Advancing Trustworthy and Socially Responsible Artificial Intelligence in Transportation Demand Modeling

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1 Introduction

1.1 Background

Creating an effective demand modeling for transportation is essential for optimizing resource distribution, enhancing service quality, guiding infrastructure development, promoting environmental sustainability, and boosting economic efficiency. Demand modeling is the process of using statistical and computational methods to predict future travel behavior and demand based on various factors, such as socioeconomic data, travel patterns, and infrastructure. Accurate modeling facilitates the allocation of resources, ensure service responsiveness, and enable eco-friendly operations, thereby augmenting the overall efficiency and sustainability of the transportation network. With the rapid development of artificial intelligence methods, especially various neural network architectures, accuracy has been well improved in the past decade [Zhang et al., 2019, Liang et al., 2023, Gao et al., 2023, Ke et al., 2021, Zhang et al., 2017, Liu et al., 2019]. Throughout the remainder of this thesis proposal, unless otherwise specified, the focus will be on demand modeling through the application of artificial intelligence techniques, including machine learning and deep learning.

However, trustworthiness and social responsibility are also important attributes but have been less studied in transportation demand modeling studies. Trustworthiness targets reliable and robust prediction results. More specifically, reliability refers to the consistent accuracy of predictions across different conditions, while robustness indicates a model's resilience to unexpected data variations and uncertainties. Social responsibility in demand modeling emphasizes social considerations, ensuring that models and their outcomes do not exacerbate social inequities but rather promote accessibility and equity. It involves actively considering the broader societal impacts of prediction decisions, aiming to benefit all community members equitably. The relationship between social responsibility and trustworthiness is intrinsic; trustworthy results are not just about accuracy and reliability, but also about ensuring that these results are achieved in a manner that is ethically sound and socially equitable. Existing transportation demand models focus on the single numerical value outputs with the emphasis on accuracy without fully leveraging those features in the outputs in a more holistic way [Ke et al., 2021, Jiang et al., 2022, Zhao and Kockelman, 2002].

To bridge the identified gaps, this thesis proposes a demand modeling framework illustrated in Figure 1. This framework not only aims for high accuracy but also emphasizes trustworthiness under external changes and a dedication to the social implications of prediction results. Specifically, we concentrate on attributes besides accuracy, such as reliability, robustness, accessibility, and equity.

In this thesis, we propose three critical areas within artificial intelligence that enhance transportation demand modeling, aiming to achieve trustworthy and socially responsible outcomes: uncertainty quantification, integration of multi-source data, and the implementation of socially-aware computational methods, as shown in Figure 1. Among them, uncertainty quantification will be the main focus of this thesis as the backbone to provide more theoretical contributions and insights. Combining theoretical frameworks and practical advancements, this thesis strives to develop demand modeling techniques that embody these values, thereby enhancing the five attributes in transportation planning.

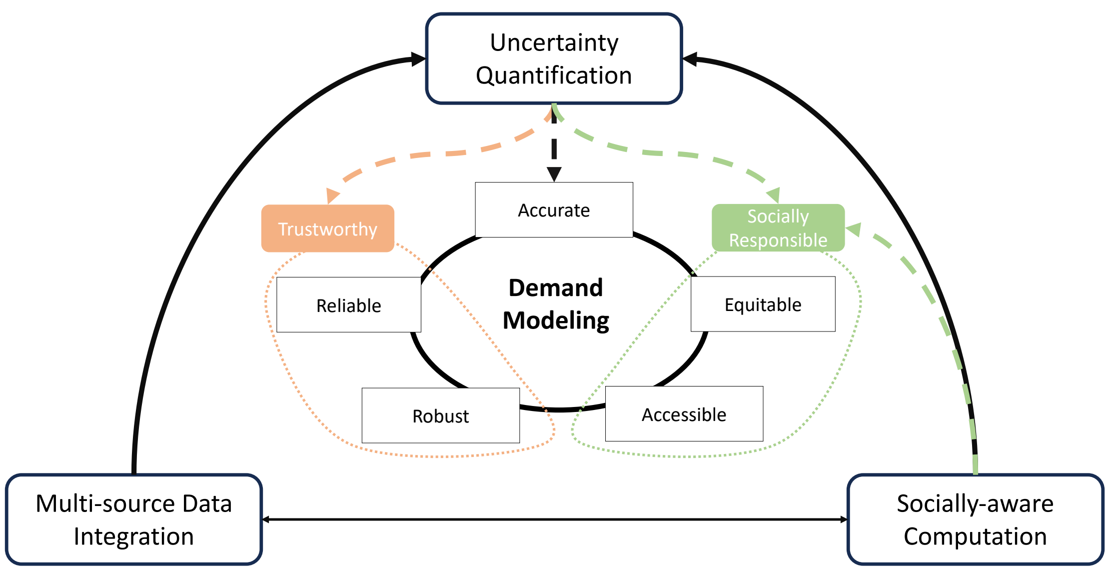

Figure 1: Envisioned transportation demand modeling framework.

1.2 Research Problems

The scope of three key areas in Figure 1 provides us with three specific research problems to solve in this thesis:

- **Uncertainty Quantification:** This is the major focus of this thesis, which emphasizes the importance of quantifying uncertainties in transportation demand modeling, addressing both data and model uncertainties as well as the calibration of uncertainty. The objective is to ensure that the models are robust and adaptable to real-world variations, thereby enhancing their reliability and trustworthiness.

- **Multi-source Data Integration:** This involves leveraging the diverse nature of transportation data, including structured spatiotemporal and socioeconomic, as well as unstructured data types, to comprehensively describe mobility dynamics and demand from various perspectives. The aim is to harness the richness of these data sources to provide a detailed and nuanced understanding of transportation needs and patterns.

- **Socially-aware Computation:** The third focus involves assessing the social impacts and implications of the transportation demand models applied. It seeks to ensure that the demand models do not exacerbate social equity issues or introduce biases, aiming instead to promote social responsibility and positive societal outcomes through transportation planning.

Addressing the three research problems in isolation is insufficient; they must be tackled collectively to develop a demand modeling framework that is both efficient and fair. For instance, when transit agencies adjust bus schedules based on real-time demand, they must account for the inherent uncertainties, the heterogeneity of urban demand, and the broader social consequences of their actions. These considerations are critical for informed policy-making, highlighting the necessity for an integrated approach in crafting demand modeling techniques. This thesis is committed to creating transportation demand modeling algorithms that embody trustworthiness and social responsibility by weaving together these three intertwined research areas.

1.3 Data

This thesis integrates datasets focusing on transportation dynamics within Chicago, New York City, and selected London boroughs. The datasets include 1) structured records of spatiotemporal travel demand and traffic incidents, sociodemographic data revealing economic, and social characteristics at the census tract level, and 2) unstructured data, which is non-tabular and non-quantitative information, like satellite images and road network topology that illustrates the built environment.

Specifically, key spatiotemporal datasets include the Chicago Data Portal[1] for analyzing ride-sharing trip patterns, the Smart Location Database[2] for studying For-Hire Vehicle trips in Manhattan, and both Chicago Traffic Crash Data[3] and Chicago Crime Records[4] for insights into traffic incidents and crime rates. These sources offer a broad overview of travel demand, enabling an examination of traffic safety and crime rates with varying spatial resolutions and temporal spans, crucial for addressing data sparsity and improving prediction accuracy. Sociodemographic insights are derived from the American Community Survey (2017-2018), detailing the diverse characteristics of Chicago's census tracts.

For unstructured data, we use road network data for Chicago supported by the OSMnx package using OpenStreetMap to accurately represent the city's infrastructure. Furthermore, this research incorporates the UK's STATS19 dataset[5] as well as the associated Google street-view images and satellite images to evaluate the impact of traffic policies such as the Ultra Low Emission Zone (ULEZ) in London boroughs like Westminster, Lambeth, and Tower Hamlets on traffic accidents.

2 Conceptual Framework

We propose the conceptual framework of the research plan shown in Figure 2 to break down the three research problems into different topics that address *trustworthiness* and *social responsibility*.

Trustworthiness: This thesis aims to enhance the trustworthiness of demand modeling techniques by developing new methods for uncertainty quantification and discussing their implementation. We also plan to mitigate the challenges raised by the consideration of data variation and inclusion of multi-source data adds complexity. We propose the Probabilistic Spatiotemporal Graph Neural Networks (STGNNs), Spatiotemporal Uncertainty Calibration, and Deep Hybrid Model (DHM) for demand modeling, integrating unstructured data with improved interpretability and reliability. Furthermore, we explore the potential of applying uncertainty quantification to event prediction in transportation systems, such as assessing traffic risk and predicting traffic accidents.

Social Responsibility: This thesis examines the social impacts of demand modeling techniques, their outputs, and the decision-making process. We introduce fairness-enhancing deep learning approaches

[1] https://data.cityofchicago.org/Transportation/Transportation-Network-Providers-Trips/m6dm-c72p
[2] https://www1.nyc.gov/site/tlc/about/tlc-trip-record-data.page
[3] https://data.cityofchicago.org/Transportation/Traffic-Crashes-Crashes/85ca-t3if
[4] https://data.cityofchicago.org/Public-Safety/Crimes-2001-to-Present/ijzp-q8t2
[5] https://www.gov.uk/guidance/road-incident-and-safety-statistics-guidance

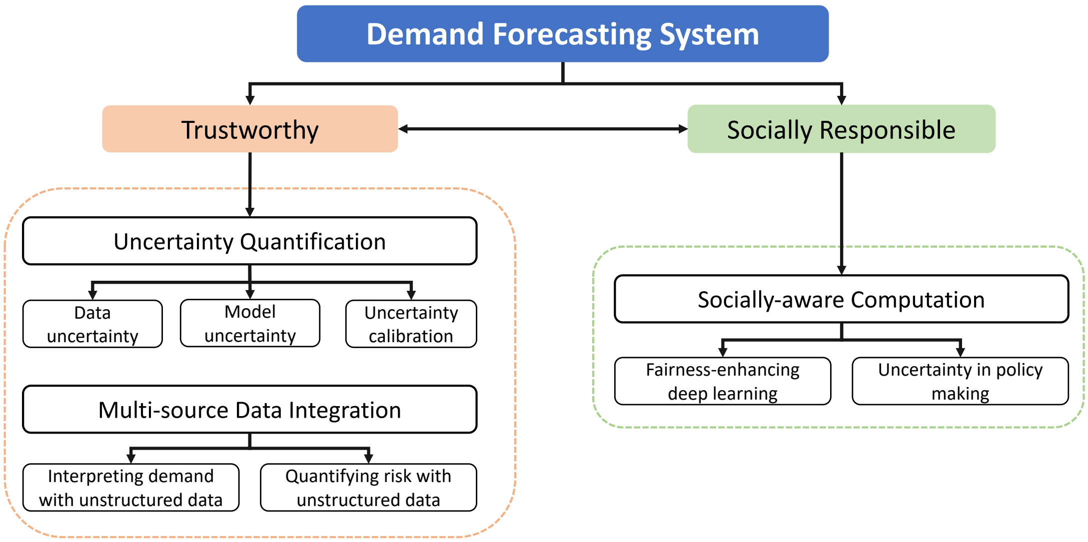

Figure 2: Conceptual framework of the thesis research plan.

that incorporate fairness interventions into the demand modeling process, addressing equity issues more effectively. Additionally, we aim to extend uncertainty quantification to the policymaking supported by the demand modeling methods, examining the variability and responses of policies to the uncertainties in the demand modeling. This approach seeks to ensure equitable access to transportation services for all community members, thereby fostering a more inclusive transportation system.

2.1 Quantifying Uncertainty in Demand Modeling

This thesis aims to advance demand modeling by addressing the limitations of traditional deterministic models, which often assume homogeneity in travel demand variability. Recognizing the complexity of travel demand, it leverages deep learning techniques, particularly STGNNs to predict demand with higher accuracy [Zhao and Kockelman, 2002, Ding et al., 2018]. However, existing demand modeling techniques do not fully address the alignment between model predictions and actual data distributions [Khosravi et al., 2011, Sankararaman and Mahadevan, 2013]. what happens if the uncertainty is not well quantified.

Ensuring such alignment is the quantification of uncertainty, distinguishing between model (epistemic) and data (aleatory) uncertainties, utilizing both Bayesian and Frequentist approaches for comprehensive analysis [Wu et al., 2021]. The Bayesian method integrates probability distributions to represent parameter uncertainty, incorporating prior knowledge and updating beliefs with new data to quantify uncertainty directly. In contrast, the Frequentist approach focuses on data variability, using confidence intervals and hypothesis testing to assess parameter uncertainty and outcome probabilities. In this thesis, we will emphasize on the Frequentist approach as the we majorly quantifying the confidence interval of our prediction outputs.

2.1.1 Quantifying Uncertainty with Probabilistic STGNN Models

In the field of transportation demand modeling, significant strides have been made with the adoption of advanced neural network architectures to capture spatial and temporal information, notably enhancing predictive accuracy. Among various neural network architectures, graph-based models, including Graph Convoltuion Networks (GCNs) and Graph Attention Networks (GATs), adeptly capture the complexities of urban transport networks in recent work [Yao et al., 2018, Ke et al., 2017, Liu et al., 2020, Wang et al., 2020a,b, Koca et al., 2021, Geng et al., 2019, Yang et al., 2019, Guo et al., 2022, Wang and Wu, 2021, Qian et al., 2023, Zhuang et al., 2022].

This thesis proposes the development of probabilistic STGNN models to accurately quantify demand uncertainty. By leveraging a Frequentist approach within the deep learning paradigm, we aim to design probabilistic STGNN models as depicted in Figure 3. This framework focuses on quantifying

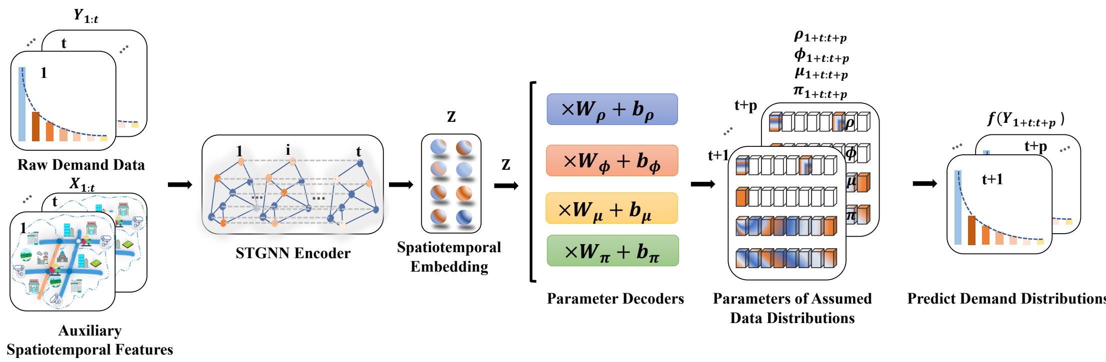

Figure 3: Conceptual framework illustrating probabilistic STGNN models for demand uncertainty quantification.

data uncertainty in travel demand, employing parametric distributions such as Gaussian or negative binomial distributions to derive spatiotemporal embeddings through STGNN encoders. Subsequent decoding processes infer distribution parameters, enabling the prediction of future demand distributions and the derivation of confidence intervals. Emphasizing the modeling of probabilistic distributions, this approach allows for the adaptation to various demand scenarios, including sparse demand or traffic incidents, by incorporating appropriate parametric distributions, like zero-inflated negative binomial models, thus enhancing the model's utility and trustworthiness in demand modeling. Kindly refer to my previous published papers on this topic [Zhuang et al., 2022, Jiang et al., 2023, Gao et al., 2023, Wang et al., 2023b].

2.1.2 Uncertainty Calibration in Demand Modeling

For demand modeling techniques, redesigning and retraining a probabilistic model for uncertainty quantification could be costly. Therefore, calibration emerges as a critical post-hoc method, striving to align model-predicted probabilities with actual outcomes, thereby enhancing uncertainty validation [Nixon et al., 2019].

While numerous strategies exist to calibrate pre-trained classifiers, addressing the calibration challenges in prediction tasks remains less studied [Thiagarajan et al., 2020, Kuleshov et al., 2018]. Post-hoc calibration techniques, such as temperature scaling, Platt scaling, and isotonic regression, initially designed for classification, have been modified for regression applications, offering a pathway to refine probabilistic model outputs [Kull et al., 2019]. Recent advancements introduce quantile regression-based calibration, proposing novel methods for more accurate probability estimations [Chung et al., 2021]. These techniques provide a versatile solution, applicable across various probabilistic models without requiring retraining, emphasizing their utility in improving model reliability.

The application of uncertainty calibration in trasportation demand modeling has been even less leveraged [Zhao et al., 2022]. The main reason is due to the complex data nature of spatiotemporal data in transportation and there is a lack of proper theoretical tools to handle with it. This thesis aims to bridge this gap by proposing novel calibration methods specifically crafted for spatiotemporal data, suitable for integration with probabilistic STGNN models. By developing specific post-hoc spatiotemporal calibration techniques, as shown in Figure 4, this thesis will enable the application of calibrated uncertainty measures across all existing STGNN models.

To be more specific with the concept, by defining distributional assumptions and STGNN encoder architectures similarly in Figure 3, we can then apply these calibration methods to obtain output distribution parameters (Bayesian approach) or confidence intervals (Frequentist approach) that more accurately reflect data variability. The two steps (modification and calibration) help existing STGNN model architectures adapt to uncertainty quantification context. Eventually, for any assumed distributions, parameterized by ρ and ϕ, we manage to align closely with the actual data percentiles upon calibration to ρ^* and ϕ^*. For a practical instance, the 5th and 95th percentiles of the calibrated distributions effectively encompass the 5th and 95th percentiles of the true data, demonstrating an accurate reflection of data variability. Note that ρ and ϕ are just example parameters for the distributions, which should be adapted according to data features. Preliminary results in our recent work have

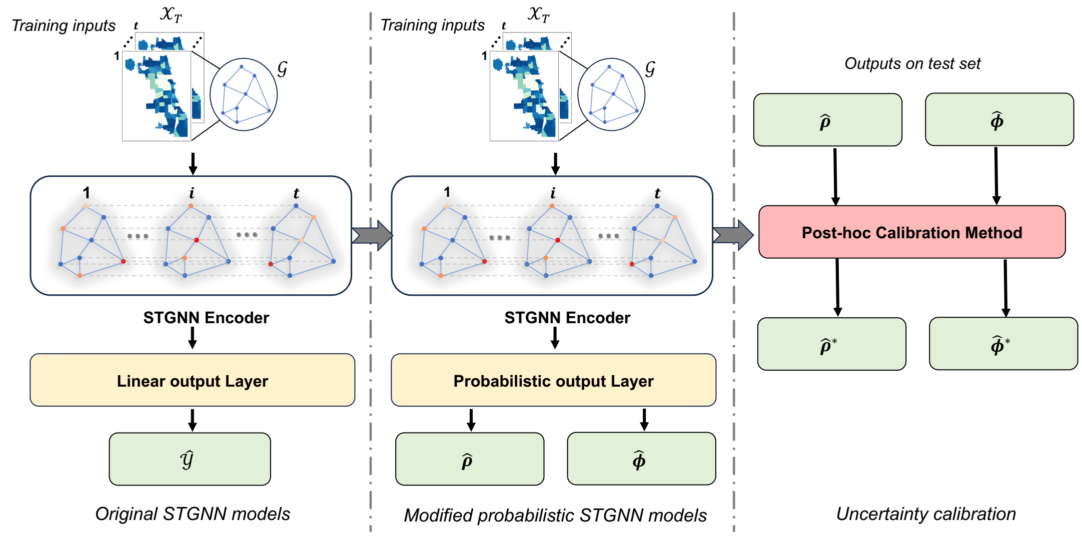

Figure 4: Conceptual framework illustrating uncertainty calibration to all existing deterministic STGNN models.

shown 20% reduction in calibration errors [Zhuang et al., 2023] for sparse travel demand prediction.

2.2 Integrating Multi-source Data in Demand Modeling

Integrating multi-source data in transportation systems provides more dimensions to design demand modeling techniques that are both trustworthy and socially responsible. Diverse data sources like images, road networks, the built environment, and documented data enrich the analysis, offering a holistic view of transportation dynamics. This comprehensive data integration enables the transportation demand modeling to capture complex patterns and interactions that traditional data forms may overlook, improving accuracy and reliability [Cheng et al., 2019, Jalili et al., 2017, Lerique et al., 2020, Ren et al., 2014, Teney et al., 2017, Wu et al., 2020].

To integrate these varied data types effectively, it's crucial to employ advanced analytical methods capable of handling and synthesizing heterogeneous information. Artificial intelligence techniques such as machine learning, deep learning, and data fusion algorithms are instrumental in processing and extracting meaningful insights from multi-source data. These methods facilitate the identification of nuanced patterns and trends, contributing to more precise and informed demand predictions.

Moreover, the inclusion of diverse data sources in demand modeling aligns with the principles of social responsibility. By considering a wide range of factors influencing transportation needs, such as environmental conditions, urban infrastructure, and social behaviors, the enriched demand modeling process can better address the needs of all community members. This approach ensures that transportation planning is inclusive, equitable, and reflective of real-world complexities, thereby enhancing the system's trustworthiness and societal value.

This thesis will cover the potential of using multi-source unstructured data for demand prediction and combine the aforementioned uncertainty quantification models for estimating the uncertainty in the transportation system.

2.2.1 Deep Hybrid Model for Travel Demand Prediction

The rapid urbanization and its impact on the built environment necessitate an advanced approach to understanding travel demand. Traditional models, focused on mode share based on demographic and trip characteristics, fall short in capturing the intricate relationship between the built environment and travel behavior. The complexity of integrating such unstructured data, especially the unstructured formats of urban road networks, satellite images, or word vocabulary, poses a significant challenge. Leveraging embedding techniques, offers a solution by converting complex unstructured data into structured vector representations, thus enabling a deeper analysis of how urban infrastructure influences travel choices. This method provides a different angle to overcome the limitations of existing models by providing a comprehensive view of the built environment's role in shaping transportation demand, paving the way for more effective and socially responsible transportation planning.

In this thesis, we introduce the Deep Hybrid Model (DHM), a novel framework that combines hybrid choice modeling with advanced machine learning and deep learning techniques to process unstructured data effectively. This model integrates diverse data types, enhancing the accuracy and comprehensiveness of urban transportation demand modeling [Wang et al., 2023a]. Figure 5 conceptually illustrates how DHM utilizes road network topological data for mode choice using graph embedding techniques.

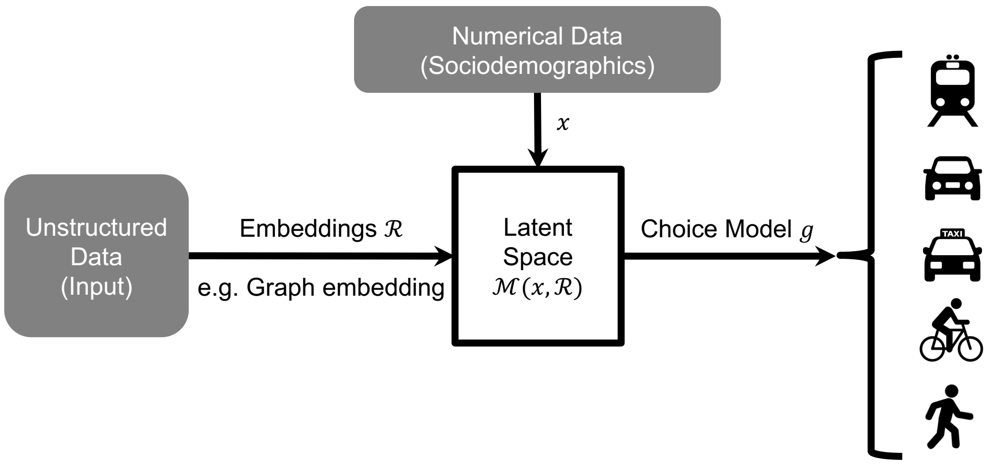

Figure 5: Conceptual framework of the Deep Hybrid Model.

The DHM is formally described as:

$$P(y_n|V_n) = g(V_n) = g(z_n) = g(\mathcal{M}(x_n, \mathcal{R}_n)), \tag{1}$$

Here, y_n and x_n represent numerical outputs and inputs for the n-th census tract, and $\mathcal{R}n$ denotes embedded variables from the unstructured data like road network topology. V_n is the utility that is generally considered in travel demand prediction. The model synthesizes these components through a *mixing operator*, $\mathcal{M}(\cdot)$, and employs a *behavioral predictor*, $g(\cdot)$, to estimate probabilities. The *mixing operator* might simply fuse x_n and $\mathcal{R}n$, while the *behavioral predictor* utilizes a generalized linear form, $g(z_n) = \sigma(\beta' z_n)$, transforming the mixed variables into predictive outputs. This setup highlights our focus on the integration mechanism, though $g(\cdot)$ is adaptable to various output types.

Like the hybrid choice model, DHM uses latent variables z_n within a latent space to capture intricate details, here specifically applying to unstructured road network data. Our proposed architecture efficiently maps this data into a high-dimensional latent space, enriching the model with the ability to incorporate and interact with additional data, such as sociodemographics. This approach not only bolsters the model's predictive capability but also enhances its versatility and applicability across different transportation contexts.

DHM's adaptability is further demonstrated in its capacity to accommodate various unstructured data forms, including images and texts, through alternative embedding techniques like CNNs, RNNs, or Transformers. This flexibility ensures that DHM is a scalable and robust solution for transportation demand modeling, capable of leveraging multi-source data to create a more trustworthy and socially responsible system.

2.2.2 Quantifying Uncertainty with Unstructured Data

The DHM is designed to effectively capture latent variables or spaces, enhancing demand prediction tasks within transportation systems. By integrating uncertainty quantification techniques, the DHM can be extended to improve the quality of demand modeling. Fundamentally, DHM leverages multiple stacks of neural network layering to extract meaningful embeddings from unstructured data, akin to spatiotemporal embeddings referenced in Section 2.1.1. It underscores the necessity of employing multi-source data not only for numerical demand prediction but also for refining uncertainty quantification.

This thesis intends to synthesize the concepts presented in Sections 2.1.1, 2.1.2, and 2.2.1. For advanced, adaptive, and reliable uncertainty quantification methods, we propose a fusion of DHM's representational strength with probabilistic STGNN models. As depicted in Figure 6, our approach innovates by integrating the embedding of unstructured data and sociodemographic information with the spatiotemporal embedding of demand data into the *mixing operator* $\mathcal{M}$. This integration enriches the latent space with comprehensive information, facilitating the downstream inference of probabilistic distributions assumed for the data.

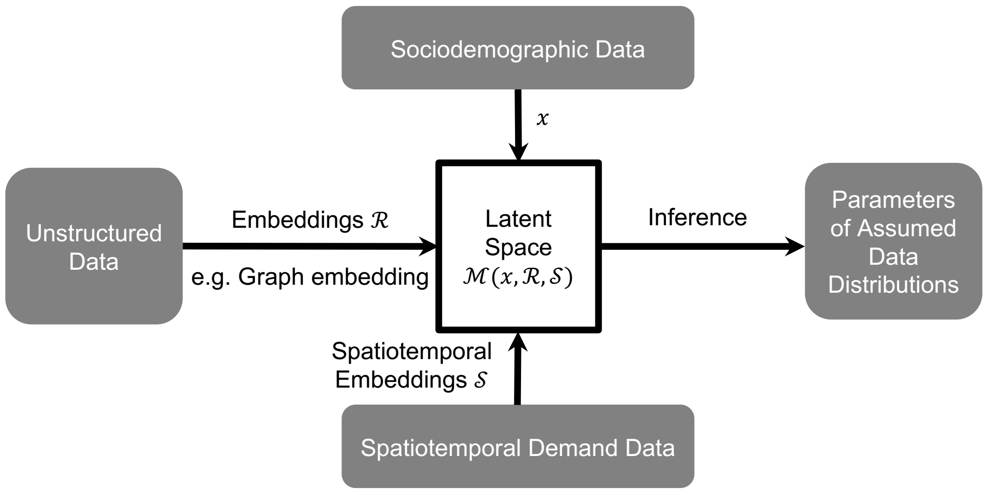

Figure 6: Conceptual framework that combines Deep Hybrid Model and the framework of probabilistic STGNN models to quantify the demand uncertainty more comprehensively.

2.3 Socially-aware Demand Modeling

Considering social impacts into demand modeling algorithms is imperative for ensuring their alignment with social responsibility principles. This integration acknowledges that transportation decisions extend beyond mere technical and economic factors, influencing equity, accessibility, and the overall welfare of communities. By examining social impacts, potential biases can be identified and addressed, promoting equitable benefits across all societal sectors. This fosters an inclusive approach to planning, taking into account the varied needs and preferences of the population, and enhancing the system's applicability and efficiency.

Furthermore, acknowledging the social aspects of transportation enables the direction of policies and initiatives towards sustainable and equitable solutions, in alignment with broader societal goals, albeit with some degree of uncertainty. Consequently, designing demand modeling methods that are aware of social impact analysis is vital for developing transportation networks that are not only operationally efficient but also equitable and beneficial to the public interest.

This thesis commits to advancing socially-aware demand modeling methods, focusing on reducing prediction biases and quantifying model uncertainty in policies derived from machine learning or deep learning models.

2.3.1 Fairness-enhancing Demand Modeling

The emergence of on-demand mobility services highlights the need for accurate and fair travel demand modeling, particularly to ensure equitable service across diverse neighborhoods. Traditional demand prediction models often prioritize accuracy without considering the social equity implications, risking service inadequacy in under-served areas [Lewis et al., 2021, Binns, 2018]. This neglect can exacerbate disparities, especially in disadvantaged neighborhoods where demand might be systematically underestimated, leading to poorer service levels. Commonly, studies have concentrated on overall accuracy, overlooking the variance in performance across socioeconomic regions and missing the unique sociodemographic dynamics of each area, which can result in biased prediction results. As an instance, in ride-hailing companies, demand prediction directly influence pricing, scheduling, and routing decisions.

Our analysis indicates that such demand-driven strategies may inadvertently disadvantage low-income areas by diminishing service focus [Guo et al., 2023]. To address these issues, this thesis proposes the development of fairness-enhancing demand modeling algorithms that account for demographic variables like race, gender, and income, aiming to balance prediction outcomes and influence policy decisions equitably.

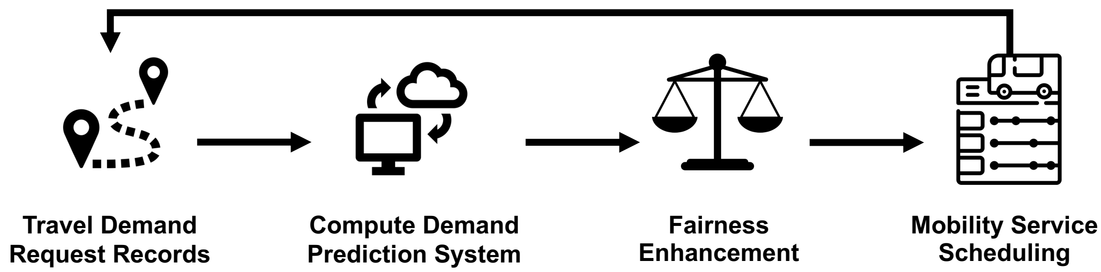

Figure 7: Conceptual framework illustrating the integration of fairness-enhanced demand modeling into mobility service scheduling guided by demand prediction results.

As outlined in Figure 7, historical travel demand request records, upon which the demand modeling algorithms are constructed, may inherently contain biases, leading to some passenger groups being underserved. Consequently, when developing the demand modeling techniques, these biases are inevitably reflected in its outputs.

To address this issue, it is imperative to introduce fairness interventions into the algorithms during both model training and output generation phases. We integrate bias mitigation strategies—including a socially aware norm in the model's objective function and an adaptive attention block—to discern and correct biases among different user groups. This approach seeks to amend inherent biases in historical travel demand data, which may underrepresent certain passenger groups, thus leading to biased prediction outcomes. Early findings show promising results, such as a 67% reduction in the prediction error gap between black and non-black communities, achieved without compromising accuracy, and a 10% decrease in the generalized entropy index, evidencing the model's capacity to lessen spatial prediction disparities [Zheng et al., 2023]. These efforts underscore our commitment to forging a demand prediction system that is both trustworthy and socially responsible, enhancing fairness in transportation policies.

2.3.2 Trustworthy Policy Making

Quantifying uncertainty is critical for enhancing the trustworthiness of transportation demand modeling, enabling policymakers to make well-informed decisions. Such quantification leads to the development of robust, adaptable policies, ensuring the reliability and robustness of transportation systems.

This thesis examines the impact of model uncertainty on transportation policies, with a focus on traffic accident predictions within London's Ultra Low Emission Zone (ULEZ). We aim to assess if ULEZ-related uncertainty in demand prediction models' parameters could potentially increase traffic accidents. To address this, we will use the Heterogeneity in Means method to analyze data variability across demographic and geographic groups with machine learning-based demand prediction models. Statistical tests, such as t-tests or ANOVA, will evaluate the significance of mean differences among groups. This method will uncover data heterogeneity and the effects of various factors on outcome distributions, facilitating the quantification of uncertainty in policymaking.

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