Predicting Trip Attraction of Urban Activity Centres in Greater London using Explainable Machine Learning on Open Data

by

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Abstract

Using explainable machine learning techniques (SHAP) on the predictions of an XGBoost model, we were able to use amenity and connectivity features extracted from open data of an area to predict with high accuracy ($R^2 > 80\%$) total arrivals by public transport in a given area in Greater London, representing the area's 'trip attractiveness'. The use of SHAP machine learning explanations further provides insights into the spatial heterogeneity of the feature importance, enabling the identification of destination hotspots for different purposes, such as urban activities or transit interchange. The methodology can be extended to analysing public transport mobility patterns in other localities since it relies on open data sources such as OpenStreetMap and the national censuses. Furthermore, it serves as a foundation to be developed and adapted to analyse trip destination hotspots from mode-agnostic mobility data to inform urban planning and policy-making decisions.

Keywords: urban mobility, explainable machine learning, XGBoost, SHAP, open data, activity hotspots, point-of-interests (POI), spatial heterogeneity, Greater London

Declaration

I, The-Huan Hoang, declare that the work presented in this dissertation is my own. Where claims, information or findings have been derived from other authors and sources, I confirm that this has herein been indicated in writing, attributing due credit. In the spirit of reproducible research, all scripts used for analysis and their outputs are made available on GitHub at https://github.com/shaunhoang/casa-tfl.

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1. Introduction

Urban mobility, a dynamic interplay of individual travel choices and collective movement patterns, profoundly shapes the fabric of modern cities. This complex phenomenon, influenced by a myriad of factors ranging from individual preferences and socioeconomic conditions to the characteristics of the built environment, serves as the lifeblood of urban areas. Understanding and predicting these intricate patterns is not merely an academic pursuit; it is fundamental to achieving sustainable urban planning and efficient transport system management.

Historically, insights into urban mobility have been gleaned through surveys and limited datasets, often characterized by their costliness and time-consuming nature. However, the advent of the digital age has ushered in a transformative era, one where open data, freely available and increasingly rich in detail, presents an invaluable resource for understanding urban dynamics. When harnessed in conjunction with advancements in machine learning, these open datasets can be transformed into powerful predictive models, shedding light on the intricate relationship between the built environment and human mobility.

This thesis embarks on a journey into this exciting frontier, seeking to predict non-commute transport demand using open data and machine learning techniques. In the face of rapid urbanization, cities worldwide are grappling with the challenges of managing escalating transport demand while ensuring the accessibility and sustainability of their transport systems. Urban planners and transport authorities require sophisticated tools to not only understand but also anticipate mobility patterns, empowering them to make informed decisions regarding infrastructure investments, service planning, and policy interventions. The confluence of open data and machine learning offers a promising avenue to address this pressing need.

At the core of this thesis lies the exploration of how features of the built environment, such as the availability of amenities and the connectivity of transport networks, influence the choices individuals make about their travel destinations and modes of transport. By constructing predictive models based on these features, we aim to forecast non-commute transport demand, providing valuable insights for urban planning and transport management.

However, we do not stop at mere prediction. We recognize that understanding the 'why' behind these predictions is equally crucial. The 'black box' nature of many machine learning models, while capable of producing accurate predictions, often obscures the underlying decision-making process. This lack of transparency can hinder their adoption in critical domains such as urban planning. To address this challenge, we employ Explainable AI (XAI) techniques. By peering into the 'black box', we strive to not only enhance trust in our models but also uncover valuable knowledge about the key drivers of non-commute transport demand.

In essence, this thesis serves as a testament to the transformative power of open data and machine learning in the realm of urban mobility research. We demonstrate how these tools can be leveraged to predict and understand non-commute transport demand, offering invaluable insights for urban planners and transport authorities. By shedding light on the complex relationship between the built environment and human mobility, we contribute to the creation of more sustainable, efficient, and livable cities.

However, we acknowledge that this research, like any other, has its limitations. The models we develop, while powerful, are inevitably simplifications of a complex reality. There is always room for improvement, whether through the incorporation of more granular data, the exploration of novel methodologies, or the expansion of our understanding of the factors influencing urban mobility.

In conclusion, we believe this thesis represents a significant step forward in harnessing the potential of open data and machine learning for urban mobility research. By demonstrating the feasibility of predicting non-commute transport demand and providing insights into the underlying factors, we pave the way for more informed and effective urban planning and transport management. As we look to the future, we are excited by the possibilities that lie ahead, and we are confident that data-driven approaches will play an increasingly central role in shaping the cities of tomorrow.

In the spirit of continued exploration and discovery, we leave you with two key research questions that have emerged from our work:

- **Can trip attractiveness (total arrivals in an area) be predicted using only amenity and transport connectivity features?** This question challenges us to refine our understanding of the relationship between the built environment and human mobility. Can we create accurate predictive models based solely on readily available open data, or do we need to incorporate more complex socio-economic factors to achieve a comprehensive understanding?

- **Can we effectively identify destination hotspots/urban activity centers using mobility data such as total arrival data?** This question invites us to explore the potential of mobility data for revealing the hidden patterns of urban life. Can we pinpoint the areas that attract the most people, and what can this tell us about the dynamics and vibrancy of our cities?

These questions, and many others that arise from this research, point towards a future where data-driven insights play an increasingly central role in shaping our cities. We are confident that the work presented in this thesis represents a significant step towards that future, and we invite others to join us in this exciting journey of exploration and discovery.

2. Literature Review

Understanding intracity non-commute travel behaviour on an aggregate scale is a crucial yet underresearched area in urban mobility planning, with more focus on commuting trips.

Estimating trip attraction constitutes an integral component of the demand forecast framework, termed the Four-Step Model (FSM), which begins with the Trip Generation step, where the number of trips generated by each traffic analysis zone is estimated, and Trip Distribution allocates these trips to their destination zones before proceeding to mode choice determination and route assignment. The task of Trip Distribution may be accomplished using a variety of spatial interaction models, most prominent among which is the classic *Gravity Model* and its derivatives inspired by Newton's law of universal gravitation (Erlander and Stewart, 1990). Formulated initially to estimate flows among cities in a region, it has been adapted to intracity mobility, suggesting that the number of trips between two locations is proportional to each location's difference in *mass* and inversely proportional to the distance between them.

However, it is worth noting that the definition of *mass* in any gravity-based spatial interaction model may depend on the research interest. The estimation of trip attraction in transport planning literature has predominantly revolved around commutes (i.e., primary travel demand) from residential zones to employment centres or education institutions. On the one hand, this choice is a practical one first and foremost, as commuting trips represent a large share of regular intracity mobility flows, whose high volume within short peak periods has important implications on road capacity management or public transit operations, among others. Due to its importance, the calibration of the spatial interaction model for commuting flows is further aided by nationwide flow datasets, such as those present in the UK Census [1], which provides detailed and explicit Origin-Destination data to serve as ground truth. Without this declared data, researchers have also turned to spatial features to calibrate commute trip distribution, as explored by Yang et al., 2014.

On the other hand, a plethora of potential trips generated for other non-commute purposes is often underresearched, partially due to the complexity of non-commute trip purpose identification, classification and quantification: Non-commute trips can be defined as trips that are not carried out to fulfil time-bound and regular work or education obligations and can include trips for shopping, leisure, and social activities. Therefore, as opposed to commuting trips, Non-commute trips are highly irregular both spatially and temporally, i.e., they can vary in terms of distance, duration, and mode of transport from one to another, even for the same destination between different days. Nevertheless, Non-commute trips are an important component of urban travel behaviour and can have a significant impact on the overall system. Advances in the field have

[1] An interactive visualisation of the UK Census 2021 origin-destination data can be found at https://www.ons.gov.uk/visualisations/censusorigindestination/

brought about improvements to methodologies such as travel diary surveys[2], which collect data on personal and household travel behaviour, including Non-commute trips, to allow for comprehensive planning. By design, however, they are limited in scale.

Overall, this reveals a gap in our understanding of the comprehensive intracity travel behaviour on an aggregate scale. With the number of trips for shopping, leisure, and social activities increasing in recent years and the number of work-related trips decreasing as flexible work arrangements become more prevalent (Wöhner, 2022), with recognised health benefits to workers (MacLeod, Cole, and Musselwhite, 2022), it is crucial to understand the factors that influence non-commute trip attraction and to incorporate them into urban and transport planning models. Within the scope of this research, we hypothesise that a given area's non-commute trip attractiveness *mass* is associated with the built environments, which include their amenity and public transport connectivity profiles.

2.1 Urban amenities as attractors

Cervero and Kockelman (1997) was one of the foundational works to provide an econometric estimation of how three groups of factors on the built environments—namely Density, Diversity and Design—are associated with travel demand to a traffic analysis zone for different purposes (work/non-work) and with different mode choices (private vehicles/public transport). This study is novel for demonstrating that changes in the built environment—such as density, diversity, and walkability have a tangible impact on travel behaviour, especially non-work one, which supports the idea that designing more compact, mixed-use, pedestrian-friendly neighbourhoods can significantly influence whereto and how people choose to travel. The components of density and diversity refer to the number and the variety of destinations available in a given area, respectively. In contrast, the design component refers to the physical layout of the area, including the presence of sidewalks, bike lanes, and other pedestrian-friendly infrastructure.

Many recent attempts have been to link the intensity of presence—or "Density"—of urban amenities to trip attraction and calibrate how we define urban attractors. Beyond the pure correlation observed between the density of points of interest (POIs) in a region and intensity of trips made to a given area (Melikov et al., 2021), the typology of the POIs differs between urban clusters that see distinct patterns of inflow trips made. For example, after Aaqib Javed et al. (2020) have clustered urban areas in one city into Global (e.g., airports), Downtown (d.g., central business district) and Residential attractors based on the volume, spatial dispersion and distance of the trips made using origin-destination information extracted from call data, they found that the differences in the types of POIs in each of these clusters were also statistically significant. The typology of amenity POIs explored in this study included not only Retail, as is common when considering the primary purpose for non-commute trips, but also hospitals, public services, restaurants, religious institutions, and other categories. This suggests that the type of urban amenities available in an area can influence the volume of trips made to that area and that different types of amenities may attract different types of trip purposes.

Regarding "Diversity", Cervero and Kockelman (1997) recognised the diversity of amenities is a factor that explains why people gravitate towards certain areas, apart from the presence of the amenities themselves. More specifically, for non-commute trips where locations are not necessarily prescribed or obligated, and the destination choice can be influenced by personal preferences and

[2]An example of these is the UK National Travel Survey, accessible at https://www.gov.uk/government/collections/national-travel-survey-statistics

circumstantial convenience, people may be more likely to visit more vibrant areas that offer a variety of services and activities where multiple tasks could be carried out, as opposed to areas where one type of destinations is overrepresented. This subjective perception of the quality of urban areas is consistent with the concept of 15-minute cities, which purports that mixed-use areas with a diversity of amenities within a 15-minute walking distance are more attractive areas to live in—and by extension, to visit—than single-use ones. (Khavarian-Garmsir et al., 2023)

2.2 Transport accessibility as attractors

If the density and diversity of amenities were the only explanatory factors for non-commute trip demand, it would be tempting to conclude that having them alone is the sole determinant of why people go to one place and not another for their diverse needs. In reality, neighbourhoods do not exist in a vacuum but are intricately connected to one another by the transportation network. In simple terms, the consideration of distance as friction in the classic Gravity Model attests to the fact that the more accessible a destination is, the more likely it is to attract travel demand, especially trips with higher elasticity of choice, such as non-commute. Public transport accessibility has been shown to contribute to the growth of intercity importance of certain areas as opposed to others and preserve travel demand variability over time (Zhong et al., 2015), which means that it reinforces the prominence of well-connected areas as urban attractors.

Jayasinghe, Sano, and Rattanaporn (2017) went one step further to purport that the network centrality property of an urban area is enough to predict travel demand to a high degree of accuracy without the need to consider other attractors such as employment centres and amenities, thanks to its high correlation. More specifically, the study looked at four centrality measures: Connectivity, Choice, Global Integration and Local Integration, which are analogous to the concept of degree centrality, betweenness centrality, closeness centrality, and closeness centrality in a confined radius, respectively. Among them, Global Integration (closeness centrality) was found to be the most significant predictor, suggesting that the role of the transport network in shaping urban travel demand at the aggregate scale is paramount, perhaps just as important as socio-economic factors (Convery and Williams, 2019). However, this study's use of car trip data does not represent all mobility patterns, especially considering public transport and walking. Therefore, it is logical to investigate the role of network centrality in conjunction with other variables.

2.3 Public transport and the walkable city

Walkability contributes to the quality of life in cities, with the "15-minute city" being one of the most prominent urban planning concepts that garnered attention in recent years. A resident living in a neighbourhood with all the amenities they need within a 15-minute walk or cycle can ideally reduce their reliance on cars and public transport to a minimum. However, this does not mean that the role of public transport is diminished within the 15-minute city vision. On the contrary, public transport is an essential component of a sustainable system, which provides an efficient and affordable way for people to travel longer distances in the city, effectively agglomerating a larger urban system made up of many 15-minute cities. In other words, public transport is the backbone of the 15-minute city, connecting neighbourhoods and enabling people to travel further than they can on foot or by bike. This, in turn, has multiple implications for the local communities:

- From the lens of urban planning and traffic management, the higher the volume of public transport trips to an area, the higher the amount of pedestrian traffic it receives on top of the

local population patronising their local amenities. Understanding the trip attraction factors can help prioritise investments in public transport capacity planning, pedestrian or cycling infrastructures and services for these individuals, leading to a virtuous cycle of increased active travel and reduced car dependency.

- From the lens of fomenting local economies, increased pedestrian traffic injected by public transport can also be seen as an additional source of footfall, invaluable for businesses with storefronts. Findings on the economic benefits of walking and cycling done by Transport for London[3] showed that retail rents increased by 7%, and office space rents increased by 4% in areas that encouraged non-motorised access, suggesting that the street improvements translated into much more desirable spaces.

It is also worth mentioning that footfall estimation is a prolific field of research within retail analytics, which counts on various technologies such as WiFi tracking, video analytics, and mobile phone data to estimate the number of people passing by a given location. The insights derived from footfall data can inform decisions on store location, opening hours, staffing levels, and marketing strategies, among others. Uncovering public transport trip attractiveness patterns, which indicate non-local pedestrian inflows, could complement traditional footfall data and provide a more comprehensive retail footfall estimate.

2.4 Explainable Artificial Intelligence for spatial systems

Up to this point, our visited literature has shown that both urban amenities and transport accessibility are important factors in determining an area's attractiveness to non-commute trips, albeit in isolation. In reality, the interaction between these two factors has yet to be well studied in conjunction. In the interest of addressing the research questions, we are presented with a dilemma of interpretability versus prediction accuracy in the choice of modelling techniques.

Spatial statistical methods, commonly used in policy analysis, can help us quantify and interpret the relationship between the dependent variables and independent variables in the form of explicit coefficients. However, even spatially aware methods such as Spatial Lag Model (SLM) or Geographically Weighted Regression (GWR) are limited in their assumptions of linearity and issues with multicollinearity (Wheeler and Tiefelsdorf, 2005), to provide robust interpretations.

In parallel, machine learning methods have gained popularity in urban mobility research due to their ability to capture complex, non-linear relationships between spatial features with high prediction accuracy. However, the lack of interpretability of machine learning models has been a significant drawback, especially in urban planning, where understanding the underlying factors that drive the model's predictions is crucial for decision-making. Among many opportunities to develop Machine Learning explanation techniques for causal inference in urban mobility is the need to evaluate causal effects of input features and derive actionable insights (Xin et al., 2022).

To address the interpretability challenge, the Machine Learning interpretation technique like **SHAP** (SHapley Additive exPlanations) is a unified approach to explain the output of any machine learning model—introduced by the seminal work of Lundberg and Lee (2017) based on the cooperative game theory of Lloyd Shapley—, and aim to provide detailed attributions of input features to individual predictions made. Its introduction kick-started a growing body of literature on interpretable machine learning with spatial systems for regression with XGBoost (Li, 2022) or classification with Light GBM (Louhichi et al., 2023). One of the most notable recent examples of

[3]https://tfl.gov.uk/corporate/publications-and-reports/economic-benefits-of-walking-and-cycling

SHAP for urban mobility in action was the development of the Deep Gravity Model introduced by Simini et al., 2021, which used SHAP to not only explain how the predictions of the deep learning model for spatial interaction were influenced by the input spatial features such as land-use mix, points of interest in the origin and destination zones.

As we approach this research with an eye on modelling the real-world phenomenon and explaining the contributing factors, instead of GWR or SLM, we will use a machine learning model to predict non-commute trip attraction in urban areas to a high degree of accuracy and then leverage SHAP to explain the predictions in an attempt to quantify the marginal importance and contribution of amenities and transport connectivity as attractors to an area's trip attractiveness.

2.5 Open data and reproducibility

Many recent advances in urban mobility research have been made possible by the availability of proprietary datasets owned by private companies, such as mobile phone data, GPS data, and social media data. Although the high data granularity has opened doors to new research opportunities and the development of new advanced techniques, its use also raises concerns about data privacy, data ownership, and data sharing. Moreover, it heightens the barrier to entry for independent researchers who would like to replicate the studies for their cities or regions. In contrast, open data not only democratises independent and participatory research in the public interest but also breaks down many reproducibility barriers when applying established methodologies to other localities (Yadav et al., 2017).

On one side, we have readily available open datasets maintained by local or federal government agencies in many countries. Conversely, we have global platforms like **OpenStreetMap** and **Overture Maps Foundation** that provide a wealth of spatial data for cities worldwide. The use of open data to encourage reproducibility will be a crucial focus of this research to ensure that the findings can be replicated, unburdened by commercial data availability and access barriers. It also enables flexible preprocessing of the amenity or transportation features to model the intracity mobility behaviour pertinent to the locality's needs while adhering to the same model training and analysis methodology. Adhering to the spirit of openness and future reproducibility across different urban contexts, all of the datasets used in this research will be entirely sourced from open data hubs and platforms. The associated scripts used for data processing, model training and prediction analytics are available on GitHub.

2.6 Summary

To address the research questions posed and informed by past literature, we set out to fine-tune and select a performant model to predict non-commute trip attractiveness, where we hypothesise that the built environment factors, including urban amenities and transport connectivity, are important trip attractors. Using a machine learning model in conjunction with explainable machine learning techniques such as SHAP allows us to capture complex, non-linear relationships and analyse contributions of input features to the predictions made to uncover underlying mobility patterns.

3. Methodology

In this chapter, we will first describe the methodology used to preprocess data from various sources to engineer the features for the predictive model, as informed by past literature. Second, we will outline the training model selection and evaluation process. Finally, we will discuss the methodology used to interpret the model predictions using SHAP techniques to answer the research questions. For ease of reference, the data preprocessing and feature engineering pipeline is summarised in Figure 3.1, and an overview of the model training and prediction interpretation methodology can be found in Figure 3.2. More detailed information on the data sources and the feature engineering process can be found in the Data Sources section of the Appendix.

Figure 3.1: Overview of the feature engineering pipeline

Figure 3.2: Overview of model training and interpretation

3.1 Defining the spatial unit of analysis

As features will be extracted and engineered from different data sources, the spatial unit of analysis—at which features are aggregated and the model is trained—is a crucial consideration. We will use 15-minute walking isochrones—i.e., the area that can be reached within a 15-minute walk from a point. They were generated based on initial seeds of 16,890 points distributed evenly across the Greater London region, using OpenStreetMap Pedestrian Network API (osmnx). The choice of using 15-minutes-walk isochrones as the spatial unit of analysis for our model is motivated by the following reasons:

- The spatial unit should reflect how individuals interact with transport nodes and amenity POIs that are pedestrian-accessible. In contrast, Euclidean distance proximity overlooks natural barriers, such as rivers or private estates.
- Human mobility in cities is not bound by administrative boundaries such as Output Areas or boroughs, and the use of overlapping isochrones allows us to capture the spatial heterogeneity of the input features and the target variables with high granularity.
- The 15-minute-walk specification of the isochrones aims to be aligned with the 15-minute city concept that characterises a desirable intra-neighbourhood mobility threshold. It serves as a standardised catchment area for the amenities and transport nodes that are likely to attract visitors to come and navigate on foot and, therefore, can also enable footfall estimation for local businesses within.
- Lastly, the density of the spatial units is a compromise between the granularity and the computational resources required to process the data. The initial seeds of 16,890 points are centroids of H3 cells at resolution 9 needed to cover the Greater London area.

The detailed methodology to generate the isochrones is illustrated in Figure 3.3, and two example isochrones in Central London can be seen in Figure 3.4, showing how these spatial units may vary in shapes and sizes. The following section will describe the data transformation and feature engineering process in more detail. Note that the terms spatial units of analysis or isochrones may be used interchangeably from this point in our discussion.

Figure 3.3: Methodology to generate 16,890 isochrones as the spatial unit of analysis

Figure 3.4: Two example isochrones as spatial units of analysis located in Central London

3.2 Data Preprocessing

3.2.1 Aggregating target variables

Total arrivals, i.e., the average number of passengers who exit a station or alight from a bus[1] within a spatial unit on a Saturday, are the target variables for our model as a proxy for trip attractiveness. The aggregation results are illustrated in Figure 3.5, which shows the total figures and the figures aggregated into the four time bands. The Total figures show an apparent concentration of passenger arrivals in Central London, with the highest number of passengers arriving

[1]The station exit and bus alighting data are provided as open data by Transport for London based on smartcard tap data and other inference methods. See Open Data Sources in the Appendix for further clarification.

at transport nodes. In contrast, the time band figures show a similar pattern, with the highest number of passengers arriving during the Midday and Evening time bands (10:00-19:00 and 19:00-22:00, respectively). Meanwhile, the Morning and Late time bands show lower numbers of passengers using the system due to early hours in the day on weekends and sparser night services, respectively. Lastly, since the target variable has a highly right-skewed distribution, we opt for a log transformation (shown in Figure 3.6) to the target variable to normalise the distribution and improve the model's performance, which will be corroborated in the Results section.

Figure 3.5: Public transport arrivals on an average Saturday, spatially aggregated to the spatial units. *Top* Total, *Bottom* By time band.

Figure 3.6: Distribution of the Total arrivals as raw count (left) and log-transformed (right). Similar transformations are carried out for arrivals by each of the four time bands

3.2.2 Feature engineering

Density-based features

The density of POIs is one of the first feature types of interest for our model, which represents the intensity of amenities or transport nodes of each type in an area that we hypothesise would attract visitors as destinations. Based on Cervero and Kockelman (1997)'s work, we expect a positive correlation between the density of POIs of all types and the total arrivals since an area with a high concentration of retail is expected to be more attractive than a similar-sized area with a low concentration of retail if the non-commute trip is for shopping purposes. Similarly, an area with a high concentration of transport facilities, such as stations and bus stops, is expected to accommodate a higher inflow volume of visitors. All density-related features are formulated by aggregating their counts for each spatial unit by type, resulting in a set of **16 features** (See Figure 3.7)

Figure 3.7: Population, Amenity and Transport POI density by type
(Source: UK Census 2021, OSM)

Diversity-based features

Diversity of Amenity POIs according to Cervero and Kockelman (1997) is also an important factor that may influence the trip attractiveness of an area for certain types of non-commute travel demand. The implication is that between two neighbourhoods, all else being equal, the area that is more diverse in its amenities will be more attractive as a destination on average because of its vibrancy and the possibility it provides visitors to accomplish different tasks in one trip.

What was left under-explored by literature is the diversity of public transport facilities present in a spatial unit, which may be an important trip attractor as it is a better proxy for transit accessibility than transport node density alone. Moreover, transport diversity can also capture the modal interchange behaviour of passengers whereby they alight in a specific area to switch between different means in order to reach their final destination elsewhere. As a hypothetical example, between two areas with a similar amenity density and diversity profile, the area that can be reached with multiple transit modes and routes should be more attractive to visitors, either because it makes that area more easily accessible or because it provides opportunities for passengers to switch between different modes of transport. The latter is of critical importance. Since there is no origin-destination matrix available for the study area, its inclusion potentially helps the model disentangle the impact of modal interchange behaviour on the total arrivals, as opposed to the trip attraction factor of the area itself as a destination.

Cervero and Kockelman (1997) conceptualised diversity in the form of *entropy*. Entropy, a concept that originated in information theory, is the average amount of information conveyed by an event when considering all possible outcomes. Batty et al. (2014) further adapted it to convey complexity in a spatial system. Interestingly, they also considered the increase of spatial entropy to be a trade-off between the density of amenity types and the unique types of amenity present, which stands in competition with other density-based features created. Therefore, including entropy as a measure of POI diversity could help us visualise this trade-off as the model is trained. We intend to replicate the approach used by both of the cited works above and adopt the formulation of entropy introduced by Shannon (1948) to calculate the diversity index of amenity POIs in each spatial unit as follows:

$$H = -\sum_{i=1}^{n} p_i \ln p_i \tag{3.1}$$

where p_i is the proportion of the i-th POI class in the total number of POIs in the spatial unit, and n is the total number of POI classes being considered. The entropy index ranges from 0 to $\ln n$, where 0 indicates no diversity and $\ln n$ indicates maximum diversity, which is then normalised to the 0-1 range. Based on this definition, we will engineer **3 features** related to the diversity of amenity POIs and transport POIs, further explained as follows:

- *Amenity POI*: 12 amenity POI classes are considered for the calculation of the diversity index for each spatial unit (see Table A.2). Looking at the 10% highest values of the diversity index in Figure 3.8, we can see that the most diverse areas are located throughout the Greater London area, which urban studies literature links to activity centres or neighbourhoods. As a whole, the distribution of the diversity index is right-skewed, indicating a pluricentric urban structure in Greater London.
- *Transport POI diversity by mode*: 3 transport POI classes (bus stops, rail stations, other hubs) are considered for the calculation of the diversity index for each spatial unit (see Table A.2). The top 10% values of the diversity index are mapped in Figure 3.8, showing that

the most diverse areas are located around important transport intermodal hubs, such as national rail stations, airports, and ferry piers.

- *Transport POI diversity by route option*: A more granular transport diversity index is calculated for the transport POIs, considering the different bus routes and train services the transport POIs in each spatial unit serve. The top 10% values of the diversity index are mapped in Figure 3.8, showing that the most transport-option diverse areas are not only intermodal hubs but also areas around arteries where many bus routes or rail services converge.

Figure 3.8: Normalised diversity indices for Amenity POIs, Transport POIs by mode and by route options. *Top*: Mapping top 10% values, *Bottom*: Distribution of diversity indices

The inclusion of both transport diversity indices aims to provide complementary information to the model, as they capture different factors to explain why an area receives more or less arriving passengers. High transport mode diversity indicates a high possibility that the area facilitates modal interchange for onward travel (such as long-distance intercity or cross-city trips), whereas high transport route diversity, in addition to that, indicates a high possibility that the area is locally well-connected with reasonable frequency. Zooming into a specific area, such as the Hammersmith and Fulham borough, we can see a slight divergence between the two transport diversity indices (Figure 3.9). The Shepherd's Bus area has a higher transport mode diversity index thanks to the existence of national rail services (Southern Railways) beyond Tube and buses. In contrast, the area around Earl's Court has a higher transport option diversity index due to the presence of multiple local bus routes converging in the area.

Figure 3.9: Top 10% values of 3 diversity indices
Borough: Hammersmith and Fulham

Centrality-based features

Whereas the public transport diversity index, previously discussed, captures the variety of transport options available in an area, it obscures one aspect of accessibility in relation to other areas in London using the public transport network. Centrality-based features add yet another layer of information to the model, capturing the importance of a bus stop or a station in relation to the whole network. For example, between two hypothetical areas with similar diversity of transport options (e.g., both are served by five bus routes), the area with a higher centrality measure may be more attractive to visitors because it is more 'accessible' from other areas on average.

Figure 3.10: Network graphs of TfL Bus (left) and Rail (right) networks
Constructed based on TfL API data

First, we construct the network graph of the TfL Bus and the TfL Tube and Rail networks from open data (See Figure 3.10), with nodes representing the stops or stations and the edges representing routes or lines. Due to the lack of data related to travel time and scheduling, we abstain from combining the two networks into a multi-layered network, which would have allowed us to consider the whole public transport network as one connected component. Instead, we will calculate the following centrality measures for all the nodes in the Rail and Bus networks separately, resulting in a set of 6 node attributes:

Figure 3.11: Mapping three centrality measures of spatial units on the Rail (left) and Bus (right) networks

- *Degree centrality*: The number of direct connections a node has. A high degree of centrality indicates that the node is well-connected to other nodes in the network (i.e., many routes available).
- *Closeness centrality*: The average shortest path length from a node to all other nodes in the network. A high closeness centrality indicates that the node is close to other nodes in the network (i.e., centrally located).
- *Betweenness centrality*: The number of shortest paths that pass through a node in the network. A high betweenness centrality indicates that the node is an important bridge between other nodes in the network (i.e., transport hubs).

Finally, to incorporate calculated attributes of the nodes into **6 features** of centrality, we will consider all the nodes in each spatial unit and extract the maximum attribute values. In other words, the centrality feature of a spatial unit has the value of the rail or bus transport node with the highest centrality measure of each of the six attributes. The mapping of the centrality measures to the spatial units is illustrated in Figure 3.11.

3.2.3 Incorporating spatial lags as a feature

In summary, the feature engineering process thus far has resulted in a total of **25 features** that will be used to train the model to predict the (log-transformed) public transport arrivals in a given spatial unit. The features are summarised in Table 3.1.

No.	Feature
1	Population density
2-13	Amenity POI density by type (12)
14-16	Transport POI density by type (3)
17	Amenity POI diversity index
18	Transport POI diversity index by mode
19	Transport POI diversity index by route option
20-25	Bus and Rail centrality measures (Degree, Closeness, Betweenness) (6)

Table 3.1: Summary of the 25 main features engineered for the model

When working with machine learning models with data in a closed spatial system such as the Greater London area, it is important to consider the spatial autocorrelation in the target variable. In the context of our analysis, the number of passengers arriving in an area is likely correlated with the number of passengers arriving in nearby areas. Although deep learning models' parameters and hyperparameters can be made more complex and tuned to reach a high degree of prediction accuracy without considering the spatial aspect of the dataset, accounting for potential spatial autocorrelation could reduce the probability of biased outcomes even with a relatively low-complexity and high-interpretability architecture, e.g. tree-based models (Meyer et al., 2019).

The indication of spatial autocorrelation in the target variables is confirmed by the Local Indicators of Spatial Association (LISA) analysis, which shows the presence of spatial clusters in the target variables (Figure 3.12), using Local Moran's I indicators. If spatial information among these spatial units is provided to the model during tuning and evaluation, we could improve accuracy further, especially in these localities that make up more than 50% of the study area.

To address this issue, Liu, Kounadi, and Zurita-Milla (2022) proposed incorporating spatial lag into the model as a feature. More specifically, the authors have concluded that when spatial features were induced in the random forest model, the global spatial autocorrelation among the predictions' residuals was significantly reduced, leading to higher validation accuracy. For our analysis, the spatial lag feature of each spatial unit is calculated as the average number of passengers arriving at neighbouring isochrones[2]. The creation of a **Spatial Lag features** is replicated for the total arrival counts, as well as for each time band, resulting in a set of additional features to be included to train the model in predicting the corresponding target variable.

[2]The choice of the distance band of 750m was calibrated to ensure all spatial units have neighbours, i.e., there are no islands.

Figure 3.12: LISA cluster map of Total arrivals showing local spatial autocorrelation
Global Moran's I: 0.742 (High spatial autocorrelation)

No.	Target variable	Main Features		Spatial Lag Feature
1	Total arrivals	Population, amenity and accessibility profile (25 features)	+	Spatial Lag - Total arrivals
2	Morning arrivals			Spatial Lag - Morning arrivals
3	Midday arrivals			Spatial Lag - Midday arrivals
4	Evening arrivals			Spatial Lag - Evening arrivals
5	Late arrivals			Spatial Lag - Late arrivals

Table 3.2: Mapping spatial lag features to predict corresponding target variables

3.3 Model selection and interpretation

As previously explored through relevant literature, we are faced with an important decision when attempting to model the non-commute travel demand in the Greater London area based on variables related to the built environments, such as the amenity profile and the connectivity profile. More specifically, the choice is between using a machine learning model—which prioritises prediction accuracy and can handle heterogeneous data, and a spatial-statistical one—which prioritises interpretability and requires more stringent requirements of the explanatory variables. Although spatial statistical models such as the Spatial Lag Model or Geographically Weighted Regression are standard for such analysis, Li (2022) has shown that machine learning models can capture spatial effects if spatial information is provided, and the appropriate Machine Learning explanation technique is used. This work aims to demonstrate the use of SHAP explanation on a fine-tuned prediction model to provide insights into the geographically varying effect of the features on the predictions. Figure 3.2 provides an overview of the model training and interpretation process.

Model evaluation

Firstly, we will compare the performance of three machine learning models: *Linear Regression, Gradient Boosting, and Neural Network* in predicting Total arrivals. As we are working within a spatial system with a high degree of spatial autocorrelation demonstrated earlier, special attention will be paid to spatial cross-validation in hyperparameter tuning and evaluation because random cross-validation and train-test splits are not able to prevent train-test data leakage, which inflates the accuracy score.

More specifically, the model tuning and evaluation process will be carried out using a nested 10-fold cross-validation approach introduced by Schratz et al. (2018), with R^2 as the performance metric. The nested cross-validation approach is illustrated in Figure 3.13, where the inner loop tunes the model's hyperparameters, and the outer loop is used to evaluate the model's performance. The spatial 10-fold cross-validation splits for our datasets (see Figure A.1 in Appendix) ensure that the training and test sets in the inner and the outer folds are spatially distinct. The model and its hyperparameters with the highest R^2 score will be selected as the best model to fit the entire dataset for further analysis[3].

Figure 3.13: Spatial vs. non-spatial nested cross-validation using 5-folds for hyperparameter tuning and performance evaluation. This technique helps ensure the training and test sets in both the inner and the outer folds are spatially clustered to avoid data leakage
Source: Schratz et al. (2018)

Model interpretation

Rooted in the work on game theory, SHAP tackles the challenge of fair credit allocation within a cooperative game. In this reimagined context, features in our data are the players, the set of features used for training represents the coalition, and a model prediction is the game. For each observation, the SHAP values quantify the average marginal contribution of a feature to achieve

[3]Although the model tuning and selection process is only performed on Total Arrivals as the target variable for simplicity, the chosen model will be applied to predict arrivals by time bands.

the final prediction, providing a nuanced understanding of each feature's impact on the model's predictions at the local level (i.e., for each observation)

Among other properties contributing to its popularity in Explainable AI research, it is model-agnostic and additive, meaning that the sum of all features' SHAP values equals the difference between the model's final and baseline predictions for each observation. In this scenario, given the model is spatially aware thanks to the addition of spatial lags as a feature, the outputs from this ML explanation technique share some similarities in interpretation with spatially varying coefficients of a geographically weighted regression model. Visualising features' SHAP values on a map can, therefore, provide insights into the spatial heterogeneity of the feature importance in the model's prediction, which can be used to identify hotspots of high trip attraction factors for non-commute travel demand.

While SHAP computation was initially a barrier, approaches like Kernel SHAP and Tree SHAP made available in the SHAP package have made estimation more efficient. SHAP's local interpretability and integration with popular machine learning libraries also make it a powerful tool for spatial data where feature attribution can be visualised geographically. These properties of SHAP allow us to derive our methodology to interpret the model's prediction in the context of the features engineered to answer the research questions:

- SHAP-based *global feature importance* will be used to identify the most important features (amenity and connectivity profiles) to the model's prediction of inflow travel demand, allowing us to understand the general patterns and relationships between the features and the target variables. Since the model in question must attain a high level of accuracy before the SHAP values can be considered insightful, due care will be taken to ensure that the model is well-tuned and evaluated before proceeding with the SHAP analysis.
- SHAP-based *local feature importance* will be used to interpret the model's prediction for individual spatial units, allowing further investigation into identifying local spatial trip attraction patterns. With spatial clustering analysis such as HDBSCAN on the local SHAP, we can also identify clusters where our main features of interest have high (or low) importance compared to others, effectively identifying hotspots of high trip attraction factors for non-commute travel demand.

The following chapter will present the results of the model training and interpretation process, followed by a discussion of the findings and their implications for the research questions and other applications.

3.4 Ethical considerations

The research exclusively utilises publicly available and anonymised data, ensuring individual privacy and confidentiality. Data sources are transparently outlined in the Appendix, and the anonymisation process mitigates re-identification risks, such as suppressing low counts in the outputs. The findings from this research may be disseminated for academic purposes to contribute to a greater understanding of urban mobility patterns, as well as with partner organisations and municipal transport authorities to inform more responsive and sustainable urban planning, transport service planning, and policy-making. The UCL Ethics Committee assessed the study's scope and methodology as minimal risk and did not require further review.

4. Results

4.1 RQ1: Predicting attractiveness from spatial features

Prediction model evaluation and selection

As previously explained, choosing a suitable machine learning model is critical, as Machine Learning explanation techniques such as SHAP would be less insightful if the predictions produced high inaccuracies. The evaluation results in Table 4.1 show that the Gradient Boosting tree-based model (XGBoost) outperforms the other models in predicting the target variable *Total arrivals (log)* with an R^2 of 0.792. Meanwhile, the simple Linear Regression model performs more poorly in comparison due to underfitting (i.e., consistently low accuracy with training data folds), and the Multilayer Perceptron Artificial Neural Network model also performs poorly but due to overfitting (i.e., high accuracy achieved with training data folds but low accuracy with validation data folds). XGBoost also outperforms itself when predicting the pre-transformed target variable with an R^2 of 0.633. This shows that while XGBoost has long been popular thanks to its fast convergence and high validation accuracy, transforming the highly right-skewed target variable can further improve prediction performance.

Model	R^2 **(raw)**	R^2 **(log)**
Linear Regression	0.576	0.697
XGBoost	0.633	**0.792**
ANN	0.526	0.410

Table 4.1: Comparing model R^2 results of 3 models predicting Total arrivals (raw) and Total arrivals (log) using spatial k-fold cross-validation for tuning and evaluation

In managing overfitting risks, XGBoost stands out among other models for its built-in L1 and L2 regularisation hyperparameters, which penalise the model for complexity and suppress highly correlated input features. This is particularly important when considering the complex patterns of correlations among our input features, as shown in Figure 4.1. Here we observe groups of highly correlated features, such as Population-Public Facilities-Religious POIs, Entertainment-Restautants-Shopping POIs, and between different public transport centrality measures. Therefore, with XGBoost, we could further fine-tune two hyperparameters *alpha* and *lambda*—which represent L1 and L2 regularisation thresholds, respectively—to achieve even better prediction results. As done previously, nested spatial k-fold cross-validation is used to fine-tune the model and validate the results. The fine-tuned XGBoost model improves R^2 up to **0.823** (an approx. 3pp increase) in predicting total arrivals from the pre-tuned model and performs consistently well in

Timeband	R^2	MSE	MAE
Total	**0.823**	0.687	0.570
Morning	**0.809**	0.614	0.571
Midday	**0.828**	0.629	0.549
Evening	**0.819**	0.687	0.593
Late	**0.824**	0.635	0.601

Table 4.2: Finetuned XGBoost model evaluation results for All target variables (log) using nested spatial k-fold cross-validation for tuning and evaluation

Figure 4.1: Correlation matrix of the input features and target variable Total arrivals (log)

predicting arrivals by time band, as shown in Table 4.2. The results suggest that the fine-tuned XGBoost model is fit for purpose and enables us to address the first research question: Built environment features engineered from open data are adequate predictors of public transport inflows (as a proxy for trip attractiveness) to a high degree of accuracy.

Before further analysis, it is important to recognise where the model falls short and what that may tell us about its potential lack of generalisability. Figure 4.2 shows the distribution of observations whose prediction residuals are Tukey's fence's 'outliers', i.e., the target variables are significantly overpredicted or underpredicted. These are primarily concentrated in Outer London where poor predictions go in both directions. While it is not easy to immediately unravel, possible

root causes include:

- *Low Spatial Autocorrelation:* There is consistency between areas with low spatial autocorrelation of the target variable (see Figure 3.12, grey regions), and where the model predicts more poorly. This may indicate that incorporating spatial lag as a feature improves the model's performance only where spatial autocorrelation is present. In its absence, the model has a higher chance of poorer predictions based on the main features alone.
- *Omitted features:* It is possible that adding variables such as car ownership and socioeconomic factors can help the model predict two hypothetical areas with the same built environment profiles but different public transport usage. This is especially true in Outer London, where car ownership is higher, and public transport services are less frequent.
- *Incomplete target variable:* It is probable that a spatial unit with its built environment profile does have the predicted public transport trip attractiveness in reality. However, since only data from TfL-operated services are considered, omitting trip data from other rail operators—more prevalent in Outer London and especially south of the Thames— may manifest as an apparent overprediction.

Figure 4.2: Observations with significant overprediction and underprediction (N=576 of 16,890) Fine-tuned XGBoost model, Total arrivals (log)

Nonetheless, these 'outliers' account for less than 3.5% of the total observations, and the model's performance is still satisfactory in explaining the large majority of the spatial units in the Greater London area.

Global feature importance

After fitting the fine-tuned XGBoost model to the entire dataset, we applied SHAP to obtain the SHAP values for each feature and observation. This allows us to evaluate the importance of each feature in predicting the target variable and understand the direction of the relationship between the feature and the target variable.

Figure 4.3 shows the summary of feature importance for the target variable *Total arrivals (log)* from most to least important (top to bottom) as distributions of the SHAP values for each feature. For each feature, the direction of the relationship between the feature value and the SHAP values is shown using a red-blue scale: For example, the higher the value of the feature *Rail transport node density (transport_rail)*, the likelier it contributes positively to the prediction (red tail on the right side). Meanwhile, the higher the value of the feature *Leisure-Active POI density (poi_leisure_active)*, the likelier it contributes negatively to the prediction (red tail on the left side). For the feature *Closeness centrality measure on the bus network (cent_bus_closeness)*, higher feature values have a weaker positive impact on the prediction, while lower feature values have a stronger negative impact on the prediction (i.e., the distribution has a longer blue tail on the left side than the red tail on the right side).

From here, we can make several observations: First, the connectivity profile features have outsized importance with the *transport route option diversity index (diversity_transp_opt)* on top in predicting trip attractiveness. This is consistent with the reality that people tend to alight/exit at transport-rich areas with multiple bus routes or rail services for onward journeys, representing the most prominent interchange behaviour. The second most important feature is the spatial lag of the target variable (i.e., mean of target variables of neighbouring), which partially corroborates its influence on the model's performance hypothesised earlier when analysing outliers. The most important amenity POI feature is *shopping POIs*, which is also consistent impact across all time bands (see Figure A.2 in Appendix), followed by *banking POIs*, *active leisure POIs*, *medical POIs*, *restaurant POIs*, *nature POIs*, and *outdoor leisure POIs*. This suggests that for the whole of Greater London, total arrivals as a proxy for trip attractiveness are driven mainly by, first and foremost, the need to interchange for onward travel and, secondly, by the availability of certain key types of amenities.

Figure 4.3: Summary of feature importance based on SHAP values. Red-Blue scale represents the feature value, and the x-axis represents the SHAP value, i.e., impact on final model prediction of Total arrivals (log)

At this point, it is important to acknowledge the effect of correlation between the input features as previously observed and how the XGBoost model learns on SHAP global explanations. Although XGBoost's regularisation hyperparameters are in place to avoid overfitting due to highly correlated features, they do not drop them from the model. Consequently, when SHAP is applied for a retroactive explanation, highly correlated features will show comparable importance. Therefore, it is more insightful to consider the SHAP values of the correlated features in clusters, as shown in Figure 4.4. We can see that there are differences from the previous graph, where the top most important features (or feature clusters) are as follows:

1. Transport route option diversity index
2. Spatial Lag
3. Population + Public Facilities (clustered, local residential amenity features)
4. Bus stop density + Bus stop closeness centrality (clustered, bus interchange features)
5. Shopping and Restaurants POI density (clustered, commercial features)

Figure 4.4: Feature importance in predicting Total arrivals (log)
Features clustered by correlation and ordered by mean absolute SHAP values

In summary, as it pertains to our first research question, the global feature importance analysis shows that built environment features are indeed important predictors of public transport inflow demand in London and that the XGBoost model can capture the complex relationships between these features and the target variable with high accuracy ($> 80\%$). There are also opportunities to improve the prediction performance by addressing possibly omitted spatial and non-spatial features. The high importance of the spatial lag feature is both an advantage and a shortcoming: While it drastically improves the model's performance overall for Greater London, it penalises the model in areas where the spatial autocorrelation is low, reducing its generalisability to predicting the trip attractiveness of an isolated area without considering its neighbours. Finally, highly correlated features should be considered in clusters when analysing importance to avoid interpreting undue importance to a single feature.

4.2 RQ2: Identifying local attractors and hotspots

One of the highlights of SHAP is its ability to provide local explanations for individual predictions. When applied to a spatial system, these local explanations offer additional insights on spatial phenomena that are not well captured in a global feature importance analysis, namely spatial heterogeneity (i.e., varying impact of the target variable across different spatial units) and spatial non-stationarity (i.e., varying impact of an input feature on the target variable across different spatial units). SHAP's additive property allows us to decompose the prediction of a spatial unit into the sum of the SHAP values of each feature and exact the contribution of each feature to the prediction.

Figure 4.5 shows the local SHAP values for two spatial units, Kew Gardens and Covent Garden, for a closer look. They represent two distinct localities with supposedly different amenity and transport profiles. Kew Gardens is a quiet residential area in the public transport network, also known for its many renowned parks and gardens, while Covent Garden is a bustling commercial and entertainment district with high connectivity in the public transport network. By design of SHAP, the baseline prediction $E[f(X)]$ for both spatial units are the same, but the contributions of the features are what enable the model to make two different final predictions $f(x)$ for the two spatial units. The local SHAP values for Kew Gardens show a higher contribution of the population density and POI classes associated with neighbourhood amenities (stores, clinics, etc.) to the prediction of total arrivals. In comparison, the local SHAP values for Covent Garden show a higher contribution of POI classes such as restaurants, entertainment venues, etc. This is consistent with the expected profiles of the two areas and demonstrates SHAP's ability to provide local explanations for individual predictions. In both cases, in line with global feature importance, the transport route option index's contribution is among the top, indicating that with the station exit and bus alighting dataset at hand, the interchange behaviour is still a significant pattern regardless of where in London the spatial unit is located.

Figure 4.5: Local SHAP values for 2 spatial units
Kew Gardens and Covent Garden

By mapping the local SHAP values for all spatial units in the Greater London area, we can

visualise the differing impact of the input features on the target variable across the region of interest. Figure 4.6 shows the local SHAP values for two features, Outdoor leisure POIs and Entertainment leisure POIs, for the target variable of *Total arrivals (log)*. The map shows that the impact of these features on the target variable is not uniform across space, with some areas showing a positive impact (red) and others showing a negative impact (blue). Central London understandably commands the highest contributions of entertainment POIs to predict trip attractiveness. Still, it also indicates secondary areas of high impact in the outer boroughs, such as Brixton and Haringey. Outdoor leisure POIs, on the other hand, have a more dispersed impact citywide, with a hotspot around Richmond.

On the temporal dimension across time bands, we can also observe the varying impact of the input features on the target variable across different time bands. Figure 4.7 depicts local SHAP values spatial distribution throughout the day normalised by the target variable (arrival by time band) to enable comparison. Entertainment POIs in Central London have the highest trip attractiveness in Midday, especially Evening time bands. In contrast, Outdoor leisure POIs show a more consistent impact across time bands, with a notable increase in the intensity of certain hotspots and coldspots in the Late time band.

It reveals the methodology's shortcoming: According to global feature importance for the Late time band (see Figure A.2 in Appendix), *density of outdoor leisure POIs* seem to have an increased impact on the prediction, contrary to the expectation that no passengers would be visiting outdoor leisure POIs after midnight. Since SHAP's goal is to ultimately approximate how a trained model makes decisions, it may overestimate the importance of existing features when omitted features could have explained the variances better. This also means that the feature selection process may not be a one-size-fits-all for temporal datasets, and additional features might be necessary to avoid overinflating the contribution of certain features for individual time bands. If feature selection is different in predicting arrival by each time band, however, comparing SHAP values across them may also be misleading.

Figure 4.6: Mapping SHAP values as hotspots for two features: Outdoor leisure POIs and Entertainment leisure POIs. Target: Total arrivals (log)

Finally, the availability of raw SHAP values also enables other manipulations for specific purposes. For example, with different types of weightage, we can observe the impact of the features on the target variable in a different light. Figure 4.8 shows the comparison of raw and

Figure 4.7: Mapping SHAP values as hotspots for two features Outdoor leisure POIs and Entertainment leisure POI (weighted by number of arrivals for comparison). Target: Arrivals by time band (log)

weighted SHAP values for two features, Outdoor leisure POIs and Entertainment leisure POIs, for the target variable *Total arrivals (log)*, weighted in two different ways:

1. Weighted by amenity diversity index: This can add more highlights to feature hotspots in areas with many other potential *contenders* for trip arrivals. Under this treatment, we can see that Entertainment POIs have an even more pronounced impact in Central London and clusters of small areas with high amenity diversity, indicating that these Entertainment POIs attract trips even though the area is saturated with other amenities.
2. Weighted by transport route option diversity index: This can add more highlights to feature hotspots in areas not well-served by many public transport routes. Under this treatment, we can see that Outdoor POIs on the outskirts of London now have a more pronounced trip attraction factor, indicating that despite the lack of public transport connectivity, these Outdoor POIs are still relatively popular.

Overall, SHAP local interpretability with individual SHAP values for each spatial unit provides a more nuanced understanding of the impact of the input features on the target variable across space and, in our case, time. In effect, it decomposes the target variable (Total arrivals) into the sum of feature contributions in the form of local SHAP values, which can be visualised spatially to identify hotspots and coldspots of feature impact. This is particularly useful for identifying activity centres in the Greater London area, as it allows us to pinpoint areas where certain features have a high impact on the prediction of trip attractiveness in the form of *Total arrivals (log)*. Limitations exist, however, in the methodology, as they are much more adept at enabling comparison of feature importance within the same model (within each time band) rather than across models (between different time bands). In our discussion, we will also consider the implications and applications of these findings on urban analytics literature and transport planning.

Figure 4.8: Raw vs. weighted SHAP for 2 features
Outdoor leisure POIs and Entertainment leisure POIs
Total arrivals (log)

5. Discussion

To recapitulate our findings thus far: First, we have established that provided with open data on population, amenity points-of-interest density and diversity, and public transportation accessibility indices, we can predict the total number of arrivals by public transport to a high degree of accuracy using an XGBoost machine learning model that is fine-tuned to overcome overfitting and converge fast. Secondly, we extracted more sophisticated feature importance indications using SHAP for machine learning model explanation than originally achievable with the XGBoost model's internal tree-path structure. Thirdly, the methodology allows us to decompose each target variable (i.e., arrivals by public transport) prediction into the sum of each feature's contribution in the form of its SHAP value.in effect, by examining local SHAP values' spatial distributions, we can identify hotspots for different POI features overall and across different time bands.

One of the benefits of using SHAP values as imperfect approximants to coefficients in a statistical model is their additive nature. This means that we can decompose the model's predictions into the sum of the SHAP values, with which we can control for unwanted effects. For example, without an explicit origin-destination matrix and dwell time data and using only station exits and bus alighting data, it is not immediately possible to say whether a person is exiting at a destination to attend an activity or to interchange to another mode of transport. Using SHAP to extract local explanations with its additive property, therefore, can help isolate the impact of the amenity profile of the destination area on the trip attractiveness of the area while controlling for the contribution of its connectivity profile based on how well the model predicts the total arrivals for each spatial unit.

One way to visualise it is by grouping local SHAP values by feature groups and visualising their spatial distribution. This can be seen in Figure 5.1 with features grouped into (1) amenity-related, (2) population, and (3) connectivity-related features. When comparing the Midday and Late time bands, representing the peak and lowest volumes, respectively, we can see that the impact of the amenity profile on trip attractiveness is significantly more pronounced in the Midday time band, whereas the impact of the connectivity profile on trip attractiveness is seemingly unchanged (i.e., they have visually similar spatial distributions). Since we can assume that the connectivity-related features in our model (density of transport nodes, centrality measures, etc.) are static and independent of time bands[1], and that the only difference between these two time bands is the trip attraction generated by amenities, this suggests that the model can isolate whether an area attracts trip because of the presence of the amenities. This is insightful for instances where we want to qualify whether certain areas are urban activity hotspots based on the availability of amenities while excluding demand generated with the purpose of interchange for onward journeys (i.e., "transit" hotspots).

[1]Service scheduling and frequency of public transport services are not considered in our model

Figure 5.1: Amenity vs. Residential vs. Transit "Hotspots"
Calculated as the sum of SHAP values for each feature group in each spatial unit
Timeband: Midday vs. Late

This can be summarised via a generalised formula for Activity Hotspot Index

$$A_i = \sum_j h_{ij}$$

where A_i is the Activity Hotspot Index of spatial unit i and h_{ij} is the local SHAP value of amenity-related feature j of spatial unit i[2]. Applying spatial clustering such as HDBSCAN on the isochrones based on spatial units' Activity Hotspot Index A effectively surfaces activity hotspots in Greater London, as shown in Figure 5.2 with the top 10% activity hotspots based on the mean activity hotspot index of all member spatial units. These hotspots are areas where the amenity profile has the highest mean SHAP values across all spatial units in the cluster, indicating that these areas are popular for non-commute activities based on the amenity profile of the area. Figure 5.3 demonstrates a closer look at Wood Green's top activity hotspot cluster, comprised of five member spatial units (isochrones). This can be useful for local urban planners to identify destination areas that are popular for non-commute activities, such as parks, shopping, dining, or entertainment.

[2]In total, there are 15 density-based amenity features and 1 amenity diversity feature. See the Methodology chapter for further clarifications.

Figure 5.2: Top 10% activity hotspot clusters in Greater London
Based on mean activity hotspot index of member spatial units

Figure 5.3: Top activity hotspot cluster in Wood Green by mean Activity Hotspot Index (left) and the centroids of the five member spatial units (right)

It is worth acknowledging the methodology's limitations, which affect its generalisability and applicability in some instances.

- *Core assumptions in the selection of target variables*: In order to approximate non-commute trip attractiveness, we opted for data on a Saturday as a typical weekend day to remove the effect of employment centres from the analysis as much as possible. However, this does not account for travel demand from those who work on weekends. Future work could consider using a more comprehensive dataset that includes trip purpose information to better understand the non-commute trip attractiveness of an area if such distinction is essential for the analysis.
- *Missing features*: The analysis of outliers suggests that other factors may influence the number of arrivals in an area not accounted for in the model. These could include socioeconomic factors, car ownership, or other urban morphological features that affect people's usage of public transport. Incorporating these features into the model could improve its accuracy and generalisability in localities with high variance in public transport usage.
- *Generalisability*: The high feature importance of the spatial lag features across the board means that the model may not accurately predict a new observation in isolation from its neighbours, nor can it be readily generalisable to other cities. Nevertheless, the model can predict the trip attractiveness of a given area in Greater London as the city changes, giving transport planners a useful tool. For example, when a neighbourhood is undergoing redevelopment, we can predict the potential inflow of public transport trips based on the planned addition of amenities or transport facilities and connectivity.
- *POI classification*: The classification of amenity and transport POIs in this analysis adheres to Geofabrik's out-of-the-box OSM data classification. Future work could attempt to reclassify these POIs more deliberately to capture the association between certain trip purposes of interest and the types of amenities that fulfil them as destinations.
- *Quality of open data*: More broadly, due to the reliance on open data as part of the methodology, the data quality used in the analysis is subject to the quality of the data sources.

Varying degrees of quality in the open data available across different localities, especially OSM data, could lead to incorrect predictions and conclusions.

Last but not least, the dissertation scope is limited to public transport trips and does not account for other types of urban mobility, such as cycling, walking, ridesharing, or driving, which would provide a more comprehensive understanding of the non-commute trip attractiveness of an area regardless of mode of transport, especially during time bands when public transport is less accessible such as late nights. As an extension of this shortcoming, activity hotspots identified so far may only hold true for public transit users. Future work could incorporate mode-agnostic mobility data and trip purpose inferences into a modified version of this methodology to provide a more comprehensive understanding of what draws people to a certain area in Greater London. Special care should be taken to ensure that the connectivity-related features, in this case, reflect the transport modes of interest. For example, to engineer connectivity-related features with active means of transport such as cycling, the density of cycle lanes and bike-sharing stations would be more relevant than the density of bus stops and rail stations.

6. Conclusion

Disentangling urban mobility patterns is a complex endeavour with a multitude of factors influencing destination and mode choice. Within that context, this work has sought to understand the relationship between the built environment of an area and the non-commute transport demand it attracts, using Greater London's public transport as a case study. We found that using a combination of amenity and connectivity features extracted from publicly available open data sources such as OpenStreetMap and the Census, we can predict the total number of arrivals as a proxy for trip attractiveness of a given area in London with a high degree of accuracy. The methodology calls for the use of an XGBoost model that has been fine-tuned to overcome overfitting and fairly evaluated using nested spatial k-fold cross-validation to avoid inflated performance due to spatial autocorrelation.

In order to inspect feature importance on both the global and local levels in the prediction of the target variable made by the machine learning model, as opposed to a more conventional approach using a statistical model's parameters, we have employed SHAP explanation values to deconstruct the model's predictions. This has allowed us to identify the most important features in the model's decision-making process, as well as to understand the spatial distribution of this feature importance. SHAP is a powerful explanation machine learning technique not only for highly complex deep learning models but also for tree-based models like XGBoost thanks to its interventional nature that can surface more sophisticated feature importance beyond XGBoost's built-in functionality.

Following this methodology, we confirmed the high feature contribution of connectivity-related features such as the diversity index of transit routes in the area to the prediction of 'trip attractiveness' —both globally and locally. However, we also found that amenity-related features such as the number of restaurants, parks, and theatres in the area are also important in predicting the target variable but with varying degrees of importance across the region of interest. This means the model and the accompanying local SHAP explanations, especially when presented cartographically, can highlight spatial heterogeneity in the impact of amenity to inflow travel demand, serving as a valuable tool for deducing other aspects of mobility, such as trip purposes. Finally, these SHAP values can be further manipulated to surface destination hotspots, which can be useful for transport urban planners to identify areas that are popular for non-commute activities. Specifically, in this study, where we focused on public transport, the predictive model can inform transit service planning and urban planning, such as in the case of redevelopment, as well as estimating pedestrian traffic surges, with applications in retail location planning and public health, among others. Since open data is at the core, the methodology can be extended to other cities and regions that lack more granular mobility datasets but have similar open data availability.

In conclusion, we have demonstrated the potential of using open data to predict non-commute transport demand in urban areas. The model's high accuracy, combined with the explanation power of SHAP, makes it a valuable tool for urban planners and transport authorities to understand the relationship between the built environment and trip attraction. Nevertheless, the work presented has limitations that could be addressed in future research. For instance, the model can

be further improved by incorporating more granular data such as the frequency of public transport services, the quality of the built environment, and the socio-economic characteristics of the area. Moreover, the model can be extended to predict other types of transport demand, such as cycling and walking, which are also important modes of non-automobile intracity trips. Lastly, it hints at new possibilities in the field of urban mobility research that could be built upon. For example, we could also explore how this methodology and these insights could be incorporated into a more comprehensive mobility model using granular origin-destination matrices that enable the prediction of aspects of urban mobility, such as trip purposes, mode choices, accessibility, and activity sequence.

A. Appendix

A.1 Open data sources

The analysis carried out will utilise the Greater London area as the working case study, serving as an example for further replications of the analysis for other localities. The Office for National Statistics (ONS) defines the Greater London metropolitan area to include the City of London and the 32 London boroughs, with a total area of 1,572 km^2 and a population of 9.4 million people, making it the largest in the United Kingdom. The choice of the Greater London metropolitan area is also motivated by the availability of open data sources from which necessary features could be derived and the complexity of the public transport network, coupled with rich usage data made available to the public. The data sources used in this analysis are summarised in Table A.1 and detailed below.

	Variables	**Sources**
Public transport arrivals (target)	Tube and Rail station exits Bus alightings	TfL network demand (NUMBAT) TfL network demand (BUSTO)
Population	Population count	UK Census 2021
Amenity Profile	POI count by type POI diversity index	OSM Amenity POIs
Public Transport (PT) Connectivity Profile	PT node count by type PT node diversity index PT network centrality	OSM Transport POIs and TfL

Table A.1: Summary of data used in the analysis and their sources

Transport for London (TfL) Open Data

We use the following GIS datasets from the TfL GIS Open Data Hub and TfL API to derive transport-related features for the study area including density of transport facilities, diversity of transport options, and accessibility in the form of centrality measures in the Rail and Bus networks separately. The networks of interest are defined as follows:

- *Rail network* includes the London Underground, London Overground, the Docklands Light Railway, and the Elizabeth Line, excluding stations and segments that are not managed by TfL or fall outside the Greater London area.

- *Bus network* includes stop locations and route data of all bus and tram services, excluding stops and route segments that are not managed by TfL or within the Greater London area.

TfL also provides annually-updated network demand datasets, which will be used to derive the target variables of our analysis. The datasets of special interest to our analysis are namely *Rail demand data (NUMBAT)* and the *Bus demand data (BUSTO)*, from which we will extract estimated counts of station exits and bus alightings at the station or stop level, respectively. The dataset's temporal granularity is also an important aspect to consider. To address non-commute trips for the analysis, we will specifically use **average Saturday demand**, representing the demand in a typical period without any major citywide disruptions or events. This Saturday travel demand may still include work trips for those working on Saturdays, albeit not concentrated into peak periods as with weekday travel demand. For the scope of this analysis, we will treat these potential work trips as non-commute.

To examine possible variations between different times of day, besides the total counts of exits and bus alightings in one day, we will aggregate the data into four larger time bands:

- *Morning* (05:00 - 10:00): Limited mobility expected due to early hours
- *Midday* (10:00 - 19:00): High daytime mobility expected
- *Evening* (19:00 - 00:00): High evening mobility expected
- *Late* (00:00 - 05:00): Minimal mobility expected due to sparser night PT services

The choice of time band delineation is a compromise between different granularity levels afforded by the TfL rail and the bus demand datasets. There are opportunities to deepen the analysis by further segmenting the time bands into finer intervals if data permits.

It is worth noting that despite the existence of the Oyster Card integrated fare system, TfL does not provide origin-destination data as open data. Therefore, station exits and bus alightings are not directly associated with the number of passengers traversing through the system but are treated as discrete events. For example, a person who takes a bus to reach a Tube station for onward travel and then exits to arrive at their destination would be counted as two separate data points, one alighting for the bus and one station exit for the Tube. Nevertheless, our model will take this into account when making poredicion and allows us to investigate patterns and the contribution of modal interchange behaviour in our interpretation.

Lastly, we need to acknowledge the particularity of the TfL bus demand dataset (BUSTO). Although passengers do not 'tap off' when alighting from busses, TfL has adopted a methodology to estimate the number of passengers alighting at each bus stop based on individuals' next actions and other statistical methods. The methodology is described in the BUSTO User Guide and Data Dictionary

UK Census Data 2021

For the estimated population datasets, we rely on the most recent United Kingdom Census data administered in 2021. The data is ingested at the Output Area (OA) level, which is the smallest geographical unit for which census data is available. Further processing will aggregate the data to the desired spatial unit of analysis.

OpenStreetMap POIs

OpenStreetMap (OSM) is a collaborative mapping project that provides a free and open-source map of the world. The version of OSM data used in this analysis is packaged by an OpenStreetMap

community project Geofabrik and provides a snapshot of the OSM database as of June 2024. Geofabrik also standardises the categorisation of POIs' amenity attributes in the OSM database into larger classes[1]. Our analysis will use this default POI classification, extracting 12 amenity POI types. Lastly, apart from amenity POIs, we also make use of the OSM transport POIs point data to derive non-TfL transport-related features, such as national rail stations, ferry piers, long-distance bus stations and airports.

Combined with transport node data acquired from TfL open data sources, all extracted Amenity and Transport POI types of interest are summarised in Table A.2.

	POI Type	**Examples**
Amenity	*Public Facilities*	Post offices, schools, universities, libraries,...
	Medical	Hospitals, clinics, pharmacies,...
	Entertainment	Theatres, Night clubs, cinemas,...
	Outdoors	Parks, playgrounds,...
	Active	Sports centres, swimming pools, stadiums,...
	Restaurants	Restaurants, cafes, pubs, bars,...
	Hotels	Hotels, motels, hostels,...
	Shopping	Supermarkets, bakeries, florists, bookshops, malls,...
	Banking	Banks, ATMs,...
	Tourism	Tourist attractions, museums, monuments, viewpoints,...
	Religious	Churches, mosques, temples,...
	Nature	Riverbanks, beaches, hills,...
Transport	*Bus stops*	Bus stops and stations (TfL)
	Rail stations	TfL rail stations (TfL) and Non-TfL rail stations (OSM)
	Other transport hubs	Airports, ferry piers, long-distance bus stations (OSM)

Table A.2: Summary of Amenity and Transport POI types used in the analysis

[1]More information about Geofabrik's OSM data product can be found in Geofabrik OSM data dictionary

A.2 Supplemental Figures

Figure A.1: Map of the spatial k-fold cross-validation splits for hyperparameter tuning and performance assessment (k=10)

Figure A.2: Summary of feature importance based on SHAP values of a sample. Red-Blue scale represents the feature value, and the x-axis represents the SHAP value, i.e., impact on final model prediction of arrivals in each time band (log)

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