1	Using Neural Network for Predicting Hourly Origin-Destination Matrices
2	from Trip Data and Environmental Information
3 4 5	Ehsan Hassanzadeh ¹ , Zahra Amini ^{*,1}
6 7	¹ Department of Civil Engineering, Sharif University of Technology, Tehran, Iran
8 9	E-mail Addresses: <u>ehsan.hassanzadeh@student.sharif.edu</u> (E. Hassanzadeh), <u>zahra.amini@sharif.edu</u> (Z. Amini)
10 11 12 13 14	Submitted for review and possible publication in Scientia Iranica
15 16 17	Corresponding author: Zahra Amini Azadi Avenue
18 19 20	Tehran Iran Email: zahra amini@sharif.edu
20 21 22 23 24	Phone:
25 26 27 28	
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45 Biography

46 Ehsan Hassanzadeh is a graduated Master's student in transportation engineering at the 47 Sharif University of Technology, Tehran, Iran. In his master's studies, he has focused on 48 transportation network modeling and traffic percolation under the supervision of Dr. Zahra 49 Amini. During his Master's career, he has also focused on applications of Machine Learning 50 methods in Transportation Engineering, specifically on the application of Neural Networks in estimating travel demands. He holds a bachelor's degree in Civil Engineering from the Ferdowsi 51 52 University of Mashhad and he has started his Ph.D. studies in Transportation Engineering at the 53 University of British Columbia (UBC). 54 Zahra Amini is currently an Assistant Professor at the Department of Civil Engineering,

Zahra Amini is currently an Assistant Professor at the Department of Civil Engineering,
 Sharif University of Technology. She completed her bachelor's degree in 2014 and her master's
 degree in 2015, in Civil Engineering at University of California, Berkeley. She obtained her
 Ph.D. in Highway and Traffic Engineering, in 2018 at University of California, Berkeley. Her

research interests are Intelligent Transportation System (ITS), traffic theory and control

59 strategies, and transportation system operation and management.

60

61 Abstract

62 Predicting Origin-Destination demand has always been a challenging problem in transportation.

63 Conventional demand prediction methods mainly propose procedures for forecasting aggregated temporal

64 Origin-Destination (OD) flows. In other words, they are primarily unable to predict short-term demands.

Another limitation of these models is that they do not consider the impact of environmental conditions on trip patterns. Furthermore, OD demand prediction requires two individual steps of modeling: trip

67 generation and trip distribution. This article presents a framework for predicting hourly OD flows using

the Neural Network. The proposed method utilizes trip patterns and environmental conditions for

69 predicting demands in single-step modeling. A case study on New York City Green Taxi 2018 trip data is

70 done to evaluate the method, and the results demonstrate that the network has reasonably accurate OD

71 flows predictions.72

73 **Keywords:** O/D demand prediction; Short-term prediction; Neural Network; Machine

- 74 Learning, Trip Generation
- 75

76 Highlights

- Short-time O/D flow prediction is proposed to be obtained by Neural Network models
- The proposed Neural Network model uses past trip and environmental condition data
- The proposed model may replace aggregate distribution models for short-time predictions
- 80

81 **1. Introduction**

In recent years, demand for public transport has increased significantly due to urban
 development and population growth. One option to meet this demand is public transportation
 network expansion, which is expensive and has many limitations [1]. A more appropriate

solution is network management with the available facilities. Network management includes

strategies and policies to fulfill demand in the system and utilize the facilities more effectively

87 [2]. A preliminary requirement if devising such management plans is predicting and modeling

88 users' travel behavior.

89 One of the most popular models in demand modeling is the Four-Step Model (FSM), which 90 contains the following steps: 1. trip generation, 2. trip distribution, 3. mode choice, and 4. route 91 choice [3]. Although this paper mainly focuses on the first two steps and assumes predicting O/D 92 demands for a single mode, some dynamic factors are considered that could alter users' mode 93 choices. The second step, trip distribution, distributes generated trips to match destinations. In 94 the third step, mode choice and trip modes proportions are specified, and the user behavior is 95 modeled using the Consumer Choice theory. Based on this theory, consumers' preference is 96 affected by utility functions, which are not deterministic [4–6]. By assuming a uniform 97 distribution for the random component of the utility function across the modes, it can be 98 concluded that the difference in utilities is only due to the difference in the systematic part. 99 However, it should be noted that researchers have assumed that the random components are 100 independent but non-identically distributed [4].

101 Nonetheless, reviewing the random component's distributions is beyond the scope of this 102 paper, and since it will not be used in this research's modeling process, the distribution is 103 assumed to be uniform to explain the impact of the systematic component. As a result, users' 104 mode choice behavior can be modeled and predicted by considering systematic utility 105 components, including consumers' socio-economic attributes, the vehicle's operational 106 characteristics, and the trip distribution table [4]. Moreover, previous studies show that 107 environmental conditions (e.g., weather data, land use, and other related parameters) have 108 substantial impacts on travel times, public transportation systems quality, and daily travel 109 behaviors [7–10]. As a result, these parameters can be considered in the consumer's utility 110 function. The relationship of these parameters with the utility function (e.g., linear or nonlinear) 111 would be determined by the Neural Network in this project by creating dummy variables in the 112 hidden layers; hence, this paper will not discuss the possible relationships with the utility 113 function. Given that the other parameters, such as the socio-economic attributes (e.g., the impact 114 of income on the mode choice), do not vary over short periods, this paper disregards such 115 parameters as they are assumed to be unchanged over the study period.

116 This paper aims to predict hourly OD flows for a single specific mode using the Neural 117 Network (NN) without users' information (e.g., income, car ownership). To predict OD flows, 118 input parameters reflecting the consumer's utility and other parameters regarding trip information 119 are used. Then to evaluate the proposed method, this study uses New York City Green Taxi 2018 120 trip data and New York City 2018 weather data. The trip data consists of 8.81 million trip information, including trips' origin and destination zones number, trip distance, and other related 121 122 trip information. Another dataset that is used for training the model includes hourly weather data 123 of the desired location.

The rest of this article is organized as follows. Section 2 reviews related works on OD prediction and studies using a similar dataset. Section 3 discusses the proposed framework to predict OD flows in detail. Then, section 4 describes datasets used to evaluate the proposed model and data verification by investigating existing trip patterns. Section 5 discusses model results, and the final section provides the conclusion.

129

130 **2. Literature review**

131 Demand modeling has been a prominent research area in transportation for years, and the 132 FSM has been one of the most comprehensive approaches for demand modeling. This approach 133 underlies methods to predict mode-specific demand [11]. The Gravity model is widely used for 134 trip distribution in the trip generation step of the FSM. This model distributes trips between zones based on the zones' relative attraction and a function of distances between zones [12]. The
model is calibrated on a single OD table, including aggregated trip data. Thus, applying the
Gravity model for estimating hourly OD flows is not practical. Moreover, the Gravity model
considers a limited number of parameters to calibrate the model. Studies have shown that the

Gravity model output has little similarity with the observed data [13]. It can be inferred from theGravity model that the origin and destination zones and a function of distances between the

141 zones (either temporal or spatial) should be considered in the modeling.

142 The third step of the FSM involves using discrete choice models to understand user behavior 143 when selecting transportation modes. The Logit and Probit models are commonly used in this 144 step, which use utility functions to determine choice probabilities [14,15]. However, collecting 145 user information to define these utility functions can be challenging. These models have 146 limitations, such as assuming a constant relationship between dependent and independent 147 variables, making them inflexible and unable to adapt dynamically. They also perform poorly 148 when input variables are multicollinear [16–18]. This paper focuses on parameters that can affect 149 user choices based on environmental conditions, rather than explicitly modeling mode choice.

150 Recent studies have explored the use of Neural Networks (NN) as an alternative to 151 traditional methods for predicting OD matrices and mode choices [19–23]. Researchers have compared the accuracy and performance of NN models with other statistical methods, such as 152 153 the Multinomial Logit Model (MNL) [24], mode choice modeling [25], and Bayesian Model Tree [26]. Xiong et al. [27], proposed a framework that used Graph Neural Networks (GNN) and 154 155 Kalman filters to predict OD flows based on historical link flows. Yaldi et al. [28] used NN 156 models with three input parameters to predict trip flows. However, these approaches have 157 limitations in considering the factors impacting OD flows and user behavior. The current paper 158 proposes a new approach that uses NN models to predict trip flows based on trip patterns, 159 environmental conditions, and consumer preferences. Like the method proposed by Xiong et al. [27], the framework used by Yaldi et al. [28] limits input parameters to trip interchange 160 attributes, ignoring environmental attributes affecting users' behaviors. In contrast, the current 161 162 paper implements the NN to predict trip flows using trip patterns and environmental conditions 163 considering consumer preferences.

164 Researchers have realized that environmental conditions may impact traffic patterns in various ways. Liu et al. claimed that weather parameters, including temperature, snowfall, and 165 166 precipitation, substantially impact travel behaviors [7]. They showed that these weather parameters affect all travel modes, including pedestrian walking, bicycle, private car, and public 167 168 transport. In another study, Rudloff et al. evaluated relations between weather conditions and trip 169 patterns using mode choice models. They estimated choice models' parameters based on 170 household survey data from Vienna, employing the maximum likelihood approach. Their results showed that weather conditions significantly influence transport choice and travel behavior [8]. 171 172 Hyland et al. investigated the effects of weather conditions on travel mode choice using a stated preference (SP) survey in Chicago and realized that commute choice patterns differ vastly in 173 174 various weather conditions. Furthermore, they claimed that the impacts of weather on mode choices vary across the community [29]. Thus, the present paper considers weather conditions as 175 176 effective environmental parameters while training the network for predicting OD flows. The NN is mainly trained on the existing trip patterns to learn future predictions. 177

- 178 Consequently, it is essential to create parameters considering different trip patterns to have a
- more accurate estimate of the future. Studies have shown that different trip behaviors are
- 180 observed on weekends and holidays compared to workdays. Dong et al. [30] used trajectory data

181 collected from ride-hailing services in Beijing, China, to investigate urban trip patterns. Their

- results showed tangible differences in trip distributions between particular zones. Specific hourly
- 183 patterns also justify considering the hour of the day as an effective parameter in network training.
- 184 They observed a notable difference between workday and non-workday trip patterns for various
- trip purposes. Other researchers have also shown the importance of the time of the day in
- 186 predicting OD flows [31–33]. These results reveal the importance of considering weekends,
- 187 holidays, and hour of the day in model training.

Another aspect of this research is dealing with big data for transportation analysis. In this regard, numerous research uses big data for various types of analysis. To name a few related research, [34,35] use big data for analyzing a specific mode of transportation. The latter also focuses on the impacts of COVID-19 on bike-sharing systems. Another similar approach to

- 192 dynamically predict trip patterns using the NN is to apply agent-based day-to-day models. In this
- 193 field, many papers focus on trip-related information and how it can impact traffic conditions by
- applying agent-based models [36,37]. Based on the nature of the problem, which includes
- various parameters impacting traffic patterns and mode choices, this paper opts to utilize the NNfor predicting OD flows.

197 This article uses 2018 New York City taxi data from NYC Open Data to evaluate the 198 proposed framework's performance. Related works on similar datasets are as follows. Deri et al. 199 used similar 2010-2013 New York City taxi data and presented a solution for estimating taxi 200 trajectories using Dijkstra's algorithm with a significantly reduced computation time [38]. In 201 another study, Freire et al. discussed cleaning Spatio-temporal data. They used 2008-2012 New 202 York City taxi data to observe the anomalies in the dataset. Results showed that data exploration 203 needs users' assistance, and the lack of adequate information about events prevents the system 204 from discerning anomalies [39]. Patel et al. proposed an approach to visually explore big OD 205 data and determine average hourly drivers' revenue. They used 2014 New York City taxi data to 206 evaluate their method. Unlike related works using a similar dataset [40], this paper aims to 207 predict OD flows considering the abovementioned parameters.

208

209 **3. Materials and Methods**

This section describes data cleaning procedures and obtaining various input and output parameters required for modeling and the network structure. Input parameters (independent parameters in modeling) indicate parameters used as the network's input to predict output parameters (dependent parameter in modeling), the OD flow per hour. In other words, hourly input data are used to predict the hourly OD flows. This section divides the proposed algorithm's procedure into four major steps, as summarized below:

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- <u>Step 1:</u> Obtaining Input Parameters (Independent Parameters) data for training and testing the NN (See Section 3.1). This step consists of the following minor steps:
 - <u>1A:</u> Obtaining OD zone IDs and hour of the day (See Section 3.1.1)
 - <u>1B:</u> Obtaining interzonal travel times (See Section 3.1.2)
 - <u>1C:</u> Obtaining binary parameters (See Section 3.1.3)
- <u>Step 2</u>: Obtaining output parameters data (number of trips for each pair of OD zones at each time step) for training and testing the NN (See Section 3.2).
- Step 3: Cleaning obtained data to remove any outliers that may deteriorate the NN accuracy (See Section 3.3).
- 226 <u>Step 4:</u> Reshaping input and output data matrices to be fed into the NN for training (See Section 3.4).

228 • Step 5: Standardize data to avoid bias in training the NN (See Section 3.5).

229 • Step 6: Building the NN's structure and training the network (See Section 3.6). 230

231 According to the possible factors affecting trips described in earlier sections, this paper 232 considers the network's input parameters as follows:

- 233 Interzonal travel times, including calculated hourly travel times for all possible OD pairs
- 234 Origin zone, defined by a unique ID •
- 235 Destination zone, defined by a unique ID •
- 236 Hour of the day, specified by a number within the range zero to 23 •
- 237 Weekend/ weekday binary classification •
- 238 Holiday/ nonholiday binary classification •
- 239 • Temperature, including hourly resolution records 240
 - Precipitation, including hourly resolution records •
- 241 Snow depth, including hourly resolution records •

242 This paper assumes that certain parameters such as passenger count and fare amount cannot be 243 determined without access to corresponding demand data or algorithms used to calculate these

244 parameters. Therefore, these parameters are not used as inputs in the model. Additionally, input

- 245 parameters with intercorrelation are omitted, such as distance between origin and destination
- 246 zones. The procedures for obtaining each parameter are explained in detail below.
- 247

248 3.1. Obtaining input data

249 As described earlier, each hourly input record comprises nine factors. Three of these nine 250 parameters, which are temperature, precipitation, and snow depth, can be obtained directly from datasets for each time step. Obtaining the remaining six requires additional steps, which are 251 252 described below.

253

254 3.1.1. Obtaining OD zone IDs and hour of the day

255 In this research, the "hour of the day" variable is defined as the departure hour for each trip. 256 This definition may raise an error since trips are not necessarily finished in the same hour as they 257 started. Since it is assumed that the desired trips only consist of urban trips, trip durations would be reasonably short; hence the error is negligible. Zone IDs can be defined as the assigned IDs 258 259 for each Traffic Analysis Zones (TAZs). Therefore, each trip's destination and origin can be determined with two IDs demonstrating its origin and destination. Traffic Analysis Zones can be 260 specified using the available datasets for the research area or by defining the TAZs using the 261 available methods [41]. 262

263

264 3.1.2. Obtaining interzonal travel times

265 The Gravity model examines how distances between zones impact OD flows, but this article 266 suggests using hourly travel times between zones to consider the impact of traffic flows. Hourly travel times can be obtained from various services like Google Maps, but the calculation of 267 268 shortest paths requires real-time traffic data. Since this research aims to predict hourly OD flows, 269 all input and output data should be aggregated into hourly records. The article proposes 270 calculating average travel times between OD pairs in each hour after removing outliers to 271 represent the hourly travel time for all the trips between the OD zones. Section 3.3 provides more details on the removal of outliers. Then, interzonal hourly travel times are obtained as a linear matrix, TT_k , according to Equation (1).

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$$TT_{k} = \left[tt_{1,1,k}, \dots, tt_{1,n,k}, \dots, tt_{i,j,k}, \dots, tt_{n,n,k} \right]$$
(1)

- 276 277
- TT_k = linear travel time matrix in the hour k, $tt_{i,j,k}$ = travel time for the *ij* OD pair for the hour k.

Depending on the dataset used, travel times for the OD pairs may be obtained using a particular method available. As will be discussed in Section 4.1, the dataset used in this study includes the start time and end time for each trip record. Therefore, each trip's travel time can be simply calculated by computing the in-time vehicle for each trip.

284 3.1.3. Obtaining binary parameters

285 As described in section 2, users have different traffic behaviors on weekends and holidays 286 than on regular weekdays. Two binary parameters are defined to address this variation: "Weekend" and "Holidays," parameters which indicate whether the trip was on the weekend or 287 288 holiday or not, respectively. These parameters' values are equal to zero if the desired day is not a 289 holiday or a weekend. It is worth mentioning that the holidays can be specified using the national 290 holidays' list for the desired database. After obtaining all parameters as discussed, linear matrices of hourly attributes, att_k can be created according to Equation (2). The data source for obtaining 291 292 these parameters will be discussed in Section 4.2.

294
$$att_k = [hr_k, weekend_k, holiday_k, temp_k, PCP_k, SD_k]$$

295 (2)

293

298

296 att_k = linear attributes matrix of the hour k, and for the hour k: hr_k = the hour k of the day, $Temp_k$ = 297 the hour k hourly temperature, PCP_k = the hour k hourly precipitation, SD_k = the hour k snow depth.

299 **3.2.** Obtaining output data

The network's output parameter for each hour is an OD flow matrix showing trip counts between each OD pair. The OD flow matrices at each hour are created by counting the trips between each pair of OD in the trips database. In this study, origins and destinations are considered Traffic Analysis Zones (TAZs), which can be specified by assigning zone IDs. The hourly OD matrix is created as shown in Equation (3).

305 306

$$307 OD_{k} = \begin{bmatrix} T_{1,1} & \cdots & T_{1,n} \\ \vdots & T_{i,j} & \vdots \\ T_{n,1} & \cdots & T_{n,n} \end{bmatrix} (3)$$

308 309

310 $T_{i,j,k}$ = trip counts from zone *i* to zone *j*, for the hour *k*. *k* = the data record index representing the hour 311 *k*

313 It should be noted that hourly trips are counted based on their start time (i.e., departure time).

These matrices are then reshaped to linear matrices, as shown in Equation (4), to simplify the network's training process since it would be less baffling to acquire one row of data per record

316 when feeding the input data to the network.

317 318

319
$$OD_k = [T_{1,1,k} \dots T_{1,n,k} T_{i,j,k} \dots T_{n,n,k}]$$
 (4)

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These matrices are then added to the final output matrix, *T*, according to the occurrence time, starting from the first hour of the initial day (k = 0) to the last hour of the last day in the period (k= t). Thus, the output matrix, *T*, would be a ($t,n \times n$) dimensional matrix according to Equation (5). Each row of the output matrix (i.e., dependent variable) indicates hourly trip counts for an OD pair. The predicted results after training the model will also follow the same format.

$$328 \quad T = \begin{bmatrix} OD_0 \\ \vdots \\ OD_t \end{bmatrix}$$
(5)

329 330

331 3.3. Data Cleaning

The existence of errors in data will result in bias in the network's training process. As a result, possible errors should be omitted from the data before using it for training. This section discusses removing outliers and possible errors from input and output data. To do so, the Z-score is calculated for each record to identify outliers in the data. The Z-score indicates the distance between the observed value and the sample's mean in the standard deviation units [42]. The Zscore can be calculated using Equation (6).

338

339 $z = \frac{x - \mu}{\sigma}$

(6)

340 341

344

342 z = the standard score, x = the observed value, $\mu =$ the mean of the sample, $\sigma =$ the standard 343 deviation of the sample

After calculating the Z-score, records with $|z| \ge 3$ are considered outliers (preserving 99.8% of

the data range). It should be noted that the threshold for removing the records is calculated after

investigating the results by examining different thresholds. This procedure should be done for all

input and output parameters with possible errors. Besides, constraints should be set for each
 parameter to ensure that all remaining data are valid. For example, travel time values should be

349 parameter to ensure that all remaining data are valid. For example, travel time values should be 350 positive and over 60 seconds. Values exceeding these ranges should be omitted based on the

350 positive and over 60 seconds. Values exceeding these ranges should be omitted based on the 351 parameter range.

353 3.4. Reshaping data matrices

So far, the origin and destination zone IDs have not been determined in the input and output matrices. As discussed before, each pair of OD has a unique traffic pattern. So, it is crucial to consider origin and destination zones as parameters for training the model. Then, input and output data are reshaped so that each row of data matrices represents dependent and independent values for a specific OD pair in a specific hour. The final output matrix, *T*, would be as shown in Equation (7).

			$T_{1,1,0}$
	$\left\lceil OD_{0} \right\rceil$]	:
	:		$T_{n,n,0}$
360	$T = OD_k$	$ \rightarrow$:
	:		$T_{i,i,k}$
	OD_t		:
		-	$T_{n,n,t}$
			L

361

To create the final input matrix, X, the travel times matrices, TT_k , should be first reshaped similar to the output matrix. Then, trip attributes parameters can be appended, including origin and destination zone IDs for each record, duplicating common attributes for all the trips in the desired hour. As a result, the final input matrix, X, is according to Equation (8).

$$367 \quad X = \begin{bmatrix} tt_{1,1,0} & i & j & hour_0 & weekend_0 & holiday_0 & temp_0 & PCP_0 & SD_0 \\ \vdots & & & \vdots \\ tt_{i,j,k} & i & j & hour_k & weekend_k & holiday_k & temp_k & PCP_k & SD_k \\ \vdots & & & \vdots \\ tt_{i,j,t} & i & j & hour_t & weekend_t & holiday_t & temp_t & PCP_t & SD_t \end{bmatrix}$$

$$(8)$$

368

369 $tt_{i,j,k}$ = calculated travel time for the origin zone *i* and the destination zone *j* in the hour *k* 370 *i*, *j* = origin and destination zone IDs for each record

371 372 3.5. Data Standardization

373 Due to the significant variances between parameter values (either the difference between 374 values of one parameter or the diversity between the data range of various parameters), the 375 network's training process may be biased. As a result, large trip counts in the OD matrix, which 376 are vital for modeling, could be recognized as outliers. All parameters' values are standardized in 377 their category to address this issue, making the mean of each parameter zero and the standard 378 deviation of parameter one. Standard values are calculated using Equation (9) [43].

$$380 x' = \frac{x - \mu}{\sigma}$$

- 381
- 382

383 x' = the standardized value, x = the observed value, μ = the mean of the sample, σ = the standard 384 deviation of the sample

(9)

386 It should be noted that the network's predicted data will be calculated in the normalized format 387 and must be converted to the original format for evaluating the model.

388

385

389 3.6. The Neural Network's structure

390 The Neural Network is a supervised machine learning method in which the network is 391 trained first using a set of data with pre-defined outputs. The network tries to minimize the 392 defined objective function to achieve the most desirable results by finding connections between 393 input and output nodes. The NN is composed of multiple layers including input, hidden, and 394 output layers. Hidden layers identify possible relations between parameters and provide a 395 representation of data with multiple layers of abstraction. Each layer has a specific activation 396 function to transmit the data format for the next layer. The NN optimizer updates weights based 397 on the gradients computed in each iteration through an iterative backpropagation process [44].

398 The NN used in this paper has two hidden layers, as illustrated in Figure 1. The input layer is 399 provided with the input parameters and transmits input data directly to the next layer via the 400 neurons. As mentioned earlier, the number of nodes in this layer equals the number of input 401 parameters, which is nine. The input and output layers' dimensions are 9 and 1, implying the 402 input feature vector's dimensionality and prediction value. The predicted value here is the hourly 403 OD flow, and each predicted value defines the predicted flow for a specific OD pair in a specific 404 hour of the desired period. To determine the number of nodes in the hidden layer, different 405 numbers of nodes can be chosen, and then the output results of the network can be compared. As 406 a general experimental rule, the number of nodes in the hidden layers is chosen close to the 407 average input and output number of nodes. After investigating the results with different counts of 408 nodes for the hidden layers, 7 and 5 nodes are finally considered for the hidden layers, 409 respectively, as shown in Figure 1.

410 Activation functions are added to the NN to convert the previous layer's output values into 411 desirable input values for the next layer. The ReLU (Rectified Linear Unit) activation function is 412 used for hidden layers in this network as it offers better performance and generalization than the 413 other activation functions used for predicting a numerical value [45]. The ReLU function can be 414 written as Equation (10).

415

416
$$ReLU(x) = \max(0, x) = \begin{cases} x, & \text{if } x \ge 0\\ 0, & \text{if } x < 0 \end{cases}$$
 (10)

- 417
- 418

As illustrated in Figure 1, the output layer connects the last hidden layer to the output values.
This layer has only one node, which is the network output value. Activation functions like the
Sigmoid function result in output values between 0 and 1 that predict categorical values. The

422 output values in this work are numerical; thus, the Linear function is used as an activation423 function for the output layer, expressed as Equation (11).

- 424 425
- 426 f(x)=ax
- 427
- 428

The Mean Squared Error (MSE) loss function is used in this study to calculate the difference
between the actual and the prediction value. This function computes the average squared
difference between the actual and predicted values using Equation (12) [43]. The MSE is also
used as the metric parameter for keeping track of performance measures (i.e., the objective
function of the NN).

(11)

434 435

436
$$MSE = \frac{1}{n} \sum_{i=1}^{n} (y_i - \hat{y}_i)^2$$
(12)

- 437
- 438
- 439
- 440

 y_i = the actual value, \hat{y}_i = the predicted value, n = number of predicted values

441 The "learning rate" is a crucial hyperparameter in NN that determines the step size for 442 weight updates during the optimization process. Overfitting is a common issue when data is 443 similar to each other in time, and to avoid it, the "shuffle" parameter should be used while 444 training the model. The Adam optimizer is used for updating weights in the network, and it can 445 adjust the learning rate with the "decay" parameter. The network's weights are updated iteratively 446 using batches, with each batch representative of the dataset, and the batch size should be large 447 enough to include non-zero values. The dataset is divided into three splits of training, testing, and 448 validation, with each containing a different percentage of the data. The optimal values for the 449 hyperparameters require evaluating different values on the dataset.

450 The process of updating the weights of a neural network is iterative and occurs over many 451 epochs. An epoch consists of one forward and backward pass of the entire dataset, which is 452 usually too large to be fed into the network at once, so it is divided into batches. It is important to 453 choose a batch size that is representative of the dataset to prevent errors. The batch size 454 parameter should be large enough to include non-zero values in a batch since multiple output 455 values are often zero. The correct values for the batch size and epoch parameters should be 456 chosen by assessing different data values. Finally, the dataset is split into three sets: training, 457 testing, and validation, with percentages of 56%, 30%, and 14%, respectively.

458

459 **4. Case Study**

460 A case study was done using open-source trip and weather datasets to evaluate the proposed 461 framework. These datasets are reviewed in detail in the following sections.

462

463 **4.1. Trip Data**

464 This study uses open-source data provided by the Taxi and Limousine Commission (TLC) 465 available on the NYC Open Data website [46]. The dataset consists of 8.81 million New York 466 Green Taxi 2018 trip records. Each record includes pickup date and time, drop-off date and time,

- trip's origin and destination zones ID, and other fields shown in Table 1 (redundant fields formodeling such as tax and distance are ditched).
- According to the City Zones dataset available on the NYC Open Data, zone IDs denoted in Table 1 represent specific taxi zones defined by the Department of City Planning [47]. As shown in Figure 2, there are 265 zones numbered from 1 to 265. Table 2 shows samples of this dataset. This study uses this definition of zones for the case study instead of TAZs for specifying origins
- This study uses this definition of zones for the case study instead of TAZs for specifying origins and destinations.
- 474

475 **4.2. Weather Data**

476 Section 2 discussed that the weather conditions substantially impact daily travel behaviors.
477 This study uses an open-source weather dataset from the National Climatic Data Center (NCDC)
478 [48]. This dataset contains hourly recorded weather information, including date and time,
479 temperature, wind speed, wind direction, 1-hour liquid precipitation, 6-hour liquid precipitation,
480 and snow depth, as shown in Table 3.

481

482 *4.3. Data Preparation*

483 Now that the datasets are explained, procedures done on the datasets described in section 3 484 are summarized here. After setting constraints for each parameter, values exceeding these 485 constraints are omitted. Then, examining the remaining data reveals that there are apparently no 486 outliers remaining in the dataset, as they were possibly removed in the last step. However, there 487 would still be outliers while calculating average travel times, which will be removed based on 488 the Z-score. Moreover, additional constraints should be set for some parameters. For example, 489 calculated travel times with minimal positive values (e.g., less than a minute) may not be omitted 490 based on the initial constraint of being positive and also may not be detected as outliers. After 491 cleaning the datasets from possible errors, only the data for the first quarter of the year (90 days) 492 is used in this study to prevent inundating the network while training. So, indices of data rows 493 considering the available 265 zones are calculated as $265 \times 265 \times 90 \times 24 = 151,686,000$ indices.

494

495 *4.4. Data Verification*

It is necessary to verify the validity of the acquired data to prevent possible errors before training the network. Data verification can be done by examining the conformity of trip patterns with previous studies. As a result, average trip patterns are investigated in this section to verify the validity of the dataset. To investigate the trip patterns, average hourly trip counts were computed for all weekends and weekdays in February 2018. To show the contrast between the trip patterns during the holidays and non-holidays, hourly trip counts of 1st January 2018 (New Year's Day) are computed as a sample. These patterns are plotted in Figure 3.

503 As illustrated in Figure 3, there are two peak hours in the morning and the evening for trip 504 counts in the weekday average trip pattern, which are 8 a.m. and 6 p.m., respectively. The 505 weekend average trip pattern shows that the morning peak hour is vanished (since there are no 506 work-based trips in the morning) and the midnight trip is increased significantly compared to the 507 average weekdays. The trip patterns from previous studies can be compared to similar hourly 508 patterns of taxi trips on weekdays and weekends to validate the results [30,49]. The main 509 difference between the holidays and non-holiday trip patterns (including non-holiday weekends) 510 is that there are numerous holidays, and generally, traffic patterns are changed based on the

holiday and related celebrations or rituals of the day. The reasons mentioned above substantially
 impact trip patterns (e.g., travel destinations change vastly). For instance, the hourly trip pattern
 on 1st January 2020 plotted in Figure 3 shows substantial differences compared to weekday and
 weekend trip patterns.

515 Trip patterns between OD zones can also be inspected to see differences in the patterns 516 between weekends, workdays, and holidays. The weekday average trip pattern shows that trips 517 between zones 74 and 75, East Harlem North and East Harlem South neighborhoods, have the 518 most frequency at different day hours, including the morning and evening peak hours. According 519 to the Office of the New York State Comptroller report, East Harlem is mainly a residential neighborhood with concentrated small businesses [50]. Weekends average trip pattern exposes 520 that trips between zones 41 and 42 (Central Harlem and Central Harlem North neighborhoods) 521 522 and internal trips of zone 7 (Astoria zone of borough Queens) have the highest frequency at 523 different hours of the day. Inspecting New York City's Zoning and Land Use Map [51] indicates 524 that Central Harlem and Astoria are commercial neighborhoods, including numerous recreational 525 places, specifically the Astoria. Internal trips of the Astoria neighborhood also showed the 526 highest frequency at different hours in the selected holiday. According to the City Zones dataset, 527 these paths are illustrated in Figure 4.

These results gave us good insights into the differences between weekdays, weekends, and holiday trip patterns and the need to use binary parameters to address these variances. It can also be derived that the demand in the origin and destination zones is a function of land use.

Therefore, it can be verified that the input data have rational patterns and can be used for trainingthe network.

534 **5. Results**

533

535 5.1 Network Results

536 "Keras is a deep learning API written in Python, running on top of the machine learning 537 platform TensorFlow. It was developed with a focus on enabling fast experimentation." [52] This 538 package provides the required functions for training the network in Python. After evaluating 539 different values for the network parameters, a summary of the chosen values for the network's 540 parameters is given in Table 4. After manually inspecting the network's prediction accuracy, 541 these values are chosen by evaluating different values for each parameter.

542 As shown in Figure 5, it is observed that the error value converges to a relatively constant 543 value after performing several epochs. Consequently, the number of epochs is chosen to be 10. 544 The NN training results indicate the presence of MSE = 0.5798 after ten epochs, which is 545 reasonable. It should be noted that these results cannot be compared directly to results from the 546 trip distribution models, including the Gravity Model and the Fratar model, since these models 547 predict aggregated trips for a period of time. On the contrary, this paper proposed a method to 548 predict hourly trip counts. However, the hourly prediction may cause an increase in error, which 549 comes from numerous possible scenarios in each hour. The output results of each epoch can be 550 seen in Figure 5, and the loss reduction trend in Figure 6. The middle oscillations in Figure 6 551 indicate the beginning of a new epoch. The error reduction trend verifies that the network is 552 working correctly. As shown in Figure 5, loss values decrease rapidly at first and then slowly 553 after the third epoch.

It can be inferred from the results that the loss value is minimized after a limited number of iterations, and there is no need to increase the number of epochs. The network performance is then investigated on one million random samples from the test dataset. It is worth mentioning 557 that the predicted results are rescaled to the original values and rounded to the nearest integer 558 since they represent trip counts. Test results are given in Table 5.

559 Test results show that the number of predicted zero values in the OD matrix and the total 560 predicted trips perfectly match the actual values, and the Mean Squared Error of 0.0348 confirms this. R Squared value of 0.453 shows the model's acceptable fit, but possible reasons for the R 561 562 Squared's relatively small value are discussed here. One million samples are approximately 563 equivalent to 14 hours of trips since there are 70,225 possible paths (a path is a possible route 564 between OD pair) between zones in an hour, and the results show that there are 15,100 trips in 565 one million random samples of the trips. It can be deduced that there is an average of 1,100 trips 566 for the available 70,225 paths in one hour, which means the average hourly trip count for each 567 path is a small value. It can also be derived from the results that the average value for non-zero 568 trip counts is approximately equivalent to 1.7 trips. Hence, slight deviations from the actual 569 value can be due to the rounded predicted values (e.g., the predicted value of 3 for the actual 570 value of 2), decreasing the Coefficient of Determination (R Squared) vastly. As a result, R 571 Squared's small value can not necessarily represent the model's inadequate goodness of fit, and 572 the MSE is a better quantifier to evaluate the model's goodness of fit. Suggested solutions to 573 reduce the existing errors are given in the discussion.

574

575 5.2 Validating Network Results

576 In this section, the NN's results are compared to the Gravity model to validate the results. As 577 mentioned before, the NN predicted hourly trips, and the Gravity model generates aggregated 578 trip predictions; therefore, these results cannot be compared directly. So, the results of the 579 Gravity model should be compared to the aggregated results of the NN. Although this study aims 580 to predict hourly flows, comparing the aggregated form of the results with the traditional models 581 is compulsory for validation. The Gravity model's general form can be expressed in Equation 582 (13) [53,54].

(13)

583 584

585	$T = \frac{P_i A_j F_i K_j \times f(c_{ij})}{P_i K_j \times f(c_{ij})}$
565	$I_{ij} = \frac{1}{\sum_{v} A_{v} F_{i} K_{v} \times f(c_{ij})}$

586

587 588

8 T_{ii} = total trips between zones *i* and *j*

589 P_i = total trips produced by zone *i*

- 590 $A_i = \text{total number of trips attracted to zone } j$
- 591 v = set of 265 zones
- 592 $f(c_{ij}) =$ decreasing function of the travel cost c_{ij}

593	F_{i}	=	balancing	factor	ensuring	$\sum_{j} T_{ij} = P_i$
594 595	(14) <i>K</i> _j	=	balancing	factor	ensuring	$\sum_{i} T_{ij} = A_j$
596 597	(15)					I

The travel cost function in Equation (13) (friction function) is any decreasing function of the travel cost (which is assumed to be the travel time in this study). Hence, the friction function can be considered as the power function shown in Equation (16) [55].

601 602

$$603 \qquad f\left(c_{ij}\right) = \frac{1}{\left(c_{ij}\right)^{n}}$$

(16)

- 604
- 605

606 607

c_{ij} = average travel time between zones <i>i</i> and <i>j</i>
n = power variable

608 609 Since the Gravity model requires total productions and attractions for the prediction period (i.e., the NN test data), they should be estimated using the trip generation models. The trip 610 611 generation models require access to socio-economic data, which are assumed to be unavailable in this study. As a result, zones' productions and attractions are estimated by applying linear 612 613 regression to the train data to predict the number of attracted (A_i) and produced (P_i) trips for the 614 test set. The training and test data in this section cannot be the same as before since the Gravity model predicts aggregated trips for the prediction period. Consequently, hourly records of the 615 dataset are aggregated into daily records. The test data includes 27 daily productions and 616 617 attractions records for all zones (30% of the whole period), and the training data includes 63 618 daily records. Although the trip generation estimation should be for the desired 27 days, the 619 training and the test data are aggregated into data points of 9 days to increase accuracy. In other 620 words, the test data is aggregated into three data points (each one including aggregated productions and attractions of all zones for nine days period), and the training data is aggregated 621 622 into seven accumulated data points. 623 Then, linear regression is applied to each zone's seven data points to predict future productions and attractions. It is worth mentioning that the linear regression equation is 624 625 calibrated for the productions and attractions of each zone separately. Hence, $265 \times 2 = 530$ 626 linear regression equations are calibrated, predicting three data points for future periods. Zones' 627 production and attraction values are then compared to the actual values. Table 6 shows R Squared values of predictions for the zones' productions and attractions. 628 629 Linear regression results show a reasonable fit of the predicted productions and attractions with an R Squared of 0.99 and a reasonable error in predicting the total trips. The three predicted 630 631 data points for each zone's attractions and productions are then aggregated to calibrate the 632 Gravity model. As shown in Equation (14), the Gravity model requires average travel times for 633 the forecasting period. The required travel times are calculated by averaging the non-zero travel 634 times after removing the outliers, as described in section 3.3. It should be noted that the average 635 travel times are calculated using the data from the 63-day training dataset. Since the zero average 636 travel times cannot be used in Equation (16), the zone pairs with an average travel time of zero 637 are assumed to have no trip interchanges. However, this assumption may increase the accuracy of the results since zone pairs with no trip interchanges in the 63 days training period are forced 638

639 to have no trips in the future.

- 640 After implying the travel times in Equation (13), the F_i and K_i balancing factors are
- calibrated through an iterative process to ensure that the conditions expressed in Equation (14)and Equation (15) are met. The stop condition of this iterative process is as follows:
- 643

644
$$\max\left\{\max_{i\in\nu}\left(\left|1-\frac{P_i}{\sum_j T_{ij}}\right|\right), \max_{j\in\nu}\left(\left|1-\frac{A_j}{\sum_i T_{ij}}\right|\right)\right\} < 0.05$$
(17)

- 645
- 646 T_{ij} = total trips between zones *i* and *j*
- 647 P_i = total trips produced by zone *i*
- 648 A_i = total number of trips attracted to zone j
- 649 v = set of 265 zones
- 650

Then, the calibration process is done with different power variables, *n*, in Equation (16) to minimize the error. Table 7 shows the Gravity model results with different values for the power variable, including the iterations needed to meet the convergence condition expressed in Equation (17).

As shown in Table 7, n = 2 had the lowest error in prediction with an MSE of 2340 and an R Squared of 0.84. However, the aggregated NN results for the same period showed an MSE of less than 25. One point worth mentioning from the above table is that the R Squared value for the power variable of 6 is negative. While the R Squared name suggests that it may always range from 0 to 1, some exceptions may also be negative. In cases where the model predictions are not being compared to the observation that were used for calibrating the model, the Total Sum of Squared Errors component (SS_{res}) is not included in the Total Sum of Squares (SS_{tot}) [56].

662 663

 $664 \qquad R^2 = 1 - \frac{SS_{res}}{SS_{tot}} \tag{18}$

665 666

 SS_{res} = Total Sum of Squares of Residuals

- $SS_{tot} = \text{Total Sum of Squares}$
- 669

670 Hence, as Equation (18) suggests, the R Squared value could also be negative in such cases. It should be noted that R Squared has been criticized for the lack of reliability as a measure of 671 672 predictive accuracy [57]. Therefore, a more suitable measure of accuracy should be used to compare the prediction results, which is MSE in this case. Moreover, the NN uses MSE as the 673 674 metric to optimize the learning process, and as a result, the network tries to reduce MSE in each 675 iteration. The results showed that the NN had a clear superiority to the Gravity model in this case, although the purpose of this study was to predict hourly OD flows, and the Gravity model 676 677 is unable to predict the flows on an hourly basis. Besides, forecasting the future trip distribution 678 using the Gravity model required additional steps to estimate the future trip generations (i.e., the 679 second step of the FSM), while the NN can predict trip distributions more precisely without 680 requiring further steps. Another point worth mentioning is that, as mentioned before, the output

681 results of the gravity may not be directly compared to those of the NN. The reason is that the

682 Gravity model predicts aggregated trips for a period of time, while the NN in this study aims to

683 predict hourly trips. Although it can be argued that the aggregated trips of the NN output results

684 can be compared to the Gravity model results, given that the NN is optimized to predict the 685

hourly hours, this study is not focusing on such comparisons using visual descriptions (e.g.,

686 comparison plots) 687

688 6. Conclusion and Discussion

689 OD matrix prediction for a specific transit mode using traditional methods has always faced 690 numerous problems, including data collection. Using traditional methods requires data collection 691 for the trip generation and trip distribution steps of the FSM. This data includes users' socio-692 economic characteristics and travel expenses information, which requires time-consuming and 693 costly collection methods, such as filling out questionnaires. Finally, due to the nature of these 694 collecting data methods, there is a significant error in the collected data, and it is also challenging 695 to update them periodically.

696 This paper aimed to facilitate this procedure using the data from data-driven transportation 697 systems. Prediction results showed proper fit and the logical dependence of the output data on 698 the input data. Other advantages of predicting trips using the NN compared to the traditional 699 modeling methods are considering more scenarios (weekends/holidays and more), quickly 700 updating the network with recent changes, and adequately forecasting OD flows on an hourly basis.

701

702 It can be inferred from the results that there are considerable differences in the number of 703 trips between zones. As a result, some output values, which are numerically significant and 704 essential to be included in predictions, are detected as outliers and have insignificant impacts on 705 model training. As a potential research extension, paths between zones can be classified based on 706 their traffic volume (e.g., low traffic, medium traffic, and high traffic) and then modeled for each 707 category separately. Creating dummy variables indicating each category can also be done 708 instead.

709 It should also be noted that the results represent the predicted part of the demand that taxi 710 drivers could handle. In other words, there would be other trip demands exceeding the taxi 711 service supply; therefore, as there are no data for the unanswered demands in the dataset, the 712 calibrated model disregards such demands. A potential research extension includes datasets 713 containing users' requests to consider the drivers' unhandled trip requests, especially during peak

714 hours.

715 As described in section 4.4, holiday trips showed various patterns depending on the 716 occasion. A potential research direction is to model each type of trip discussed in this article 717 separately (e.g., separate modeling for weekdays and weekends) to increase accuracy. Using 718 algorithms to detect abnormal trip patterns (e.g., gatherings, special occasions that are not 719 officially registered, and social events) and separating them from other data used for training the 720 network can also improve results. Trip data used in this study included origin and destination 721 zones for each trip, including precise longitude and latitude of origins and destinations, resulting 722 in more accurate travel times and improved results. 723

724 **Conflict of Interest**

All the authors have no conflict of interest with the funding entity and any organization mentioned in this article in the past three years that may have influenced the conduct of this research and the findings.

728

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732

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- 870

871 Captions

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890

Figure 2. Structure of the Neural Network in this study





893

Figure 2. New York City taxi zones



Figure 3. Weekday, Weekend and Holiday hourly trip patterns Holiday trip data as of 1st January 2018, Weekend and Weekday trip data are average trip counts of all weekends and all weekdays of February 2018 respectively.





Figure 4. Paths with highest trip counts



Figure 5. Optimum loss values in each epoch



Table 8 - Trip record	fields sample
-----------------------	---------------

	Field	Pickup Date Time	Dropo Date Ti	off PU Locat ime ID	ion DO Location ID	Passenger Count	Trip Distan	ce
	Description	Passenger pick-up date and time	Passeng drop-c date au time	ger off Destinati nd zone II	on Origin zone D ID	Number of passengers	Distance trave from origin t destination	eled to
	Sample	01/01/2018 12:18:50 AM	01/01/20 12:24:39	018 43 AM	75	2	3.5 mi	
908 909 910	Table 9 zones datas	9 – et 7 0	ne ID	12	46	94	165	New York City sample
911			cation	Manhattan- Battery Park	Manhattan- Chinatown	The Bronx- Fordham South	Brooklyn- Midwood	
912								
913								

Field	YR	DIR	SPD	SPD SKC		PCP01	
	MODAHRMN						
	Year-Month-	Wind direction	Wind	Sky cover	Temperature	1-hour liquid	Sn
Description	Day-Hour-	in compass	speed	(Nominal	in Eahranhait	precipitation in	dep
	Minute in GMT	degrees	(mph)	classification)	III Famelinen	inches	inc
Sample	201801281151	990	6	SCT	49	0.01	0
		Tabl	e 11. Netwo	ork parameters v	values		
	Parameter	Learning rate	Decay	Batch size	Number	of epochs	
	Value	0.0005	1*10-6	256	1	0	
		Table 12. Te	st results on	one million rar	idom samples		
-		Total Trip	Nu s	umber of zero values	R Squared	MSE	
-	Predicted Values	s 14721		991384	0.452	0.0248	
-	Actual Values	15127		991324	_ 0.453	0.0348	
			Tot	al Trips	R Squared		
			Predicted	d Actual			
	_	Zones Productions	692585	693364	0.9921		
	_	Zones Attractions	692565	693364	0.9922		
	—						
		Table	e 14 - The G	ravity model res	sults		
Number of zero							
	Power varia	bie valu	values		MSE	Iterations	
	(n)	Actual	Predicted				
	1		18057	0.5933	6098 768	9	
			17780	0.8439	2340 261		
			16584	0.7714	3248.935	13	
	<u></u>	19112	13502	0.7714	7866 803	16	
			10164	0.1162	13254 1566	19	
	 6		7950	_0 22/18	18370.005		
	0		1730	-0.2240	103/0.003	44	