel flow, a significant portion of parcels deviate from these patterns in reality. To address this challenge, we employ a specific machine learning model called the Field-weighted Embedding-based Neural Network (DeepFwFm) (Deng et al. 2021). This model is utilized to predict the next hop of a parcel based on features extracted from the parcel itself, the origin-destination (O-D) path, and the current hop.

Under this setup, experiments have been conducted using the historical record in several consecutive days, where the proposed method demonstrates superior prediction accuracy compared with a set of classic baselines, while effectively reducing the mean average percentage error (MAPE) of simulation by 4.83% than rule-based method. In summary, the contributions of this work can be highlighted as follows:

- This work introduces a novel paradigm that leverages machine learning as a data-driven decision engine to replace hard-coded rules in simulation. By emulating internal decision-making mechanisms using data-driven strategies, this approach enhances accuracy, flexibility, and transparency.
- A specific Discrete Event Simulation (DES) model, simulating parcel processing in logistics systems, is implemented to validate the proposed method. Machine learning is embedded as a decision module to predict the next hop of each parcel based on volatile context features.
- Experiments have been conducted using historical records of parcel processing in real-world logistics systems. Results demonstrate that the proposed method outperforms a set of classic baselines, leading to a substantial reduction in simulation Mean Absolute Percentage Error (MAPE).

The remainder of this paper is organized as follows. The related works for applications of machine learning in simulation are reviewed in Section 2. The background of the considered simulation framework is introduced in Section 3. The technical details of the proposed method are presented in Section 4. The experimental results are discussed in Section 5. Finally, we conclude in Section 6.

2 RELATED WORKS

In modern simulation systems, the major applications of machine learning are devoted to input data modeling, surrogate modeling, and customized solutions in specific simulation scenarios, as depicted in Figure 1(a), (b), and (c).

As input data modeling is the interface of simulation programs to obtain knowledge about the external world, the accuracy of simulation critically relies on the quality of input data modeling. In order to capture the key characteristics of real-world data, machine learning techniques have been utilized to establish connections between the input data and potential impacting factors, thereby appropriately estimating their distributions (Liu et al. 2020; Barra Montevechi et al. 2021; Reed and Löfstrand 2022; Cen et al. 2020). For instance, the sorting time is estimated based on the spatial-temporal features of parcel volume distribution in (Liu et al. 2020) to catch the impact of further dynamics. Similarly, distributional random forest is utilized in (Reed and Löfstrand 2022) to model the multi-variant nature of event outcomes instead of simple approximations using expected values. In (Barra Montevechi et al. 2021) and (Cen et al. 2020), the potential of generative models, such as adversarial generative networks (GANs) and variational autoencoder (VAE), are explored to emulate the complex distributions, and generate high-quality synthetic data for simulations.

While simulation is an important tool to validate the impact of decisions, the simulation program usually need to be rapidly executed to support the evolutionary optimization of decision strategies, which is known as simulation-based optimization. As it is usually expensive to execute the simulation program repeatedly especially for the simulation of large-scale systems, surrogate modeling uses machine learning model as a substitute evaluation function to map the simulation input directly to the corresponding outcomes (Cen and Haas 2022; Feng et al. 2018; Zhao et al. 2021). A precursor in this direction (Feng et al. 2018) establishes a neural network to emulate the outputs of DES given the candidate configurations of building construction. Reinforcement learning and co-evolutionary algorithms are further incorporated in (Zhao et al. 2021) to train the surrogate model, thereby adapting to new operational conditions. Graph neural network is utilized in (Cen and Haas 2022) to represent structural characteristics of the physical system, and consequently achieve a superior simulation accuracy.

Apart from the aforementioned applications, machine learning is also used to construct customized solutions to address the problems in specific scenarios of simulations. In (Montevechi et al. 2022), GAN has been employed to validate the outputs of simulation programs through discriminating it from real world data using the discriminator. An innovative application has been proposed in (Wozniak et al. 2022) to detect the errors induced by scaling up the code for network simulation through parallelism. It transforms the simulation traces into image formats, and leverages computer vision techniques to examine the correctness of implementation.

3 SIMULATION FRAMEWORK

Based on the real-world logistics system, we consider the simulation of an end-to-end logistics network as depicted in Figure 2. It consists of a set of facility nodes, including warehouses, distribution centers, terminal stations, and the transportation routes connecting them (Liu et al. 2020). Through the simulation program, we aim to emulate the end-to-end processing of each parcel, evaluate the performance of operations, and finally achieve feedback on the efficacy of actions.

As the logistics network is a sophisticatedly designed hierarchical architecture, a parcel being shipped will go through a series of standard operations before delivered. Taking retailing logistics as an example. Once an order is placed, the corresponding items will be picked and packed in the warehouse, and a shipping bill will be created correspondingly in the system. Subsequently, it will be forwarded by a series of distribution centers to the local region of the receiver. Finally, it will arrive at the terminal station, and be delivered to the receiver by the courier. The shipping bill can also be created from a personal shipment order, in which the courier needs to collect the parcel from the sender, and let it go through the same procedure as retailing parcels.

In order to emulate the working conditions of the real-world logistics system and obtain the key performance indicators (KPIs), the workload of the system needs to be simulated based on the practical scenarios. To reach this goal, a set of shipping bills will be generated for each day, with the distribution of their volumes, weights, origins, destinations and total numbers appropriately controlled, to match the reality. Given the generated workload, the parameters related to the processing in each component of the logistics network, such as sorting time and transportation time, are also estimated to approximate the response of the system (Liu et al. 2020). Based on the aforementioned configurations on input parameters,

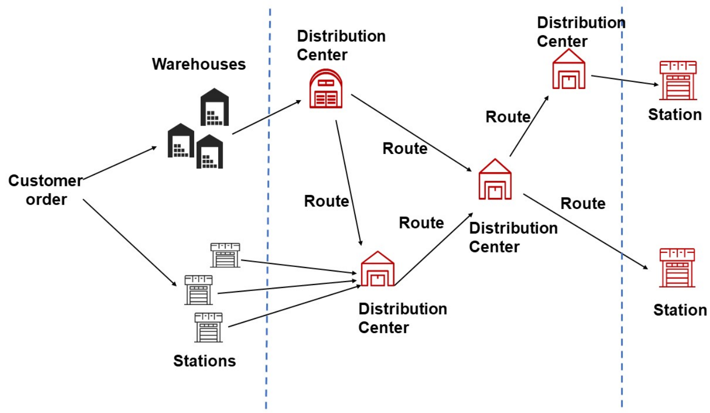

Figure 2: An end-to-end logistics network is considered in the simulation framework, which consists of warehouses, distribution centers, terminal stations, and the routes connecting them.

we would like to evaluate the time efficiency and recognize bottlenecks in resources both globally in the entire logistics network and locally in each component.

Given the aforementioned configurations, this work studied the method to emulate the decision strategies in logistics operations for approximating the characteristics of the real-world. While the specific approaches for processing the parcels need to be determined by decision makers, their assignments on logistics operations directly affect the processing efficiency and utilization of resources. Hence, the quality of simulation critically depends on the accuracy for modeling the behaviors of decision makers. However, this only has been investigated in a few existing literature due to practical difficulties despite its importance (Kandemir et al. 2022; Wu et al. 2008; Lang et al. 2022). In specific, the strategies for item picking have been modeled in (Lang et al. 2022) using empirical assumptions and rules. The behavior of decision makers is usually complicated, which can be impacted by a wide variety of external factors and personal preference. Hence, it can hardly be modeled by trivial rules and mathematical formulations. For instance, the specific routing of a parcel needs to be determined after the origin and destination are known to assign the sequence of distribution centers in the corresponding O-D path. This can be implemented straightforwardly by directly taking the shortest path. However, the practical parcel routing usually needs to consider various other factors such as the capacity of routes and distribution centers, and the availability of other resources. Given a set of distribution centers $\mathscr{D}$, suppose that a parcel is at distribution center $d_i \in \mathscr{D}$, and next hop in the shortest path is $d_j \in \mathscr{D}$. However, the capacity of d_j can be exceeded due to the large workload during promotions (e.g., Black Friday), and the parcel will suffer from severe sorting delay if assigned to d_j. In this scenario, the decision maker must consider re-arranging next hop, which cannot be appropriated approximated by trivial rule-based simulation strategies.

In order to address the aforementioned issues, this work proposes to investigate the correlations between operational decisions and potential impacting factors through historical records using machine learning. This can help develop data-driven insights to understand the philosophies behind the manual decisions, thereby generating more realistic decisions in the simulation program given corresponding context. In specific, we take the routing of parcels as an example to illustrate the utilization of data-driven decision strategies for logistics system simulation. To reach this goal, we extract representative features to capture the characteristics of the parcels, distribution centers, and transportation routes. A machine learning model is subsequently established, which takes these features as input and generate the prediction on next hop as output. In order to learn the behavior of decision makers, we train the machine learning model using historical data before deploying it in the simulation program. Finally, the machine learning model is used to predict next hop of each parcel given the specific context once it is created, until it is delivered.

4 PROPOSED METHOD

Based on the simulation framework described in Section 3, this section is dedicated to the construction of the machine learning model for next-hop prediction. A straightforward approach to implement this can be directly mapping the features representing the current state of the parcel to the most probable next hop, which can be cast into a multi-class classification problem, with each candidate next hop defined as a class. However, this can induce variations on the output dimensions since the number of candidate next hops for different distribution centers are not guaranteed to be consistent. It means that we need to establish an individual model for each distribution center, which can hardly be reused. In order to tackle this difficulty, we adopt the common practice in the recommendation system community, where the information of the user and candidate item are fed into the machine learning model simultaneously to generate a click-through rate (CTR). Inspired by that, we propose to feed the features corresponding to both the current hop and candidate next hop into the machine learning model simultaneously, and generate the probability that the solution is selected by the decision maker. This approach offers significant flexibility, such that it can evaluate if a route can be selected as long as the pair of current/next hop distribution centers are given, regardless the topology of any specific logistics network. Hence, the machine learning model proposed in this work can be presented by

$$y = f(\mathbf{x}), \tag{1}$$

where the the feature vector $\mathbf{x}$ contains the features extracted from the current state of the parcel and the context of candidate next hop, and y is the probability that the route can be selected by a decision maker.

4.1 Feature Selection

In order to include enough key foundations that can facilitate decision making, we adopt 4 types of information in the input feature vector $\mathbf{x}$ as follows.

- **Parcel Information** For each parcel, we consider its basic attributes including weight, volume, and the number and types of items, as they can impact the efficiency of sorting and transportation. Furthermore, we also consider the origin, destination, and time efficiency-related features as they are important basis for decision makers to determine their routing.
- **Current Hop Information** For the distribution center corresponding to the current hop, we consider the regional features as it represents the topological information. We also consider the workload information of the distribution center as the decision maker may tend to assign the parcels to more down-stream distribution centers if its workload is high.
- **Candidate Next Hop Information** Similar to the current hop, we consider the regional and workload-based information of candidate next hop as well, as they will impact the expected time efficiency.
- **Candidate Route Information** Given the current hop and candidate next hop, the candidate route is automatically fixed. For the route, we consider the availability of resources such as the number of vehicles, time-efficiency-related information such as transportation time, and the recent workload.

For each distribution center and route, their indices are included in the feature set as well, to investigate high-order correlations with decision making. According to the above categorization, the feature vector $\mathbf{x}$ can be divided into 4 groups, such that

$$\mathbf{x} = [\mathbf{x}_P, \mathbf{x}_{DC}, \mathbf{x}_{DN}, \mathbf{x}_R], \tag{2}$$

where $\mathbf{x}_P$, $\mathbf{x}_{DC}$, $\mathbf{x}_{DN}$, and $\mathbf{x}_R$ are the segments corresponding to the parcel, current hop, candidate next hop, and candidate route, respectively. Among these groups of features, $\mathbf{x}_P$ and $\mathbf{x}_{DC}$ represent the current state of the parcel, and $\mathbf{x}_{DN}$ and $\mathbf{x}_R$ represent the information of candidate next hop. The considered features can be classified into numerical ones (e.g., the weight of parcel) and categorical ones (e.g., indices of distribution centers). While the numerical ones are directly taken as the input of the machine learning model, the categorical ones are one-hot encoded before being used. In practice, these factors can be jointly considered to determine the routing of parcels.

4.2 Model Construction

In order to investigate the underlying patterns of input features, recognize their correlations with the decisions, and make full use of their prediction power, this work adopts the recent advance of recommendation system, i.e., the DeepFwFm model (Deng et al. 2021), for the construction of $f(\cdot)$. The DeepFwFm model comprises two components including a deep neural network (DNN) component and an FwFm component. Before entering these components, the sparse one-hot formats of the categorical features need to pass through a embedding network to obtain the compressed format. As the decision maker will jointly consider the impact of multiple factors to the efficiency of logistics operations when selecting the routing of parcels, their contributions to the final decision is usually highly complicated. Taking advantage of the highly nonlinear architecture, the DNN component takes all numerical features and the embedded formats of the categorical features to explore their manifold correlations with final decisions. In contrast to the DNN component, the FwFm component only absorbs the embedded formats of categorical features to learn their representations based on their interactions. While a numerical feature usually has an explicit physical meaning, a majority of categorical features are indices, whose values cannot be directly compared. However, their contributions to the final decision can be reflected in their historical interactions. For instance, the frequency that distribution centers d_i and d_j have been selected as adjacent hops of a parcel can provide useful insights on the decision strategy. In our proposed model, this is investigated using the FwFm component. Finally, the outputs of these two components are summed to construct the output of the DeepFwFm model.

For a feature vector $\mathbf{x}$, let the set of numerical and categorical features be denoted by Θ and Φ, respectively. Thus, the value of numerical feature $\theta \in \Theta$ is denoted by s_θ, and the embedding vector of categorical feature $\phi \in \Phi$ is denoted by $\mathbf{e}_\phi$. Furthermore, we denote the DNN and FwFm components by $f_{Deep}(\cdot)$ and $f_{FwFm}(\cdot)$, respectively. Among these components, the input of $f_{Deep}(\cdot)$ is the concatenation of two vectors $\mathbf{s}$ and $\mathbf{e}$, where $\mathbf{s} = [s_1, \dots, s_\theta, \dots, s_\Theta]$, such that each dimension corresponds to a numerical feature, and $\mathbf{e} = [\mathbf{e}_1, \dots, \mathbf{e}_\phi, \dots, \mathbf{e}_\Phi]$, such that each segment corresponds to a categorical feature. f_{FwFm} can be mathematically represented as

$$f_{FwFm}(\mathbf{e}) = w0 + \sum_{\phi=1}^{\Phi} \langle \mathbf{e}_\phi, \mathbf{v}_\phi \rangle + \sum_{\phi=1}^{\Phi} \sum_{\phi'=\phi+1}^{\Phi} \langle \mathbf{e}_\phi, \mathbf{e}_{\phi'} \rangle R_{\phi,\phi'}, \tag{3}$$

where w_0, $\mathbf{v}_\phi$ and $R_{\phi,\phi'}$ are learnable model parameters. Finally, the output of the DeepFwFm model is computed by

$$f(\mathbf{x}) = f_{Deep}(\mathbf{s}, \mathbf{e}) + f_{FwFm}(\mathbf{e}). \tag{4}$$

4.3 Training and Inference

In order to train the model, we sample a set of processing records denoted by $\mathcal{N}$, where each record corresponds to a combination of parcel and its current distribution center. Among these records, each record is combined with its next-hop distribution center to create a positive sample. It is also combined with other available distribution centers to create negative samples. Thus, the positive and negative samples can reflect the choice of decision makers under specific contexts, thereby enabling the learning of decision strategies. The sets of positive and negative samples are denoted by $\mathcal{N}_p$ and $\mathcal{N}_n$, respectively. Based on these samples, the DeepFwFm model is trained through minimizing the cross-entropy loss (Mao et al. 2023) using Adam (Kingma and Ba 2015) optimizer. Note that the embedding network for compressing categorical features is treated as a component of the machine learning model, whose parameters are learned simultaneously with the weights of the DeepFwFm model.

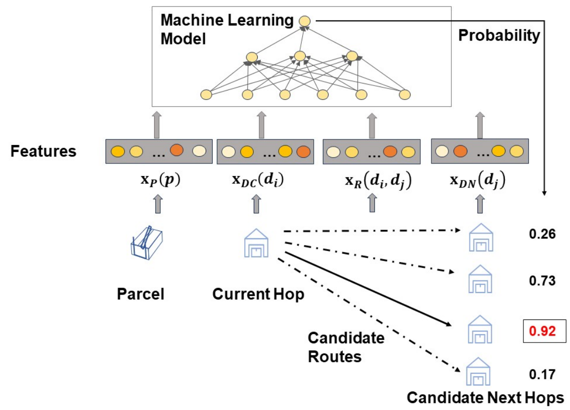

Figure 3: When a parcel arrives at a distribution center d_i, it first generates a set of candidate next hops. For each candidate distribution center, a feature vector is created according to Equation (2), and fed into the DeepFwFm model to compute the probability that it will be selected by a decision maker.

After the DeepFwFm model is fully trained, it is integrated into the simulation program to emulate the behavior of decision maker on determining the routing of parcels. In the simulation system, a set of parcels will be generated along with their basic attributes such as volume, weight, type, origin and destination. For each parcel, the simulation system sequentially determines the next-hop routing in its O-D path. As depicted in Figure 3, when a parcel p arrives at a distribution center d_i, it first generates a set of candidate next hops by gathering the distribution centers have appeared to be the next hop of the current one in history, denoted by $\mathscr{D}_{cand}$. For each candidate distribution center $d_j \in \mathscr{D}_{cand}$, a feature vector $[\mathbf{x}_P(p), \mathbf{x}_{DC}(d_i), \mathbf{x}_{DN}(d_j), \mathbf{x}_R(d_i, d_j)]$ is created according to Equation (2), which is subsequently fed into the DeepFwFm model to compute the probability that it will be selected by a decision maker. Among all the candidate distribution centers, the one with the largest probability is chosen as next hop of parcel p. Subsequently, the state of parcel p is updated by setting the selected next hop as the current hop, and predict next hop using the DeepFwFm model until it arrives the destination.

5 EXPERIMENTAL RESULTS

In this section, experiments are conducted to evaluate the efficacy of the proposed method. We consider a logistics network with 1100 routes and 1061 distribution centers, and sample the records of 1,450,189 parcels in several consecutive days. For each of them, a set of positive samples and negative samples are created as mentioned in Subsection 4.3. For training data, we down-sample the negative data samples to mitigate the imbalance issue between positive and negative data. The details of constructed datasets are shown in Table 1. After the DeepFwFm model is fully trained, it is applied in the simulation program for next-hop selection. Based on the above setup, the experiments in this work are divided into the following two parts.

- In the first part, the proposed method is compare with three other machine learning techniques, i.e., catBoost (Prokhorenkova et al. 2018), DeepFM (Deng et al. 2021), and FwFm (Pan et al. 2018)), for prediction accuracy. Through this set of experiments, we intend to demonstrate the capability of the proposed method to emulate the behavior of decision makers.
- In the second part, the outputs of machine learning models are compared with conventional rule-based simulation strategy for estimating the workload in each route, where the rule-based simulation strategy determines the O-D routing of each parcel by selecting the series of hops with minimum processing time. As route-wise workload is critical to evaluate the performance of logistics system,

we intend to demonstrate the capability of the proposed method on improving simulation accuracy. Totally 53.4 million parcels are created for the simulation.

The machine learning models are implemented using Python language, and deployed on a cloud server with 4 2.3GHz CPUs, 20G RAM and 3 NVIDIA TESLA P40 GPUs. The simulation program is implemented using Java, and runs on another cloud server with 8 2.4GHz CPUs and 50G RAM. When integrating the outputs of machine learning models for decisions in simulation, the machine learning models interact with the simulation program through http protocol.

Table 1: Dataset construction.

Dataset	Num. Parcels	Num. Positive Sample	Num. Negative Sample
Training	1256041	1282024	4446775
Testing	194148	196666	1049871

The accuracy for prediction and simulation are presented in Table 2. As next-hop prediction is essentially a binary classification task, the accuracy is evaluated using area under curve (AUC). The target of the simulation program is to evaluate the workload of each route, i.e., the number of parcels processed by each route. Hence, we compare the simulation accuracy using MAPE. We also note that the rule-based simulation strategy determines the complete O-D path of each path at the beginning, and cannot generate the prediction for all considered parcel-hop combinations. Hence, the prediction accuracy of rule-based simulation is not presented. We can observe from Table 2 that DeepFwFm, DeepFm, and FwFm can achieve an AUC above 0.92, while catBoost leads to an inferior AUC of 0.8560. This attributes to the fact that catBoost fails to investigate the interactions between features, and cannot effectively utilize the underlying patterns of categorical features. Within the methods considering the interactions between features, DeepFwFm slightly outperforms DeepFm and FwFm, due to the appropriate trade-off between deep- and interaction-based knowledge. We can also observe from the table that the methods with higher prediction AUCs also result in lower simulation MAPEs for route-wise workload estimation. Furthermore, all machine learning-based methods outperform rule-based simulation on the MAPE for workload estimation, where the MAPE achieved by DeepFwFm is 28.89%-24.06%=4.83% lower than rule-based simulation.

Table 2: The prediction and simulation accuracy of the machine learning techniques and rule-based simulation.

Methods	DeepFwFm	DeepFm	FwFm	catBoost	Rule-Based Simulation
Prediction AUC	0.9289	0.9279	0.9287	0.8560	-
Simulation MAPE	24.06%	24.47%	24.64%	26.82%	28.89%

In order to gain more details, we assign the routes considered in the simulation into bins based on the difficulty level for workload estimation using rule-based simulation. As there are totally 1100 routes, we divide them into 5 groups based on the MAPE of rule-based simulation, where the ranges of simulation MAPEs are $[0,0.2]$, $(0.2,0.4]$, $(0.4,0.6]$, $(0.6,0.8]$, and $[0.8,\infty]$, respectively, such that the estimation difficulty is increasing as the index of group increases. Correspondingly, the number of routes contained in these groups are 550, 154, 90, 17, and 289. We show the simulation MAPE within each group in Figure 4, where we can observe that the machine learning-based techniques demonstrate substantial advantages compared with rule-based simulation when the difficulty level is high. That is because these routes are associated with high uncertainty, which cannot be appropriately captured by hard-coded rules. In contrast, the machine learning-based methods can develop data-driven insights on the strategies of historical decisions, and apply them to make more accurate predictions in future scenarios.

While the DeepFwFm method outperforms the conventional rule-based simulation by 4.83% in total on the MAPE for estimation the route-wise workload, the dispatch error can be reduced by 860 trucks for the 53.4 million parcels if the capacity of each truck is 3000 parcels. Apart from the significant reduction

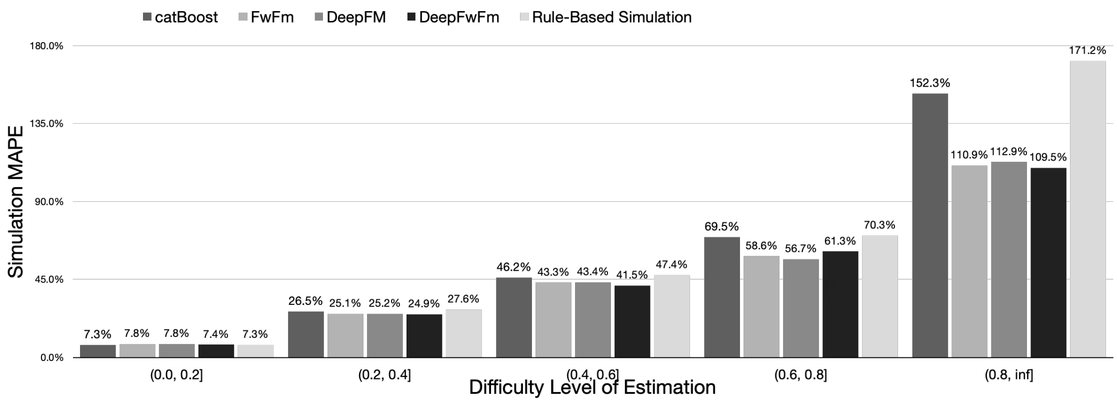

Figure 4: Machine learning-based techniques demonstrate substantial advantages compared with rule-based simulation when the difficulty level for estimation is high.

of economic cost for truck usage, this also mitigates the potential risk on transportation delay. In order to assess the cost for employing the data-driven decision strategies, we also compare the execution time length for rule-based simulation and data-driven simulation using DeepFwFm. Through optimizing the simulation program architecture, it takes 157 seconds for rule-based simulation and 1690 seconds for data-driven simulation. The increase on execution time is acceptable in real-world applications especially when considering the granted benefits.

6 CONCLUSION

In this work, we proposed a new paradigm for utilizing machine learning in logistics system simulation. In specific, we utilize machine learning to emulate practical operations in logistics systems through data-driven decision strategies, thereby improving the simulation accuracy. It is validated via establishing a machine learning model to predict the routing of parcels given the features extracted from current states and candidate next hops of parcels, where the proposed method demonstrates substantial improvement of simulation accuracy compared with rule-based approaches. Furthermore, the proposed method is also characterized by the high flexibility and transparency, and all of these underscore the great potential to facilitate the high-quality logistics system simulation in practical scenarios.

REFERENCES

Aerts, J. C. J. H., W. J. Botzen, K. C. Clarke, S. L. Cutter, J. W. Hall, B. Merz, *et al*. 2018. "Integrating human behaviour dynamics into flood disaster risk assessment". *Nature Climate Change* 8(3):193–199.

Barra Montevechi, J. A., A. T. Campos, G. T. Gabriel, and C. H. dos Santos. 2021. "Input Data Modeling: An Approach Using Generative Adversarial Networks". In *Proceedings of 2021 Winter Simulation Conference (WSC)*, 1–12.

Cen, W. and P. J. Haas. 2022. "Enhanced Simulation Metamodeling via Graph and Generative Neural Networks". In *Proceedings of 2022 Winter Simulation Conference (WSC)*, 2748–2759.

Cen, W., E. A. Herbert, and P. J. Haas. 2020. "NIM: Modeling and Generation of Simulation Inputs Via Generative Neural Networks". In *Proceedings of 2020 Winter Simulation Conference (WSC)*, 584–595.

Deng, W., J. Pan, T. Zhou, D. Kong, A. Flores and G. Lin. 2021. "DeepLight: Deep Lightweight Feature Interactions for Accelerating CTR Predictions in Ad Serving". In *Proceedings of ACM International Conference on Web Search and Data Mining*, 922–930.

Feng, K., S. Chen, and W. Lu. 2018. "Machine Learning Based Construction Simulation and Optimization". In *Proceedings of 2018 Winter Simulation Conference (WSC)*, 2025–2036.

Gerrits, B. and P. Schuur. 2021. "Parcel Delivery For Smart Cities: A Synchronization Approach For Combined Truck-Drone-Street Robot Deliveries". In *Proceedings of 2021 Winter Simulation Conference (WSC)*, 1–12.

Ghorpade, T. and C. G. Corlu. 2020. "Selective Pick-up and Delivery Problem: A Simheuristic Approach". In *Proceedings of 2020 Winter Simulation Conference (WSC)*, 1468–1479.

Hao, S., Y. Liu, Y. Wang, Y. Wang and W. Zhe. 2022. “Three-Stage Root Cause Analysis for Logistics Time Efficiency via Explainable Machine Learning”. In *Proceedings of ACM SIGKDD Conference on Knowledge Discovery and Data Mining*, 2987–2996.

Herrera, E., J. Panadero, A. A. Juan, M. Neroni and M. Bertolini. 2021. “Last-Mile Delivery of Pharmaceutical Items to Heterogeneous Healthcare Centers with Random Travel Times and Unpunctuality Fees”. In *Proceedings of 2021 Winter Simulation Conference (WSC)*, 1–12.

Kandemir, C., C. Reynolds, Q. Tom, K. Fisher, R. Devine, E. Herszenhorn, *et al*. 2022. “Using discrete event simulation to explore food wasted in the home”. *Journal of Simulation* 16(4):415–435.

Kingma, D. P. and J. Ba. 2015. “Adam: A Method for Stochastic Optimization”. In *Proceedings of International Conference on Learning Representations*.

Lang, L., L. Chwif, and W. Pereira. 2022. “Decision-Making Impacts of Originating Picking Waves Process for a Distribution Center Using Discrete-Event Simulation”. In *Proceedings of 2022 Winter Simulation Conference (WSC)*, 1509–1520.

Liebler, K., U. Beissert, M. Motta, and A. Wagenitz. 2013. “Introduction OTD-NET and LAS: Order-to-delivery network simulation and decision support systems in complex production and logistics networks”. In *Proceedings of 2013 Winter Simulations Conference (WSC)*, 439–451.

Liu, B., Y. Liu, S. Hu, and W. Zhe. 2023. “Opportunities and Challenges of Scheduling in Logistics Industrial Park Cyber-Physical Systems”. *IEEE Transactions on Industrial Cyber-Physical Systems* 1:322–334.

Liu, Y., X. Tao, X. Li, A. W. Colombo and S. Hu. 2023. “Artificial Intelligence in Smart Logistics Cyber-Physical Systems: State-of-The-Arts and Potential Applications”. *IEEE Transactions on Industrial Cyber-Physical Systems* 1:1–20.

Liu, Y., L. Yan, S. Liu, T. Jiang, F. Zhang, Y. Wang *et al*. 2020. “Enhancing Input Parameter Estimation by Machine Learning for the Simulation of Large-Scale Logistics Networks”. In *Proceedings of 2020 Winter Simulation Conference (WSC)*, 608–619.

Lundberg, S. M. and S.-I. Lee. 2017. “A Unified Approach to Interpreting Model Predictions”. In *Proceedings of Advances in Neural Information Processing Systems*, Volume 30.

Mao, A., M. Mohri, and Y. Zhong. 2023. “Cross-entropy loss functions: theoretical analysis and applications”. In *Proceedings of the 40th International Conference on Machine Learning*.

Montevechi, J. A. B., G. T. Gabriel, A. T. Campos, C. H. dos Santos, F. Leal and M. E. F. H. S. Machado. 2022. “Using Generative Adversarial Networks to Validate Discrete Event Simulation Models”. In *Proceedings of 2022 Winter Simulation Conference (WSC)*, 2772–2783.

Nag, B. and R. Pal. 2022. “Simulation Optimization for Supply Chain Decision Making”. In *Proceedings of 2022 Winter Simulation Conference (WSC)*, 2853–2863.

Onggo, B. S., X. Martin, J. Panadero, C. G. Corlu and A. A. Juan. 2022. “Solving Facility Location Problems for Disaster Response Using Simheuristics and Survival Analysis: A Hybrid Modeling Approach”. In *Proceedings of 2022 Winter Simulation Conference (WSC)*, 1497–1508.

Pan, J., J. Xu, A. L. Ruiz, W. Zhao, S. Pan, Y. Sun *et al*. 2018. “Field-weighted Factorization Machines for Click-Through Rate Prediction in Display Advertising”. In *Proceedings of World Wide Web Conference*, 1349–1357.

Paul, S. and G. Doreswamy. 2021. “Simulation and Optimization Framework for On-Demand Grocery Delivery”. In *Proceedings of 2021 Winter Simulation Conference (WSC)*, 1–12.

Pedrielli, G., A. Vinsensius, E. P. Chew, L. H. Lee, A. Duri and H. Li. 2016. “Hybrid order picking strategies for fashion E-commerce warehouse systems”. In *Proceedings of 2016 Winter Simulation Conference (WSC)*, 2250–2261.

Peyman, M., Y. Li, R. D. Tordecilla, P. J. Copado-Mendez, A. A. Juan and F. Xhafa. 2021. “Waste Collection of Medical Items Under Uncertainty Using Internet of Things and City Open Data Repositories: A Simheuristic Approach”. In *Proceedings of 2021 Winter Simulation Conference (WSC)*, 1–11.

Prokhorenkova, L., G. Gusev, A. Vorobev, A. V. Dorogush and A. Gulin. 2018. “CatBoost: Unbiased Boosting with Categorical Features”. In *Proceedings of International Conference on Neural Information Processing Systems*, 6639–6649.

Rabe, M., M. Ammouriova, and D. Schmitt. 2018. “Utilizing domain-specific information for the optimization of logistics networks”. In *Proceedings of 2018 Winter Simulation Conference (WSC)*, 2873–2884.

Ramírez-Villamil, A., J. R. Montoya-Torres, and A. Jaegler. 2020. “A Simheuristic for the Stochastic Two-Echelon Capacitated Vehicle Routing Problem”. In *Proceedings of 2020 Winter Simulation Conference (WSC)*, 1276–1287.

Reed, S. and M. Löfstrand. 2022. “Discrete Event Simulation Using Distributional Random Forests to Model Event Outcomes”. In *Proceedings of 2022 Winter Simulation Conference (WSC)*, 689–700.

Ribeiro, M. T., S. Singh, and C. Guestrin. 2016. “"Why Should I Trust You?": Explaining the Predictions of Any Classifier”. In *Proceedings of ACM SIGKDD International Conference on Knowledge Discovery and Data Mining*, 1135–1144.

Rushton, A., P. Croucher, and P. Baker. 2006. *The Handbook of Logistics and Distribution Management*. 3rd ed. London: Kogan Page.

Tordecilla, R. D., J. Panadero, A. A. Juan, C. L. Quintero-Araújo and J. R. Montoya-Torres. 2020. "A Simheuristic Algorithm for the Location Routing Problem with Facility Sizing Decisions and Stochastic Demands". In *Proceedings of 2020 Winter Simulation Conference (WSC)*, 1265–1275.

Tripathy, M., R. Ahmed, and M. Kay. 2021a. "On-Demand Logistics Service for Packages: Package Bidding Mechanism vs. Platform Pricing". In *Proceedings of 2021 Winter Simulation Conference (WSC)*, 1–12.

Tripathy, M., R. Ahmed, and M. Kay. 2021b. "On-Demand Logistics Service for Packages: Package Bidding Mechanism vs. Platform Pricing". In *Proceedings of 2021 Winter Simulation Conference (WSC)*, 1–12.

Urzua, M., A. Mendoza, and A. González. 2019, 12. "Evaluate The Impact of Order Picking Strategies on The Order Fulfillment Time: A Simulation Study". *Acta logistica* 6:103–114.

van Steenbergen, R., M. Brunetti, and M. Mes. 2021. "Network Generation for Simulation of Multimodal Logistics Systems". In *Proceedings of 2021 Winter Simulation Conference (WSC)*, 1–12.

Wozniak, M. K., L. Liang, H. Phan, and P. J. Giabbanelli. 2022. "A New Application of Machine Learning: Detecting Errors in Network Simulations". In *Proceedings of 2022 Winter Simulation Conference (WSC)*, 653–664.

Wu, S., L. Shuman, B. Bidanda, M. Kelley, K. Sochats and C. Balaban. 2008. "Agent-based Discrete Event Simulation Modeling for Disaster Responses". In *Proceedings of Industrial Engineering Research Conference*.

Zhang, J., G. Adomavicius, A. Gupta, and W. Ketter. 2020. "Consumption and Performance: Understanding Longitudinal Dynamics of Recommender Systems via an Agent-Based Simulation Framework". *Information Systems Research* 31(1):76–101.

Zhao, Y., E. Hemberg, N. Derbinsky, G. Mata and U.-M. O'Reilly. 2021. "Simulating a Logistics Enterprise Using an Asymmetrical Wargame Simulation with Soar Reinforcement Learning and Coevolutionary Algorithms". In *Proceedings of the Genetic and Evolutionary Computation Conference Companion*, 1907–1915.

AUTHOR BIOGRAPHIES

SHIQI HAO received her M.S. degree in Big Data from Peking University. Currently, she holds the position of Senior Machine Learning Engineer at JD Logistics, where her work is dedicated to the application of artificial intelligence in logistics scenarios. Her expertise has led to the deployment of several exploratory algorithms that are now actively enhancing logistical operations, and peer-reviewed publications on premier conferences such as ACM SIGKDD. Her e-mail address is haoshiqi@jd.com.

YANG LIU received the Ph.D. degree from Michigan Technological University. He is currently a Senior R&D Manager at the Department of X of JD Logistics, where he is leading the research and applications of artificial intelligence and operations research techniques in the logistics domain. His research has been applied in multiple logistics-based industrial solutions. Before joining JD Logistics, he has been with Duke University as a Postdoctoral Research Associate. He has been serving as a Guest Editor of IEEE Transactions on Industrial Informatics for the Special Section Artificial Intelligence in Logistics Systems. His current research interests mainly focus on smart logistics, smart supply chain and cyber-physical systems. He is the corresponding author of this article. His e-mail address is liuyang130@jd.com.

YU WANG is the Director of Operations Research at JD Logistics, leading a R&D team to develop intelligent decision tools to optimize the design, planning and operations of complex logistics networks. He received his Ph.D. degree from the University of Pittsburgh, and his B.S. & M.S. from Tsinghua University. His e-mail address is bjwangyu3@jd.com.

XIAOPENG HUANG recieved the Ph.D. degree in operational research and cybernetics from Academy of Mathematics and Systems Science, Chinese Academy of Sciences. He currently serves as an algorithm engineer at JD Logistics, where his primary research focuses on logistics simulation, digital twinning, and network optimization. His research has successfully applied in the practical production processes of JD Logistics. His e-mail address is huangxiaopeng5@jd.com.

MUCHUAN ZHAO received the M.S. degree from Nanjing University, Nanjing, Jiangsu, China. He is currently an algorithm engineer at JD Logistics, Beijing, China, where his work focuses on simulation research and digital supply chain construction. Before joining JD Logistics, he has been a process engineer at China Aerospace Science and Industry Corporation. His e-mail address is zhaomuchuan1@jd.com.

XIAOTIAN ZHUANG serves as the senior director of intelligent supply chain at JD Logistics of China since 2019 and is in charge of intelligent supply chain demand forecasting, inventory optimization, network planning, and transportation scheduling. Previously, he worked as a strategic consulting advisor for IBM's Global Enterprise Services, then as a senior scientist at Amazon's Global Supply Chain Technology Department. He received his Ph.D. degree at Arizona State University. His e-mail address is zhuangxiaotian@jd.com.