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Real-Time Estimation of Origin–Destination Matrices Using a Deep Neural Network for Digital Twins

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Abstract

The digital twin, a real-time replica of physical systems, has garnered attention as a promising tool to strategize and evaluate solutions for complex real-world issues. However, developing digital twins in the field of transportation faces significant challenges related to the real-time estimation of dynamic origin–destination (OD) matrices constrained by computation time. To bridge this gap, microscopic traffic simulations with real-time synchronization are being researched. Nonetheless, the computational issue persists, emphasizing the need for more efficient OD estimation methods. In this regard, our objective is to reduce computation time in simulation-based methods by developing a data-driven metamodel using a deep neural network. The proposed model serves to map the correlation between the OD matrix and detector data. This model simplifies the computational process using hidden layers, rather than calculating complex interactions between vehicles in the traffic simulation. Compared to conventional methods, we evaluate the capability to estimate a reasonable OD matrix within a restricted time and validate our approach using detector data from Daejeon City, South Korea. The findings indicate that by combining our data-driven metamodel with the simultaneous perturbation stochastic approximation, it becomes feasible to estimate a reasonable OD matrix within a stipulated time frame, compared to the conventional method. Given a 1-min time frame, the proposed method outperforms the conventional simulation-based method by improving the calibration performance of traffic flow by 44.5 percentage points. This paper proposes a practical and versatile approach for real-time OD estimation, laying the foundation for extending microscopic traffic simulation into the digital twin.

Keywords

digital twin, real-time microscopic traffic simulation, dynamic origin-destination estimation, data-driven metamodel

Driven by the surge in population, transportation issues such as traffic congestion have emerged as significant challenges in the world. Therefore, innovative solutions are being developed to enhance transport system efficiency and address these intricate problems. For example, solutions such as dynamic traffic assignment (*1*), traffic signal control (*2*), and variable speed limits (*3*) have been acknowledged as crucial elements in real-time traffic operations and management. However, implementing and evaluating these strategies in the real world presents significant challenges. These difficulties often arise from constraints such as limited budget and insufficient time for the establishment of infrastructure. As a result, the concept of the digital twin, a virtual world for strategic implementation, has gained increasing attention in recent years (*4*). While there is no absolute definition of the digital twin, it is generally understood as a real-time replica created through synchronization with the physical world, using real-world data (*5*).

Traditionally, microscopic traffic simulation has been utilized to serve a similar role to the digital twin. Despite the absence of synchronization and real-time elements,

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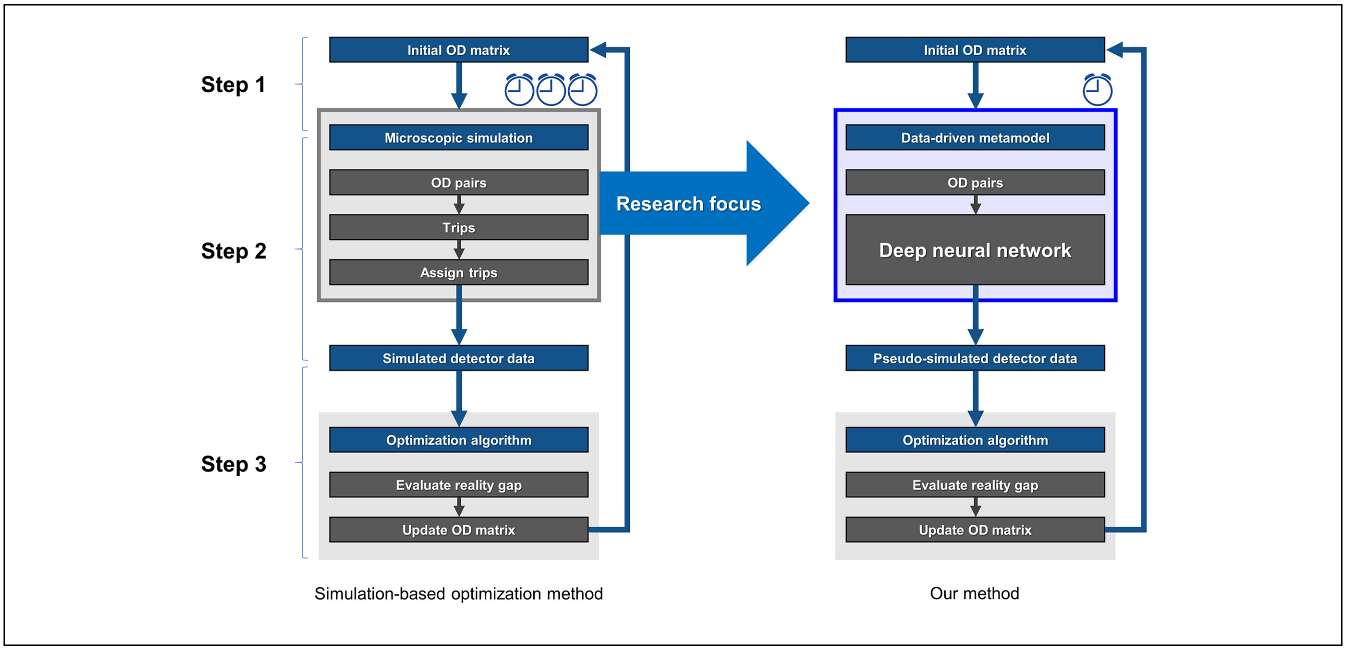

Figure 1. Simulation-based optimization method and our research focus.
Note: OD = origin–destination.

microscopic traffic simulation effectively portrays the dynamics in traffic, with the objective of gaining a deeper understanding and replicating real-world transportation systems. Recently, scholarly efforts have been initiated to infuse real-time synchronization into the microscopic traffic simulation, aiming to expand its benefits (*6*).

There are several challenges to be addressed when it comes to estimating the origin–destination (OD) matrix. The first challenge stems from the limitations of the data sources. Historically, household and roadside surveys served as tools for OD matrix estimation. These methods are inefficient with respect to time and cost and fail to adequately represent the dynamic and high-dimensional OD matrix. Acknowledging these limitations, researchers have shifted their focus to detector data of transportation systems as an alternative data source. However, utilizing detector data to estimate the OD matrix also has its limitations, because of its stochastic, high-dimensional, and spatiotemporally dependent relationship with the matrix itself (*7–9*). Often referred to as the dynamic origin–destination matrix estimation (DODE) problem, traditional approaches aimed to analytically formulate the relationship between the collected detector data and the OD matrix. However, because of the complexity of the problem, alternative methods are being explored, such as a simulation-based approach (*8–9*). Nonetheless, even with advancements, estimating a realistic OD matrix solely from detector data remains challenging, often requiring a significant amount of time to find an appropriate solution.

The second challenge arises from the limitation of computation time associated with real-time synchronization. The core concept of the digital twin revolves around an online virtual world created through synchronization, enabling the application and evaluation of potential transportation planning and operational strategies. To achieve this, it is necessary to synchronize the traffic simulation with the real world under real-time conditions. In other words, it is necessary to complete the OD matrix estimation process using currently collected data within a certain computation time before the next collected data is updated. This requirement of completing tasks in given intervals obliges us to consider the computation time of the algorithms. For example, recent research has been directed toward developing more efficient algorithms, including those based on simultaneous perturbation stochastic approximation (SPSA) (*10–13*) and the Bayesian optimization (BO) method (*7*).

In light of these identified challenges, the primary focus of the previous studies was to design algorithms that can reduce the computation time of the OD estimation process. Shifting away from this conventional paradigm, our study presents an alternative pathway for consideration. In this paper, we introduce a simple approach designed to expedite the OD estimation process by reducing the runtime of the traffic simulation. Specifically, our primary objective is to develop a data-driven metamodel that employs a deep neural network (DNN), thereby substituting the microscopic traffic simulation. Figure 1 illustrates the conventional OD matrix estimation process and identifies our research focus in the process. Firstly, a randomly created initial OD matrix is input into the traffic simulation. Secondly, the traffic simulation calculates the trips of travelers and their interactions based on the given network and OD matrix. As a result of interactions among travelers including their route choices, detector data such as link flow is generated in the traffic simulation. Thirdly, this simulated detector data is evaluated against real-world detector data and, based on this comparison, a new OD matrix is updated according to optimization algorithms such as SPSA. Our research specifically targets the second step in the Figure 1. In other words, rather than improving the OD estimation process through algorithm design, we focus on reducing traffic simulation runtime by replacing the simulation with a neural network.

The substitution of intricate dynamical relationships within traffic simulations with neural networks is a contemporary approach gaining traction in diverse disciplines, including physics (*14–17*). Similarly, our model simplifies the relationship between the input (OD matrix) and the output (detector data). Importantly, employing a data-driven metamodel based on a DNN can greatly reduce the computation time required for a single iteration of the conventional OD matrix estimation process. To assess its performance, we compare the results and computation time of our method and the simulation-based OD estimation method. Moreover, we present potential options for hyperparameters and algorithmic settings that can benefit implementing our methodology. For validation, we utilize real-world data on 5-min interval link traffic flow data obtained through closed-circuit television (CCTV) detectors in Daejeon City, South Korea.

The remainder of this paper is structured as follows: the second section reviews the evolution of OD estimation methods and acknowledges the significant contributions of the research community. In this section, we also present the progressive contributions of our methodology. The third section offers a comprehensive understanding of the problem and the approach we chose to resolve it. The fourth section discusses the experimental results and explores the implications of OD matrix estimation methods, emphasizing the potential value of our model. The fifth section concludes the study, reflecting on our findings and suggesting potential directions for future exploration.

Literature Review

Conventionally, several research studies have been performed to understand and address issues related to the transportation system by analyzing traffic demand, often described with respect to the OD matrix. The direct method to estimate the OD matrix involves conducting surveys, such as roadside or home interviews. However, these methods have proven to be inefficient with respect to time and cost (*18*). As a result, researchers have been exploring alternative approaches to economically estimate a reasonable OD matrix.

Initially, researchers developed methods based on macroscopic indicators such as socio-economic variables to understand how traffic demand is generated and distributed without considering the assignment of the demand. However, there have been considerable doubts about the reasonableness of the estimated OD matrix because of its inability to accurately reflect real-world data (*19*). As an alternative, assignment-based methods, capable of verifying the validity of the estimated OD matrix based on real-world data, have been developed (*20*). Through these methods, the estimated OD matrix is appropriately assigned to the network, which subsequently transforms it into a format to detector data, such as traffic flow data. Consequently, by comparing this to real-world detector data, the reasonability of the OD matrix can be evaluated.

However, as the temporal and spatial resolution of the traffic data increases, estimating OD matrix has become more dynamic and higher-dimensional. In this context, the problem of estimating the OD matrix has expanded into the DODE problem, an issue gaining attention among recent researchers (*7–9*). This problem can be divided into two levels: the upper-level problem of estimating the OD matrix and the lower-level problem of transforming such OD pairs to link flows (*21*). In both problems, a common approach is to optimize the objective function to reduce the discrepancy with real-world data. Assignment-based methods addressing the bi-level DODE problem can be largely categorized into two main approaches.

The first approach involves mathematical modeling. Methods such as the ordinary least squares estimator, constrained optimization, recursive estimation formula, and Kalman filtering were employed (*22*). More recently, analytical methods have been proposed to find reasonable OD matrices in more complex transportation systems. For instance, in relation to the lower-level problem, researchers have considered the effects of congestion when setting up the response functions required for OD matrix estimation (*23*). Efforts have also been made to address the problem more realistically by considering some nonlinear relationships between the OD matrix and the flow (*24*). Despite these efforts, analytical methods have limitations in estimating OD matrices in large-scale networks because mathematical modeling-based methods struggle to reflect the stochastic traffic flow, dynamic changes in the system, and complex interactions between individual vehicles.

Therefore, as a second approach, simulation-based methodologies have been coming to the fore recently (*25*). In this context, simulation refers to a model that iteratively computes inputs and outputs to mimic the

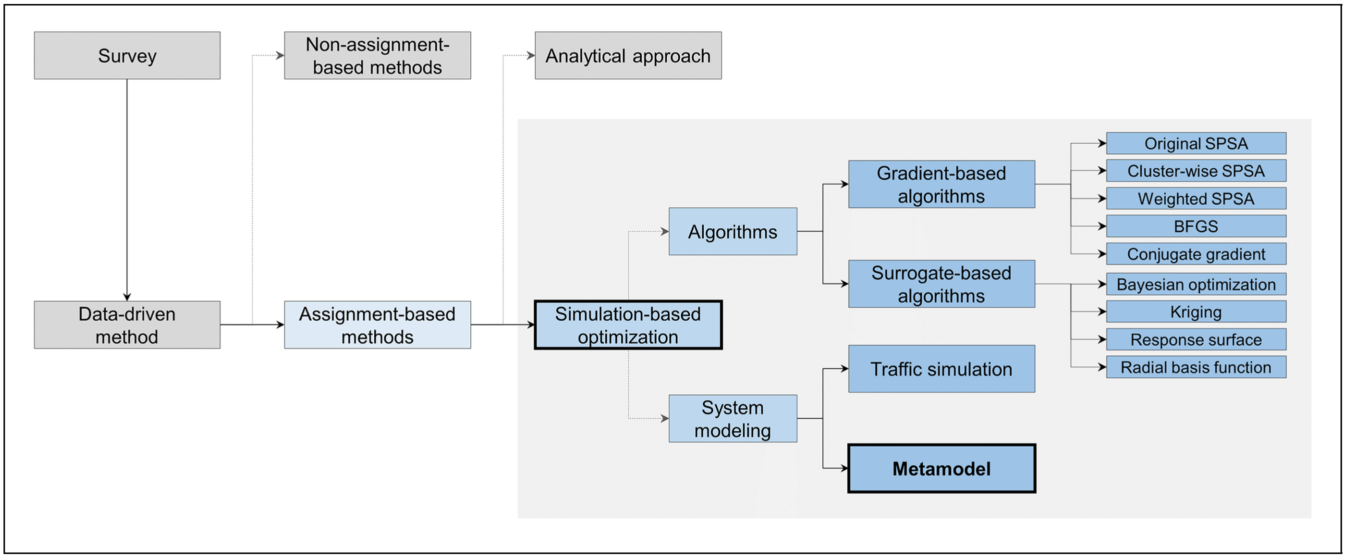

Figure 2. Literature review on origin–destination matrix estimation methods.
Note: SPSA = simultaneous perturbation stochastic approximation; BFGS = Broyden–Fletcher–Goldfarb–Shanno.

dynamics of a particular system. To avoid confusion, this paper clearly differentiates between the traffic simulation and the simulation used in optimization methods. Traffic simulation, a common tool for representing traffic systems, can be used as one of the tools in simulation-based optimization. In particular, microscopic traffic simulations, which incorporate various detailed models such as route choice, lane-changing, and car-following models, can represent dynamic traffic scenarios. This approach can handle the lower-level problem realistically in the bi-level DODE problem (*7*). To solve this problem, researchers could utilize the input and output values of the traffic simulation. The SPSA algorithm, one of the state-of-the-art algorithms, operates in a sequential manner by iteratively evaluating the objective function and utilizing the obtained results to estimate the gradient of the objective function. Its widespread application is observed in methods for estimating OD matrix through simulation-based approaches (*10*).

However, solving the DODE problem with a simulation-based approach using traffic simulations presents a significant computational challenge for researchers, especially when dealing with high-dimensional OD matrices or large networks. Researchers have improved the design of algorithms to estimate the OD matrix more quickly. For example, c-SPSA, which improves the convergence performance of the conventional SPSA (*26*), and W-SPSA, which considers the weight matrix based on the correlation between variables, have been proposed (*12*). The Broyden–Fletcher–Goldfarb–Shanno (BFGS) algorithm and the conjugate gradient method were also used (*27*). In addition, algorithmic solutions based on surrogate models, such as BO, which aim to evaluate the objective function less frequently, have emerged. BO, based on Bayesian statistics, assists in efficient solution search with fewer samples by creating a surrogate model that approximates the objective function (*28*). Methods such as kriging, response surface, and radial basis function were also employed (*29*). Figure 2 presents an overview of the seminal works in the DODE problem, demonstrating the evolution of this concept (*7*).

To our knowledge, there are two primary ways to reduce computational time in a simulation-based approach to solving the DODE problem. The first is to efficiently design the algorithm. As discussed in the literature review above, a well-structured algorithm with a solid theoretical foundation can reduce computation time. The second is to decrease the time required for runtime of the system modeling. The calculation involved in finite element analysis of physical simulations generally takes a considerable amount of time. Recently, methods that dramatically reduce computation time by using approximation of the physical simulation have emerged and are receiving considerable attention in various engineering fields, including the field of transportation (*14–17*).

In this study, we propose changing the tool to represent traffic dynamics in a conventional simulation-based approach from a traffic simulation to a metamodel. A metamodel is a model that provides an approximation to the objective function of a simulation-based approach. Unlike traffic simulation, which involves numerous computations, a metamodel achieves high computational efficiency by providing an approximation of the output as a function of the input through a simplified function. For example, stationary network model-based metamodels (*9*, *30*), gradient-based metamodels (*31*), and bi-modal macroscopic fundamental diagram-based metamodels

(*32*) have been used as alternatives to traffic simulations to represent traffic dynamics. In this paper, we extend this line of research to data-driven metamodels at the microscopic level. This model is pre-trained using data reflecting the dynamics of microscopic traffic simulations. This approach can reduce the runtime of the simulation while accounting for detailed interactions between vehicles. Thus, by using a data-driven metamodel that approximates the input–output relationships of microscopic traffic simulations, we can quickly collect sample data for real-time OD matrix estimation, which can be applied directly to a microscopic-level DODE problem.

The objective of our research is to develop a data-driven metamodel using a DNN to replace microscopic traffic simulations. DNNs are capable of approximating various functions, including probability distributions (*33*), making them well-suited for the data-driven metamodel imitating the microscopic traffic simulation that reflects interactions among various interactions of travelers. This work reduces unnecessary runtime, thereby facilitating the simplification of the subproblem of DODE. Accordingly, we establish a foundation for extending microscopic traffic simulations to digital twins and present the following contributions.

1. The proposed data-driven metamodel reduces the time required for the runtime of the microscopic traffic simulation. It is possible to estimate a reasonable OD matrix within a shorter time span.
2. For digital twins, we emphasize the practicality of our model through a comparison of calibration performance and computation time with conventional simulation-based methodologies within a limited time frame.
3. This approach is developed independently without disrupting the conventional academic flow, such as algorithm design. Thus, it provides a wide versatility, as it allows for the application of various algorithms considered for the OD matrix estimation problem.

Methods

Problem Statement

The OD matrix represents demand occurring over a specific time interval in a given traffic network, denoting the number of trips made up of OD pairs. For example, the vector of OD matrices can be expressed as shown in Equation 1:

$$m(N, |T|) = [O_1D_1, O_1D_2, \cdots, O_iD_j, \cdots, O_ID_{J-1}, O_ID_J] \tag{1}$$

where m is the vector of the OD matrix, N is the given target network, T is the set of time interval indices, O_iD_j is the flow rate from zone i to zone j, I is the number of zones from which departure is possible, and J is the number of zones to which arrival is possible.

The DODE problem is formalized as a bi-level optimization problem divided into upper and lower levels. The upper-level problem we aim to solve is as depicted in Equations 2 and 3:

$$\begin{aligned} \min_m f(d_r, m) &= \min_m |d_r \odot d_s(m)| \\ &= \min_m \sqrt{\frac{1}{|T||L|} \sum\nolimits_{t \in T} \sum\nolimits_{l \in L} \left| d_{t,l}^r - d_{t,l}^s(m) \right|^2} \end{aligned} \tag{2}$$

subject to:

$$G(m) \leq 0 \tag{3}$$

where f is the objective function to minimize the difference between d_r and d_s, G represents the constraints on m, m is the vector of the OD matrix, d_r is the vector of real-world detector data in time $|T|$, d_s is the vector of simulated detector data in time $|T|$, $d_{t,l}^r$ is the real-world value collected from detector l during time interval t, $d_{t,l}^s$ is the simulated value collected from detector l during time interval t, T is the set of time interval indices, L is the set of indices of detectors, and $\odot$ is the operator for the performance measure.

The upper-level problem is one that minimizes the discrepancy between the detector data obtained from the real world and that from the simulation, using this difference as an objective function. We measure the difference between the real world and simulation using the root mean squared error (RMSE). The lower-level problem describes the relationship between the OD matrix, which is the input of the simulation, and the detector data, which is the output. As mentioned in the literature review section, considering the complex relationship between OD matrix and detector data, and its stochastic nature, recent research tends to use microscopic traffic simulation for solving the lower-level problem. In the same way, we address the lower-level problem using SUMO, a microscopic simulation software. The formulation of the lower-level problem can be written from the perspective of individual travelers, as shown in Equations 4 and 5:

$$\max_{a_i} U_i(a_i,\ b_i) \tag{4}$$

subject to:

$$g(a,\ b) \leq 0 \tag{5}$$

where U_i is the objective function for traveler i, aiming to maximize utility, g represents the constraints on a, b, a_i is the environment of the simulation that traveler i can control (e.g., route choice behavior), and b_i is the environment of the simulation that traveler i cannot control (e.g., traffic flow, signal).

In the microscopic traffic simulation, each traveler has a personal objective function and behaves to maximize their utility. They act in a manner that optimizes their utility in the given environment. In this study, all settings that can influence the behaviors of travelers, such as car-following, lane-changing, and route choice models, utilize the default models of SUMO. Details are described in the *Simulation Settings* section. Consequently, traffic flows in the traffic system are created according to the behavior of travelers, and this flow is linked to the simulated detector data called variable $d^s_{t,l}$ in the upper-level problem. As a result, the OD matrix comprising individual travelers' trips is assigned to the network and subsequently transformed into numerical values corresponding to the detector data.

Data-Driven Metamodel Using a Deep Neural Network

According to the literature review, previous studies show a constrained interest in the lower-level problem. To our knowledge, conventional methods redesign algorithms to solve the upper-level problem. This is because running the traffic simulation can be regarded as a mandatory step in the lower-level problem. However, we focus on the idea that resolving the lower-level problem by executing the traffic simulation is not necessarily an efficient solution. Microscopic traffic simulations can be inefficient because they have to calculate the behavior of every traveler at each time step. Also, in urban areas, where traffic signals exist and changes in the OD matrix have a significant impact on the traffic system, it is challenging for the traffic simulation to provide a sufficient number of samples for OD matrix estimation within a reasonable time.

For these reasons, synchronization for digital twins has been seen as a challenge for researchers. Real-time OD matrix estimation must complete all processes within at least the time interval when the next detector data is collected. Typically, this time interval can range from 5 to 15 min (*34–35*), and there are limitations to using conventional methods. Therefore, we operate the microscopic traffic simulation in advance to prepare input–output pairs, based on which we develop a DNN-based data-driven metamodel that can approximate the input–output relations of the simulation. Our model is trained to predict what detector data will come out when a certain OD matrix is given. This approach generates an approximation of detector data without calculating the locations, speeds, accelerations, or routes of every vehicle at each time step. In other words, this study embeds the lower-level problem into the upper-level problem using an approximation approach, thereby bypassing the need for separate traffic simulations, as demonstrated in Equations 6–8:

$$\min_m f(d_r,\ m) = \min_m |d_r \odot d_s(m)| \approx \min_m |d_r \odot d_s{}^*(m)| \quad (6)$$

$$\min_m \sqrt{\frac{1}{|T||L|}\sum_{t\in T}\sum_{l\in L}\left|d^r_{t,\ l} - d^s_{t,\ l}(m)\right|^2} \approx \min_m \sqrt{\frac{1}{|T||L|}\sum_{t\in T}\sum_{l\in L}\left|d^r_{t,\ l} - d^s_{t,\ l}{}^*(m)\right|^2} \quad (7)$$

subject to:

$$G(m) \leqslant 0 \quad (8)$$

where f is the objective function to minimize the difference between d_r and d_s, G represents the constraints on m, m is the vector of the OD matrix, d_r is the vector of real-world detector data in time $|T|$, d_s is the vector of simulated detector data in time $|T|$, $d_s{}^*$ is the vector of the data-driven metamodel's output approximating the vector d_s, $d^r_{t,l}$ is the real-world value collected from detector l during time interval t, $d^s_{t,l}$ is the simulated value collected from detector l during time interval t, $d^s_{t,l}{}^*$ is the data-driven metamodel's output approximating the value $d^s_{t,l}$, T is the set of time interval indices, L is the set of indices of the detectors, and $\odot$ is the operator for the performance measure.

The key difference from the conventional methods is that we simplify the process of collecting detector data from individual travelers, as shown in Equations 4 and 5. Our data-driven metamodel is composed of a DNN, which is a powerful approximator for various nonlinear functions (*33*). To approximate the complex models of microscopic traffic simulation, we constructed our model using multiple fully connected layers, forming a multilayer perceptron, as illustrated in Figure 3. In other words, the proposed model employs a feedforward architecture, wherein the input vector is propagated in a unidirectional manner through multiple layers to the output vector. This architecture is simple and powerful in its ability to approximate unknown functions via backpropagation. It also has the advantage of being scalable and generalizable, making it applicable to various problems (*36*). There are three specific structures: firstly, it could be organized in hidden layers with decreasing perceptrons from the input to the output. This structure represents the sequential compression of important information as trips are assigned to the network. Secondly, the layers could be arranged as a rhombus, with the middle layer having the highest number of perceptrons. This is the most common structure in DNNs, where the initial layer recognizes simple features of the OD matrix and uses them to learn more complex features in the middle layers. Thirdly, the layers could be organized so that the number

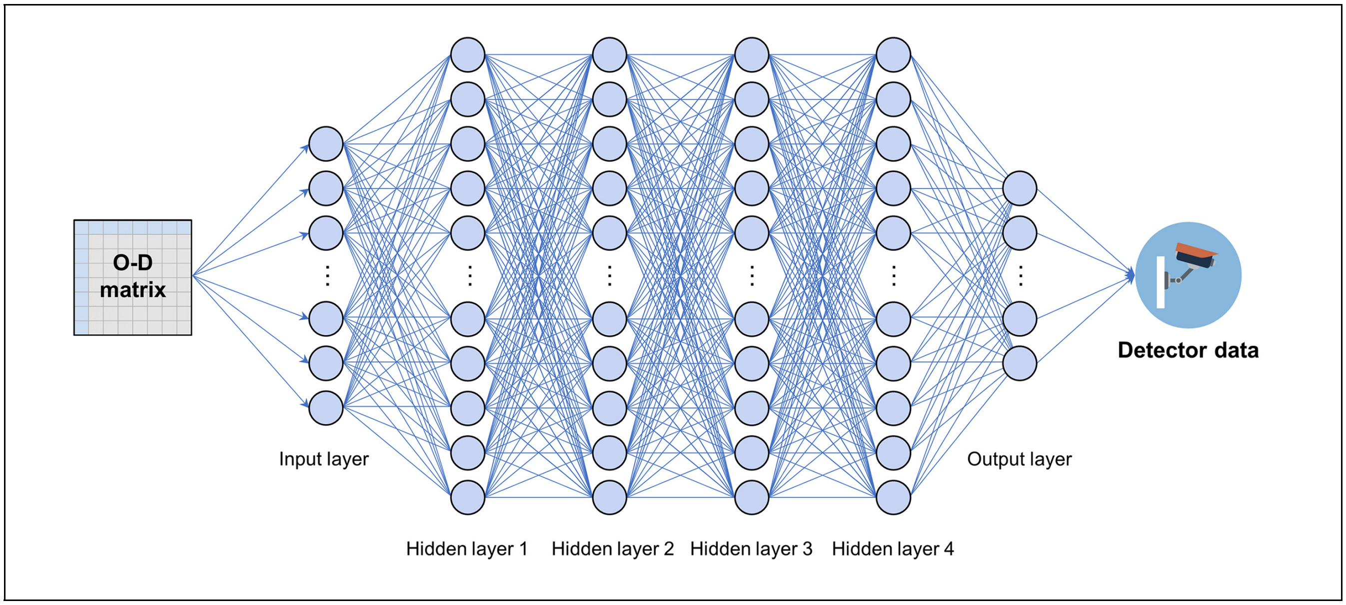

Figure 3. Data-driven metamodel to surrogate the microscopic traffic simulation.
Note: OD = origindestination.

of perceptrons gradually increases close to the output. This progressive representation structure models increasingly complex patterns from simple ones.

The OD matrix is vectorized and then inputted into the model's input layer. The input vector passes through the first hidden layer. It then goes through the second, third, and fourth hidden layers. Finally, it passes through the output layer, yielding an output as a vector of the detector data. We build the three structures presented above for the hidden layers, train on each structure, and measure the test loss. The alternatives are subdivided into a structure with 256-128-128-16 dimensions, a structure with 64-128-128-64 dimensions, and a structure with 16-128-128-256 dimensions. We also apply hyperbolic tangent, rectified linear unit (ReLU), and leaky ReLU with a negative slope of 0.01 for the activation function applied between each layer. Losses are recorded for each neural network. Finally, we adopt the structure with the lowest loss. We also apply the dropout technique between layers to prevent overfitting and apply normalization to the input data to ensure the stability of the learning. Further details on the training process and data are discussed in the *Experimental Design* section, and the adopted model is presented in the *Results* section.

Experimental Design

In addressing the OD matrix estimation problem, our experimental framework unfolds as follows: firstly, the target network of our experiment is defined, along with a brief overview of the related data. This is followed by creating training and test data sets and training the data-driven metamodel through a DNN. Subsequently, we review previous literature to determine the most suitable algorithm for our study. After that, OD matrices are estimated within constrained time frames, employing conventional and our proposed methods. Lastly, the derived OD matrices are reintroduced into the microscopic traffic simulation to evaluate their similarity with real-world data.

Data Description. In our study, we selected a network within the Wolpyeong-dong area of Daejeon, South Korea, as the analysis network. To evaluate the accuracy of our OD matrix estimation, the generated detector data through traffic simulations based on this OD matrix and compared these results with real-world detector data collected from this network. The network covers an area of about 1.1 km^2 and consists of streets that allow vehicles to choose alternative routes when necessary. A total of 16 zones are divided into five zones (Z1, Z2, Z5, Z10, Z11) that can be traveled in the outer area and 11 inner zones (Z3, Z4, Z6–9, Z12–16). Since we consider all possible directions, each zone interacts with all zones except itself. Therefore, there are 240 OD pairs in this network, which translates to 240 dimensions of input vectors in the model. In a given network, CCTV detectors measure traffic flow in each direction based on the four major intersections. These detectors measure the traffic flow data by accumulating the number of vehicles passing every 5 min. As a result, the detector data is a 16-dimensional vector, corresponding to our model's output vector. The network elements have been adjusted to have

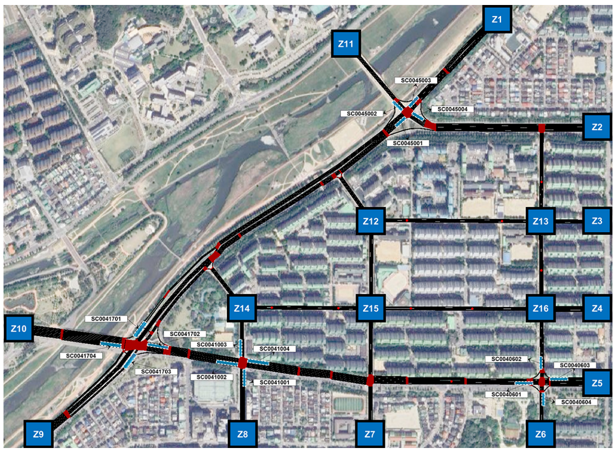

Figure 4. Target network of the experiment.

the exact physical measurements as in the real world. This network is configured as shown in Figure 4.

Real-world traffic flow data collected on March 27, 2022, from CCTV detectors was used for validation. We use data in 5-min increments collected from 06:00 a.m. to midnight. Therefore, the total number of time steps is 216. The traffic flow from CCTV detectors is 16-dimensional, so the total validation data is 3456. According to the average speed data of the most major arterial road connecting Z5 and Z10, the level of service (LOS) of the target network is mainly from C to E, as shown in Figure 5, with the distribution of LOS as follows: A is 0.00%, B is 0.56%, C is 15.14%, D is 37.64%, E is 36.85%, and F is 9.81%. The speed distribution indicates that the data set covers a wide range of traffic conditions within the network.

Training Process. The purpose of both the microscopic traffic simulation and our data-driven metamodel is fundamentally identical. Both describe what detector data will be produced at the next time step when certain OD matrix is entered at a certain time step in a given network. In other words, they are black-box models that produce the output vector depending on the input vector. To achieve this goal, the data-driven metamodel is trained almost similarly to the internal logic of the simulation. Therefore, it is necessary to build sufficient training data by running the simulation randomly in advance.

Note that in the OD matrix estimation problem, a true OD matrix is unknown, so the training data of our model is inherently synthetic data, which is used to train our neural network to capture the relationship between the input OD matrix and the resulting observations of the detectors.

However, several issues need to be considered. In particular, when generating the demand for OD pairs randomly, it can be inefficient to simply generate an OD matrix with a uniform upper bound for all OD pairs. For example, if the wrong upper bound is chosen or includes unrealistic demand, it can result in an unrealistic solution, and the training data set can be time-consuming to build.

At this point, it is important to have a baseline for how our synthetic data set should be built to ensure the practicality of the model and the efficiency of the training. Therefore, to address these limitations, it is necessary to determine a baseline demand for which our synthetic data set should be built to ensure the practicality of the model and the efficiency of the training. We use the gravity model, a simple and powerful tool for describing the distribution of trips with the assumption that traffic demand between zones decreases as a function of distance (*37*). The singly constrained gravity model used in this study is shown in Equation 9:

$$T_{ij} = A_i O_i D_j C_{ij}^{\alpha} \tag{9}$$

where T_{ij} represents the trips from origin i to destination j, A_i is the balancing factor of origin i; $A_i = \frac{1}{\sum_j D_j C_{ij}^{\alpha}}$, O_i represents trips generated in origin i, D_j represents trips

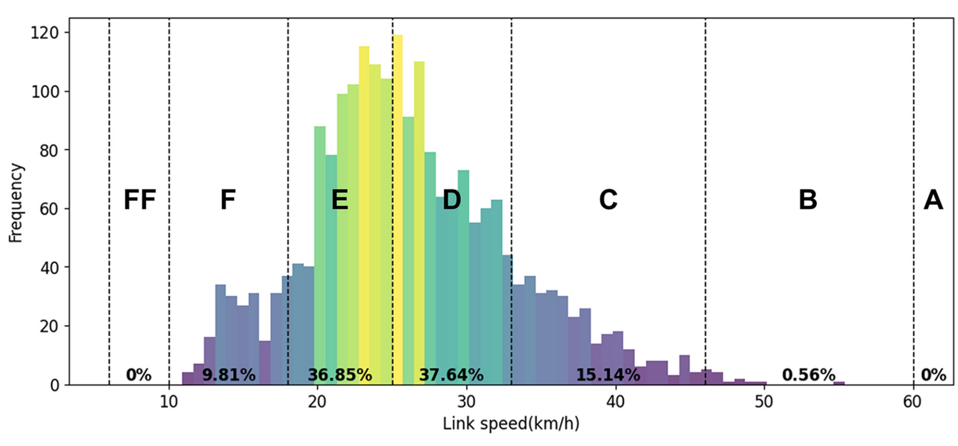

Figure 5. Histogram of speed data with percentages.

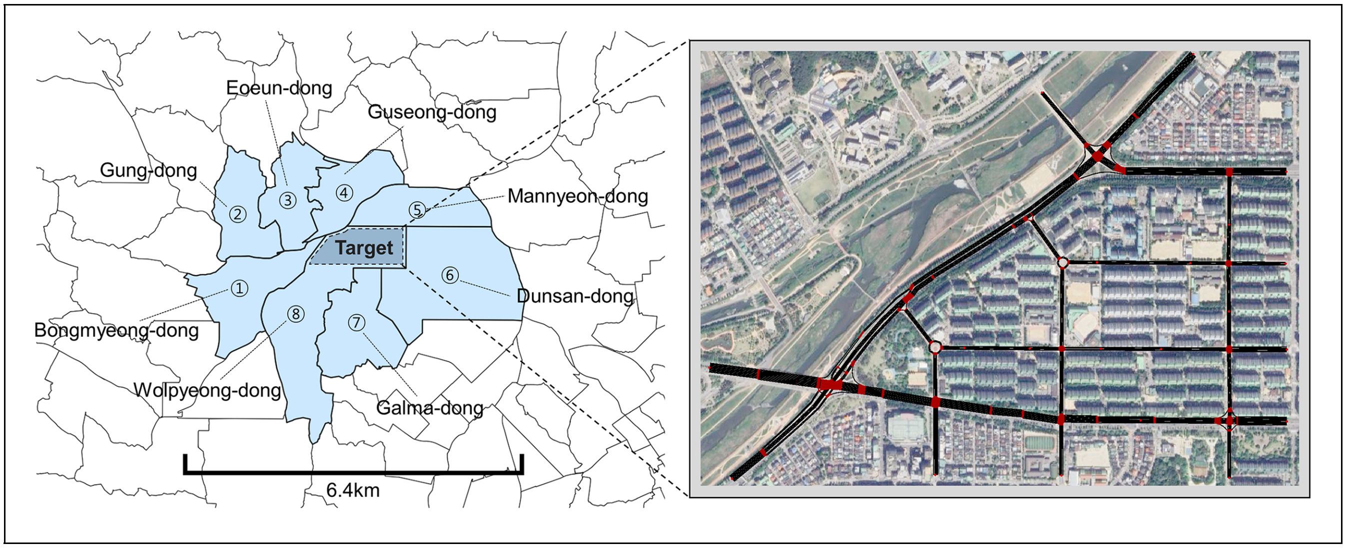

Figure 6. Target network and the surrounding administrative regions.

Table 1. Shortest Distance Between Centroids of Administrative Regions (km)

Region index	1	2	3	4	5	6	7	8
1	0	2	3.5	3.6	5.1	4.9	3.2	2.1
2	2.2	0	1.6	3.7	3.1	4.4	2.3	3
3	3.7	1.6	0	3.4	4.8	5.8	4.4	3.4
4	3.3	3.6	3.3	0	3.1	4.4	4.1	3.2
5	3.7	4.1	4.1	2.1	0	3.6	3.4	2.4
6	4.7	5.6	5.6	4.7	3	0	2.3	3.5
7	2.9	4.8	4.1	4.2	3.8	3.1	0	1.8
8	1.6	4.4	3.8	4.4	4.6	3.8	1.5	0

Table 2. Vehicle Trip Generation in Administrative Regions Based on the Gross Floor Area by Use

	Gross floor area by use								
Region index	1	2	3	4	5	6	7	8	Trip generation rate (vehicles/ 1000 $m^2 \cdot$ day)
Residential (apartment, m^2)	293,921	45,003	369,460	10,268	361,377	2,263,502	741,149	1,554,775	27.06
Educational (university, m^2)	na	429,242	123,920	568,947	na	8505	na	na	35.02
Office building (m^2)	3504	16,732	na	16,976	95,970	1,107,723	23,700	160,937	45.9
Public office (m^2)	na	na	na	na	na	15,017	2735	na	131.8
Retail (m^2)	na	na	na	na	23,023	227,652	24,648	127,034	188.7
Factory (m^2)	na	na	na	na	na	na	na	3857	36.4
Sum of trips (vpd)	**8114**	**17,018**	**14,338**	**20,982**	**18,528**	**157,329**	**26,154**	**73,570**	na

Note: vpd = vehicles per day; Sum of trips = the sum of the gross floor area by use multiplied by the trip generation rate.

attracted in destination j, C_{ij} is the distance between origin i and destination j, and α is the discount factor.

Figure 6 shows the administrative regions surrounding the target network. The target network is part of the eighth region (Wolpyeong-dong). Table 1 shows the shortest distance between zone centroids. To calculate the trip generation of each region, we used the publicly available data of gross floor area by use and vehicle trip generation rate by use, as shown in Table 2 (*38–39*). Thus, the vehicle trip generation of all regions is calculated.

As a result, the number of trips passing through and entering the target network was calculated. The trips were allocated based on the shortest paths. For simplicity of calculation, it was assumed that the production

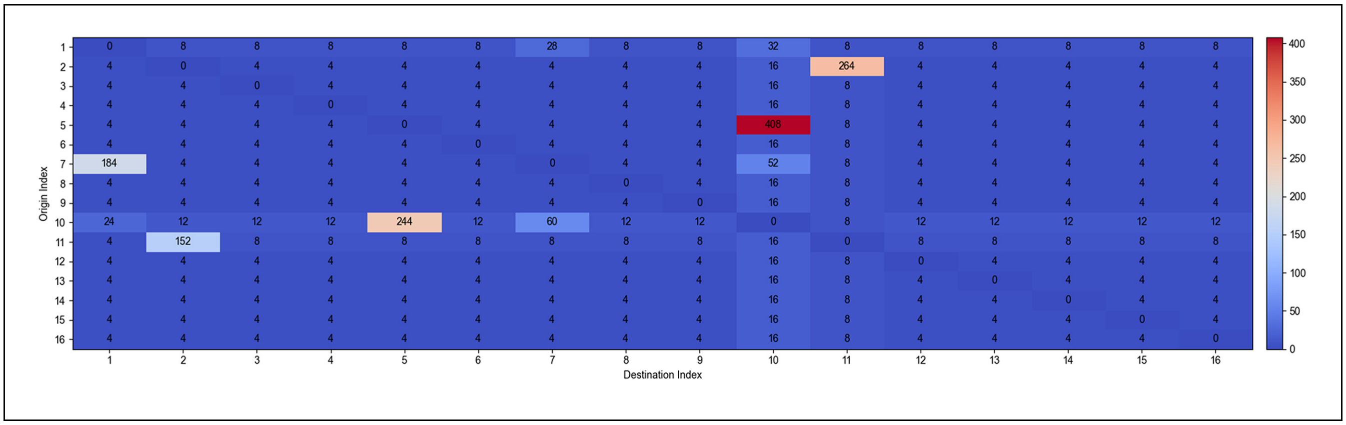

Figure 7. Upper limits for each origin–destination pair's traffic demand (vehicles/5 min).

and attraction were the same, and the distance factor α was set to 0.5. The entering trips were evenly distributed among 11 zones (Z3, Z4, Z6–9, Z12–16). The values are shown in Figure 7 and were used as the upper limits for each OD pair's traffic demand. We converted the daily demand values into 5-min intervals by dividing them by 288 and assigned a value of 1 to the empty demand. Next, a constant $\tau = 4.0$ was multiplied across the matrix to cover unexpected peak demands. The peak constant τ could vary depending on the characteristics of the network and is higher as the demand spikes in a short time.

Furthermore, given that microscopic simulations encompass random variations inherent in individual driver behaviors and traffic dynamics, it is crucial that the proposed model is equipped to manage such stochasticity. To address this issue, we employ the sample average approximation method, which generates multiple samples from a single input data set and calculates the mean of these outputs to derive a representative single sample (*40*). Similarly, in this experiment, detector data was generated repeatedly over multiple simulation runs for the same OD matrix. We ran 30 simulation runs per OD matrix and averaged the detector data to create a row of data with one OD matrix paired with one detector data. We used a warm-up time of 10 min to allow the given traffic demands to affect the network uniformly.

Following these procedures, we prepared 5000 input–output (OD matrix to detector data) pairs: 80% were split as training data and 20% as test data. We trained the DNN model with the normalized data for 10,000 epochs. The Adam optimizer was used, with a learning rate of 0.0001. The mean absolute error (MAE) was used to calculate the loss between the predicted and actual values. The MAE is commonly used to build robust models that are less influenced by outliers, unlike the mean squared error (MSE). The detector data in this study has 16 dimensions, and each dimension typically has a different data range. Therefore, we used the MAE to provide uniform weights for all detector data. The batch size used for learning is 64. To develop a robust model and reduce overfitting, the dropout technique and L2 regularization were used. Perceptrons of the neural network were trained by arbitrarily dropping out with a probability of 0.1, and a penalty proportional to the sum of squared weights of the model was added to the loss. The hyperparameter for regularization strength λ should be chosen with consideration for the model's structure and its generalization performance. It numerically represents the importance of generalization. Setting this value too high can hinder the training process, resulting in lower overall performance, so it is important to choose an appropriate value. In this study, the regularization strength was set to a small value of 0.00001 to take a conservative approach to model training. Equation 10 represents the loss function that the proposed model aims to minimize:

$$\text{loss} = \frac{1}{N}\sum_{i=1}^{N}|y_i - \hat{y}_i| + \lambda\sum_{j} w_j^2 \tag{10}$$

where N is the total number of data points, y_i is the actual value of the ith dimension, $\hat{y}_i$ is the predicted value of the ith dimension, λ is the hyperparameter of regularization strength ($=0.00001$), and w_j is the jth weight of the model. Finally, the results of training on different structures and activation functions based on these settings are presented in the *Results* section:

Algorithm for OD Estimation. The use of the already discussed algorithms is thought to be able to emphasize the strengths of our approach under limited computation time conditions. Therefore, we adopt the SPSA algorithm, which is one of the methods of stochastic approximation that emerged to solve stochastic problems. Instead of approaching the objective function analytically, this algorithm approximates the objective function using only the input and output of the function. The SPSA algorithm aims to find θ^* that satisfies $\frac{\partial L}{\partial \theta} = 0$,

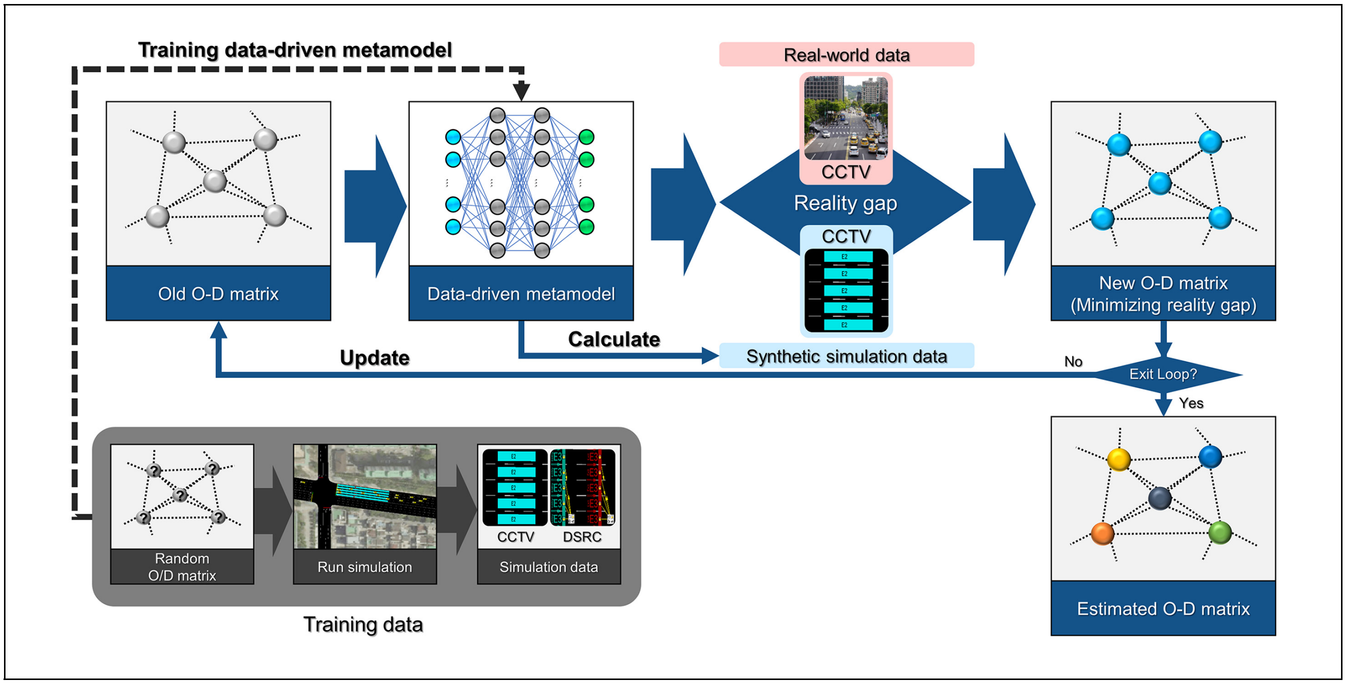

Figure 8. Experiment framework.
Note: OD = origin–destination; CCTV = closed-circuit television.

which is the gradient of the loss function $L(\theta)$ where θ is a decision vector, that is, it minimizes the loss function. Specifically, the SPSA algorithm follows Equations 11 and 12 (*10*). In this optimization problem, since the search space is different for each dimension, a scale vector s is utilized to explore solutions at variable rates corresponding to the magnitude of the search space in each dimension:

$$\hat{\theta}_{k+1} = \hat{\theta}_k - a_k \hat{g}_k(\hat{\theta}_k) \tag{11}$$

where $\hat{\theta}_k$ is an estimate of the decision vector at the k th iteration of the algorithm, $\hat{g}_k(\hat{\theta}k)$ is an estimate of the gradient at $\hat{\theta}_k$, a_k is the step size vector at the k th iteration; $a_k = \frac{a}{(k+1)^{\delta}} s$, δ is a constant greater than zero, and s is a scale vector indicating the size of the search space per dimension:

$$\hat{g}_{ki}(\hat{\theta}_k) = \frac{y(\hat{\theta}_k + c_{ki}\Delta_{ki}) - y(\hat{\theta}_k - c_{ki}\Delta_{ki})}{2c_{ki}\Delta_{ki}} \tag{12}$$

where $\hat{g}_{ki}(\hat{\theta}_k)$ is the i th element of the gradient vector $\hat{g}_k(\hat{\theta}_k)$, $y(\cdot)$ is the stochastic loss function defined in Equation 6, including noise, c_{ki} is the i th element of the perturbation vector at the k th iteration; $c_{ki} = \frac{c}{(k+1)^{\delta}} s_i$, Δ_{ki} is the i th element of the unit vector at the k th iteration that takes value $+1$ or -1, δ is a constant greater than zero, and s_i is the i th element of the scale vector.

The hyperparameters of the SPSA algorithm used in this paper are $a = 0.001$, $c = 0.1$, $\delta = 0.1$. Using a common algorithm, we compare the results of the optimization using the microscopic traffic simulation used in previous research and the proposed data-driven metamodel.

Experiment Framework. The overall experiment framework can be summarized as in Figure 8. In this paper, we solve the DODE problem by replacing Equation 2 with Equation 6 using the data-driven metamodel to complete the OD matrix estimation process within a short computation time. Before the experiment, we vectorized 240 OD pairs as inputs and 16 detector data as outputs in our set target network. Following the established rules, we randomly run the traffic simulation to generate 5000 data, ensuring that our model can sufficiently learn the input–output relation of the simulation. Using the trained model, we estimate the OD matrix that can best reproduce the given detector data according to the SPSA algorithm. Our primary interest is how well various methods can reproduce real-world detector data and the computation time required to derive each performance. For the reality gap, we utilized the RMSE.

Simulation Settings. All experiments are conducted in the microscopic traffic simulation software, SUMO (*41*). The value assigned per OD pair is the mean of a Poisson distribution and vehicles are generated stochastically based on the distribution. Also, to obtain a reasonable solution to the lower-level problem, microscopic simulation uses a variety of driving behavior models and assumptions that

Table 3. Parameters of the Simulation Used in this Study

Parameter	Value
Vehicle type	Passenger car
Car-following model	Krauss
Lane-changing model	LC2013
Acceleration (m/s^2)	2.6
Maximum deceleration (m/s^2)	9.0
Deceleration (m/s^2)	4.5
Sigma of car-following model	0.5
Tau of car-following model	1.0

Table 4. Final Mean Absolute Error Loss Depending on the Structure and Activation Function of the Model

	Structure of the model		
	256-128-128-16	64-128-128-64	16-128-128-256
Activation function			
tanh	50.29	29.01	7.41
ReLU	8.18	6.46	5.24
Leaky ReLU	8.45	6.63	5.73

Note: ReLU = rectified linear unit; tanh = hyperbolic tangent.

reflect domain knowledge (*42*). In our simulation, OD matrices are assigned to the network as individual trips, all of which are assumed to be passenger cars. The driving behavior models of the individual vehicles are set to the default models in SUMO. For example, the car-following model is based on the Krauss model (*43*). For the lane-changing model, the LC2013 (*44*) model is utilized, which allows strategic lane changes while considering safe velocity. Every 10 s, vehicles can be rerouted to minimize their travel time. The detailed values are provided in Table 3.

Results

The key element of our approach is a data-driven metamodel using a DNN. This model simplifies the relationship between the OD matrix and detector data by replacing the traffic simulation with the conventional simulation-based method. In other words, this model significantly reduces the computation time of the lower-level problem. Before starting the OD matrix estimation process, we train the data-driven metamodel. All experiments were conducted on a personal computer equipped with an Intel Core i7-8700 and 32 GB DDR4 memory.

Figure 9*a* shows the training results by the structure and activation functions. On the test data set, the MAE loss decreases over 10,000 epochs. For a neural network structure with dimensions of 256-128-128-16, where the activation functions are the hyperbolic tangent, ReLU, and leaky ReLU with a negative slope of 0.01, the final MAE losses were 50.29, 8.18, and 8.45, respectively. Similarly, for the structure of 64-128-128-64, the losses were 29.01, 6.46, and 6.63. Finally, the structure of 16-128-128-256 yielded losses of 7.41, 5.24, and 5.73. The MAE losses for each model at the end of training are shown in Table 4. In conclusion, the best model in this study is the one that utilizes the 16-128-128-256 dimensions and the ReLU as the activation function. This finding suggests that a structure in which information scales from simple to increasingly complex is appropriate when describing the relationship between the OD matrix and detector data in our experiments. Our data-driven metamodel effectively predicts test data sets of the microscopic traffic simulation. A box plot of the test data and predicted data is shown in Figure 9*b*. Since the average data from 30 detector data obtained for one OD matrix were used for training, the proposed model can reflect the stochastic relationship between the OD matrix and detector data in the simulation.

Applying our data-driven metamodel to the OD matrix estimation process offers a computational advantage over conventional simulation-based methods. This advantage is even more pronounced under time-limited conditions. As mentioned above, we compare the performance of two methods: the SPSA with traffic simulation and the SPSA with our model. In this method, the initial solution used random integers of 0 or 1. Since we do not know what traffic situation the given data represents, we start from a conservative initial solution to find the optimal solution.

Figure 10 shows the results of an experiment to estimate OD matrices within 1 min. The x-axis signifies real-world data, and the y-axis corresponds to simulated data. Consequently, the closer the points are to the black dashed line, the better the OD matrix represents the real-world data. The gray points were produced by the initial solution. The red points were made by the SPSA method using traffic simulation, and the blue points were made by the SPSA method using the proposed metamodel.

As observed in the figure, our proposed method outperforms the conventional simulation-based method with respect to calibration performance. The RMSEs for the flow are as follows: 63.04 (initial solution), 55.34 (SPSA with the traffic simulation), and 27.31 (SPSA with the proposed metamodel). According to these results, using the conventional approach led to a 12.2% decrease in errors, whereas the proposed approach resulted in a 56.7% decrease. In other words, our method has improved the calibration performance with respect to traffic flow by 44.5 percentage points over the existing method within 1 min. Since the initial solution is set to a small size, the initial simulated data is typically underestimated. In all methods, the points move upward and closer to the black dashed line with each iteration. However, in the case of the conventional simulation-based method, an iteration takes a few seconds, making

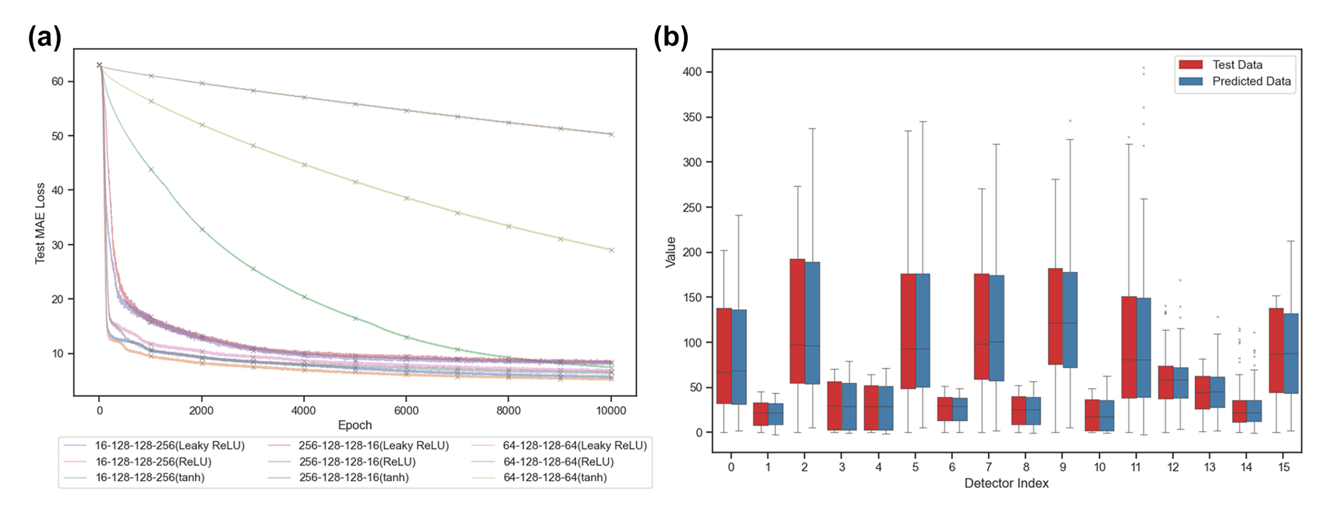

Figure 9. Training results of the data-driven metamodel with test loss (*a*) and box plot (*b*).
Note: MAE = mean absolute error; ReLU = rectified linear unit.

it difficult to perform sufficient repetitions within 1 min. In contrast, our method takes a few milliseconds per iteration, allowing us to estimate a reasonable OD matrix in a relatively short time.

In general, detectors with a low coefficient of variation and significant traffic flows tend to calibrated accurately: SC0040601, SC0040603, SC0041002, SC0041004, SC0041702, SC0041704, SC0045003, and SC0045004. From this result, the data of the above detectors are prioritized for calibration. This is because the smaller the coefficient of variation of the detector data, the easier it is for the estimation algorithm to identify patterns between the OD matrix and the detector data, and also because the algorithm uses a RMSE that is sensitive to large values. Conversely, for detectors with a high coefficient of variation and minor traffic flows, the estimated flows tend to be overestimated: SC0041001, SC0041003, SC0040602, SC0040604, SC0045001, and SC0045002. In addition, data of detectors with unsignaled merging flows are overestimated, which is a limitation of the simulation, as it needs to reflect the delays at merging areas that often occur in real world: SC0041701 and SC0041703. These features are crucial to interpreting the results from our experiments as they affect the outcome of OD estimation. Figure 11 illustrates the trend in a scatter plot.

Figure 12 displays the min-max scaled detector data when estimating the OD matrix at each time step within 1 min, presented as a heatmap. The top four figures show the results for traffic flow data in the following order: the real world, our method (SPSA with the proposed metamodel), conventional method (SPSA with the traffic simulation), and the initial solution. In these figures, the x-axis is the time step in units of 5 min, and the y-axis is the index of a detector. When considering the traffic flow at peak hours, along with the consistency in adjacent time periods, an analysis of the color distribution in the heatmaps indicates that the heatmap generated by our method aligns more closely with real-world patterns compared to those produced by the conventional method.

In the same vein, Figures 13 and 14 shows the result of estimating the OD matrix when the time constraint is extended to 5 min. In a practical context, given that the temporal resolution of detector data is set at 5-min intervals, extending the time constraint beyond this limit for completing the OD matrix estimation process before the subsequent data update presents significant challenges. Interestingly, it has been observed that when more than a minute is allocated to the conventional simulation-based method, its results commence to align with those derived from our method. This suggests that our approach accomplishes commensurate results with conventional methods but within a shorter time span. Despite the inherent error tied to the data-driven metamodel, our method presents a distinct advantage because of its capacity to facilitate a larger quantity of iterations, thus proving more effective in addressing the DODE problem under time constraints.

Figure 15 illustrates the variation in computation time based on different methods. To simplify the comparison, this figure specifically addresses the traffic flow of SC0041004. This detector is located in the center of a major street in the target network. Under a 5-min time constraint, after undergoing the OD matrix estimation process using our method, we focus on a specific time step from 09:05 to 09:10 a.m., where the absolute error of the traffic flow reaches a median value. At this time step, the error for the flow is 38.0 with the conventional

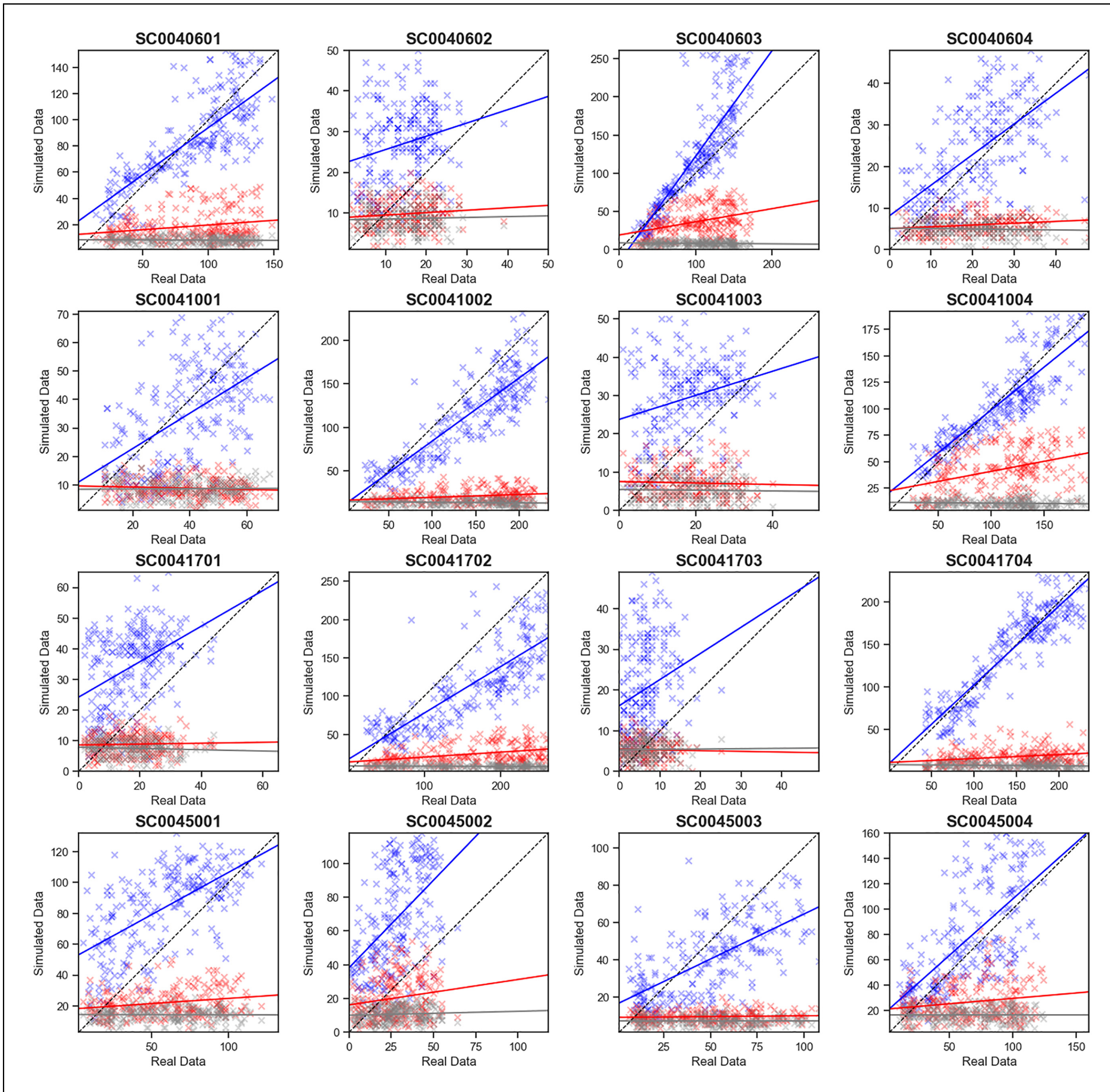

Figure 10. Origin–destination matrix estimation performance within 1 min with scatter plots.
Note: Color online only.

simulation-based method and 15.0 with our method. Considering the randomness in the experiment, separate from the experiments mentioned above, we conducted the same process for this time step under a 5-min constraint on 10 separate occasions. The shaded area depicts the range between the minimum and maximum error, while the line within this area represents the average value. In summary, this figure illustrates the average trend of the error in relation to computation time for the given detector and time step. These findings indicate that our approach is substantially more time-efficient compared to the conventional method. This efficiency is attributed to the significant reduction in the time required for each iteration of the algorithm.

Conclusions

This paper introduces an approach using a data-driven metamodel for the DODE problem, a crucial step in expanding microscopic traffic simulations into digital

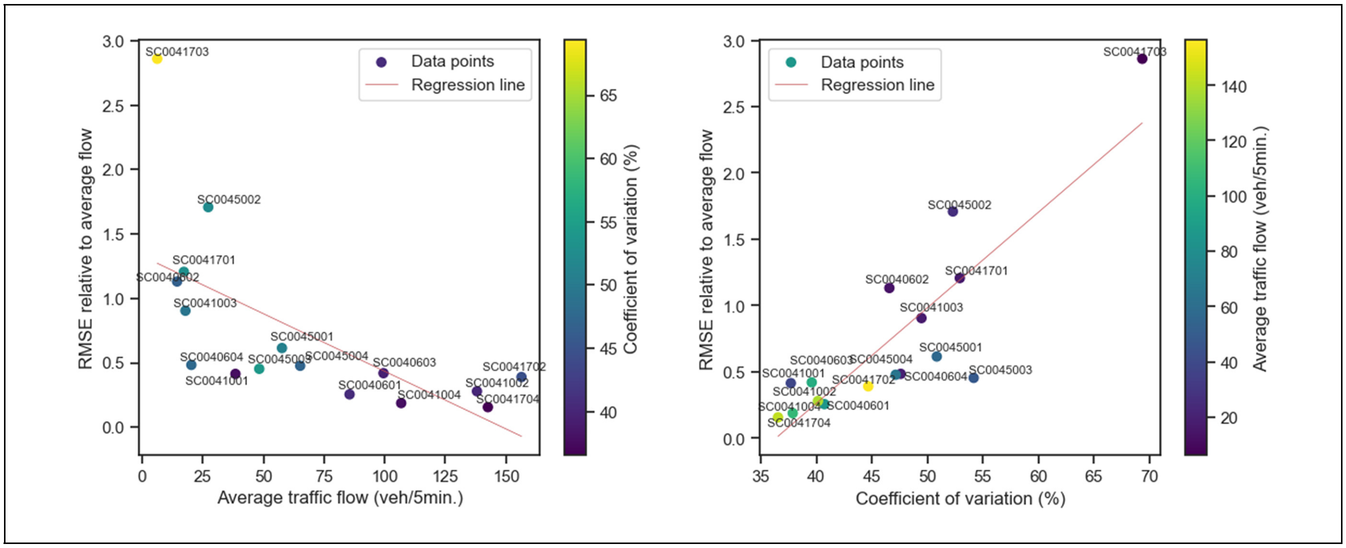

Figure 11. Trends in relative root mean squared error (RMSE) by average traffic flow and coefficient of variation.

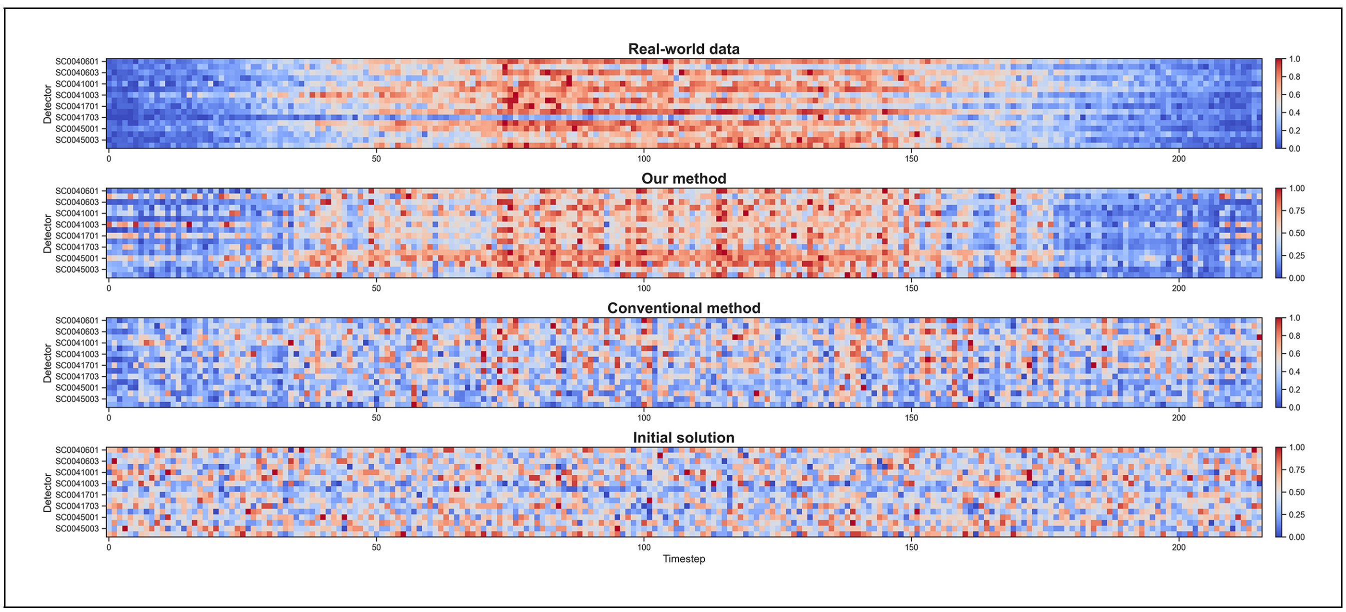

Figure 12. Origin–destination matrix estimation performance within 1 min with heatmaps.

twins. To achieve this, the OD matrix estimation process must be completed within a given time. We use a DNN to develop a data-driven metamodel, integrating the lower-level task of the bi-level DODE problem into the upper-level task. This model simplifies the relationship between the OD matrix and detector data, negating the need to compute the behaviors and routes of all vehicles at each time step, unlike microscopic simulations. As a result, our model provides sufficient samples for estimating a reasonable OD matrix within a constrained time frame. We develop a data-driven metamodel using a DNN, and incorporate the lower-level problem of the bi-level formulated DODE problem into the higher-level problem.

The proposed model and method are validated based on real-world detector data. According to our experimental results, our DNN-based data-driven metamodel effectively approximates the relationship between the OD matrix and detector data. Moreover, the SPSA method with our model offers accurate calibration performance and computational efficiency within minutes, compared to the conventional method. Therefore, our data-driven metamodel is practically superior to conventional simulations for digital twins. We focus on real-time operation

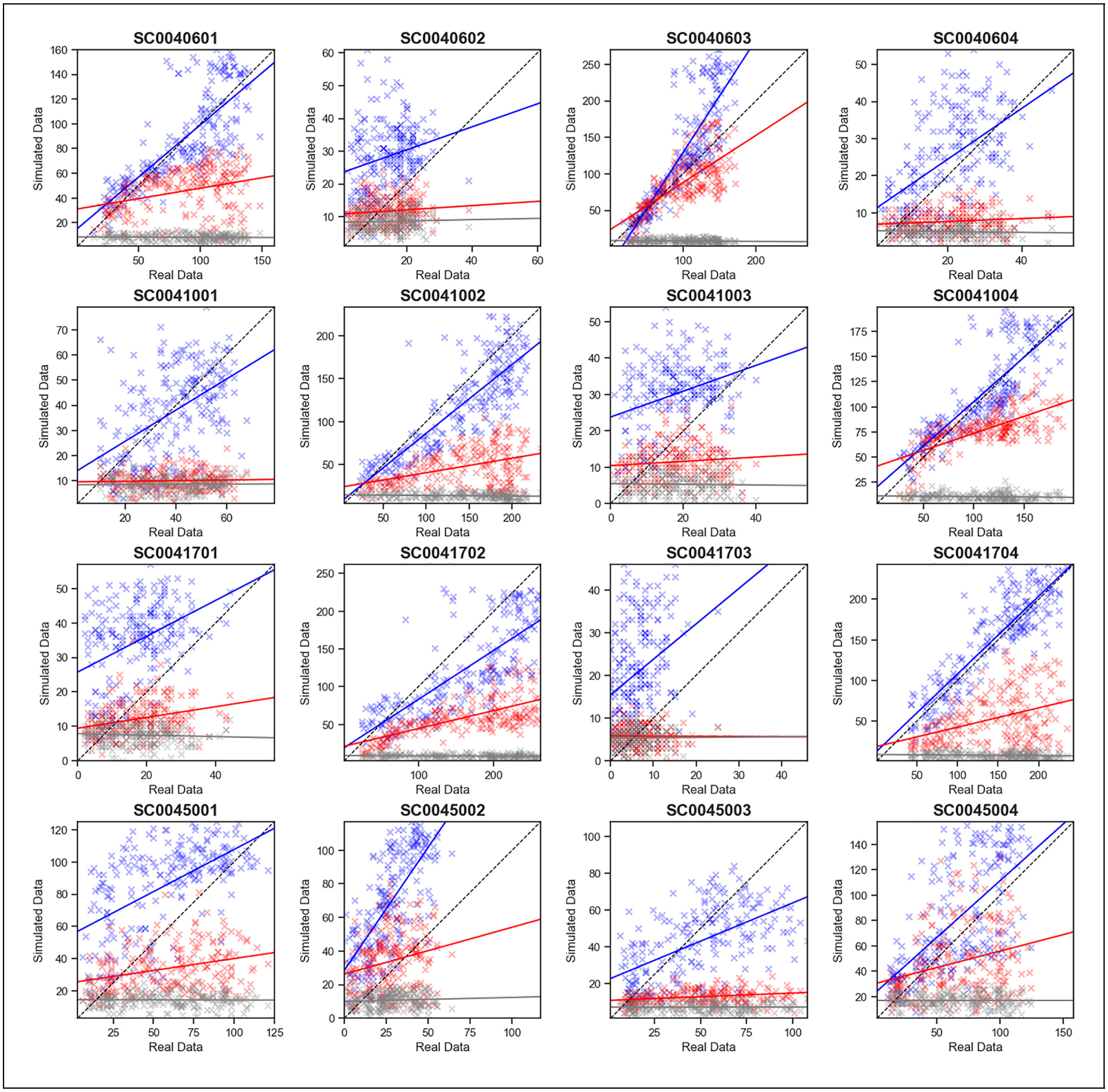

Figure 13. Origin–destination matrix estimation performance within 5 min with scatter plots.

through the data-driven metamodel, offering a practical method for extending microscopic traffic simulations to digital twins.

This study contributes a practical method that significantly cuts down the runtime of traffic simulation, previously overlooked in the conventional simulation-based methods for handling the DODE problem. The proposed data-driven metamodel, using a DNN, tackles challenges that must be addressed for the expansion of microscopic traffic simulations into digital twins. Therefore, we provide a practical and efficient OD matrix estimation framework for digital twins. Furthermore, the versatility of our approach allows the application of various algorithms considered at the upper level, which are researched from the algorithm design for solving the DODE problem. Ultimately, the practical contribution of this research lies in the development of digital twins. By updating traffic demand in real-time at the micro-level, digital twins are capable of accurately depicting real-world traffic dynamics. This enables decision-

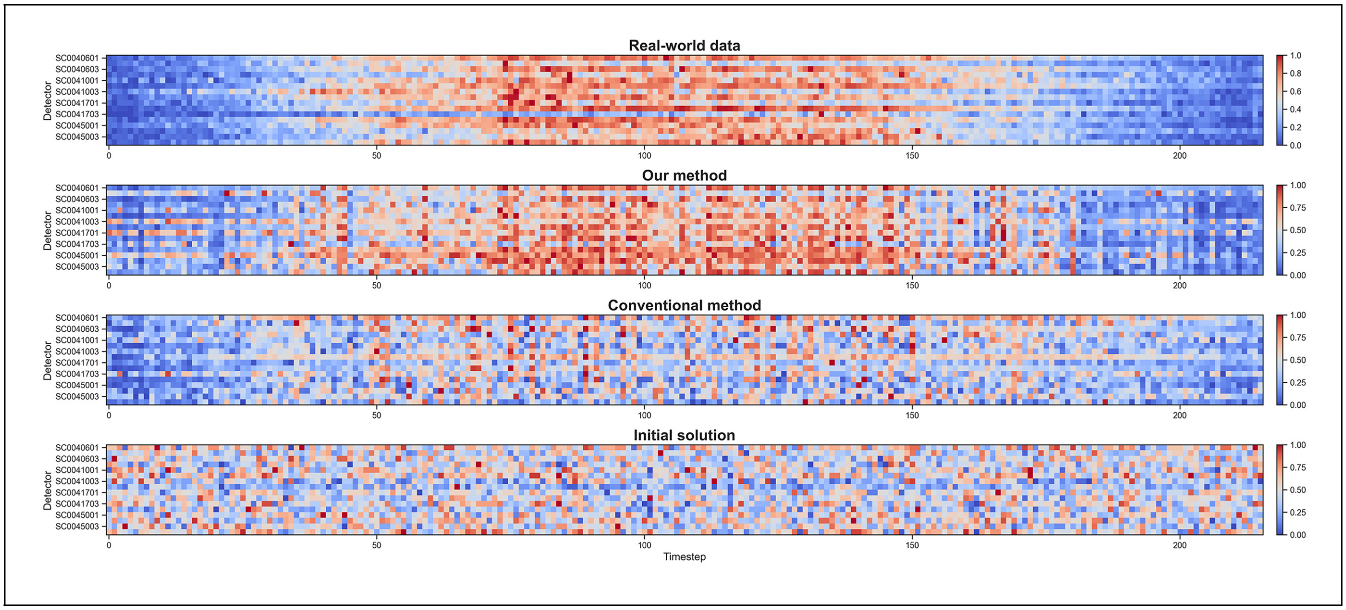

Figure 14. Origin–destination matrix estimation performance within 5 min with heatmaps.

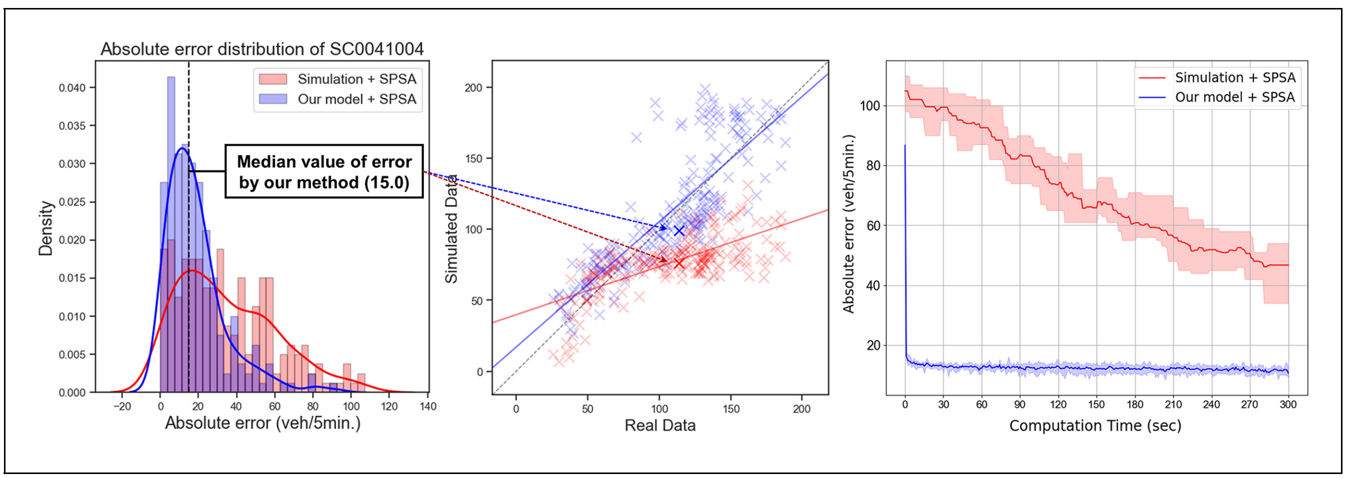

Figure 15. Variation of error with computation time at the median error point for SC0041004.
Note: SPSA = simultaneous perturbation stochastic approximation.

makers to simulate and understand the potential impacts of their actions on actual traffic conditions before implementing new policies or strategies. Furthermore, an accurate microscopic traffic simulation can generate virtual data for areas lacking detectors, providing valuable information to drivers or service providers. This can lead to significant economic benefits, such as reducing individual and network-wide travel costs, and lowering expenses related to the installation of detectors.

While the proposed method provides valuable insights, there remain aspects that need further enhancement in subsequent studies. Firstly, our approach has been validated on relatively small-scale networks. The purpose of this paper is to introduce a new approach by comparing it with conventional methods. For this study, we selected a small-scale network to mitigate the high dimensionality and stochasticity of the experiments, thereby facilitating a clearer comparison. However, future research on large-scale networks is essential to broaden the practical implications of our findings. In large-scale networks, microscopic traffic simulations may have more complex input–output relations, making it challenging to approximate the simulation's internal logic with a simple model structure, as done in this paper. Therefore, using advanced neural network structures that can handle more high-dimensional OD matrices and detector data is an important direction for future research. For instance, mixture density networks (MDNs) are capable of stochastically predicting multiple potential outputs from a single input. This capability allows us to potentially expand our research findings to encompass large-scale network applications. Furthermore, to effectively apply our methods in complex and large-scale networks, ensuring the model's interpretability by incorporating domain knowledge is crucial. For example, insights into route-switching behavior at intersections or route choice models could be incorporated into model architectures. It would also be beneficial to analyze the impact of OD matrices on detector data and to develop model architectures that reflect these spatiotemporal patterns. These tasks can significantly contribute to the theoretical design and analysis of the proposed data-driven metamodel using neural networks.

Secondly, we assumes all network components are fixed. If minor changes occur in the network (e.g., signal timing adjustment), the reliability of our model may be questioned. A natural extension of this is to propose an efficient method to rebuild the model using the information of the already trained model. For instance, we could employ techniques such as transfer learning, utilizing the weights from our pre-trained model. This approach has the potential to decrease both the training time and the computational resources necessary for developing a model that accurately represents the dynamics of the new network. In addition, the data utilized in this experiment were limited to information on traffic flow. A significant advantage of microscopic traffic simulation is its ability to incorporate additional metrics, such as queue lengths at intersections and travel times for networks or individual vehicles. Future studies, enhanced by advanced vehicle detection techniques, could leverage more detailed data to more accurately simulate microscopic traffic flow within the network. Consequently, we anticipate that integrating methodologies from various fields, alongside insights from prior transportation studies, will yield meaningful directions for future research.

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Author Contributions

The authors confirm contribution to the paper as follows: study conception and design: D. Min, D.-K. Kim; data collection: D. Min; analysis and interpretation of results: D. Min, D.-K. Kim; draft manuscript preparation: D. Min, H. Yun, S.W. Ham; All authors reviewed the results and approved the final version of the manuscript.

Declaration of Conflicting Interests

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