Comparative Analysis Of Gravity Model, Neural Network, And Graph Neural Network For Traffic Demand Modeling In Urban Areas

Keivan Jamali, Nassrin Sharifi

***Abstract*—**

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I. Introduction

TRansportation systems are infrastructures of cardinal importance in modern societies [1]. As these systems get more and more complex, traffic prediction becomes more essential in urban management and traffic engineering [2].Over the past decades, various models have been developed to estimate traffic flows, among which the Four-Step Model (FSM) , consisting of the steps: trip generation, trip distribution, modal split, and trip assignment, has gained significant popularity [2].Trip distribution modeling (TDM) is the second step and a crucial component of the 4-step transportation planning model which provides valuable insights into the spatial allocation of trips from origins to destinations within a given area.

Various models have been developed and examined for predicting trips distributed in transportation networks. Trip distribution modelling mostly utilizes statistical methods like time-series, regression and the gravity model (GM), which is a very popular one [3]. The gravity model, despite its widespread use in TDM, has its own limitations . Overestimation of short trips, underestimation of long trips, and data deformity caused by transforming to linear equations are some of the drawbacks of GM mentioned in [4]. According to [5], GM usually needs large amount of data and high calibration percentage in order to perform well. Also, traditional GM doesn't give good results for networks with low homogeneity [6].

Machine learning (ML) is a branch of artificial intelligence that focuses on the development of algorithms and models capable of automatically learning from data and making predictions or decisions without being explicitly programmed. It involves the utilization of statistical techniques and optimization algorithms to enable computers to improve their performance on specific tasks through experience and data-driven learning. Various ML models have been compared to traditional models such as GM in previous articles, including neural network (NN), artificial neural network (ANN), random forest (RF), and generalized regression neural network (GRNN). In [7], the GM has shown a poor performance in commuting trip distribution at the census tract level in NYC, compared to RF and ANN in terms of mean square error (MSE) and R^2. Also, the GRNN model conducted in [4] has a lower average Root Mean Square Error (RMSE) and higher R^2 compared to GM.

The rise of machine learning (ML) has improved problem-solving and prompted researchers in various fields to adopt this new method. ML methods can effectively handle nonlinearities, discontinuities, and polynomial aspects and it makes them suitable for a wide range of fields including transportation systems [3]. For example, Intelligent Transportation Systems (ITS), have been positively impacted by the growth of machine learning [8]. Additionally, ML techniques are crucial in driving advancements in areas such as advanced driver assistance systems (ADAS) [1], traffic prediction, and optimization [5], [9]. Deep Learning (DL), a specific type of machine learning, has become popular in transportation systems due to the increased availability of data and advancements in computational techniques [8] . Traffic networks often have a graph-like structure so new deep learning techniques called graph neural networks (GNNs) have been developed to handle graph data [10]. GNNs have demonstrated remarkable performance in diverse applications ; for example, traffic congestion [11], travel demand [12], transportation safety [13], traffic surveillance [14], and autonomous driving [10], [15]. GNNs are particularly well-suited for traffic forecasting tasks due to their capability to capture spatial dependencies, which are often represented using non-Euclidean graph structures [1]. In the field of TDM, there have been several studies focusing on neural network (NN) approaches. Initially, the results obtained from these NN models were not satisfactory [5]. However, with further research and advancements, the performance of NN models improved over time [3], [4], [16]. Despite these improvements, there is currently a lack of research specifically exploring the adoption of GNNs in TDM.GNNs possess several features that make them highly suitable for TDM. The spatial modeling capabilities, understanding of location-level and network-level information, handling of heterogeneous data, make GNNs well-suited for TDM. Given the powerful features of GNNs, it is presumed that this model has the potential to outperform NN models in this domain. Therefore, the objective of this paper is to investigate the potential benefits of employing GNNs in TDM and evaluate their performance compared to traditional NN and GM models.

In TDM, GNNs excel at capturing spatial dependencies between transportation entities, such as origins, destinations, and their connections. By considering the graph structure of the transportation network, GNNs can learn and leverage the

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relationships between different locations, including their proximity, connectivity, and traffic patterns [17]–[20]. Moreover, TDM often requires the integration of diverse data sources, such as traffic counts, land use characteristics, socio-economic factors, and transportation infrastructure details. GNNs can handle heterogeneous data by incorporating features associated with each node and edge in the graph representation [21], [22]. This allows for the simultaneous consideration of multiple data types, leading to more comprehensive and accurate modeling compared to the gravity model or traditional NNs. Additionally, GNNs have the advantage of learning end-to-end representations from raw input data. They can automatically discover relevant features and patterns within the transportation network, reducing the need for manual feature engineering [23], [24]. This is particularly beneficial in scenarios where the underlying relationships and dependencies are complex and not easily captured using traditional models like the gravity model or NNs. While traditional neural network relies on complete data for training and prediction, GNN have the potential to handle missing data. this missing data may lead to biased or inaccurate gravity model estimates. However, the impact of missing rates on the accuracy of the gravity model may be relatively low compared to GNNs or NNs.¬

II. Literature

Various methods have been employed to predict travel distribution in the literature . Traditional approaches often rely on statistical models, such as regression analysis [25] and the gravity model [6], [26] to estimate travel patterns based on historical data. The widely used GM method fails to predict well on heterogeneous networks thus Almog et al. [6] have developed an enhanced GM model to address this shortcoming. These methods typically focus on aggregate-level information, assume static relationships between variables, and do not handle nonlinearities well [5], [7]. However, with the advent of machine learning techniques, new approaches have emerged. Machine learning algorithms, including random forests [7], and support vector machines [27] , have been applied to travel distribution prediction. These methods leverage the power of data-driven models to capture complex relationships and patterns in travel behavior. In recent studies, neural networks have been widely explored and compared to previously used models, particularly GM, in trip prediction. Tillema et al. [5] have developed a NN model that outperformed GM when data was scarce. In [16], the accuracy of the NN model is twice that of the direct demand model. The major limitation of neural networks as mentioned in [5] and [4] is that they are black boxes. It is not easy to understand the process happening inside the network and the relationships between parameters.

Additionally, deep learning has emerged as a powerful tool in various domains, and its potential in transportation has gathered significant attention. The utilization of deep learning methods in the transportation sector has yielded encouraging outcomes, paving the way for improved transportation systems and services. The papers collectively suggest that deep learning methods, including recurrent neural networks (RNNs) [10], generalized regression neural networks (GRNN) [4], and convolutional neural networks (CNNs) [9], [28], have shown promising results in predicting travel distribution. In [4], the GRNN model slightly outperforms the GM in terms of average Root Mean Square Error (RMSE) and R2. Nguyen et al. [29] provide a review of deep learning applications in transportation, highlighting its potential but also noting limitations in its current utilization. Varghese et al. [30] investigate the impact of spatial and temporal granularity on demand prediction using deep learning models, finding that the granularity of space and time can improve prediction performance. Yao et al. [31] propose a Deep Multi-View Spatial-Temporal Network (DMVST-Net) framework that considers both spatial and temporal relations for taxi demand prediction, demonstrating its effectiveness over existing methods. Markou et al. [32] explore the combination of time-series data and semantic information using machine learning and deep learning techniques for travel demand prediction in event areas, showing significant error reduction in forecasts.

Recently, GNNs have gained attention for their ability to model the spatial and relational aspects of travel distribution [1], [10], [33]. These methods enable more accurate predictions by considering the interconnections between different locations and their influences on travel patterns. Recent studies suggest that GNNs are a promising tool for traffic demand modeling. In their comprehensive survey, Jiang et al. [1] provide a comprehensive survey of recent research using GNNs in various traffic forecasting problems, demonstrating that GNNs have achieved state-of-the-art performance. Diehl et al. [34] specifically evaluate GNNs for modeling traffic participant interaction and find that GNNs can effectively take the interaction between traffic participants into account. In comparison to other modeling techniques, Golshani et al. [35] find that NNs offer better predictions for travel mode and departure time decisions, suggesting that GNNs may also outperform other modeling techniques. However, none of the papers directly compare GNNs to NNs or GMs in traffic demand modeling, so further research is needed to fully address this research gap.

III. Method

1. Trip Distribution: Trip distribution modeling involves the study of spatial interaction, which encompasses the movement of goods, individuals, money, or information across geographical space (Fotheringham and O'Kelly, 1989). At its core, trip distribution involves the examination of travel behavior to discern the likelihood of trips originating from specific zones to terminate at others. For doing this, a better understanding of the pattern of trip making other than productions and attractions is needed. Although productions and attractions provide a general idea of the level of trip making in a study area, they are often inadequate for modeling and decision-making purposes. It is necessary to have a better understanding of the pattern of trip making in order to create an accurate and usable travel demand model. An intriguing challenge arises when information is available on the number of trips originating and ending in each zone. In such cases, the total number of trips produced in a zone should correspond to the total interaction flows exiting that zone. Spatial interaction models are categorized based on the constraints imposed on the predicted trip matrix, which captures prior knowledge about the total interaction flows entering and/or exiting specific zones.

When information is available on the number of trips originating and ending in each zone, an important consideration arises. The total number of trips originating from a particular zone, referred to as trip production, should be equal to the total number of interaction flows exiting that zone:

$$\sum_j T_{i,j} = O_i.\forall_j. \tag{1}$$

Similarly, the total number of trips ending in a particular zone, known as trip attraction, should be equal to the total number of interaction flows entering that zone:

$$\sum_j T_{i,j} = D_i.\forall_j. \tag{2}$$

When both Equation 1 and Equation 2 are satisfied, the model is referred to as a doubly constrained gravity model:

$$T_{i,j} = A_i O_i B_j D_j f(c_{i,j}). \tag{3}$$

Here, A_i and B_j are balancing factors, c_ij represents the travel impedance, O_i and D_j represent production and attraction, $f(c_ij)$ denotes the distribution function, and T_ij represents the estimated flow or interaction between origin zone i and destination zone j.

In trip distribution modeling, the balancing factors A_i and B_j, along with the travel impedance c_ij and the distribution function $f(c_ij)$, play significant roles. Various constraints can be applied to model trip distribution. Studies have demonstrated that the doubly constrained gravity model provides the most accurate results for estimating spatial interaction (Ortuzar and Willumsen, 2001). Therefore, in this article, the doubly constrained model is used as the benchmark.

3.1 Calibration of Gravity Model: The calibration process of the gravity model follows a general form discussed in [1], which can be expressed using Bayes' theorem as:

$$p_{i,j} = a_i b_j f(\mu, C_{i,j}) \tag{4}$$

In Equation (4) a_i, b_j, and μ represent the model parameters, while $C_(i,j)$ represents constants. The function f is a specified smooth function. Different decay functions, such as the exponential model and power model, can be utilized. The decay functions are defined as follows:
For the exponential model:

$$f(\mu, C_{ij}) = \exp(-\mu C_{ij}) \tag{5}$$

For the power model:

$$f(\mu, C_{ij}) = \exp(-\mu C_{ij}) \tag{6}$$

According to [1], using Equations (4) and (5), the exponential model can be expressed as:

$$T_{ij} = \beta P_i A_j \exp(-\mu C_{ij}) \tag{7}$$

Similarly, utilizing Equations (4) and (6), the power model is given by:

$$T_{ij} = \beta P_i A_j C_{ij}^{-\mu} \tag{8}$$

Here, P and A represent production and attraction, while C denotes travel impedance. The objective of calibration is to determine the optimal values for the β and μ parameters in the above equations.

To facilitate calibration, Equations (7) and (8) can be transformed into a linear regression model in the form of $y = mx + b$ (Least Square Method).

For the exponential model, we have:

$$\ln\left(\frac{T_{ij}}{P_i A_j}\right) = \ln(\beta) - \mu C_{ij} \implies m = -\mu, \quad b = \ln(\beta) \tag{9}$$

For the power model, we have:

$$\ln\left(\frac{T_{ij}}{P_i A_j}\right) = \ln(\beta) - \mu \ln(C_{ij}) \implies m = -\mu, \quad b = \ln(\beta) \tag{10}$$

By fitting a line through the data obtained from Equations (9) or (10), we can calculate the slope (m) and intercept (b) of the line. These values correspond to the parameters μ and $\ln(\beta)$, respectively.

Hence, the gravity model can be calibrated by estimating the values of m and b through the linear regression process.

3.2 Neural Network: The process of modeling with a neural network consists of two main parts. The first part involves choosing a proper neural network architecture based on the available data. In trip distribution problems, three distinct inputs and one output are typically used to construct the neural network's structure. However, in cases where the inputs lack discriminatory information, the number of inputs may decrease to two or even one.

Input: trip attraction, trip production, impedance
Output: trip distribution

The second part of building a neural network is specifying hyperparameters, including the number of layers, the number of units in each layer, activation functions, epoch number, batch size, and learning rate, among others.

For optimal results, we propose a neural network with 2 hidden layers, each containing 8 units. These numbers are determined through careful examination, allowing the model to learn faster and better while preventing overfitting and underfitting. We assume 500 epochs with an early-stopping strategy to stop the model earlier and prevent overfitting. Each epoch comprises several batches, with each batch containing 512 data points. Batch sizes are usually set to 32 or 16, but in this case, as the region is large with hundreds of thousands of training data, a higher batch size yields excellent results. A learning rate of 0.0001 is chosen to ensure a gradual and stable learning process.

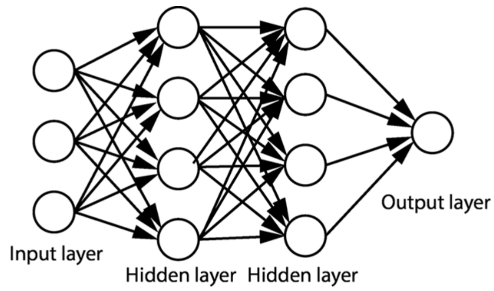

Fig. 1. Neural Network

The neural network architecture can be described mathematically as follows:

Input Matrices: Let X be the input matrix with dimensions (m, n), where m represents the number of data points and n represents the number of features. The input matrix is defined as: $X = [x_1, x_2, \ldots, x_m]$ where x_i represents the feature vector for the ith data point.

Hidden Layers: The neural network consists of 2 hidden layers, each containing 8 units. The activation function used in the hidden layers is the rectified linear unit (ReLU), which introduces non-linearity and helps the model learn complex patterns. The output of the first hidden layer can be represented as: $H_1 = \mathrm{ReLU}(W_1 \times X + b_1)$ where W_1 represents the weight matrix of dimensions $(8, n)$, b_1 represents the bias vector of dimensions $(8, 1)$, and the ReLU function applies element-wise non-linearity.

Similarly, the output of the second hidden layer can be represented as: $H_2 = \mathrm{ReLU}(W_2 \times H_1 + b_2)$ where W_2 represents the weight matrix of dimensions $(8, 8)$, b_2 represents the bias vector of dimensions $(8, 1)$.

Output Layer: The output layer is a linear layer that produces the predicted trip distribution. It can be represented as: $Y_{\text{pred}} = W_{\text{output}} \times H_2 + b_{\text{output}}$ where W_{output} represents the weight matrix of dimensions $(\text{output\_dim}, 8)$, b_{output} represents the bias vector of dimensions $(\text{output\_dim}, 1)$, and Y_{pred} represents the predicted trip distribution.

During training, the neural network optimizes the mean squared error (MSE) loss function, which measures the average squared difference between the predicted trip distribution and the ground truth values. The Adam optimizer is employed to update the network's weights and biases, utilizing adaptive learning rates for each parameter.

The training process involves feeding the input data (trip attraction, trip production, and impedance) into the neural network and obtaining the predicted trip distribution as the output. The predicted values are then compared to the ground truth trip distribution, and the model's parameters are adjusted through backpropagation and gradient descent to minimize the MSE loss.

By defining the matrices for the input data, specifying the layers and activation functions, and outlining the training process, we establish a comprehensive understanding of the mathematical operations occurring within the neural network architecture.

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