Modeling and Forecasting the Impact of Major Technological and Infrastructural Changes on Travel Demand

By

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Abstract

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The transportation system is undergoing major technological and infrastructural changes, such as the introduction of autonomous vehicles, high speed rail, carsharing, ridesharing, flying cars, drones, and other app-driven on-demand services. While the changes are imminent, the impact on travel behavior is uncertain, as is the role of policy in shaping the future. Literature shows that even under the most optimistic scenarios, society’s environmental goals cannot be met by technology, operations, and energy system improvements only – behavior change is needed. Behavior change does not occur instantaneously, but is rather a gradual process that requires years and even generations to yield the desired outcomes. That is why we need to nudge and guide trends of travel behavior over time in this era of transformative mobility. We should focus on influencing long-range trends of travel behavior to be more sustainable and multimodal via effective policies and investment strategies. Hence, there is a need for developing policy analysis tools that focus on modeling the evolution of trends of travel behavior in response to upcoming transportation services and technologies. Over time, travel choices, attitudes, and social norms will result in changes in lifestyles and travel behavior. That is why understanding dynamic changes of lifestyles and behavior in this era of transformative mobility is central to modeling and influencing trends of travel behavior. Modeling behavioral dynamics and trends is key to assessing how policies and investment strategies can transform cities to provide a higher level of connectivity, attain significant reductions in congestion levels, encourage multimodality, improve economic and environmental health, and ensure equity.

This dissertation focuses on addressing limitations of activity-based travel demand models in capturing and predicting trends of travel behavior. Activity-based travel demand models are the commonly-used approach by metropolitan planning agencies to predict 20-30 year forecasts. These include traffic volumes, transit ridership, biking and walking market shares that are the
result of large scale transportation investments and policy decisions. Currently, travel demand models are not equipped with a framework that predicts long-range trends in travel behavior for two main reasons. First, they do not entail a mechanism that projects membership and market share of new modes of transport into the future (Uber, autonomous vehicles, carsharing services, etc). Second, they lack a dynamic framework that could enable them to model and forecast changes in lifestyles and transport modality styles. Modeling the evolution and dynamic changes of behavior, modality styles and lifestyles in response to infrastructural and technological investments is key to understanding and predicting trends of travel behavior, car ownership levels, vehicle miles traveled (VMT), and travel mode choice. Hence, we need to integrate a methodological framework into current travel demand models to better understand and predict the impact of upcoming transportation services and technologies, which will be prevalent in 20-30 years.

The objectives of this dissertation are to model the dynamics of lifestyles and travel behavior through:

- Developing a disaggregate, dynamic discrete choice framework that models and predicts long-range trends of travel behavior, and accounts for upcoming technological and infrastructural changes.
- Testing the proposed framework to assess its methodological flexibility and robustness.
- Empirically highlighting the value of the framework to transportation policy and practice.

The proposed disaggregate, dynamic discrete choice framework in this dissertation addresses two key limitations of existing travel demand models, and in particular: (1) dynamic, disaggregate models of technology and service adoption, and (2) models that capture how lifestyles, preferences and transport modality styles evolve dynamically over time. This dissertation brings together theories and techniques from econometrics (discrete choice analysis), machine learning (hidden Markov models), statistical learning (Expectation Maximization algorithm), and the technology diffusion literature (adoption styles). Throughout this dissertation we develop, estimate, apply and test the building blocks of the proposed disaggregate, dynamic discrete choice framework. The two key developed components of the framework are defined below.

First, a discrete choice framework for modeling and forecasting the adoption and diffusion of new transportation services. A disaggregate technology adoption model was developed since models of this type can: (1) be integrated with current activity-based travel demand models; and (2) account for the spatial/network effect of the new technology to understand and quantify how the size of the network, governed by the new technology, influences the adoption behavior. We build on the formulation of discrete mixture models and specifically dynamic latent class choice models, which were integrated with a network effect model. We employed a confirmatory approach to estimate our latent class choice model based on findings from the technology diffusion literature that focus on defining distinct types of adopters such as innovator/early adopters and imitators. Latent class choice models allow for heterogeneity in the utility of adoption for the various market segments i.e. innovators/early adopters, imitators and non-adopters. We make use of revealed preference (RP) time series data from a one-way carsharing system in a major city in the United States to estimate model parameters. The data entails a complete set of member enrollment for the carsharing service for a time period of 2.5 years after being launched. Consistent with the technology diffusion literature, our model identifies three latent classes whose utility of adoption
have a well-defined set of preferences that are statistically significant and behaviorally consistent. The technology adoption model predicts the probability that a certain individual will adopt the service at a certain time period, and is explained by social influences, network effect, socio-demographics and level-of-service attributes. Finally, the model was calibrated and then used to forecast adoption of the carsharing system for potential investment strategy scenarios. A couple of takeaways from the adoption forecasts were: (1) highest expected increase in the monthly number of adopters arises by establishing a relationship with a major technology firm and placing a new station/pod for the carsharing system outside that technology firm; and (2) no significant difference in the expected number of monthly adopters for the downtown region will exist between having a station or on-street parking.

The second component in the proposed framework entails modeling and forecasting the evolution of preferences, lifestyles and transport modality styles over time. Literature suggests that preferences, as denoted by taste parameters and consideration sets in the context of utility-maximizing behavior, may evolve over time in response to changes in demographic and situational variables, psychological, sociological and biological constructs, and available alternatives and their attributes. However, existing representations typically overlook the influence of past experiences on present preferences. This study develops, applies and tests a hidden Markov model with a discrete choice kernel to model and forecast the evolution of individual preferences and behaviors over long-range forecasting horizons. The hidden states denote different preferences, i.e. modes considered in the choice set and sensitivity to level-of-service attributes. The evolutionary path of those hidden states (preference states) is hypothesized to be a first-order Markov process such that an individual’s preferences during a particular time period are dependent on their preferences during the previous time period. The framework is applied to study the evolution of travel mode preferences, or modality styles, over time, in response to a major change in the public transportation system. We use longitudinal travel diary from Santiago, Chile. The dataset consists of four one-week pseudo travel diaries collected before and after the introduction of Transantiago, which was a complete redesign of the public transportation system in the city. Our model identifies four modality styles in the population, labeled as follows: drivers, bus users, bus-metro users, and auto-metro users. The modality styles differ in terms of the travel modes that they consider and their sensitivity to level-of-service attributes (travel time, travel cost, etc.). At the population level, there are significant shifts in the distribution of individuals across modality styles before and after the change in the system, but the distribution is relatively stable in the periods after the change. In general, the proportion of drivers, auto-metro users, and bus-metro users has increased, and the proportion of bus users has decreased. At the individual level, habit formation is found to impact transition probabilities across all modality styles; individuals are more likely to stay in the same modality style over successive time periods than transition to a different modality style. Finally, a comparison between the proposed dynamic framework and comparable static frameworks reveals differences in aggregate forecasts for different policy scenarios, demonstrating the value of the proposed framework for both individual and population-level policy analysis.

The aforementioned methodological frameworks comprise complex model formulation. This however comes at a cost in terms of prolonged computation and estimation times. Due to the non-convex nature of the objective function, direct maximization of the likelihood could become
difficult and highly unstable. An alternative approach would be to use the Expectation Maximization (EM) algorithm instead of traditional gradient descent algorithms. This particular statistical learning technique is more stable, and requires fewer iterations to converge by taking advantage of the conditional independence structure of the model framework. This dissertation will provide rigorous derivation, formulation and application of the EM algorithm for mixture models and hidden Markov models with logit kernels, which constitute the building blocks of the generalized dynamic framework. Using such a statistical learning technique, i.e. the EM algorithm, model estimation time will be reduced from the order of many hours to minutes.

The line of work initiated throughout this dissertation is critical in this era of transformative mobility in terms of developing a generalized model that accounts for adoption styles and dynamic modality styles. The proposed dynamic, disaggregate discrete choice framework models the evolution of travel and activity behavior over time in addition to the adoption and diffusion of new transportation services. The proposed framework can be integrated with current travel demand models through the construct of adoption styles and modality styles, which shall provide a deeper understanding of behavioral dynamics and trends of travel behavior in an attempt to better inform long-range policy making. This dissertation provides the building blocks to advance the field of travel demand modeling in order to guide transformative mobility into the envisioned sharing economy future.
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Chapter 1

Introduction

1.1 Motivation

The growth in population and urban development has impacted societies in one way or another from air pollution to greenhouse gas emission, climate change and traffic congestion. This in turn encouraged more investments in infrastructure and technological services to take place. Behavioral change in terms of motivating people towards the use of more sustainable modes of transport is necessary to achieve the required reductions in traffic congestion and efficient usage of the available infrastructure. And as we know people are at the heart of most of the issues in metropolitan studies, in which prime objectives are to better understand and improve the urban environment. The behavioral and decision-making process that individuals and consumers undergo can’t be overlooked when it comes to evaluating a set of investment strategies or policies aimed at improving sustainable mobility and multimodality. Modeling this decision-making process is key to (1) identifying the most effective policy or investment strategy catered towards behavioral change, (2) predicting and forecasting the demand of policies and investment strategies for a certain population in a more representative manner, and (3) specifying sources of heterogeneity in tastes and preferences.

Major investments in technology and infrastructure are expected to occur over the next decades such as the introduction of autonomous vehicles, connected vehicles, high speed rail, carsharing and ridesharing. This shall induce potential paradigm shifts in the cost, speed, safety, convenience and reliability of travel. Together, they are expected to influence both short-term travel and activity decisions, such as where to go and what mode of travel to use, and more long-term travel and activity decisions, such as where to live and how many cars to own. This transformative mobility trend, whether in the form of sharing economy, connected vehicles, autonomous and app-driven on-demand vehicles and services will impact travel and activity behavior through disrupting the need to travel and the disutility of travel. While the changes are imminent, the impact on travel behavior is uncertain as is the role that policy can play in shaping the outcome. We want the future to consist of sustainable and efficient systems, which cannot be attained by technology, operations, and energy system improvements only – behavior change is needed. Developing quantitative behavioral analysis tools that focus on modeling and influencing trends of travel behavior to guide transformative mobility and set it on the right track is a key ingredient. This is a critical component in the design of smart cities that need to be shaped with the correct set of policies and regulations to attain the desired goals and outcomes.

Moreover, the automobile has long been the preeminent mode of transportation, more so in the United States (US) than anywhere else. However, the last decade has heralded a generational change within much of the developed world in terms of attitudes towards the car. Between 2000 and 2010, in the US alone, car sales went down by 35.8 percent, per capita highway passenger vehicle miles traveled (VMT) decreased by 6.7 percent, while the proportion of the driving age population that is licensed to drive declined from 88.0 percent to 86.4 percent (Office of Highway Policy Information). Researchers have referred to this process or phenomenon as “peak auto” with
the reversal in the car dependence being variously attributed to factors that include a stagnant economy, an aging population, rising oil prices, a renewed interest in urbanism, growth in e-commerce, the spread of online social network, and the smart phone revolution.

Figure 1.1: Current and Upcoming Infrastructural and Technological Investments

The impact of comparable changes in technology and infrastructure in the past has thus far been examined retrospectively. A framework for predicting long-range trends in travel behavior, such as the peak auto or the rise of carsharing and ridesharing, remains lacking. As a consequence, transportation specialists, practitioners and policy-makers have been historically forced to be more reactionary than visionary. That is why it is essential to develop quantitative methods for travel demand analysis that can be used to understand and predict long-range trends in travel and activity behavior in response to major infrastructural and technological changes affecting both the transportation and land use system. Over time, travel choices, attitudes, and social norms will result in changes in lifestyles and travel behavior. That is why understanding dynamic changes of lifestyles and behavior in this era of transformative mobility is central to modeling and influencing trends of travel behavior, and improving long-range forecasting accuracy.

1.2 Activity-based Travel Demand Models

Activity-based travel demand models are the commonly-used approach by metropolitan planning agencies to predict 20-30 year forecasts of traffic volumes, transit ridership, biking and walking market shares brought about from large scale transportation investments and policy decisions. These models try to assess the impacts of transportation investments, land use and socio-demographic changes on travel behavior with the main objective of predicting future mode shares, auto ownership levels, etc. These forecasts are critical in assessing the viability of any infrastructure investment or policy (e.g., parking, HOV lanes, etc.) as they predict how decisions now will play out in the future. Furthermore, results from these models will: (1) provide insight to locations and corridors bound to suffer from congestion in future years, (2) identify impacts of a
certain infrastructure investment or policy in mitigating congestion along congested spines or corridors, and (3) assess increase/reduction in greenhouse gas emissions (GHG). This dissertation contributes to efforts that aim at addressing shortcomings of current activity-based travel demand models in order to account for transformative technological and infrastructural changes.

This section provides a brief overview of the various components of activity-based travel demand models. The strong relationship that exists between travel and activities comprises the basis for these types of models (Bhat and Koppelman, 1999). Travel is assumed to be a derived demand whereby people travel to participate in certain activities (shopping, work, recreational, etc.). The figure below displays the modeling framework of the San Francisco Chained Activity Modeling Process (SF-CHAMP). It is evident that several interdependent models make up the travel demand modeling framework. Some of the key sub-models are described below:

a- **Population Synthesizer**

This component comprises microsimulation techniques as opposed to the traditional sample enumeration methods. Microsimulation focuses on modeling the behavior of a sample of individuals and households that are representative of the target population. A sample is created that entails decision-makers and households with a set of socio-demographics and other characteristics that match the designated population. The synthesized individuals are assigned respectively to households, which have a defined list of characteristics (number of workers, number of vehicles owned, etc.). Following that, households are mapped to various residential locations that are in turn divided into travel analysis zones (TAZ).

b- **Vehicle Availability Model**

This component evaluates the auto ownership level for each of the households. The choice of owning zero or multiple vehicles is modeled as a function of characteristics of the household.

c- **Full-Day Tour Pattern Models**

These types of models predict the tour patterns for each of the individuals in the population synthesizer. Five types of tours are included in the SF-CHAMP framework:

1. Home-based work primary tours
2. Home-based education primary tours
3. Home-based other primary tours
4. Home-based secondary tours
5. Work-based sub-tours

A home-based tour comprises the entire set of trips conducted by the time a decision-maker leaves his/her house until he/she gets returns home. Primary versus secondary tours vary based on the trip purpose. For example, education, work, shopping, personal business, social/recreation, and serve passengers are considered as primary tours (Primerano, 2008). The remaining trip purposes are considered as secondary.
Figure 1.2: SF-CHAMP Modeling Framework
d- **Time of Day Models**

This component models the start time, end time, and duration of all trips in a certain tour (Abou Zeid et al., 2006). Models are estimated at two different levels. First level entails “modeling the joint choice of arrival time at a primary destination of the tour and departure time from the primary destination of the tour” while the second level comprises “modeling the arrival time at or departure time from the intermediate stop and consequently its duration” (Abou Zeid et al., 2006).

e- **Tour/Trip Mode Choice Models**

This component models travel mode choice for various tours and trips. In other words, probabilistic models are developed to predict the primary mode used for each of the available tours in addition to each of the conducted trips. Choice set consideration for the trip mode choice consists of available modes of transport.

The aforementioned models are typically specified as binary, multinomial or nested logit choice models. Random utility models and in particular discrete choice analysis constitute the building blocks of activity-based travel demand models.

### 1.3 Discrete Choice Analysis and Random Utility Models

Discrete choice analysis (Ben-Akiva and Lernam, 1985) focuses on modeling a dependent variable that takes on discrete values. Discrete choice modeling is widely used in the transportation industry for travel demand modeling and forecasting. However, models of this kind are applicable to a wide variety of businesses and public organizations, with the objective of better understanding and predicting the demand and market shares for goods and services. These techniques are widely used in market research and quantitative marketing. Of great interest is the identification of key variables that shape the demand of a certain good/service, which include, but are not limited to, characteristics of the decision-maker, attributes of the available alternatives, attitudes and perceptions, as well as social influences.

Random utility models are based on the notion that decision-makers associate a “utility” with each of the available alternatives in their consideration set. Utility is an abstract concept that tries to quantify the level of attractiveness of a certain alternative (McFadden, 2001; Ben-Akiva and Lerman, 1985). The decision-maker is postulated to choose the alternative that maximizes his/her random utility. Other decision rules exist but utility maximization has been the decision rule of choice for studies on individual and household travel and activity behavior. Note that utility is not observed by the analyst, which is why it is treated as a random variable. Random utility is broken down into an observable deterministic component and an unobservable component (adapted from Walker, 2001):

\[
U_{in} = V(X_{in}; \beta) + \varepsilon_{in}
\]

where:

- \(U_{in}\) denotes the random utility of an alternative \(i\) for individual \(n\)
- \(V\) denotes the function that expresses the systematic/observable component of utility as a function of explanatory variables
$X_{in}$ denotes explanatory variables; attributes of alternative $i$ and characteristics of individual $n$

$\beta$ denotes the parameter vector to be estimated

$\varepsilon_{in}$ denotes the random/unobservable component of random utility

The most common class of discrete choice models is the multinomial logit (MNL), which assumes the following (McFadden, 2001; Ben-Akiva and Lerman 1985):

- Utility maximization decision rule
- $\varepsilon_{in}$ are i.i.d. and follow an extreme value type I (Gumbel) distribution across individuals and alternatives with a certain scale parameter and location parameter
- Set scale parameter $\mu$ to 1 and location parameter of the distribution to 0

The specification of the model is as such:

$$ U_{in} = V(X_{in}; \beta) + \varepsilon_{in} $$

structural equation

$$ y_{in} = \begin{cases} 1 & \text{if } U_{in} = \max_j \{ U_{jn} \} \\ 0 & \text{otherwise} \end{cases} $$

measurement equation

Those assumptions lead to the following individual choice probabilities:

$$ P(y_{in} = 1 \mid X_n; \beta) = \frac{e^{V(X_{in}; \beta)}}{\sum_{j \in C_n} e^{V(X_{jn}; \beta)}} $$

where:

$C_n$ denotes the choice set available to decision-maker $n$

The logit model is characterized by the following property: Independence from Irrelevant Alternatives (IIA). IIA implies that for a given decision-maker, the ratio of the choice probabilities for any two alternatives is completely unaffected by the systematic utilities of any of the remaining alternatives. Alternative choice models such nested logit, cross-nested logit, multinomial probit models and mixture logit models account for the IIA restriction and formulate a less constrained variance co-variance matrix structure of the disturbances. The nested logit (NL) model accounts for possible correlations that could exist between alternatives in the form of correlations between the error terms. The proposed method in NL models is to group correlated alternatives together in one nest. Cross-nested logit (Vovsha, 1997) is a generalization of the NL model as it relaxes the correlation structure among alternatives even further whereby an alternative can belong to multiple nests at the same time. The multinomial probit (MNP) model exhibits the least restricted structure of the variance co-variance matrix of the error terms, whereby all alternatives depict some sort of correlation. This specification flexibility comes at a cost, which is computation time especially with an increase in the number of available alternatives.

Finally, mixture models try to model and capture unobserved heterogeneity in the decision-making process. Mixture models can be divided into two categories: discrete versus continuous. Discrete mixture models in the choice modeling world are referred to as Latent Class Choice Models
(LCCMs). These types of models assume that discrete market segments exist in the population, which are latent (unobserved). Those latent segments are characterized by different sensitivities to attributes of the alternatives and socio-demographic variables, in addition to possible distinct decision rules and choice sets (Kamakura and Russel 1989; Gopinath, 1995). Continuous mixture models on the other hand, assume that parameters associated with attributes of the alternatives are not fixed point estimates. Rather, different individuals have different sensitivities to attributes of the alternatives or other explanatory variables. This could be accounted for by allowing parameters to follow a certain distribution (normal, log-normal, etc.).

1.4 Behavioral Theory and Discrete Choice Analysis
The basic adopted discrete choice framework in the literature and in practice is represented in the figure below. Causal relationships are represented by solid arrows while measurement relationships are represented by dashed arrows. The derived utility for each of the alternatives is a function of explanatory variables: attributes of the alternatives and characteristics of the decision-maker that try to capture significant variables that influence the decision-making process. The choices made by a consumer comprise the manifestation of preferences as denoted by Random Utility Maximization (RUM) principle.

![Figure 1.3: Standard Discrete Choice Framework](image)

There is a gap between the adopted standard discrete choice framework and the actual behavioral decision process. Many psychological factors play a role in defining a consumer’s decision process such as perceptions, beliefs, attitudes, motives, etc. The figure below (McFadden, 1999) highlights the complexity of the decision-making process. In order to address some of the complexity of the behavioral process, Walker and Ben-Akiva (2002) developed an extension to the existing discrete choice modeling framework. They proposed integrating discrete choice and latent variable models. The model comprises two components: the first is the standard discrete choice model while the latter is a latent variable model. This integrated framework provides a richer behavioral dimension by incorporating the effects of psychometric and psychological constructs of attitudes and perceptions into the decision-making process.

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Based on the above figure, it is evident that preferences affect the choice of a certain decision-maker. At the same time, preferences are influenced by choices, attitudes, beliefs and other exogenous variables. One of the neoclassical assumptions in discrete choice models constitutes the fact that preferences, which denote taste parameters and the respective choice set, are stable over time. This limitation has been criticized across multiple disciplines since it serves as a major setback in capturing behavioral response to changes in the built environment in a representative manner (Hirschman, 1982; Pollak, 1978; Tversky and Thaler, 1990). Literature claims that preferences could evolve over time due to changes in socio-demographics, life cycle events, attitudes, perceptions, values, normative beliefs, and alternative attributes (for example due to changes in the transportation and land use systems). Literature also suggests that preferences and choices in previous time periods can in turn influence preferences and choices in future time periods (Bronnenberg et al., 2012; and Aarts et al., 1997). In this era of transformative mobility, the range of travel choices will be wider over time, which in turn influences lifestyles, preferences and travel behavior. That is why dynamic modeling of changes in lifestyles, preferences and behavior in response to infrastructural and technological investments is central to modeling trends of travel behavior and improving long-range forecasting accuracy. However, current travel demand models do not reflect such dynamics, which becomes questionable in times such as the present, with transformative mobility potentially revolutionizing travel and activity behavior. In this dissertation, we do account for this limitation by developing a structural approach for modeling and forecasting the dynamic evolution of preferences and lifestyles over time.

1.5 Limitations of Activity-based Travel Demand Models in Capturing Trends of Travel Behavior

Current travel demand models are unable to predict long-range trends in travel behavior for the following four reasons. First, existing models are estimated using cross-sectional travel diary datasets collected over the course of a day or two. These observation periods are not long enough
to capture the variability in the transportation and land use system that might be observed over long-range forecasting horizons spanning 20-30 years into the future, particularly in the wake of major technological and infrastructural changes.

Second, existing models employ static frameworks which assume that individuals are unaffected by past experiences and future expectations. This overlooks the relationship between decisions made at different points in time. Studies on cohort analysis have repeatedly demonstrated how individuals in similar circumstances when faced with similar choices may respond differently, based on differences in their past. For example, Bush (2003) identifies cohort differences in travel behavior between senior citizens in the US who grew up after the end of the Second World War (baby boomers). A static framework would assume that the behavior of senior citizens from the silent generation could be used as a predictor of senior citizens from the baby boomers. A dynamic framework on the other hand would recognize that differences in past experiences and future expectations could result in very different outcomes for senior citizens across the two generations. As mentioned earlier, over time, travel choices, attitudes, and social norms will result in changes in lifestyles and travel behavior. That is why incorporating a dynamic framework into existing travel demand models is key for modeling and forecasting changes in trends of travel behavior, and improving long-range forecasting accuracy.

Third, existing models fail to account for the influences of deeply ingrained lifestyles built around the use of a particular travel mode or set of travel modes or in other words, modality styles (Vij, 2013), on different dimensions of travel behavior. In the context of travel mode choice, different modality styles may be characterized by the set of travel modes that an individual considers, and his/her sensitivity to different level-of-service attributes of the transportation and land use system. For example, research on modality styles in the Bay Area for the year 2000 finds that 29 percent of the population is entirely dependent on the automobile for mobility requirements (Vij and Walker, 2014). On one hand, advances such as increases in fuel efficiency or the introduction of autonomous vehicles could reinforce existing modality styles built around the car. On the other hand, newer technology services such as ridesharing and carsharing could help overturn car-dependent modality styles and encourage more multimodal behavior. When evaluating their impact, it is therefore important to have an understanding of the distribution of modality styles in the population. Modality styles are indeed critical determinants of observable behavior. A greater understanding of dynamic changes in modality styles in response to infrastructural and technological investments is central to understanding any and all trends in travel behavior, including car ownership, vehicle miles traveled and travel mode choice.

Fourth, existing travel demand models do not entail a mechanism that projects membership and market share of new modes of transport (Uber, Lyft, autonomous vehicles, etc.) into the future. According to Guerra (2015), “only two metropolitan planning organizations in the 25 largest metropolitan areas mention autonomous or connected vehicles in their long-range regional transportation plans”. It is important to develop quantitative methods to project membership of those upcoming modes of transportation in this era of transformative mobility as their market share forecasts are critical from a planning and policy perspectives. Assessing future market shares of existing and upcoming modes is necessary to quantify the impacts of a certain investment in infrastructure and technology. In other words, current travel demand models lack a methodological framework that caters for those upcoming transportation services and technologies and their impact on travel behavior, which will be prevalent in 20-30 years.
1.6 Objectives
My overall objective in this dissertation is to develop a disaggregate, dynamic discrete choice framework to understand and predict long-range trends in travel behavior, specifically:

1- Trends of evolution of preferences, lifestyles and transport modality styles in response to changes in socio-demographic variables and the built environment.
2- Trends of technology and service adoption, in order to gain insight about the projected market shares of upcoming modes of transport.

This dissertation will also provide the derivation and formulation of all required steps of the Expectation Maximization (EM) algorithm in the context of discrete mixture models and hidden Markov models with logit kernels to save on computation and estimation time. Throughout the dissertation, empirical results are presented to highlight findings and to empirically demonstrate and test the proposed framework in the case of transformative mobility.

1.7 Methodological Framework
The proposed methodological framework in this dissertation tries to capture the impact of transformative technologies and infrastructural changes within the transportation and land use systems on trends of travel and adoption behavior. The figure below displays the proposed disaggregate, dynamic discrete choice framework, which associates a direct relationship between the transportation network level-of-service at time period t+1 and the travel and activity behavior during the previous time period t.

As we typically assume in these types of models, we are conditioning on the transportation network level-of-service (LOS). In order to model the evolution of preferences over time, we will use the construct of modality styles to denote preference states. Modality styles are defined as lifestyles built around the use of a travel mode or set of travel modes people consider when making mode choice decisions. Modality styles try to capture distinct segments of the population with different preferences i.e. modes considered in the choice set and sensitivity to level-of-service attributes. This construct addresses one of the neoclassical limitations behind traditional travel demand models that assume decision-makers consider all available modes of transport in their respective consideration set when making travel and activity decisions. An individual’s modality style is hypothesized to be some function of his/her characteristics, for example: age, gender, level of education, household auto ownership level, etc., in addition to his/her past experiences and the transportation system level-of-service.

The dynamic evolution of preferences and lifestyles over time focuses on modeling how a decision-maker transitions from one preference state, modality style in the context of travel behavior, to another when faced with changes in the built environment or socio-demographic variables. As an example, this could be brought about by the introduction of a new rail system or mode of transport. A shock to the transportation system shall force individuals to reconsider their current travel behavior. This will in turn cause a change in the share of people in different modality styles in response to the emergence of newer ways for travel and activity engagement. Conditioned on an individual’s modality style, the travel and activity preferences denoted by utilities are unobserved but are assumed to be some function of the transportation and land use system in addition to the choice set at his/her disposal. The travel and activity behavior i.e. choice a consumer
Figure 1.5: Proposed Disaggregate, Dynamic Discrete Choice Framework
makes comprises the manifestation of those preferences via the Random Utility Maximization (RUM) principle.

Individual adoption styles on the other hand describe the latent adoption behavior of an individual to new technologies or services. Similarly, adoption styles are hypothesized to be some function of the individual’s socio-economic and demographic variables. We are assuming that adoption styles are not dynamically dependent over time. Adoption styles are innate characteristics of the decision-maker and will only be influenced by socio-demographic variables.

Now, conditional on both modality styles and adoption styles, the decision to adopt a new technology or service is some function of the attributes of the innovation and socio-demographic variables. We are hypothesizing that an individual’s modality style influences the adoption of newer technologies and services in addition to decisions concerning travel and activity behavior as mentioned above. The adoption utility at a certain time period is a function of the attributes of the new technology at that time period. Other explanatory variables can influence the adoption utility such as social influences whether in the spatial proximity spectrum i.e. an individual’s neighbors that live in a defined radius away from him/her or in the socio-demographic spectrum i.e. peers and individuals with similar socio-demographics. Finally, network effect shapes the adoption behavior in a particular direction. By network effect, we necessitate capturing the influence of the size of the transportation network to which the new transformative technology can reach out to. The choice of whether a decision-maker adopts a certain technology or not is observed and is assumed to be a manifestation of the adoption utility according to RUM principle.

There are three exogenous inputs to the above framework: socio-demographic characteristics of the population of interest, transportation level-of-service (LOS), and attributes of the new technology. Changes in socio-demographics, for example an increase in income or auto ownership levels will influence modality styles and incur changes in travel and activity behavior. Moreover, these changes will influence adoption styles, which together with changes in modality styles shall impact adoption behavior. Changes in the transportation system brought about from investments in infrastructure shall influence modality styles, which will in turn impact travel and activity behavior. Finally, changes in the attributes of the new technology, will have a direct impact on the adoption behavior.

1.8 General Overview of Model Framework in This Dissertation
The building blocks of the proposed dynamic, disaggregate discrete choice framework are estimated on two different datasets. First, we will estimate a disaggregate technology adoption model with a discrete choice kernel. This model tries to understand the technology adoption process of upcoming modes of transport and project their market shares for certain policies and investment strategies. Second, we will focus on estimating hidden Markov models with a discrete choice kernel to model and forecast the evolution of preferences and behaviors over time in response to changes in socio-demographic variables and the built environment. Together, those frameworks provide a structural approach to project market shares for various modes of transport in a more representative manner in the long run.
We will build on the following four areas of the literature to address the problem statement of this dissertation: technology diffusion (both aggregate and disaggregate), travel demand models that build on the construct of modality styles to capture heterogeneity in the decision-making process, preference instability in discrete choice models, and dynamic choice models. To develop a methodological framework to address the first component of our research motivation, we focus on technology adoption models that employ a microeconomic utility-maximizing representation of individuals. This framework is of interest to us as it could be integrated with disaggregate activity-based models. We are also interested in capturing the impact of social influences and network effect (spatial spectrum) of the new technology on the adoption process. In order to model the evolution of preferences and lifestyles over time, which is the second component of this dissertation, we focus on the construct of modality styles (Vij, 2013) to denote preference states. Finally, dynamic discrete choice models are of interest to us and in particular hidden Markov models (Baum and Petrie, 1966) as they provide a structural approach to model the evolution of preferences over time as a function of socio-demographic variables and the built environment.

The first piece of our methodological framework is governed by disaggregate technology adoption models. We build on the formulation of discrete mixture models and specifically Latent Class Choice Models (LCCMs), which allow for heterogeneity in the utility of adoption for the various market segments i.e. innovators/early adopters, imitators and non-adopters. We integrate our LCCM with a network effect model. The network effect model quantifies the impact of the spatial/network effect of the new technology on the utility of adoption. We make use of revealed preference (RP) time series data for a one-way car sharing system in a major city in the United States. The data entails a complete set of member enrollment ever since the service was launched. Consistent with the technology diffusion literature, our mixture model identifies three latent classes (market segments) with utilities of adoption that have a well-defined set of preferences that are statistically significant and behaviorally consistent. The technology adoption model focuses on assessing the effects of social influences, network effect, socio-demographics and level-of-service attributes on the adoption process of an individual. This model is extremely helpful as it allows us to communicate with each market segment and forecast adoption into the future for several investment strategies or policies. The model was calibrated and used to forecast adoption for certain policies and investment strategies. Major findings from the technology adoption model are: (1) a decision-maker is more likely to be a non-adopter, high-income groups and men are more likely to be early adopters or innovators; (2) placing a new station/pod for the carsharing system outside a major technology firm will increase the expected number of monthly adopters the most; and (3) no significant difference is observed regarding the expected number of monthly adopters for the downtown region between having a station or on-street parking.

The second piece of the framework focuses on estimating hidden Markov models (HMMs) with logit kernels to model and predict the evolution of individual preferences, lifestyles and behaviors over time. The dataset used comes from Santiago, Chile (Yañez, 2010). During February 2007, the city of Santiago introduced Transantiago, a complete redesign of the public transit system in the city. The dataset is longitudinal as it entails four one-week pseudo travel diaries throughout a twenty-two month period that overlapped with the introduction of Transantiago. This dataset offers the opportunity to investigate the effects of a sudden change in the transportation network and socio-demographic variables on preferences and lifestyles. We use the construct of modality styles to denote preference states. It is these modality style preference states that dynamically evolve
over time. This dynamic discrete choice model identifies the following modality styles (market segments) in the population: drivers, bus users, bus-metro users and auto-metro users. The modality style classes differ in terms of their choice set consideration and their sensitivity to level-of-service attributes (travel time, travel cost, etc.). The transition probability model identifies how preferences, which are captured by the construct of modality styles, evolve over time due to changes in socio-demographic variables and the built environment. Parameter estimates across all sub-models and in particular the class specific mode choice model were behaviorally consistent and statistically significant. Indeed, preferences of individuals in the population have shifted over time in terms of the choice set consideration and sensitivities to level-of-service attributes. This is denoted by an increase in the share of drivers, auto-metro users, and bus-metro users across the population after the introduction of Transantiago as opposed to a decrease in the share of bus users. Finally, a comparison between the proposed dynamic framework and comparable static frameworks reveals differences in aggregate forecasts for different policy scenarios, demonstrating the value of the proposed framework for both individual and population-level policy analysis.

1.9 Dissertation Outline
The dissertation is organized in the following manner:

- Chapter 2 focuses on the formulation and estimation of the disaggregate technology adoption model. We motivate disaggregate technology adoption models as they could be easily integrated with activity-based travel demand models. In addition to that, disaggregate models allow us to quantify the impact of the spatial component of the new technology and its attributes on the adoption behavior for various types of adopters. We also motivate discrete mixture models and in particular latent class choice models (LCCMs) that try to capture unobserved heterogeneity in the decision-making process. The model’s specification tries to assess the impact of socio-demographics, social influences, network effect (spatial component) and attributes of the new technology on the adoption behavior. Empirical results are presented using revealed preference data from a carsharing service in a major city in the United States. Forecasts of adoption of this new technology are presented for several policies and investment strategies to highlight the value and importance of the proposed model.

- Chapter 3 focuses on the specification and estimation of hidden Markov models (HMMs) with discrete choice kernels. The proposed methodological framework models and forecasts the evolution of individual preferences, lifestyles and transport modality styles over time in response to changes in socio-demographics and the transportation system level-of-service. The proposed specification of our HMM evaluates how the share of individuals in different preference states or modality styles will evolve over time, which will in turn impact travel and activity behavior. This methodological framework will also provide the means to: (1) forecast trends of travel behavior that are bound to occur as a result of investments in technology and infrastructure; and (2) predict market shares for modes of transport in the long-run more accurately.
Chapter 4 entails the derivation and formulation of the Expectation Maximization (EM) algorithm for the two types of models used in this dissertation: discrete mixture models and hidden Markov models with logit kernels.

Chapter 5 provides a comprehensive summary of the research motivation, objective, adopted methodological frameworks and corresponding findings. This chapter also focuses on identifying future research directions for the proposed disaggregate, dynamic discrete choice framework that caters for transformative technological and infrastructural investments in the transportation and land use systems.

1.10 Contributions
This dissertation focuses on the enhancement of current travel demand models by addressing the need for demand models for newly-emerging paradigms in travel, such as carsharing and ridesharing. The proposed methodological framework shall enhance our understanding of the future of transformative mobility. The proposed quantitative methods shall also improve our understanding of latent demand in the wake of system improvements where we interpret latent demand as the unrealized desire for travel that shall occur in the future due to major technological and infrastructural changes. This dissertation provides the building blocks to advances in travel demand modeling required to guide transformative mobility to a sustainable and efficient system via effective policies and investment strategies.

This dissertation makes contributions along three directions. First, the study contributes to the existing body of literature on technology diffusion through the development of a disaggregate technology adoption model that caters for the adoption behavior and uptake of new services/technologies by various market segments. A disaggregate technology adoption model was developed as it can: (1) be integrated with current activity-based travel demand models; and (2) account for the spatial/network effect of the new technology to understand and quantify how the size of the network, governed by the new technology, influences the adoption behavior. Our technology adoption model accounts for the effects of social influences, network/spatial effect, socio-demographics and attributes of the technology on the adoption behavior of each of the market segments. This entails a behaviorally richer dimension as we try to account for taste heterogeneity in the adoption process for different types of adopters, which will in turn improve forecasting accuracy. The proposed framework could be used to predict future market shares of upcoming modes of transport for various policies and investment strategies.

Second, our work contributes to the discrete choice modeling literature by extending the application of hidden Markov models to model and forecast the evolution of preferences over time in response to changes in socio-demographics and the built environment. Our framework also accounts for the influence of past experiences on present preferences. Quantifying the evolution of preferences is a key ingredient in modeling and predicting trends of travel behavior in response to transformative technologies and services. Our proposed HMM will enable practitioners and policy makers to influence and nudge trends of travel behavior to be more sustainable and multimodal. The proposed dynamic framework shall also improve the accuracy of market share forecasts in the long-run for various transportation investments and policy decisions.
Third, this dissertation tackles a major issue that is bothersome when it comes to estimating advanced discrete choice models. Advanced models are prone to prolonged computation and estimation time. In this dissertation, we provide the derivation, formulation, and application of the Expectation Maximization (EM) algorithm in the context of mixture models and hidden Markov models with logit kernels. This shall enable travel demand and behavioral modelers to estimate such advanced models while saving on computation time. Using such a statistical learning technique i.e. the EM algorithm, model estimation time will be reduced from the order of many hours to minutes.
Chapter 2

A Discrete Choice Framework for Modeling and Forecasting the Adoption and Diffusion of New Transportation Services

2.1 Introduction
The growth in population and urban development has impacted societies in one way or another from air pollution to greenhouse gas emission, climate change and traffic congestion. This made policy makers more inclined towards the development of smart cities that promote sustainable mobility, connectivity and multimodality. As such, major technological and infrastructural changes are expected to occur over the next decades such as the introduction of autonomous vehicles, advances in information and communication technology, California high speed rail, carsharing and ridesharing. This will induce potential paradigm shifts in the cost, speed, safety, convenience and reliability of travel. Together, they are expected to influence both short-term travel and activity decisions, such as where to go and what mode of travel to use, and more long-term travel and activity decisions, such as where to live and how many cars to own. This transformative mobility, whether in the form of sharing economy, connected vehicles, autonomous and app-driven on-demand vehicles and services will revolutionize travel and activity behavior.

Travel demand models are the commonly-used approach by metropolitan planning agencies to predict 20-30 year forecasts of traffic volumes, transit ridership, walking and biking market shares across transportation networks. These models try to assess the impacts of transportation investments, land use and socio-demographic changes on travel behavior with the main objective of predicting future mode shares, auto ownership levels, etc. These models focus on a behaviorally richer approach to modeling travel mode choice as opposed to the traditional four step travel demand models. Travel demand models evaluate travel and activity behavior as a series of interdependent logit and nested logit models that entail travel mode choice as opposed to the traditional four step travel demand models. Travel demand models are unable to predict long-range trends in travel behavior as they do not entail a mechanism that projects membership and market share of new modes of transport (Uber, Lyft, autonomous vehicles, etc). According to Guerra (2015), “only two metropolitan planning organizations in the 25 largest metropolitan areas mention autonomous or connected vehicles in their long-range regional transportation plans”. That is why current travel demand models lack a methodological framework that caters for those upcoming transportation services and technologies and their impact on travel behavior which will be prevalent in 20-30 years.

Our objective is to develop a methodological framework tailored to model the technology diffusion process by focusing on quantifying the effect of the spatial configuration of the new technology and socio-demographic variables. Moreover, we are also interested in capturing the effect of social influences and level-of-service attributes of the new technology on the adoption process. The methodological framework used in our analysis entailed an integrated latent class choice model
(LCCM) and network effect model that was governed by a destination choice model. Our approach was confirmatory as the latent classes used in the analysis (innovators/early adopters, imitators and non-adopters) are rooted in the technology diffusion literature across multiple disciplines. These latent classes are able to capture heterogeneity in preferences towards technology adoption. Our research is motivated by existing work in technology adoption modeling which employs a microeconomic utility-maximizing representation of individuals. This framework is of interest to us as it could be easily integrated with our disaggregate activity-based models. Our proposed disaggregate technology adoption model shall help planners and policy makers gain insight regarding the projected market shares of upcoming modes of transport for various policies and investment strategies at the public and private levels.

Most diffusion models employ an aggregate framework, for example the Bass model (Bass, 1969). While recent aggregate models have further enriched the specification of the Bass model, they still do not account for a range of policy variables (including the spatial configuration) that can be used to rank policies and investment strategies needed to maximize the expected number of adopters of a new technology in future time periods. Our methodological framework is different than other disaggregate models in the diffusion and transportation literature as it accounts for (1) heterogeneity in the decision-making process across distinct market segments that have a different adoption behavior; and (2) the spatial configuration effect of the new technology in terms of quantifying how an increase in the size of the network governed by the new technology will impact adoption.

This chapter contributes to the existing body of literature in providing a unique methodology to model the adoption behavior and uptake of new products/technologies by various market segments. Our model caters for the effects of social influences, network effect, socio-demographics and level-of-service attributes of the product on the adoption behavior of each of the market segments. The following framework could be used to predict future market shares of upcoming modes of transport as one specific type of application. The chapter is organized as follows: Section 2 provides a literature review of existing technology adoption and diffusion models. Section 3 provides the adopted methodological framework used to model technology adoption and details the framework of the dynamic Latent Class Choice Model (LCCM) and the network effect model. Section 4 explains the dataset used in the study. Section 5 discusses model results and model applications. Section 6 focuses on comparing forecasts between our proposed generalized adoption model and the Bass aggregate diffusion model for three different policy scenarios. Section 7 concludes the findings of this chapter.
2.2 Literature Review

Autonomous vehicles are on the horizon, not to mention the transformative mobility trend that is occurring in our transportation system via the introduction of electric vehicles, ridesharing, carsharing, and many other new technologies. In order to quantify the effect of transportation policies and investment strategies in a representative manner, travel demand models should be able to model and forecast market shares for those new modes of transportation. However, current travel demand models do not entail a mechanism to do so, which in turn provides the core motivation behind this chapter. We believe that models of technology adoption and diffusion, which are widely used across multiple industries and cultures to forecast uptake of new technologies, will bridge this gap in the transportation literature. Diffusion models are popular in a variety of disciplines such as: agriculture (Sunding and Zilberman, 2001; and Ward & Pulido-Velazquez, 2008), consumer durables (Delre et al., 2007; and Schramm et al., 2010), pharmaceutical industry (Desiraju et al., 2004), and the automobile industry and in particular aggregate diffusion patterns of car ownership (Dargay and Gately, 1999). Also, diffusion models have been estimated and used in forecasting across different cultures such as: United States, France, Spain and many other countries (please refer to Tellis et al., 2003).

Over the course of the next few paragraphs we will describe the central piece of the framework governed by the model of technology adoption. The adoption and diffusion of new technologies have received attention across multiple disciplines within economics and social sciences over the years. As defined by Rogers (1962), “diffusion is the process by which an innovation is communicated through certain channels over time among the members of a certain social system”.

Any innovation may be defined in terms of the relative advantage offered by the innovation over existing alternatives, the degree to which the innovation is consistent with existing needs and values, the measure of difficulty associated with using the innovation, the extent to which the innovation can be tried on a limited basis, and the ease with which the benefits of the innovation are tangible to others. Differences in social systems may be characterized by the pattern of relationships among members of the system, established norms of what constitutes acceptable and unacceptable behavior, and the degree to which individual agents are able to influence the behavior of others. Communication channels can be broadly classified as either mass media, such as the television, or interpersonal channels that require a direct exchange between two or more individuals.

Diffusion models are widely used in the marketing science domain and many other industries, as mentioned above, as they capture the dynamics behind the uptake of a new product in addition to forecasting its demand. Forecasting accuracy with diffusion models varies depending on the type of dataset being used, whether it’s homogenous or heterogeneous i.e. from different sources (Meade and Islam, 2006). Improvement with respect to specification of the diffusion models such as incorporating non-parametric parametrization and enhancing flexibility has helped increase forecasting accuracy across multiple disciplines (Meade and Islam, 2006).

Rogers (1962) defines the following five classes of adopters that influence the uptake of a certain technology across various disciplines: innovators, early adopters, early majority, late majority and laggards. Based on the mathematical formulation of the diffusion model of Bass (1969), adopters can be divided into two distinct groups: innovators and imitators with the latter comprising the remaining four classes of adopters listed above. The technology diffusion literature stresses on the importance of the role of those two different types of adopters in shaping the market penetration
rate of a new good or service (please refer to Mansfield, 1961; Mahajan et al., 1990; and Cavusoglu et al, 2010). Innovators are individuals that “decide to adopt an innovation independently of the decisions of other individuals in a social system” while imitators are adopters that “are influenced in the timing of adoption by the pressures of the social system” (Bass, 1969).

Throughout the next few paragraphs, we will describe the assumptions and formulations of aggregate and disaggregate technology adoption models, and motivate why disaggregate models are a better methodological approach to our research question. Aggregate models of technology diffusion formulate the percentage of the total population that has adopted an innovation at some time period as some function of the characteristics of the population and the attributes of the innovation. The empirical research on aggregate models was pioneered by Griliches (1957), Mansfield (1961), and Bass (1969). The Bass model is well-known in the marketing science literature and it formulates the probability that a certain consumer will make an initial purchase at a given time t given that no purchase has been yet made by that specific consumer denoted as $P_t$ in the equation below as a linear function of the number of previous buyers:

$$P_t = p + \frac{q}{M} Y(t)$$

$p$: Coefficient of innovation; $q$: Coefficient of imitation; $M$: Total potential market for the technology

$Y(t)$: Cumulative number of individuals that adopted the new technology by time t (number of previous buyers)

The term $\frac{q}{M} Y(t)$ reflects the “pressures operating on imitators with an increase in the number of previous buyers” (Bass, 1969) while $p$ reflects the percentage of adopters that are innovators.

Using this formulation, sales of a certain technology/product could be forecasted into the future via a closed form solution. We are interested in the formulation of the Bass model as it identifies the two types of adopters of a new technology in addition to capturing the effect of social influence onto the probability of adoption. The figure below depicts the sales of a product over time (bell-shaped curve, $S(t)$) and cumulative sales over time (“S”-shaped curve, $Y(t)$) according to Bass (1969). The plot below uses a value of 0.005 for the coefficient of innovation $p$, 0.3 for coefficient of imitation $q$, and 100 for total potential market $M$. Those values were chosen arbitrarily to display the shape of the $S(t)$ and $Y(t)$ curves and provide useful insights. It is evident from the “S”-shaped diffusion curve that once a certain good or service is introduced in a market, it exhibits a low adoption rate followed by takeoff whereby the market experiences high adoption rates. After the takeoff period, technology adoption slows down until it reaches market saturation.

Mansfield (1961) on the other hand formulates the cumulative sales of a good/service using a logistic model, which is a special case of the Bass model ($p=0$). Extensions of the Bass model and more recent enhancements to aggregate diffusion models (see for example Kamakura and Balasubramanian, 1988; and Meade & Islam, 2006), have incorporated the effects of price, advertising and other marketing variables into the model parametrization in an attempt to increase forecasting power. Furthermore, aggregate models have been developed to assess the diffusion levels of a certain technology across different countries. Recently, agent-based modeling and simulation methods are becoming more popular in the technology diffusion discipline as they are estimated on an individual level. This will in turn address some of the shortcomings of aggregate
Diffusion models and cater for heterogeneity among consumers and explicit social structure (Kiesling et al., 2012; and Schramm et al., 2010).

Disaggregate models of technology adoption on the other hand formulate the probability that an individual or household adopts an innovation as some function of the characteristics of the decision-maker, attributes of the alternative, communication channels (both interpersonal networks and mass media) and time in order to cater for the temporal dimension of the diffusion process. These models have been used to predict the adoption of a wide variety of technologies and innovations that include color televisions, genetically modified crops, irrigation technology, computers, diapers and drill bits (Zilberman et al., 2012). Disaggregate models are of interest to us for the following reasons: (1) they employ a microeconomic utility-maximizing representation of individuals that provides insight into the decision-making process underlying the adoption or non-adoption of different innovations by consumers, which is consistent with the framework typically employed by travel demand models; (2) they capture various sources of heterogeneity in the decision-making process that will drive different consumers to adopt at different times; (3) they can be transferable across different geographical, social and cultural contexts with pertinent model calibration; and (4) they can account for a range of policy variables that can be used to rank policies and investment strategies in terms of maximizing the expected number of adopters of a new technology in future time periods. Moreover, we are interested in understanding how the spatial configuration of a new transportation service and the different socio-demographic variables of decision-makers can influence the adoption behavior. The aforementioned aggregate models cannot cater for those two key variables in their formulation to project future market shares of a

**Figure 2.1:** Sales vs. Cumulative Sales over Time
new technology in a more representative manner. In addition to that, model application is a key component in our analysis as it provides policy makers and transportation specialists with the means to quantify the expected number of adopters for a set of policies and strategies at the metropolitan levels. Aggregate models do suffer from a limited degree of policy sensitivity and can only account for a narrow range of policy variables which make them less appealing to our analysis.

There are various disaggregate diffusion models, each focusing on different aspects of the decision making process and behavior. One dominant disaggregate adoption model is the threshold model which was first introduced by David (1969) in an attempt to study the technology adoption of grain harvesting machinery and was further explored by Sunding and Zilberman (2001). The threshold model incorporates heterogeneity among decision-makers in the adoption process and could be used in conjunction with discrete choice models (logit or probit) to represent the utility maximization behavior of decision-makers. The sources of heterogeneity that affect the adoption process may include various variables depending on the available data and what the analyst is trying to capture. At every time period, the critical level of each source of heterogeneity in the model is determined. Decision-makers equipped with a value of that source of heterogeneity, say income, that is larger than the critical level at a certain time period will choose to adopt the new technology/product at that time period. The critical level of a source of heterogeneity shall decrease over time which induces more consumers to adopt due to principles of “learning by doing” and “learning by using” (please refer to Sunding and Zilberman, 2001). One application of this consisted of using a disaggregate utility function model of household vehicle choice using the threshold model in its aggregate context with income, household structure, and comfort/quality being three critical sources of heterogeneity (Liu, 2010). Advances in the threshold model incorporate dynamic optimization in their analysis, such that a decision-maker is making a trade-off between the expected decrease in price of a certain technology in the future and the current benefits from purchasing it which will dictate the timing of adoption (McWilliams and Zilberman, 1996).

As we are interested in capturing various sources of heterogeneity in the decision-making process, the threshold model does not seem to be a good fit to the methodological framework we want to adopt. As previously mentioned, the literature focuses on two different types of adopters (early adopters and imitators). We are interested in modeling the adoption behavior of those two distinct market segments in addition to the non-adopters market segment that chooses to never adopt a new technology. The formulation of the disaggregate utility function of the threshold model can be used as a starting point in the development of our methodological framework of technology adoption for the three different market segments.

What about the transportation industry? The transportation industry has been trying to develop quantitative methods rooted in the technology diffusion literature to try and predict market shares of those upcoming modes of transportation. One study (Li et al., 2015), focused on defining variables that influence ridership of the Taiwan High Speed Rail System (THSR) using econometric time series models and revealed preference (RP) data of monthly ridership from January 2007 till December 2013. Two models were estimated: (1) seasonal autoregressive integrated moving average and (2) first order moving average model to explore the influence of explanatory variables on ridership.
Moreover, studying the market diffusion of electric vehicles has received worldwide attention these past few years. For example, Plötz et al. (2014), estimated an agent-based simulation model of the diffusion process of electric vehicles using real-world driving data that captured heterogeneity among decision-makers, psychological factors and attributes of the new technology. Another study, please refer to Gnann et al. (2015), used an Alternative Automobiles Diffusion and Infrastructure (ALADIN) diffusion model to forecast market penetration of plug-in electric vehicles through simulation techniques. Their proposed methodology incorporated an agent-based simulation model that catered for different types of users in addition to their respective decision making processes to make it behaviorally richer. Other studies focused on using agent-based simulation models alone while others integrated them with discrete choice methods to account for a richer behavioral interpretation (Eppstein et al., 2011; Brown, 2013; Zhang et al, 2011). For example in Eppstein et al. (2011), an integrated agent-based and consumer choice model was estimated that tried to capture the effect of social interactions and media on the market penetration of plug-in hybrid electric vehicles.

The adoption of new transportation services has primarily focused on using stated preference (SP) data in the context of alternative fuel vehicles. Some studies were interested in assessing sensitivities to attributes of the new technology (Ito et al., 2013 and Hirdue et al., 2011) while other studies focused on both model estimation and forecasting the market share of alternative fuel vehicles under certain policy scenarios (Glerum et al., 2013, & Mabit and Fosgerau, 2011). The SP approach does capture sensitivities to attributes of the new technology in a representative way. However, using SP data does require solid model calibration and validation to enhance the model’s forecasting power. In order to account for this, integrating SP with revealed preference (RP) data would be a better approach (see for example Brownstone et al., 2000). Ideally, one should be interested in using RP data as it represents actual market demand. An SP approach entails hypothetical scenarios which hinders a model’s forecasting power. In addition to that, the analyst will not be able to capture the dynamic aspect of the diffusion process over time with respect to the social influence and spatial component dimensions of the new technology. In previous SP studies, projected market shares for electric vehicles and alternative fuel vehicles were over estimated. That is due to the fact that the adoption and diffusion of a new technology is a temporal and social process and these previous studies did not account for this.

Also, a current developed model focuses on forecasting adoption of electric vehicles using an integrated discrete choice and diffusion models (Jensen et al., 2016). This model builds on the previous work of Jun and Park (1999) whereby they specify the utility of adopting a certain good at time t as a function of the attributes of the technology, and difference between time t and the time period at which the product was introduced in the market. The parameter associated with the aforementioned second variable in the utility of adoption will account for the effect of the diffusion process. The probability of adoption at a certain time period could be computed using the logit closed form. Following that, the sales of electric vehicles at different time periods could be computed respectively. To forecast the demand of electric vehicles, data was collected from a stated preference (SP) survey conducted in Denmark in 2012 and 2013 for the choice between electric vehicles and internal combustion engines. The specification of the utility of choosing either mode included purchase price, propulsion costs, driving range, emissions, number of battery stations, and characteristics of public charging facilities. The utility equation of choosing an electric vehicle also entailed a parameter that portrays the effect of the diffusion process while assuming that internal combustion engines have reached market saturation. The model was used
to forecast market share of electric vehicles for several policy scenarios. Our proposed methodological framework is different as it caters for (1) heterogeneity among decision-makers and in particular among distinct discrete market segments in the population that have different adoption behavior; (2) effect of various socio-economic and demographic variables on the diffusion process; (3) spatial or network effect of the new technology whereby we are interested in assessing how an increase in the size of the network that is covered by the new mode of transportation will impact adoption behavior; and (4) social influences and how that will influence the utility of adoption.

2.3 Methodological Framework

The methodological framework we want to develop builds on the aggregate diffusion literature and in particular the concepts of consumer heterogeneity towards the adoption process i.e. innovators versus imitators, and social influences as described in the Bass model. We are interested in disaggregate diffusion models as they can be easily integrated with the activity-based travel demand models of interest. Also, with disaggregate models, we can account for the impact of socio-demographics and social influences on the diffusion process in addition to spatial effects. By spatial effects we are referring to increasing the relative size of potential destinations that one can reach out to via the new mode of transport. While there have been disaggregate models developed in the literature, they seem to be based on different behavioral assumptions (for example the previously mentioned threshold model) or do not cater for heterogeneity in the specification of the utility of adoption. Most studies in the literature focus on the role of three defined distinct market segments in their analysis that differ in their respective adoption behavior towards a new technology. Those market segments are: innovators/early adopters, imitators and non-adopters. We will be building on these findings using a disaggregate technology diffusion approach.

The specification we are interested in developing is unique as it tries to model how technology adoption and use is influenced by socio-demographics, attributes of the new technology/service, spatial effect (or network effect) and finally social influences. The aggregate diffusion literature mainly refers to two types of adopters (innovators and imitators). In order to assess the adoption behavior of a certain population we need to take into account those decision-makers that will choose to never adopt the new technology/service. We are interested in modeling the adoption behavior of each of the following three market segments (innovators/early adopters, imitators, and non-adopters) to try and capture heterogeneity in the adoption behavior of each of those market segments. Innovators or early adopters denote the market segment that determines whether a new technology will pick up in market share or not after being introduced in the market. They define how steep or flat the “S” cumulative diffusion curve can be during the early stages. Innovators comprise the biggest fraction of adopters of a new technology during the initial time periods. Imitators on the other hand come into play as time elapses since the introduction of the new technology. They will determine the rate at which the market will adopt the new product or service and will in turn shape the steepness of the “S” cumulative diffusion curve at later stages in the diffusion process. Non-adopters will define the time period at which the cumulative diffusion curve reaches a plateau. For example, as the number of non-adopters increases the faster the “S” curve attains a plateau.

However, we do not observe what type of a person any given individual is i.e. we do not have information about which market segment each decision-maker belongs to. In order to account for
this, discrete mixture models and in particular latent class choice models (LCCM) are found to be the most appropriate framework. Latent class choice models comprise two components: a class membership and a class-specific choice model as depicted in the figure below.

The class-specific choice model formulates the probability of technology adoption of a certain individual conditional on that individual either being an innovator, imitator or non-adopter. This component captures variation across classes with respect to choice set, tastes and sensitivities, decision protocol and covariance structure of the error term (Gopinath, 1995).

![Figure 2.2: Latent Class Choice Model Framework](image)

As we are interested in modeling the adoption process for each market segment, we should cater for the temporal dimension of technology diffusion as decision-makers will adopt the new technology at various time periods according to the aforementioned explanatory variables. Hence, the probability that individual n during time period t after the new technology was available in the market adopted or chose to not adopt could be written as:

\[
P(y_{ntj}|Z_{nt}, X_{ntj}, q_{ns}) \forall j \in \{0,1\} y_{n(t-1)j}
\]

where \(y_{ntj}\) equals one if individual n during time period t chose to adopt the new technology (j=1) and zero otherwise, conditional on the characteristics of the decision-maker during time period t denoted as \(Z_{nt}\) and attributes of the new technology (j=1) during time period t denoted as \(X_{ntj}\), and conditional on the decision-maker belonging to latent class s (\(q_{ns}\) equals one and zero otherwise).

Now, evaluating the probability of adoption or non-adoption will be based on a binary logit formulation that transforms the utility specification into probabilities. Let \(U_{ntj,s}\) denote the utility of adoption (j=1) or not (j=0) of the new technology during time period t for individual n conditional on him/her belonging to latent class s which is expressed as follows:
where $V_{ntjs}$ is the systematic utility that is observed by the analyst, $z'_{nt}$ is a row vector of characteristics of the decision-maker $n$ during time period $t$, $x'_{ntj}$ is a row vector of attributes of the new technology $(j=1)$ during time period $t$ for individual $n$, $\beta_s$ and $\gamma_s$ are column vectors of parameters specific to latent class $s$ and $\epsilon_{ntjs}$ is the stochastic component of the utility specification. Since we have prior assumptions about the behavior of the two various types of adopters (innovators versus imitators) based on the existing technology diffusion literature, the systematic utility of adoption for each of the three latent classes was specified according to the following rationale. The systematic utility of adoption of innovators shall include characteristics of the decision-maker and attributes of the new technology as we are interested in assessing the significance of those explanatory variables on the decision process of adopting or not. The systematic utility of adoption for imitators is also modeled as a function of the characteristics of the decision-maker and attributes of the new technology. However, this is the latent class whose adoption behavior is influenced by the extent of social influence and accumulating pressure with the increase in the previous number of adopters (Bass, 1969). That is why we are interested in determining the effect of the previous number of adopters on the utility of adoption of imitators at a certain time period. Finally, the systematic utility of adoption of the third latent class (non-adopters) consists of an alternative specific constant (ASC) only. Ideally, this ASC should attain a highly negative value via estimation to ensure that this class will most likely never adopt the new technology. The systematic utility of adoption / non-adoption for innovators, imitators and non-adopters is specified in the following manner:

\[
\begin{align*}
V_{\text{adopt}, nt|s=\text{innovator}} &= z'_{nt}\beta_1 + x'_{ntj}\gamma_1 \\
V_{\text{non-adopt}, nt|s=\text{innovator}} &= 0 \\
V_{\text{adopt}, nt|s=\text{imitator}} &= z'_{nt}\beta_2 + x'_{ntj}\gamma_2 + \Delta(t-1)\alpha_2 \\
V_{\text{non-adopt}, nt|s=\text{imitator}} &= 0 \\
V_{\text{adopt}, nt|s=\text{non-adopter}} &= \lambda \\
V_{\text{non-adopt}, nt|s=\text{non-adopter}} &= 0
\end{align*}
\]

where $\Delta(t-1)$ depicts the cumulative number of adopters of the new technology during time period $(t-1)$, and $\lambda$ is an alternative specific constant.

Now, in order to assess the impact of the spatial/network effect of the new technology on the utility of adoption, we were interested in quantifying the level of accessibility brought about by the new mode of transportation. Accessibility is defined as the “ease with which any land-use activity can be reached from a location, using a particular transport system” (Dalvi et al., 1976). There are several types of accessibility measures: cumulative opportunities measures, gravity-based measures, and utility-based measures (Handy and Niemeier, 1997). We will focus on utility-based measures for the assessment of accessibility through developing a destination choice zone-based model. Utility based measures of accessibility have desirable advantages over other methods as they account for flexibility in travel purposes and sensitivity to travel impedance measures in terms of time and cost. Also, they capture individual-level preferences and socio-demographic influences on travel behavior. In those types of models, we assume that given a certain origin, each decision-maker associates a utility to each of the available destinations in his/her respective choice set $C_n$. 

\[
U_{ntjs} = V_{ntjs} + \epsilon_{ntjs} = z'_{nt}\beta_s + x'_{ntj}\gamma_s + \epsilon_{ntjs}
\]
and will end up choosing the alternative i.e. destination which maximizes his/her utility. Accessibility is defined as the logsum measure of those destination choice models as it “measures the expected worth of certain travel alternatives” (Ben-Akiva and Lerman, 1985).

Let $U_{nij}$ denote the utility of individual $n$ conducting a trip from origin $i$ to destination alternative $j$. Determining the systematic utility specification requires assessing the explanatory variables that influence an individual’s decision to conduct a trip from a certain origin to a certain destination. Travel impedance whether in terms of travel distance or cost is an important variable as travelers prefer conducting shorter trips. Second, since travel is a derived demand whereby an individual goes from a certain origin to a destination to conduct an activity, evaluating the available number of opportunities or attractions at the destination is important. In addition to that, an individual is more likely to use the new technology (mode of transport in our case) if it provides a relatively close destination spot to his/her home. Finally, socio-demographic variables can play a role in defining some characteristics that can drive individuals into conducting certain trips. Accordingly, $U_{ni}$ was specified in the following manner:

$$U_{ni} = V_{ni} + \varepsilon_{ni} = d_{ij}\beta + \ln(size_j)\alpha + Z_n\gamma + X_{nj}\theta + home_n\delta + \varepsilon_{ni}$$

where $V_{ni}$ is the systematic utility observed by the analyst, $d_{ij}$ denotes a friction factor of traveling from origin $i$ to destination alternative $j$ which is the travel distance associated with origin-destination pair (i,j), $size_j$ represents the attractions associated with destination $j$ which will be governed by the employment rate at the destination (number of employees per square mile) as it is considered to be the driver behind trip attractions, $Z_n$ represents socio-demographic characteristics of decision-maker $n$, $X_{nj}$ denotes attributes of the new technology at destination alternative $j$ for individual $n$, $home_n$ is a dummy variable which will be equal to one if decision-maker $n$ resides within a certain proximity from his/her corresponding destination alternative and zero otherwise, $\beta$, $\alpha$, $\gamma$, $\theta$, and $\delta$ are parameters associated with the explanatory variables, and $\varepsilon_{ni}$ is the stochastic component of the utility specification.

Assuming that all individuals are utility maximizers and that $\varepsilon_{ni}$ follows an i.i.d. Extreme Value Type I distribution across individuals, origin and destination alternatives with mean zero and variance $\frac{\pi^2}{6}$, the accessibility measure is expressed as the following logsum measure:

$$Accessibility_{n,i,t} = \ln \left[ \sum_{j=1}^{J_t} e^{V_{ni}} \right]$$

where $i$ denotes an origin alternative and $J_t$ is the total number of distinct destination alternatives available at time period $t$.

Accessibility changes over time due to an increase/decrease in the number of distinct destination alternatives $J_t$ or changes in any of the explanatory variables of the destination choice model systematic utility. Changes in the employment rate, socio-demographics, or attributes of the new technology will induce changes in the accessibility measure over time.

Based on the above formulation, the difference in the utility of adoption for the two types of adopters (early adopters and imitators) comprises different sensitivities to characteristics of the decision-maker and attributes of the new technology. In addition to that, the adoption process for
imitators is affected by the social influence aspect of the new technology while early adopters are not. Let us focus on a carsharing service as an example. Assume a decision-maker resides in a certain area where the accessibility measure of the new technology is unattractive mainly because the individual resides in an area that is far away from zones that have a station for this carsharing service. Also, the nearest station for this service is relatively far from the decision-maker’s home. In this case, the attributes of the new technology are undesirable, and that individual is unlikely to adopt. However, as the technology evolves and becomes more attractive, that individual is more likely to adopt. This decision-maker is an early adopter in his/her local context even though he/she adopted at a later point in time. Our methodological framework caters for this as it deals with the micro-level disaggregate decision-making process. Aggregate models on the other hand, such as the Bass model, examine the diffusion process at a system level whereby they would consider this particular decision-maker to be an imitator.

Now that we have defined the formulation of the network effect model denoted by accessibility, we return to the formulation of the class-specific choice model. Assuming that all individuals are utility maximizers and that \( \varepsilon_{ntj|s} \) follows an i.i.d. Extreme Value Type I distribution across individuals, time periods, alternatives and latent classes with mean zero and variance \( \frac{\pi^2}{6} \), the class-specific choice model could be formulated as such:

\[
P(y_{ntj}|Z_{nt}, X_{ntj}, q_{ns}) = P(U_{ntj|s} \geq U_{ntj'|s} \forall j' \in C) = \frac{e^{U_{ntj|s}}}{\sum_{j'=1}^{J} e^{U_{ntj'|s}}}
\]

where \( C \) denotes the choice set i.e. either adopting to the new service or not which is common to all individuals.

Assuming that the class-specific choice probabilities for individual \( n \) across all choice situations are conditionally independent given that he/she belongs to latent class \( s \), then the conditional probability of observing a vector of choices \( y_n \) becomes:

\[
P(y_n|q_{ns}) = \prod_{t=1}^{T_n} \prod_{j \in C} P(y_{ntj}|Z_{nt}, X_{ntj}, q_{ns})^{y_{ntj}}
\]

where \( T_n \) is the total number of time periods available for individual \( n \) until he/she adopts. The class membership model on the other hand predicts the probability that decision-maker \( n \) with characteristics \( Z_n \) belongs to latent class \( s \) and is defined as such:

\[
P(q_{ns}|Z_n)
\]

Let \( U_{ns} \) denote the utility for individual \( n \) from latent class \( s \) which is expressed as follows:

\[
U_{ns} = V_{ns} + \varepsilon_{ns} = z_n' \tau_s + \varepsilon_{ns}
\]

where \( V_{ns} \) is the systematic utility, \( z_n' \) is a row vector of socio-economic and demographic variables for decision-maker \( n \), \( \tau_s \) is a column vector of parameters, and \( \varepsilon_{ns} \) is the stochastic component of the utility specification. Again, assuming that all individuals are utility maximizers and that \( \varepsilon_{ns} \) follows an i.i.d. Extreme Value Type I distribution across individuals and latent classes with mean zero and variance \( \frac{\pi^2}{6} \), the class membership model could be formulated as such:
\[ P(q_{ns} | Z_n) = P(U_{ns} \geq U_{ns'} \forall s' = 1,2, \ldots, S) = \frac{e^{\nu_{ns}}}{\sum_{s'=1}^{S} e^{\nu_{ns'}}} \]

where \( S \) denotes the total number of distinct latent classes which is equal to three in our case.

Now, to put things in perspective with respect to our methodological framework, the figure below displays all three components in our analysis.

![Generalized Technology Adoption Model](image)

**Figure 2.3:** Generalized Technology Adoption Model

The destination choice model will dynamically feed into the class-specific adoption model in terms of evaluating the accessibility measure at different time periods. Afterwards, joint estimation of the class-specific adoption model and class membership model will take place.

The marginal probability \( P(y) \) of observing a vector of choices \( y \) for all decision-makers is:

\[ P(y) = \prod_{n=1}^{N} \sum_{s=1}^{S} P(y_n | q_{ns}) P(q_{ns} | Z_n) = \prod_{n=1}^{N} \sum_{s=1}^{S} P(q_{ns} | Z_n) \prod_{t=1}^{T} \prod_{j \in C} P(y_{ntj} | Z_{nt}, X_{ntj}, q_{ns})^{y_{ntj}} \]

Finally, the technology adoption model predicts the probability that a certain individual will adopt the new technology/service at a certain time period, and is explained by social influences, network effect, socio-demographics and level-of-service attributes. The model was estimated via the Expectation-Maximization (EM) algorithm. This optimization technique enhances the computation power of model estimation by making use of conditional independence properties that exist in our model.
2.4 Dataset
We will use revealed preference (RP) time series data to estimate the integrated discrete choice and technology adoption model from a one-way carsharing system in a major city in the United States. The name of the carsharing company is withheld for confidentiality reasons. Our data focuses on the adopters of the service ever since it was launched. Signing up to be a member of this carsharing system requires a membership fee but no monthly nor annual fees. Currently, there are 14 pods/stations in addition to 5 locations for on-street pick-up/drop-off locations. The dataset entails zip code information about members of the new transportation service which drove our analysis to be zip code focused. In total, there are 16 zip code based stations for the car sharing service as some of the on-street pick-up/drop-off locations exist in the same zip code as other stations.

The dataset consists of all individuals that have signed up for the service for a time period of 2.5 years after being launched in addition to their registration date, gender and zip code associated with their residential location or zip code at which the registration payment was performed. Moreover, travel patterns via the carsharing service for a period of 6 months were recorded. Information about which user conducted a trip was recorded in addition to the origin and destination carsharing stations used. Our main focus revolves around the technology adoption behavior of residents of that major city and hence we are only interested in those adopters that had a location zip code affiliated with it which summed up to 1847 adopters. Initially, we had information about all members of the carsharing service but we limited our analysis to members that used the service during the last six months of the data collection period. An adopter is an individual that has signed up for the carsharing service and that has conducted at least one trip during the last six months of the data collection period. The figure below highlights the cumulative number of adopters over the entire time period that are active users of the service in order to project where exactly on the “S” diffusion curve the carsharing system’s current market share is.

![Figure 2.4: Cumulative Number of Adopters of Carsharing Service](image)

Figure 2.4: Cumulative Number of Adopters of Carsharing Service
Finally, in order to have a representative sample of the population, we wanted to enrich the sample with a random draw of 2724 observations from the Household Travel Survey (2013) of the same state to which the city we are working with belongs. We will also assume that the individuals from this random sample are non-adopters i.e. did not adopt to the new service for the entire data collection time period (2.5 years). The prior probability of being an adopter in the city of interest is $3 \times 10^{-4}$ given the number of adopters and the population. Hence, the expected number of adopters in the random sample is approximately one.

The figure below displays the growth in the number of pods/stations and on-street pick-up/drop-off locations for the 2.5-year time period.

![Figure 2.5: Growth in Number of Pods/Stations and On-Street Parking over Time](image)

Our technology adoption model shall assess the impact of socio-demographics, carsharing supply (fleet and pricing), social influences and network effect on the adoption behavior of innovators, imitators and non-adopters. Identifying network effect that is governed by the construct of accessibility shall be restricted to be zip code based for the same reason mentioned above. We would like to identify the level of accessibility associated with each zip code based station of the carsharing system depending on the spatial distribution of potential destinations i.e. stations. The origins and destinations entail the full set of the carsharing system’s stations. The destination choice model will be estimated based on trips that were conducted by users over a period of 6 months. For our formulation with this dataset, the accessibility measure will be non-zero only for users that have a home zip code associated with one of the stations or on-street parking locations. To account for that, we wanted to assign an accessibility measure for zip codes which do not entail a station/pod or on-street parking. We were interested in imputing the accessibility for those zip codes from the accessibility of the nearest zip code that had either a station or on-street parking while taking a friction factor into consideration, distance in our case. The accessibility measure for individual $n$ with home zip code $i$ which does not have a station or on-street parking at time $t$ could be defined as follows:
\[ \text{Accessibility}_{n,i,t} = \frac{\text{Accessibility}_{n,k,t} \text{ nearest active station } k \text{ at time } t}{(\text{distance}_{i,k})^\varphi} \]

where \( \varphi \) denotes the degree of the distance friction effect which will be estimated in the model.

Moreover, the sample population we are working is choice-based whereby each choice in the available choice set (adopt, not adopt) corresponds to a separate stratum (carsharing members versus household travel survey sample). However, the sampling fractions are not equal to the population shares especially that we have accounted for all adopters of the carsharing system and hence are highly over-represented in our sample. To cater for that and yield consistent parameter estimates, each observation needs to be weighted by \( \frac{W_g}{H_g} \) where \( W_g \) is the population fraction and \( H_g \) is the sample fraction of members of stratum \( g \) (Ben-Akiva and Lerman, 1985). Accordingly, the marginal probability \( P(y) \) of observing a vector of choices for all decision-makers should be expressed as follows:

\[
P(y) = \prod_{n=1}^{N} \left( \sum_{s=1}^{S} P(q_{ns}|Z_n) \prod_{t=1}^{T_n} \prod_{j \in \mathcal{C}} P(y_{ntj}|Z_{nt}, X_{ntj}, q_{ns}) y_{ntj} \right) \frac{W_g}{H_g}
\]

### 2.5 Estimation Results and Discussion

The destination choice model is conditional on adoption as it will be estimated from observations pertinent to adopters and users of the carsharing service. As we are assuming that individuals from the Household Travel Survey (HTS) are non-adopters, the destination choice model was estimated using data from the carsharing service and in particular the travel patterns via the carsharing service for a period of six months. The following section entails results of the destination choice model which will be used to compute the accessibility measure that is then used as an explanatory variable in the technology adoption model. Followed by that, results of the technology adoption model will be presented. Results of the destination choice model for the 16 zip code based stations are tabulated below including parameter estimates (and t-statistics).

We included 4 alternative specific constants (ASCs) for 4 stations as we considered them to be hubs for trips conducted using the carsharing service. The four exogenous variables used were distance, employment rate, home dummy, and on-street parking. The on-street parking variable was introduced in the destination choice model utility specification in order to quantify and understand the effect of having on-street parking versus stations on the projected number of adopters. The on-street parking variable used was a dummy variable which will be equal to one if the destination alternative (zip code) entails on-street parking structure for the new transportation service and zero otherwise.

We did not include ASCs in all 16 utility equations because that will be problematic when evaluating accessibility when new stations are introduced as it will be difficult to assess the ASC of the new destination i.e. station. In addition to that, a dummy variable between a major technology firm’s headquarters and a major airport in the city was introduced which takes a value of one if a trip takes place between the technology firm and the airport stations and zero otherwise. That dummy variable was of interest as 46% of the total trips of the carsharing service had either
that technology firm or airport as an origin or destination. Finally, a dummy variable between the major technology firm and the city’s downtown region was introduced which takes a value of one if a trip takes place between the technology firm and downtown, and zero otherwise.

**Table 2.1: Destination Choice Model**

<table>
<thead>
<tr>
<th>Variable</th>
<th>Parameter Estimate</th>
</tr>
</thead>
<tbody>
<tr>
<td>Distance in 100 Kilometers</td>
<td>-0.24 (-2.06)</td>
</tr>
<tr>
<td>Employment in Zip Code (employees/miles$^2$)</td>
<td>0.18 (10.06)</td>
</tr>
<tr>
<td>Home</td>
<td>1.55 (20.51)</td>
</tr>
<tr>
<td>On-street Parking</td>
<td>0.34 (5.47)</td>
</tr>
<tr>
<td>Trip between Major Technology Firm and Downtown</td>
<td>1.00 (14.18)</td>
</tr>
<tr>
<td>Trip between Major Technology Firm and Major Airport</td>
<td>2.78 (45.46)</td>
</tr>
<tr>
<td>Alternative Specific Constant</td>
<td></td>
</tr>
<tr>
<td>Technology Firm</td>
<td>1.10 (13.27)</td>
</tr>
<tr>
<td>Airport 1</td>
<td>1.76 (23.07)</td>
</tr>
<tr>
<td>Airport 2</td>
<td>0.61 (5.90)</td>
</tr>
<tr>
<td>Airport 3</td>
<td>0.93 (10.32)</td>
</tr>
</tbody>
</table>

Using the parameter estimates from the destination choice model, the logsum measure of accessibility was calculated for all observations in the carsharing service data and the HTS data. The HTS data does recognize household characteristics but in our case we were only interested in the following variables: home zip code, gender and work TAZ. Finally, both datasets (HTS and carsharing service) were integrated together and used to estimate the disaggregate diffusion model.

Since we had apriori hypothesis regarding the number of latent classes in our model, determining the final model specification was based on varying the utility specification for both sub-models i.e. class membership and class-specific choice models. The table below presents detailed parameter estimates (and t-statistics) for the class membership of the technology adoption model.
Table 2.2: Class Membership Model

<table>
<thead>
<tr>
<th>Variable</th>
<th>Class 1 Innovators</th>
<th>Class 2 Imitators</th>
<th>Class 3 Non-Adopters</th>
</tr>
</thead>
<tbody>
<tr>
<td>Alternative Specific Constant</td>
<td>--</td>
<td>7.00 (37.09)</td>
<td>7.51 (56.78)</td>
</tr>
<tr>
<td>Monthly Income ($1000)</td>
<td>--</td>
<td>-0.23 (-13.01)</td>
<td>-0.04 (-3.86)</td>
</tr>
<tr>
<td>Male</td>
<td>--</td>
<td>-0.77 (-8.70)</td>
<td>-1.72 (-23.56)</td>
</tr>
</tbody>
</table>

-- Not applicable

The rho-bar-squared ($\tilde{\rho}^2$) measure for this technology adoption model is almost 1.0 with a total number of 4571 individuals and 120,665 observations. $\tilde{\rho}^2$ has such a high value because of the weights applied to each of the observations and the fact that the market share of the carsharing adopters is very minimal compared with the rest of the population, which forces the increase in model fit.

The class membership model includes parameter estimates which correspond to the influence of socio-demographic variables on class membership. The class membership model results reveal that all else equal, an individual is more likely to be a non-adopter, high-income groups and men are more likely to be early adopters (innovators). The monthly income used in our analysis was the average zip code based income since that socio-demographic variable was not provided in the data. Sample enumeration results denote the following split in the population across the three classes: 0.22% innovators, 16.80% imitators, and 82.98% non-adopters.

The table below presents detailed parameter estimates (and t-statistics) for the class-specific model corresponding to the adoption behavior of the new technology. Parameter estimates for the utility of adoption for the two types of adopters have the right sign and are significant at the 1% level except for the major technology firm employee variable for the innovators latent class. This agrees with the behavioral interpretation of the adoption process for each class. Early Adopters’ utility of adoption increases with an individual being an employee of the major technology firm and having a station or on-street parking for the new transportation service in his/her corresponding zip code.

Also, an increase in the accessibility of a certain home zip code that has neither a station nor on-street parking will in turn drive an innovator to adopt. A similar behavioral interpretation applies for home zip codes that do have stations or on-street parking. Imitators’ utility of adoption increases with an individual being an employee of the major technology firm and with an increase in the cumulative number of adopters in the previous time period. This is the class which is highly influenced by previous adopters. Moreover, as the accessibility of the home zip code which has neither a station nor on-street parking increases, an imitator is more likely to adopt. The same rationale also applies for home zip codes that do have stations or on-street parking. The behavior of the non-adopters latent class is deterministic as the probability of non-adoption is almost equal to one for each individual that belongs to this market segment at each time period.
Table 2.3: Class-specific Technology Adoption Model

<table>
<thead>
<tr>
<th>Variable</th>
<th>Parameter</th>
<th>Class 1 Innovators</th>
<th>Class 2 Imitators</th>
<th>Class 3 Non-Adopters</th>
</tr>
</thead>
<tbody>
<tr>
<td>Alternative Specific Constant (Adoption)</td>
<td>$\lambda$</td>
<td>-7.88 (-78.08)</td>
<td>-14.71 (-78.63)</td>
<td>-23.46 (-0.01)*</td>
</tr>
<tr>
<td>Major Technology Firm Employee</td>
<td>$\beta$</td>
<td>1.33 (1.89)*</td>
<td>7.10 (46.43)</td>
<td>--</td>
</tr>
<tr>
<td>Station in Zip Code</td>
<td></td>
<td>1.38 (3.61)</td>
<td>--</td>
<td>--</td>
</tr>
<tr>
<td>On-street Parking in Zip Code</td>
<td></td>
<td>1.18 (3.99)</td>
<td>--</td>
<td>--</td>
</tr>
<tr>
<td>Accessibility for Zip Codes Containing a Station or On-street Parking</td>
<td>$\gamma$</td>
<td>0.44 (5.29)</td>
<td>0.68 (55.39)</td>
<td>--</td>
</tr>
<tr>
<td>Accessibility for Zip Codes Containing neither a Station nor On-Street parking</td>
<td></td>
<td>0.91 (22.77)</td>
<td>0.59 (22.64)</td>
<td>--</td>
</tr>
<tr>
<td>Cumulative Number of Adopters at (t-1) in 100’s</td>
<td>$\alpha$</td>
<td>--</td>
<td>0.14 (24.21)</td>
<td>--</td>
</tr>
<tr>
<td>Degree of Distance Friction Effect for Accessibility</td>
<td>$\varphi$</td>
<td></td>
<td>1.00 (--)</td>
<td></td>
</tr>
</tbody>
</table>

-- Not applicable; * Insignificant at the 5% level
Finally, the degree of distance friction effect for accessibility, $\phi$, was not directly estimated as our LCCM evaluates the gradient and standard errors for linear-in-parameter utility equations. In order to account for this, we estimated several models by varying the value of $\phi$ and selected the value that maximized the final log-likelihood. This approach is similar to a grid search.

In order to evaluate the performance of our disaggregate adoption model, we will compare its performance against a multinomial logit (MNL) model. The MNL model comprises two utility equations: adoption and non-adoption. The adoption utility specification entails all of the explanatory variables used in the LCCM while the non-adoption systematic utility specification is constrained to zero. Parameter estimates for the MNL model were behaviorally consistent and significant. The same dataset that was used to estimate model parameters for the LCCM was used for the MNL model. The final log-likelihood values for the LCCM and MNL models after accounting for choice-based sampling were -14.74, and -156.53 respectively. The table below shows the rho-bar-squared ($\bar{\rho}^2$), AIC and BIC values for the two models. It is clear that our proposed disaggregate adoption model has a slightly higher $\bar{\rho}^2$ and lower AIC and BIC values. That is why it has a better statistical fit as compared with the MNL model. It is interesting to note that both models have an extremely high $\bar{\rho}^2$ value because the marginal probability of adoption in the population is very small.

<table>
<thead>
<tr>
<th>Model</th>
<th>Log-Likelihood</th>
<th>$\bar{\rho}^2$</th>
<th>AIC</th>
<th>BIC</th>
</tr>
</thead>
<tbody>
<tr>
<td>MNL</td>
<td>-156.53</td>
<td>0.99</td>
<td>329</td>
<td>407</td>
</tr>
<tr>
<td>LCCM</td>
<td>-14.74</td>
<td>1.00</td>
<td>65</td>
<td>240</td>
</tr>
</tbody>
</table>

Finally, in order to assess model performance on a hold-out sample, we estimated the parameters of the disaggregate adoption model using observations for the first 24 months. We calibrated the model to minimize discrepancy between the predicted number of adopters and the actual number of adopters for the 25th month. We then used our calibrated model to forecast adoption for months 26-30. We performed simulation using 1000 draws by bootstrapping parameter estimates of the disaggregate adoption model at each draw. Accordingly we can generate a confidence interval that bounds the predicted number of adopters. The figure below displays boxplots for the 1000 bootstrap samples in addition to the actual number of adopters for months 26-30.

It is evident that the actual number of adopters for months 27, 28 and 29 fall inside their corresponding box, which spans the first quartile to the third quartile. As for month 26, the actual number of adopters falls within the “whiskers”, which is acceptable to a certain extent. This is a good indication regarding the confidence interval bound of the model’s predicted number of adopters. That is definitely not the case during the 30th month as the actual number of adopters is located outside the boxplot’s “whiskers”. It is important to note that a new station for the carsharing service was introduced at the beginning of the 30th month. However, the actual number of adopters is much lower than previous months. That could be due to unobserved competition in the market or some issues in the carsharing service itself, which are not accounted for in our model due to limitations of the data.
Now that we have estimated a technology adoption model, we want to use it to forecast adoption into the future for various potential scenarios. More specifically, we are interested in using the model to understand the potential effectiveness of new pods and on-street parking facilities placed in different locations. In order to do so, we should calibrate our model first by adjusting the values of the alternative specific constants (ASCs) of the utility of adoption for innovators and imitators. That will minimize the difference between projected and actual demand. In order to do so, we will perform sample enumeration on the entire population of the major city using our estimated model in order to predict the number of adopters that joined the service during the last month of the data’s time horizon. We will adjust the ASCs in order to equate the predicted number of adopters for the last month from the model with the actual number of adopters for that month from the data itself.

There were three scenarios that we were interested in assessing their impact on the adoption of the new transportation service besides the base case scenario. The base case scenario comprises not investing in any new station or on-street parking facility in any of the zip codes. The three scenarios are:

- a- Stations/pods outside a second major technology firm
- b- Stations/pods in a new zip code in the downtown region
- c- On-street parking facilities instead of stations/pods in the same zip code as in scenario b

Figure 2.6: Boxplots for Predicted Number of Adopters for Months 26-30
The figure below displays how the cumulative adoption “S” diffusion curve will be projected into the future under the aforementioned potential scenarios.

![Cumulative Adoptions for New Transportation Service](image)

**Figure 2.7**: Cumulative Adoptions for New Transportation Service

Also, the figure below identifies the forecasted cumulative monthly adoptions of the new transportation service for the next year on a month to month basis. It is evident that investing in stations/pods outside another major technology firm will increase the monthly number of new adopters the most. There is no significant difference in the number of new monthly adopters for the downtown region between having a station or on-street parking. That is because, the only way we were able to incorporate the effect of each was via dummy variables. Ideally, we would have been interested in incorporating the number of cars in each station/pod or total area allocated for on-street parking but that information was not available. That said, the power of the integrated discrete choice and adoption model we developed lies in projecting adoption into the future and identifying the most effective policy that will cater for behavior change and maximize adoption.
In order to define confidence intervals for the predicted cumulative number of adopters for each of the four aforementioned scenarios, we performed simulation using 1000 draws by bootstrapping estimates of the adoption model at each draw. The figures below display the boxplots for the 1000 bootstrap samples for the predicted cumulative number of adopters for each of the four scenarios. It is evident that the bound of the confidence interval increases with time. This indicates that predictions become more stochastic over time, which is a reasonable argument. Again, investing in stations/pods outside a major technology firm yields the highest number of forecasted adopters. Moreover, no significant difference is depicted in the predicted cumulative adopters for the downtown region for an on-street parking facility versus a station/pod.
Figure 2.9: Boxplots for Predicted Cumulative Number of Adopters for Base Case Scenario
Figure 2.10: Boxplots for Predicted Cumulative Number of Adopters for Downtown On-Street Parking Scenario
Figure 2.11: Boxplots for Predicted Cumulative Number of Adopters for Downtown Station Scenario
Figure 2.12: Boxplots for Predicted Cumulative Number of Adopters for Major Technology Firm
We were also interested in assessing the aggregate technology adoption process using the Bass model to highlight the advantages of our adopted methodological framework. The three variables that need to be calculated which define the “S”-shaped diffusion curve of the cumulative number of adopters of the one-way carsharing service are: the coefficient of innovation p, for coefficient of imitation q, and total potential market M. In order to compute the values for those three variables, we need to define the following formulation (Bass, 1969):

\[ S(t) = pM + (q - p)Y(t) - \frac{q}{M}Y^2(t) \]

S(t) depicts sales of a product over time which is the expected number of adopters of the carsharing service at time period t. The discrete time series data was used to run the required regression analysis in order to estimate p, q and M that attained the following values respectively: 0.0051, 0.2108 and 2200. The figure below displays how the number of adopters S(t) and cumulative number of adopters Y(t) will evolve over time. The cumulative number of adopters will plateau and attain a value of 2200 adopters. This value is predicted by the Bass model and will disregard any changes in the attributes of the technology or its spatial configuration that could occur at future time periods. The Bass model suffers from the following limitations: (1) lack of including important policy variables into model parametrization which hinders its forecasting power in terms of identifying effective policies and investment strategies that maximize the expected number of adopters; (2) absence of key variables that shape the adoption process of a new transportation service such as the spatial configuration of the service; and (3) absence of incorporating the effect of socio-demographic variables onto the diffusion process which should be accounted for to capture heterogeneity in the decision making process across different consumers. That is why, the Bass diffusion model forecasts displayed below, will be identical across each of the aforementioned three potential investment strategies / policies.

![Figure 2.13: Adopters vs. Cumulative Adopters over Time Using Bass Model](image_url)
2.7 Conclusion

Major technological and infrastructural changes over the next decades, such as the introduction of autonomous vehicles, implementation of mileage-based fees, carsharing and ridesharing are expected to have a profound impact on lifestyles and travel behavior. However, the commonly-used approach for predicting the 20-30 year forecasts across transportation networks suffers from its inability to project membership of upcoming modes of transport. The methodological framework used in our analysis to study technology adoption consisted of an integrated latent class choice model (LCCM) and network effect model that was governed by a destination choice model. The latent classes used in the analysis are supported by the technology diffusion literature across multiple disciplines and are defined as: innovators/early adopters, imitators and non-adopters. These latent classes are able to capture heterogeneity in preferences towards technology adoption. Each class entails a distinct set of sensitivities and parameter estimates pertinent to the exogenous variables used in estimation. The adopted methodological framework focuses on understanding the relative impact of the following set of covariates: social influences, network/spatial effect, socio-demographics and level-of-service attributes.

One major contribution for this chapter is defining a methodology to capture the impact of the network/spatial effect of the new technology. We were interested in understanding how the size of the network, governed by the new mode of transportation, would influence the adoption behavior of the different market segments as the ability of reaching out to multiple destination increased i.e. the size of the network grew bigger. This is a critical component in our analysis as it will quantify the effect of placing stations or on-street parking facilities in different locations and prioritize locations in the transportation network that will maximize the expected number of adopters. Our generalized technology adoption model has two other major advantages whereby it employs a microeconomic utility-maximizing representation of individuals and captures various sources of heterogeneity in the decision-making process.

The empirical results look promising in terms of defining the adoption behavior of the three classes. Finally, the model was calibrated and used to project adoption into the future for various potential scenarios. Some findings from our technology adoption model are: (1) a decision-maker is more likely to be a non-adopter, high-income groups and men are more likely to be early adopters or innovators; (2) network/spatial effect, socio-demographics, social influences and level-of-service attributes of the new technology have a positive set of sensitivities in the utility of adoption across latent classes which is consistent with our a-priori hypotheses and the diffusion literature; (3) placing a new station/pod for the carsharing system outside a major technology firm will increase the expected number of monthly adopters the most; and (4) no significant difference is observed regarding the expected number of monthly adopters for the downtown region between having a station or on-street parking.

Acknowledgements

We would like to thank UCCONNECT (USDOT and Caltrans) for supporting our research project. We would also like to thank Susan Shaheen for her assistance in helping us get the data from the one-way carsharing system. Finally, we would like to show our gratitude to the one-way carsharing system team that was helpful in answering our questions and concerns.
Chapter 3

Modeling and Forecasting the Evolution of Preferences over Time: A Hidden Markov Model of Travel Behavior

3.1 Introduction
Discrete choice analysts have devoted much attention to the subject of preference heterogeneity. Preferences, as denoted by taste parameters and consideration sets in the context of utility-maximizing behavior, are regularly modeled as functions of demographic and situational variables. For example, value of travel time, or the marginal rate of substitution between travel time and cost in the context of travel mode choice, is frequently formulated as a function of income, and separate values of time are usually estimated for work and non-work travel (c.f. Parsons Brinkerhoff Quade & Douglas, Inc., 2005; Cambridge Systematics, 2002). Recent interest in the influence of latent psychological, sociological and biological constructs, such as attitudes, normative beliefs and affective desires, has led to the additional inclusion of these variables within existing representations of individual preferences (e.g. Bahamonde-Birke, 2015). Some studies have even contended that preferences are an endogenous function of the decision-making environment, as characterized by available alternatives and their attributes (e.g. Vij and Walker, 2014). Implicit to each of these representations is the following assumption: as these explanatory variables change over time, so should corresponding preferences.

However, most existing frameworks employ static representations of individual behavior that do not capture preference dependencies over time for the same individual. In addition to the variables identified previously, an individual’s preferences in the present are expected to be a function of their preferences in the past, as evidenced by findings across multiple contexts, including transportation (Carrel et al., 2015), finance (Kaustia and Knüpfer, 2008), health (Gum et al., 2006), tourism (Sönmez and Graefe, 1998), sustainable development (O’Hara and Stagl, 2002), etc. Notwithstanding this evidence, discrete choice frameworks that capture such temporal dependencies are rare in the literature. Part of the limitation is empirical: most studies use cross-sectional data, and longitudinal data of the kind that is needed is not always available.

The ability to understand and predict how individual preferences evolve over time offers the potential to address transportation policy questions of great interest. Who is more likely to use shared mobility services: individuals who currently drive, or those who take public transport? Will the adoption of driverless cars be led by individuals with significant past exposure to other new technologies, or individuals with the greatest need for access to self-driving car technology? How do changes to the public transport system impact individuals that are differently predisposed towards available travel modes? Transport system use and policy will vary, often considerably, depending upon the answer to each of these questions. In fact, it is this last question that motivates the empirical application in this study.
The objective of this study is to develop an econometric framework that can model preference dependencies over time for the same individual. Our proposed framework constitutes a hidden Markov model (HMM) with a discrete choice kernel. Decision-makers are assumed to be utility-maximizing, and the unobserved states denote different preferences, as denoted by differences in taste parameters and consideration sets. Transitions between preferences are expressed as a function of time-varying covariates, namely socio-demographic variables and alternative attributes. The evolutionary path is hypothesized to be a first-order Markov process such that an individual’s preferences during a particular time period are dependent on their preferences during the previous time period. The framework is empirically evaluated using data from the Santiago Panel (Yáñez et al., 2010), which comprises four one-week waves of pseudo travel-diary data spanning a twenty-two month period that extends both before and after the introduction of Transantiago, a major redesign of the public transport system in Santiago, Chile.

HMMs were first proposed nearly five decades ago (Baum et al., 1970; Baum and Petrie, 1966). They have a rich history of application in machine learning, with particular regards to the subject of speech recognition (Rabiner, 1989). They have also been applied, albeit limitedly, to the study of individual behavior in the applied disciplines of education (e.g. Hong and Ho, 2005; George, 2000), marketing (e.g. Netzer et al., 2008) and transportation (e.g. Xiong et al., 2015; Choudhury et al., 2010; Goulias, 1999). Our contribution in this chapter is to develop, apply, and test an HMM framework that captures, models and forecasts the evolution of individual preferences and behaviors over long-range forecasting horizons.

The remainder of this chapter is organized as follows: Section 2 motivates the study through a discussion of previous findings on the evolution of individual preferences over time; Section 3 reviews dynamic discrete choice model frameworks that have been used in the past to model temporal interdependencies in preferences and behavior, and how they relate to our proposed HMM framework; Section 4 outlines the proposed methodological framework; Section 5 discusses the initial conditions problem in dynamic discrete choice models, and if and how it applies to HMMs; Section 6 describes the dataset that constitutes our empirical application; Section 7 presents results from the model framework; Section 8 demonstrates the benefits of the framework for policy analysis; and finally, Section 9 concludes with a discussion of key findings, limitations and directions for future research.
3.2 Motivation: Evolution of Individual Preferences over Time

Most economists would agree that individual preferences, as denoted by taste parameters and consideration sets in the context of utility-maximizing behavior, can and do change over time. However, most would also contend that understanding why particular preferences exist in the first place, and consequently, how they change over time, ought not to be the concern of mainstream economics. While the view has been challenged over the years (notable examples include Becker, 1996 and Elster, 2016), most contemporary economic representations of individual behavior continue to treat preferences as exogenously determined, and attention is usually limited to understanding and predicting policy implications under any given set of preferences.

Preferences may change over time in response to changes in, among others, demographic and situational variables, psychological, sociological and biological constructs, and available alternatives and their attributes. Changes in preferences have been observed across a broad spectrum of behavioral contexts, from the personal to the public. For example, Buss et al. (2001) examined the evolution of mate preferences between 1939 and 1996 at geographically different locations in the United States. Their findings indicate that mate preferences did indeed change. When looking for a potential partner over time, both males and females increased the importance of physical attraction and financial status, and males decreased the importance of domestic skills. At the other end of the spectrum, Page and Shapiro (1982) studied the evolution of preferences on matters of domestic and foreign policy, such as civil liberties, abortion, etc., between 1935 and 1979 in the United States. They found that significant shifts in preferences were rarely the case over short time periods. However, when opinions and preferences did actually change, that was the outcome of changes occurring in the decision-making environment, whether in the social and economic spectrum or in the lives of decision-makers.

In the context of transportation, perhaps the ‘peak car’ phenomenon best represents the notion of changing preferences over time. The turn of the twenty-first century has witnessed stagnant or declining levels of car use across much of the developed world (Goodwin and Dender, 2013; Garceau et al., 2014). The shift in preferences away from the car as a mode of transportation has been attributed to a combination of economic, social and technological factors that include a recessionary global economy, fluctuating oil prices, ageing national populations, shifts in cultural values, advances in information and communications technology, etc. (see, for example, Vij et al., 2017; McDonald, 2015; Kuhnimhof et al., 2013; Collet, 2012).

What about travel behavior in the era of transformative mobility? Why would one expect preferences to change over time in response to major changes in the transportation system, such as the introduction of autonomous vehicles? There may be changes in consideration sets. Individuals unwilling or unable to drive themselves may be willing and able to use autonomous vehicles. There may be changes in taste parameters. Being in an autonomous vehicle will allow decision-makers to multitask, which may cause them to be: (1) less sensitive to driving during peak hours and getting caught up in congestion; (2) not worried about finding a parking spot in congested cities nor paying parking fees; and (3) more flexible in terms of residential choice location as they might consider residing outside dense urban cities and commute via the autonomous vehicle since driving has become less onerous. These factors may lead to changes in value of time (VOT). The assumption that preferences are stable may be valid when forecasting over short-term periods.
However, when forecasting over long-term horizons, we need to take into account that various shocks/changes in the built environment and investments in technologies and services are bound to happen, and that these shocks/changes will likely impact preferences.

Preferences may additionally depend upon past experiences. Though most neoclassical frameworks assume that preferences are inter-temporally separable, studies on the formation and persistence of habits have questioned the validity of the assumption (Muellbauer, 1988; von Weizsäcker, 1971; Pollak, 1970). Past experiences provide a ready yardstick for comparison, serving both to magnify differences under certain contexts, and reduce contrasts in others. As Becker (1992) writes, “a given standard of living usually provides less utility to persons who had grown accustomed to a higher standard in the past. It is the decline in health, rather than simply poor health, that often makes elderly persons depressed. And what appeared to be a wonderful view from a newly occupied house may become boring and trite after living there for several years.”

Past experiences can also serve as anchors, dampening the ability of external events to force commensurate shifts in individual preferences. Two individuals with completely exchangeable current circumstances may still differ in terms of their preferences, due to corresponding differences in their personal histories and the life paths that brought them here. For example, Bronnenberg et al. (2012), in their study on the long-run evolution of brand preferences among individual consumers, concluded that “brand capital evolves endogenously as a function of consumers’ life histories and decays slowly once formed”. Their findings are echoed by studies in other behavioral contexts. Travel behavior in particular, due to its repetitive nature, is especially prone to habit formation (Thøgersen, 2006; Gärling and Axhausen, 2003; Sönmez and Graefe, 1998; Aarts et al., 1997). “Habits, once formed, become regularized and the market mechanism virtually ceases to operate”, and “consequently, if these habits can be identified, choices made at any future decision point can be predicted with a fairly high degree of accuracy” (Banister, 1978). As an extreme example, some studies have speculated that the use of active modes of transportation (i.e. walking and bicycling) as children can promote more sustainable travel behavior practices as adults (see, for example, Mitra et al., 2010; Faulkner et al., 2009; Roberts, 1996).

However, hypotheses such as these have rarely been tested in the literature, due largely to limitations on available data. Transportation planning has typically relied on cross-sectional mobility data for understanding and predicting different dimensions of travel and activity behavior. Cross-sectional studies can provide population snapshots at a point in time; by extension, repeated cross-sections can show broad population trends over time. However, cross-sectional studies cannot measure changes at the level of the individual over time. As mentioned before, the ability to understand and predict changes in individual-level preferences and behaviors offers the potential to address transportation policy questions of great interest.

Consider, for example, the peak car phenomenon. A 5% decrease in driving mode shares at the population level over time could imply that 5% of the population has stopped driving, or that the entire population is driving 5% less, or some combination of the two (Hanson and Huff, 1988). The nature and impact of transport policy will depend on which of these competing hypotheses is true; unfortunately, a traditional cross-sectional study would be unable to distinguish between these hypotheses. Similarly, consider the case of new transportation technologies and services,
such as autonomous and/or alternative-fuel vehicles and shared mobility services, that promise to transform mobility. The diffusion of new technologies and services is a temporal process (Rogers, 2010). The key to understanding the future of mobility is not only to study the immediate impact of current policies, services, and nudges; but also how these impacts influence trends and their evolution over decades, particularly as new technologies and services are introduced. For example, is the growth in carsharing and ridesharing services being led by individuals who have always been multimodal, or do these services also appeal to car-dependent households? Will self-driving cars be subject to the constraints of an ownership-based economy, or will gradual changes in preferences imply that access and use is facilitated primarily through shared services? Cross-sectional studies that use static frameworks cannot address these questions. Where such insight is required, longitudinal studies that use dynamic frameworks are necessary.

3.3 Methodological Basis: Dynamic Models for Discrete Choice Analysis

Dynamic discrete choice models try to account for the influence of past experiences on present choices. According to Kenneth Train (2009), current choices affect future choices, as past choices affect current choices, and this causality provides the basis for dynamic discrete choice modeling. There are two broad paradigms in the literature (for an excellent synthesis on the subject, the reader is referred to von Auer, 1998). Both paradigms assume that present preferences and behavior are impacted by past experiences; they differ in the ascribed importance of expected future utility on present behavior.

The first paradigm assumes that individuals, when making a decision at a given time period, behave as if they are forward-looking agents that maximize their present and expected future discounted utility over the entire time horizon. Perhaps the most famous example of such a representation of dynamic discrete choice behavior is the study by Rust (1987) on the optimal replacement of bus engines. Rust’s representation has since been applied to many contexts, including car ownership (see for example Cirillo and Xu, 2011; and Glerum et al., 2013), and it is in this context that we describe the framework. A car is considered a durable good that yields utility over time. An individual’s choice of whether to purchase a car at a certain time period or postpone the purchase depends on how that individual expects to use the car both now and in the future.

The second paradigm assumes a more myopic view of behavior, where individuals are assumed to maximize their present utility, and future expected utility is completely discounted. In other words, the individual cares only about the current time period, and choices in later time periods are deemed irrelevant. For theoretical treatments of such myopic representations of individual behavior, the reader is referred to, among others, Gorman (1967), Pollak (1970) and von Weizsäcker (1971). The HMM conforms to this second paradigm, where an individual’s preferences in the present are assumed to be dependent on their preferences in the past, but at any given point in time, the individual is assumed only to maximize present utility.

Depending on the empirical context, one or the other paradigm may be preferred. When studying medium and long-term travel and activity behaviors, such as car ownership and residential location, it may be more reasonable to assume that individuals are forward-looking. Decisions
such as whether to buy a car and where to live have implications that extend well beyond the present. However, when studying short-term travel and activity behaviors, such as travel mode choice, it may be more reasonable to assume that individuals are myopic. The impact of these decisions is typically short-lived and readily reversible. Since our model framework will be applied to the study of short-term behaviors, we will be adopting a myopic view of decision-making, articulated through the HMM framework.

As mentioned before, HMMs have been used previously to study the dynamics of travel and activity behavior. Goulias (1999) used HMMs to study the dynamics of household time allocation where the dependent variable is continuous. Choudhury et al. (2010) used HMMs to represent the evolution of latent plans over time, and their consequent impact on actions at any particular point in time. Their framework does make an explicit link with discrete choice analysis. They apply their framework to model the “evolution of unobserved driving decisions as drivers enter a freeway.” Their model is described very generally; extensions such as incorporating the expected maximum utility are not implemented and applications to long-range modeling and forecasting are not investigated. Perhaps the empirical application that is closest to the work presented here is the study by Xiong et al. (2015), who used HMMs to study the dynamic nature of travel mode choice behavior over time. Their framework does not allow for heterogeneity with regards to consideration sets, the transition model is not sensitive to changes in available alternatives and their attributes, and the value of the framework for policy analysis, beyond improvements in fit, is unclear. Our objective is to build upon these previous studies to develop a methodological framework capable of modeling the dynamics of preferences over time in a manner that is theoretically grounded, behaviorally meaningful and practically useful.
3.4 Methodological Framework

Our methodological framework builds on dynamic models, which are becoming more popular in the field of travel behavior. For example, Van Acker et al. (2014) highlight the need for incorporating dynamics into models of behavior by stating that “it will almost inevitably be the case that the range of travel choices open to people will be wider over time periods in which lifestyles can also change, than in the short run when the constraints will be more prominent. As such, the whole way of thinking about travel and lifestyle must be seen as a process of change over time, not as a fixed state”.

We propose using a hidden Markov model (HMM) with a discrete choice kernel, where the following two key assumptions are made: (1) we assume a myopic view of behavior, such that observed choices at a certain time period are only dependent on corresponding preferences during that time period, and future expected utility is completely discounted; and (2) the hidden states denote different preferences, and the evolution of preferences over time is assumed to be a first-order Markov process such that an individual’s preferences during a certain time period is dependent on their preferences during the previous time period. Figure 3.1 illustrates the HMM assumptions. It is important to note that 'preference state at time 1’ determines the effects of inertia and past experiences on the probabilistic assignment of each individual to a particular set of preferences during the first time period.

![Figure 3.1: Hidden Markov Model Structure (figure adapted from Choudhury et al., 2010)](image)

Hidden Markov models comprise three components: initialization model, transition model, and observed output model (Jordan, 2003). The initialization model predicts the probability that a decision-maker belongs to a certain hidden state during the first time period. The transition model predicts the probability of observing a certain evolution of hidden states between successive time periods. Lastly, the observed output model predicts the probability of observing a vector of choices for a decision-maker at a given time period, conditional on belonging to a certain hidden state during that time period.

We operationalize the HMM in the context of travel mode choice behavior by relying on the construct of modality styles. The construct has been introduced in the literature to refer to overarching lifestyles, built around the use of a particular set of travel modes, that influence all dimensions of an individual’s travel and activity behavior (Vij et al., 2013). In the context of travel mode choice behavior, we use modality styles to refer to distinct segments in the population with
different travel mode preferences, i.e. modes considered in the choice set, and sensitivity to level-of-service attributes. For example, modality style models have shown that in 2000, 42% of the San Francisco Bay Area’s population exclusively considered driving, whereas this share reduced to 23% in 2012 (Vij et al., 2017). Investment in technologies and services are expected to influence both the travel modes considered and the sensitivity to level-of-service attributes. Consider, for example, the case of autonomous vehicles. A fully autonomous vehicle that is capable of navigating itself without human input might prompt changes in the value of time, through its ability to allow passengers to engage in whatever tasks they wish to while inside the car. Similar changes in preferences can be imagined in response to other changes in the transportation system. Modeling what types of modality styles have flourished or declined over time is key to understanding and predicting mode share shifts in response to policies, services, technologies and nudges.

Accordingly, in the context of travel mode choice behavior, the unobserved states in the dynamic framework shall be represented by modality styles. Through the remainder of the chapter, we will use the terms modality styles and (travel mode) preferences interchangeably. The transition model quantifies the evolution of modality styles over time to capture structural shifts in preferences. Our dynamic framework requires a transition model that can capture shifts in modality styles brought about by major changes to the transportation system (sharing, automation, transit on demand) or by shifts in attitudes (e.g. towards/away from auto-orientation), or changes in socio-demographic variables.

![Proposed Dynamic Discrete Choice Framework](image)  

**Figure 3.2:** Proposed Dynamic Discrete Choice Framework
We are interested in forecasting, and thus require a structural model for the transition probabilities that captures the influence of transportation and societal changes. For this we will employ a homogenous HMM, which assumes that the transition model between modality styles (preferences) from one time period to the other is consistent/static i.e. the parameters entering the transition model between subsequent waves are time-invariant. Any differences in transition probabilities over waves are assumed to arise due to changes in the explanatory variables entering the transition model. Figure 3.2 displays the dynamic nature of our framework. Over following subsections, we explain each of the constituent sub-models in greater detail.

3.4.1 Class-specific Mode Choice Model
The class-specific mode choice model predicts the probability that individual \( n \) during time period \( t \) made a set of choices \( y_{nt} \), conditional on the individual belonging to modality style, or class, \( s \) during that time period. Note that \( y_{nt} \) is a vector whose element \( y_{ntk} \) equals one if the individual chose travel mode \( j \) during choice situation \( k \) over time period \( t \), and zero otherwise. The model allows more than one choice situation per individual and time period, and correlation between these choice situations is captured through the assumption that an individual’s modality style remains stable over a single time period.

Let \( U_{ntk|s} \) denote the utility of travel mode \( j \) during choice situation \( k \) over time period \( t \) for individual \( n \), conditional on the individual belonging to modality style \( s \), and is expressed as follows:

\[
U_{ntk|s} = V_{ntk|s} + \varepsilon_{ntk|s} = x'_{ntk} \beta_s + \varepsilon_{ntk|s}
\]

where \( V_{ntk|s} \) is the systematic utility. \( x'_{ntk} \) is a row vector of attributes of alternative \( j \) during choice situation \( k \) over time period \( t \) for individual \( n \), \( \beta_s \) is a column vector of parameters specific to modality style \( s \) and \( \varepsilon_{ntk|s} \) is the stochastic component of the utility specification. Now, assuming that all individuals are utility-maximizers and \( \varepsilon_{ntk|s} \) follows an i.i.d. Extreme Value Type I distribution across individuals, time periods, choice situations, alternatives and modality styles with location zero and scale one, the probability that individual \( n \) chooses travel mode \( j \) during choice situation \( k \) over time period \( t \), conditional on belonging to modality style \( s \), is as follows:

\[
P(y_{ntk} = 1|q_{nts} = 1) = P(U_{ntk|s} \geq \min_{j' \in C_{ntk|s}} U_{ntkj'}) = \frac{e^{x'_{ntk} \beta_s}}{\sum_{j' \in C_{ntk|s}} e^{x'_{ntk} \beta_s}}
\]

where \( P(y_{ntk} = 1|q_{nts} = 1) \) denotes predicting the probability that individual \( n \) over wave \( t \) and choice situation \( k \) chooses alternative \( j \) (implying \( y_{ntk} \) equals one and zero otherwise) conditional on belonging to modality style \( s \) during wave \( t \) (\( q_{nts} \) equals one and zero otherwise), and \( C_{ntk|s} \) denotes the choice set available for individual \( n \) at wave \( t \) and choice situation \( k \) conditional on modality style \( s \). Preference heterogeneity is captured by allowing both the taste parameters \( \beta_s \) and the consideration sets \( C_{ntk|s} \) to vary across modality styles.
Assuming that choice probabilities for individual $n$ across all choice situations belonging to time period $t$ are conditionally independent, given that the individual belongs to modality style $s$ during time period $t$, the conditional probability of observing a vector of choices $y_{nt}$ for a certain time period $t$ becomes:

$$P(y_{nt} | q_{nts} = 1) = \prod_{k=1}^{K_{nt}} \prod_{j \in C_{ntk}} P(y_{ntkj} = 1 | q_{nts} = 1)^{y_{ntkj}}$$

where $K_{nt}$ is the number of distinct choice situations observed for individual $n$ over time period $t$.

### 3.4.2 Initialization Model

The initialization model predicts the probability that individual $n$ belongs to modality style $s$ during the first time period. The probabilities are expressed as a function of individual characteristics during that time period, denoted by the column vector $z_{n1}$. Characteristics may include observable socio-economic and demographic variables, such as income and gender, or later psychological, sociological or biological constructs, such as attitudes, normative beliefs or affective desires. In our case, information on latent constructs was not available across all observation periods, and characteristics include observable socio-economic and demographic variables only. Depending on the analyst’s assumption, the model may be formulated as a multinomial logit, multinomial probit, mixed logit or some other model form. We assume that the initialization model is multinomial logit.

Let $U_{n1s}$ denote the utility of modality style $s$ during the first wave for individual $n$ which is expressed as follows:

$$U_{n1s} = V_{n1s} + \varepsilon_{n1s} = z'_{n1s} \tau_s + \varepsilon_{n1s}$$

where $V_{n1s}$ is the systematic utility that is observed by the analyst, $z'_{n1s}$ is a row vector of socio-economic and demographic variables for individual $n$ during the first wave and $\tau_s$ is the associated column vector of parameter estimates for modality style $s$, and $\varepsilon_{n1s}$ is the stochastic component of the utility specification. Now, assuming that all individuals are utility maximizers and that $\varepsilon_{n1s}$ follows an i.i.d. Extreme Value Type I distribution across individuals, first wave, and modality styles with location zero and scale one, the initialization model could be formulated as such:

$$P(q_{n1s} = 1 | Z_{n1}) = P(U_{n1s} \geq U_{n1s'} \forall s' = 1, 2, \ldots, S) = \frac{e^{z'_{n1s} \tau_s}}{\sum_{s'=1}^{S} e^{z'_{n1s'} \tau_{s'}}}$$

where $P(q_{n1s} = 1 | Z_{n1})$ represents the probability that individual $n$ has modality style $s$ during the first wave conditional on his/her socio-demographic variables during the first wave, and $S$ denotes the total number of modality styles in the sample.
3.4.3 Transition Model

Analogously, the transition model predicts the probability that individual \( n \) transitions to modality style \( s \) during time period \( t \), conditional on the individual belonging to modality style \( r \) during the previous time period \((t-1)\). Ordinarily, the probabilities may be expressed as a function only of individual characteristics during that time period (see, for example, Xiong et al., 2015), as was the case with the initialization model. Depending on the analyst’s assumption, the transition model may be formulated as a multinomial logit, multinomial probit, mixed logit or some other model form. We assume that the transition model is multinomial logit.

Let \( U_{nts}(t-1|r) \) denote the utility derived from transitioning into modality style \( s \) at wave \( t \) conditional on individual \( n \) belonging to modality style \( r \) during the previous wave \((t-1)\), which is expressed as follows:

\[
U_{nts|(t-1)r} = V_{nts|(t-1)r} + \epsilon_{nts|(t-1)r} = z'_{nt}\gamma_{sr} + \epsilon_{nts|(t-1)r}
\]

where \( V_{nts|(t-1)r} \) is the systematic utility, \( z'_{nt} \) is a row vector of observable socio-economic and demographic characteristics of individual \( n \) over wave \( t \) and \( \gamma_{sr} \) is a column vector of parameters specific to modality style \( s \) at wave \( t \) given that the individual belonged to modality style \( r \) during wave \((t-1)\), and \( \epsilon_{nts|(t-1)r} \) is the stochastic component of the utility specification.

Assuming that all individuals are utility maximizers and that \( \epsilon_{nts|(t-1)r} \) follows an i.i.d. Extreme Value Type I distribution across individuals, waves and modality styles with location zero and scale one, the transition probability could be formulated as such:

\[
P(q_{nts} = 1|q_{n(t-1)r} = 1) = P(U_{nts|(t-1)r} \geq U_{nts'|(t-1)r} \forall s' = 1,2,...,S) = \frac{e^{z'_{nt}\gamma_{sr}}}{\sum_{s'=1}^{S} e^{z'_{nt}\gamma_{s'r}}}
\]

where \( P(q_{nts} = 1|q_{n(t-1)r} = 1) \) denotes one entry of the transition probability matrix, which involves predicting the probability that individual \( n \) belongs to modality style \( s \) during wave \( t \), for \( t > 1 \), conditional on modality style \( r \) during the previous wave \((t-1)\).

Now, the transition model is merely a function of socio-demographic variables. However, wouldn’t changes in the level-of-service of the transport network, such as reductions in travel times or travel costs, influence the transition from one modality style to the other? Changes in the level-of-service of different travel modes will affect different modality styles differently. For example, increased freeway congestion will make car-oriented modality styles less attractive, and a reduction in transit services will have a similar effect on transit-oriented modality styles. These changes will likely impact whether and how individuals change their modality styles, and should be accordingly captured by the transition model. We account for these changes by formulating transition probabilities as an additional function of the consumer surplus each individual would derive by belonging to different modality styles (building off the static framework forwarded by Vij and Walker, 2014).

Given that individuals are assumed to be utility-maximizing, the consumer surplus offered by modality style \( s \) to individual \( n \) during time period \( t \) is given theoretically by the total expected maximum utility derived by the individual over all observations for that time period, also referred
to as the inclusive value. When the class-specific choice model is assumed to be multinomial logit, expected maximum utility reduces to the familiar logsum measure, and the average consumer surplus is given by:

$$CS_{nts} = \frac{1}{K_{nt}} \sum_{k=1}^{K_{nt}} \log \left( \sum_{j \in C_{ntk \mid s}} e^{x'_{ntk} \beta_j} \right)$$

The transition probability we are proposing is defined as follows:

$$P(q_{nts} = 1 | q_{n(t-1)} = 1) = \frac{e^{z'_{nt} \gamma_{sr} + CS_{nt} \alpha_{sr}}}{\sum_{s' = 1}^{S} e^{z'_{nt} \gamma_{s' \mid r} + CS_{nt} \alpha_{s' r}}}$$

where $\alpha_{sr}$ is a parameter associated with the consumer surplus specific to modality style $s$ at wave $t$ given that the individual belongs to modality style $r$ over wave $(t-1)$. For the model to be consistent with utility-maximizing behavior, $\alpha_{sr} \geq 0$.

The inclusion of consumer surplus in the transition model provides a basis for understanding and predicting how individual preferences might change over time in response to corresponding changes in the transportation system. Consider, for the sake of illustration, that the local public transport agency introduces a temporary free pass for all services. The introduction of such a pass would change the consumer surplus offered by different modality styles differently. For modality styles that do not include public transport in their consideration set, the consumer surplus will be unchanged. For modality styles that do include public transport, consumer surplus will be higher, making individuals more likely to belong to these modality styles in the subsequent time period. In particular, the greatest change will likely be for a modality style that both considers public transport and is highly sensitive to travel costs (since the free pass will impact travel costs). Therefore, the introduction of the free pass might not only lead individuals to expand their consideration sets, it may cause them to become more sensitive to travel costs. Similar changes could potentially be modeled for other scenarios. This is a key benefit to our framework.

### 3.4.4 Likelihood Function of the Full Model

Now, the marginal probability $P(y_n)$ of observing a sequence of choices $y_n$ for decision-maker $n$ over $T$ time periods is expressed as follows:

$$P(y_n) = \sum_{s_1 = 1}^{S} \sum_{s_2 = 1}^{S} \ldots \sum_{s_T = 1}^{S} \prod_{t=1}^{T} P(y_{nt} | q_{nts} = 1) P(q_{n1s_1} = 1 | Z_n) \prod_{t=2}^{T} P(q_{nts} = 1 | q_{n(t-1)s_{t-1}} = 1)$$

HMMs are traditionally estimated via the Expectation-Maximization (EM) algorithm (forward-backward algorithm) that provides a computationally robust method of optimization by taking advantage of the conditional independence properties of the model framework. The EM algorithm is particularly useful for HMMs because in the M-step, each of the class-specific choice models, the initialization model and transition probability model can be maximized independently.
However, for HMMs that incorporate feedback to the transition model through the construct of consumer surplus, that will no longer be the case. The class-specific choice model and the transition model can no longer be maximized independently in this case, since the class-specific taste parameters are common to both sub-models. Consequently, the EM algorithm is not useful in this case, and we resorted to using traditional batch gradient optimization techniques.

3.5 Initialization Problem in Dynamic Models

Dynamic models may exhibit what is referred to as the initial conditions problem, first discussed by Heckman (1981). The initial conditions problem refers to how the dynamic process is initialized. Heckman (1981) illustrates the problem with the following functional form:

\[ U_{nt} = f(x_{nt}, y_{n1}, y_{n2} \ldots y_{n(t-1)}) + \varepsilon_{nt} \]

where \( U_{nt} \) denotes the utility during time period \( t \) for individual \( n \), \( f \) denotes the function that expresses the observable components of utility, \( x_{nt} \) entails explanatory variables for time period \( t \) for individual \( n \), \( y_{n(t-1)} \) represents the choice that individual \( n \) made during time period \((t-1)\), and \( \varepsilon_{nt} \) is the stochastic error component of the utility specification. We can clearly see that this general dynamic model captures the effect of previous choices on current ones.

One main assumption in this model formulation entails serially correlated error structure. According to Heckman (1981), initial conditions can only be treated as exogenous variables if at least one of the following two conditions is met: (1) serially independent error structures in the model framework (\( \varepsilon_{nt} \)) whereby the error components are assumed to be independently and identically distributed over time; or (2) if the data includes observations since the dynamic process started. If one of these two conditions is met, then we can treat initial conditions as exogenous variables or “fixed”. However, if neither of those assumptions is met, then initial conditions cannot be treated as exogenous variables, and assuming that they are will lead to inconsistent parameter estimates. The latter condition is almost never going to be met, since the analyst frequently only observes a dynamic process after it first began. Therefore, in our case, in order to treat the initial conditions as exogenous, the first condition must hold true.

Heckman (1981) discusses this issue in the context of a fixed effect probit model. Let us reframe our proposed hidden Markov model using the notation employed by Heckman’s general dynamic model. The initial conditions problem, in the case of HMMs, is associated with the initialization model with left-censored datasets. The class-specific choice model could be expressed as follows:

\[ U_{nt} = f(x_{nt}, q_{nt}) + \varepsilon_{nt} \]

where \( x_{nt} \) entails explanatory variables for time period \( t \) for individual \( n \), \( q_{nt} \) denotes the modality style for decision-maker \( n \) during time period \( t \).
However, according to the aforementioned transition model, one could express the following:

\[ q_{nt} = g(z_{nt}, q_{n(t-1)}) + \tau_{nt} \]

where \( g \) denotes the function that models the transition of modality styles over time, \( z_{nt} \) entails socio-demographic variables for time period \( t \) for individual \( n \), and \( \tau_{nt} \) is the stochastic error component. Accordingly, we can express the class-specific choice model utility equation as such:

\[ U_{nt} = f'(x_{nt}, z_{nt}, q_{n(t-1)}) + \epsilon_{nt} \]

We can recursively iterate by replacing the expression of modality styles at different time periods all the way until the first time period, ending up with the following equation:

\[ U_{nt} = f''(x_{nt}, z_{1}, ..., z_{nt}) + \epsilon_{nt} \]

We are assuming that the choice probabilities that comprise the class-specific choice model for a certain individual are conditionally independent over choice situations and time periods, given the modality style they belong to and the set of explanatory variables that affect the choice process. Thus, the error components in this choice model are independently and identically distributed across time, i.e. no serial correlation. Therefore, by assuming serially independent error structures, which is standard in HMMs, initial conditions could be treated as exogenous variables or “fixed” for the aforementioned reasons.

Conditional on an individual’s modality style, how valid is it to assume that the utilities of different choice alternatives over time are serially uncorrelated? Factors that lead to serially correlated error terms entail habit or inertia whereby choices (travel patterns in the case of travel behavior) could repeat themselves over time (Cantillo et al., 2007; Gärling and Axhausen 2003). The construct of modality styles tries to capture profound individual variations in preferences and attitudes and “higher-level orientations, or lifestyles that influence all dimensions of an individual’s travel and activity behavior” (Vij, 2013). We assume that by conditioning on those higher-level lifestyle orientations, or modality styles, we are fully accounting for habit or inertia effects.

Another factor behind serial correlation in the case of panel data comprises multiple choice decisions made by the same individual. This is what we refer to as specification bias, which encompasses excluding important determinants of choice decisions that are unobserved by the analyst but are common across multiple choice decisions for the same individual. These determinants could include unobserved attitudes, missing socio-demographic variables, etc., which become confounded with the error terms over time and could induce the main source of correlation between choice decisions made by the same individual over time. Our hypothesis is that this shared correlation is captured through the construct of modality styles. That is why, once we control for those higher-level orientations, it becomes reasonable to assume that choices are serially independent.

For a hidden Markov model, the evolutionary path, i.e. the transition model, is depicted by a first-order Markov process, which follows the property:
\[ \pi^n = \pi^1 \prod_{t=2}^{T} \Omega_{t-1,t} \]

where \( \pi^n \) denotes the vector of marginal probabilities for the available modality styles at time period \( n \), \( \pi^1 \) has the same definition as \( \pi^n \) but is associated with the first time period, and \( \Omega_{t-1,t} \) denotes the transition probability matrix between time period \((t-1)\) and \( t \).

If the data is left-censored whereby the time periods which were observed correspond to: \( \{ J, J+1, \ldots, T \} \), such that \( J > 1 \), then the initialization model will be biased. Using the above Markov chain equation, the initialization probabilities evaluated at \( t=J \) equal the product of the initialization probabilities at \( t=1 \) and all the transition probabilities up until \( t=J \). In other words, \( \pi^J = \pi^1 \times \prod_{t=2}^{J} \Omega_{t-1,t} \), and the magnitude of the bias is given by the difference between \( \pi^J \) and \( \pi^1 \). However, the transition model and the class-specific choice models will remain unbiased. Our main objective in this chapter is to develop a framework for modeling and forecasting the evolutionary path of preferences over time. In order to do so, it is important that parameter estimates associated with the transition model and class-specific choice model remain unbiased. Therefore, the initial conditions problem that exists in other types of dynamic models is not of concern here.

We conducted a Monte Carlo simulation experiment to corroborate our arguments. For our Monte Carlo simulation, we simulated 5000 observations. Each of the observations entailed 10 time periods. There were two available states \( (s_1, s_2) \) that each observation could belong to at each time period. There were also two available outcomes at each time period. The distribution of the initialization model, during the first time period, is 0.4 and 0.6 across the two states i.e. \( \pi^1 = [0.4, 0.6] \). The transition probability matrix between two successive time periods is \( \Omega_{t-1,t} = \begin{bmatrix} 0.8 & 0.2 \\ 0.3 & 0.7 \end{bmatrix} \). The class-specific choice probabilities were assumed as follows: conditional on being in the first state, the probability of choosing the first outcome is 0.5, and the probability of choosing the second outcome is 0.5. However, conditional on being in the second state, the probability of choosing the first outcome is 0.7, and the probability of choosing the second outcome is 0.3. We first estimated the hidden Markov model parameters for \( N=5000 \) observations over the entire time periods associated with the dynamic process i.e. \( T=10 \). We then re-estimated the HMM parameters by truncating the dataset by removing the first 5 time periods for each of the 5000 observations. Table 3.1 summarizes the results from the model estimation using the Expectation–Maximization algorithm. The initialization model for \( N=5000 \) and \( T=5 \) could be computed as such: \( \pi^6 = \pi^1 \times \prod_{t=2}^{5} \Omega_{t-1,t} = [0.59, 0.41] \). We can clearly observe that the transition matrix and class-specific choice models remained unbiased.
Table 3.1: Monte Carlo Simulation Results

<table>
<thead>
<tr>
<th>Variable</th>
<th>True Value</th>
<th>N = 5000 &amp; T = 10</th>
<th>N = 5000 &amp; T = 5</th>
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</thead>
<tbody>
<tr>
<td>Initialization Probability (class 1)</td>
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<td>0.39</td>
<td>0.58</td>
</tr>
<tr>
<td>Initialization Probability (class 2)</td>
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<td>0.61</td>
<td>0.42</td>
</tr>
<tr>
<td>Transition Probability (class 1</td>
<td>class 1)</td>
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<td>0.78</td>
</tr>
<tr>
<td>Transition Probability (class 2</td>
<td>class 1)</td>
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<td>0.22</td>
</tr>
<tr>
<td>Transition Probability (class 1</td>
<td>class 2)</td>
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<td>0.29</td>
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<tr>
<td>Transition Probability (class 2</td>
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<td>0.71</td>
</tr>
<tr>
<td>Probability (outcome 1</td>
<td>class 1)</td>
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<td>0.49</td>
</tr>
<tr>
<td>Probability (outcome 2</td>
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<td>0.51</td>
</tr>
<tr>
<td>Probability (outcome 1</td>
<td>class 2)</td>
<td>0.70</td>
<td>0.71</td>
</tr>
<tr>
<td>Probability (outcome 2</td>
<td>class 2)</td>
<td>0.30</td>
<td>0.29</td>
</tr>
</tbody>
</table>

3.6 Dataset

Parts of the following section are adapted from Vij (2013). In February of 2007, Santiago, Chile introduced Transantiago, a complete redesign of the public transit system in the city. Before the introduction of Transantiago, public transport in Santiago comprised a privately operated and uncoordinated system of buses and shared taxis, and the publicly run underground Metro lines. The old bus system was characterized by a large and inefficient fleet of 8,000 buses operating 380 lines, competition among buses on streets to gain passengers, higher than required frequencies along the busiest corridors and inadequate service along the less travelled ones, low quality vehicles, high accident rates, rude drivers, high levels of air and noise pollution, fractured ownership, and many empty buses circulating during off peak hours (Yáñez et al., 2010). The Metro system, though considerably safer, faster and more reliable than the bus system, only accounted for 8% of the city’s trips under the old system, due largely to sparser network coverage and the high cost of transfers between buses and the Metro.

With the aim of addressing these problems and stemming the decline in the public transportation system, the city assembled a team of Chilean specialists and consultants in 2005 to come up with a design for Transantiago (Fernández et al., 2008). Under the new system, the metropolitan region in and around Santiago was divided into ten zones and operations were taken over by a group of ten new companies. Bus routes were consolidated into a hierarchical system of trunk and feeder routes. The feeder routes connected each of these zones to the Metro lines, which served as the backbone of the new system. The trunk routes complemented the Metro lines by connecting different zones of the city. Benefits envisaged under Transantiago included the elimination of route redundancies, increased safety through the introduction of new low-floor buses, approximately half of them articulated, an integrated fare collection system through the means of a contactless smart card, lower travel times, a smaller fleet size, and reduced levels of air and noise pollution.
Though the system succeeded in achieving many of these goals, as a result of poor implementation it inadvertently created several new problems. First, the system was introduced in a ‘big-bang’ fashion with no pilot studies or public information campaigns leading up to the change. As a consequence, the first few weeks following the change resulted in great chaos and confusion among users of the city’s public transportation system. Second, the system was designed under the assumption that by the time of its introduction, certain critical bus-only lanes would have been constructed and all buses in the public transit fleet would have been fitted with on-board GPS tracking systems. Neither of these goals was achieved in time, and as a consequence buses ran well below design speeds, introducing significant unreliability into the system. Third, most new bus routes were confined to run along major arterials, increasing the access and egress distances to bus stops, particularly in the suburban corners of the city. And finally, given the hierarchical nature of the new bus system, most bus routes were limited to run within the boundary of a single zone, increasing the number of transfers for trips that required traversing multiple zones. These four factors combined drove a number of passengers to alternative modes of travel, most notably the Metro, which, unlike the bus system, ran at least as reliably as before, resulting in extreme overcrowding on Metro trains, with average occupancy levels during peak hours on certain routes of 5-6 passengers per square meter. As one can imagine, Transantiago generated considerable ill will among city residents, some of which has persisted to this day.

The dataset for the study comes from the Santiago Panel, comprising four one-week waves of pseudo travel-diary data collected over a span of twenty-two months that extends both before and after the introduction of Transantiago. The first wave was conducted in December 2006, three months before Transantiago was introduced, and the next three waves were implemented in May 2007, December 2007 and October 2008, respectively. Survey respondents were drawn from full-time employees working at one of six campuses of Pontificia Universidad Católica de Chile spread across Santiago. Each wave of data collection had an observation period of one week, and survey respondents were asked to report the travel mode(s) that they used for their morning commute to work each day during that week. Therefore, each wave contains up to five observations per individual (corresponding to the five-day working week). Though this limits the number of destinations to just these six campuses, the panel was fortunate in that the distribution of origins was well spread across the city. In all, the Panel interviewed 303 individuals during the first wave, 286 individuals during the second wave, 279 individuals during the third wave, and 258 individuals during the final wave. Considering that the four waves were spread across nearly two years, the Panel has a comparatively low attrition rate. Each of the respondents was asked questions regarding their socioeconomic characteristics; attributes of their morning trip to work; additional activities before, during and after work and their influence, if any, on the respondent’s choice of travel mode; subjective perceptions about the performance of the new system (collected only during the second and third waves); and their level of agreement with attitudinal statements about different aspects of the transportation system, such as safety, reliability and accessibility (collected only during the fourth wave). For more details about the dataset, the reader is referred to Yáñez et al. (2010).

The dataset offers a unique opportunity to investigate the effects of systemic changes in the transportation network on the evolution and persistence of individual preferences. For the purpose of our analysis, we will be restricting our attention to 220 respondents, each of whom has at least
one recorded observations in each of the four waves that constitute the Panel. We aggregate the modal alternatives into seven travel modes: auto, metro, bus, walk, bike, auto/metro (for individuals that drive to the metro station, and take the metro from there), and bus/metro (for individuals that take the bus to the metro station, and the metro from there).

![Figure 3.3: Mode Shares across All Waves](image)

Figure 3.3 plots mode shares across the four waves for all 220 individuals. It is evident that there was a big reduction in choosing the bus system as a mode of transport for work trips after wave one (post introduction of Transantiago). Bus mode shares declined from 40.6% during wave one to 18.2% during wave three, before marginally rebounding to 21.6% during wave four. Mode shares for auto/metro and bus/metro increased dramatically after the introduction of Transantiago. The major shifts in the mode choices occurred between waves one and two, as one would expect. Shifts tend to stabilize over time as people get more adjusted with their new work trips mode choice habits.

The reader should note that a plot like figure 3.3 could also have been plotted using repeated cross-sectional data. Longitudinal data allows us to analyze where these changes in mode shares are coming from. Figure 3.4 plots the number of trips where individuals switched travel modes between any two subsequent waves of the Panel. The scale of the vertical axes for each of the three plots is the same, to make the comparison easier. As one would expect, the majority of the shift occurs from wave 1 to wave 2, immediately in the wake of the introduction of Transantiago, and most of it away from “bus” and towards “bus/metro”. However, as the system stabilizes over time, so does the behavior of its users, with significantly less movement across travel modes between waves 2 and 3 and waves 3 and 4. Given the nature of the differences between the old and the new
system, this is not surprising. The more interesting question is: does the shift in observable travel mode choice behavior indicate a corresponding shift in latent travel mode preferences? And does this latter shift, if any, persist beyond the first wave? We address these related questions using the HMM framework in the next section.

Figure 3.4: Shifts across Travel Modes between Subsequent Waves of the Panel
Finally, when estimating HMMs, time periods should ideally be evenly spaced. In our case, the time periods are denoted by each wave of data collection. As mentioned before, the interval between waves is not evenly spaced: five months between waves 1 and 2, seven months between waves 2 and 3, and ten months between waves 3 and 4. Given that the main objective of this chapter is to develop a framework for modeling and forecasting the evolution of preferences over time, we need to assume that the transition model parameters are stable. With unevenly spaced time periods, we need to account for these differences in the transition model specification, explicitly or implicitly. One could estimate a heterogeneous HMM, where the transition model parameters are specified as an explicit function of the time interval between waves. Alternatively, one could estimate a homogenous hidden Markov model with time independent transition model parameters, such that the parameters are implicitly averaged over the different time intervals. For the sake of simplicity, we adopted the implicit approach. Therefore, when using the model to forecast changes in preferences and behaviors beyond wave four, the time intervals between future waves will be taken as the average time interval between successive waves for the first four waves.
3.7 Estimation Results and Discussion

The following section presents results from the hidden Markov model. Our proposed dynamic discrete choice framework models the evolution of preferences over time in response to changes in socio-demographic variables and the level-of-service of the transportation network. Determining the final model specification was based on varying the utility specification for all sub-models: initialization model, transition model and class-specific choice model. The method for identifying the number of distinct preference states i.e. modality styles that exist in the sample population, is iterative. The models were built incrementally: we first estimated a model with two modality styles, using that as a starting point for the model with three modality styles, and so on. The final number of modality styles in our sample was determined based on a comparison across measures of statistical fit, such as the rho-bar-squared ($\bar{\rho}^2$), Akaike Information Criterion (AIC) and Bayesian Information Criterion (BIC), and behavioral interpretation.

We first estimated the models by varying the number of modality styles excluding the effect of the level-of-service of the transportation network on the modality style transition model, as captured through the construct of consumer surplus (i.e. the average expected maximum utility, or inclusive value). We made use of the power of the EM algorithm in estimating model parameters while saving on computation time. The EM algorithm provides a statistically robust approach for model estimation by taking advantage of the conditional independence structure of the model framework. We estimated models with two, three and four modality styles. Table 3.2 enumerates the statistical measures of fit for each of these models. While the AIC and the BIC decrease as the number of classes increases, the rho-bar-squared value is highest for the three class model. However, a joint comparison across both statistical measures of fit and behavioral interpretation led us to select the four class model as the preferred specification. The four class model was subsequently reestimated, adding the measure of consumer surplus from the class-specific mode choice models to the transition model.

Table 3.2: Measures of Model Fit

<table>
<thead>
<tr>
<th>Number of Modality Styles</th>
<th>Log-Likelihood</th>
<th>$\bar{\rho}^2$</th>
<th>AIC</th>
<th>BIC</th>
</tr>
</thead>
<tbody>
<tr>
<td>Two</td>
<td>-2365</td>
<td>0.514</td>
<td>4798</td>
<td>5015</td>
</tr>
<tr>
<td>Three</td>
<td>-1599</td>
<td>0.636</td>
<td>3328</td>
<td>3743</td>
</tr>
<tr>
<td>Four</td>
<td>-1287</td>
<td>0.601</td>
<td>2740</td>
<td>3270</td>
</tr>
</tbody>
</table>

Tables 3.3, 3.4 and 3.5 present detailed parameter estimates (and t-statistics) of the class-specific travel model choice model, initialization model and transition model, respectively, for the final specification. The four classes, or modality styles, differ from each other in terms of the travel modes that they consider, their sensitivity to the level-of-service of the transportation system, and their socio-demographic composition over time. The tabulated model results are behaviorally consistent, i.e. parameter estimates across all sub-models, and in particular the class-specific travel mode choice model, have the expected sign and are statistically significant. Over subsequent paragraphs, we summarize key characteristics of each of the classes. To underscore behavioral differences between classes, a sample enumeration is carried out across the four waves, and the results are incorporated in our description of the classes.
### Table 3.3: Class-specific Travel Mode Choice Model Results

<table>
<thead>
<tr>
<th>Variable</th>
<th>Class 1 Drivers</th>
<th>Class 2 Bus Users</th>
<th>Class 3 Bus-Metro Users</th>
<th>Class 4 Auto-Metro Users</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Alternative Specific Constant Auto</td>
<td>0.000 (-)</td>
<td>-</td>
<td>-</td>
<td>0.000 (-)</td>
</tr>
<tr>
<td>Metro</td>
<td>-3.925 (-10.134)</td>
<td>-</td>
<td>0.000 (-)</td>
<td>2.293 (208.455)</td>
</tr>
<tr>
<td>Bus</td>
<td>-4.259 (-13.437)</td>
<td>0.000 (-)</td>
<td>-7.644 (-19.739)</td>
<td>-</td>
</tr>
<tr>
<td>Walk</td>
<td>1.935 (6.158)</td>
<td>-</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td>Bike</td>
<td>-0.710 (-3.214)</td>
<td>-</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td>Auto-Metro</td>
<td>-3.440 (-11.576)</td>
<td>-</td>
<td>-</td>
<td>4.441 (753.179)</td>
</tr>
<tr>
<td>Bus-Metro</td>
<td>-3.618 (-9.750)</td>
<td>-</td>
<td>2.208 (6.965)</td>
<td>-</td>
</tr>
<tr>
<td>Travel Time (mins)</td>
<td>-0.028 (-2.968)</td>
<td>-0.042* (-0.275)</td>
<td>-0.091* (-0.290)</td>
<td>-0.069 (-3.043)</td>
</tr>
<tr>
<td>Walk Time (mins)</td>
<td>-0.041 (-3.761)</td>
<td>-0.002* (-0.019)</td>
<td>-0.127* (-0.574)</td>
<td>-0.103* (-0.073)</td>
</tr>
<tr>
<td>Travel Cost (CLP)</td>
<td>-0.006* (-1.072)</td>
<td>-0.061* (-0.280)</td>
<td>-0.102* (-0.344)</td>
<td>-0.080* (-0.074)</td>
</tr>
<tr>
<td>Waiting Time (mins)</td>
<td>-0.024* (-1.065)</td>
<td>-0.038* (-0.042)</td>
<td>-0.293* (-0.790)</td>
<td>-0.053* (-0.940)</td>
</tr>
<tr>
<td>Number of Transfers</td>
<td>-</td>
<td>-2.633 (-13.894)</td>
<td>-1.136 (-118.488)</td>
<td>-</td>
</tr>
</tbody>
</table>

- Not applicable; * Insignificant at the 5% level

### Table 3.4: Initialization Model Results

<table>
<thead>
<tr>
<th>Variable</th>
<th>Class 1 Drivers</th>
<th>Class 2 Bus Users</th>
<th>Class 3 Bus-Metro Users</th>
<th>Class 4 Auto-Metro Users</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Alternative Specific Constant</td>
<td>0.000 (-)</td>
<td>2.993 (5.951)</td>
<td>-0.073* (-0.160)</td>
<td>0.139* (0.229)</td>
</tr>
<tr>
<td>Household Income (100,000s CLP)</td>
<td>0.000 (-)</td>
<td>-0.510 (-4.621)</td>
<td>-0.060* (-1.313)</td>
<td>-0.190 (-2.008)</td>
</tr>
<tr>
<td>Male</td>
<td>0.000 (-)</td>
<td>0.223* (0.521)</td>
<td>0.635* (1.176)</td>
<td>0.519* (0.821)</td>
</tr>
<tr>
<td>Number of Vehicles</td>
<td>0.000 (-)</td>
<td>-0.992 (-3.159)</td>
<td>-0.739 (-1.979)</td>
<td>-0.295* (-0.736)</td>
</tr>
</tbody>
</table>

- Not applicable; * Insignificant at the 5% level
Table 3.5: Transition Model Results

<table>
<thead>
<tr>
<th>Variable</th>
<th>Class 1 Drivers</th>
<th>Class 2 Bus Users</th>
<th>Class 3 Bus-Metro Users</th>
<th>Class 4 Auto-Metro Users</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>Transition Model (Given Class 1 in Wave t-1)</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Alternative Specific Constant</td>
<td>0.000 (-)</td>
<td>0.900 (28.746)</td>
<td>1.351 (12.388)</td>
<td>-2.175 (-44.022)</td>
</tr>
<tr>
<td>Household Income (100,000s CLP)</td>
<td>0.000 (-)</td>
<td>-0.170* (-0.002)</td>
<td>-0.610* (-0.010)</td>
<td>-0.080* (-0.001)</td>
</tr>
<tr>
<td>Male</td>
<td>0.000 (-)</td>
<td>0.671 (21.067)</td>
<td>-1.178 (-21.928)</td>
<td>0.359</td>
</tr>
<tr>
<td>Number of Vehicles</td>
<td>0.000 (-)</td>
<td>-0.385 (-5.752)</td>
<td>-0.416* (-2.626)</td>
<td>-0.365* (-2.021)</td>
</tr>
<tr>
<td>Consumer Surplus (utils)</td>
<td>0.594* (0.303)</td>
<td>1.000 (-)</td>
<td>0.264</td>
<td>-</td>
</tr>
<tr>
<td></td>
<td>Transition Model (Given Class 2 in Wave t-1)</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Alternative Specific Constant</td>
<td>0.000 (-)</td>
<td>4.833 (7.617)</td>
<td>2.060 (163.711)</td>
<td>1.223 (382.495)</td>
</tr>
<tr>
<td>Household Income (100,000s CLP)</td>
<td>0.000 (-)</td>
<td>-0.680 (-10.155)</td>
<td>-0.310* (-0.003)</td>
<td>-0.500* (-0.005)</td>
</tr>
<tr>
<td>Male</td>
<td>0.000 (-)</td>
<td>1.831 (3.014)</td>
<td>1.056* (1.477)</td>
<td>0.999* (1.506)</td>
</tr>
<tr>
<td>Number of Vehicles</td>
<td>0.000 (-)</td>
<td>0.595* (1.135)</td>
<td>-0.130* (-0.100)</td>
<td>-0.378* (-0.248)</td>
</tr>
<tr>
<td>Consumer Surplus (utils)</td>
<td>0.330 (110.466)</td>
<td>0.500 (256.703)</td>
<td>0.155* (0.114)</td>
<td>0.317* (0.253)</td>
</tr>
<tr>
<td></td>
<td>Transition Model (Given Class 3 in Wave t-1)</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Alternative Specific Constant</td>
<td>0.000 (-)</td>
<td>2.480* (1.371)</td>
<td>0.936 (414.323)</td>
<td>1.391 (626.478)</td>
</tr>
<tr>
<td>Household Income (100,000s CLP)</td>
<td>0.000 (-)</td>
<td>-1.150 (-2.811)</td>
<td>-0.090* (-0.001)</td>
<td>-0.930* (-0.012)</td>
</tr>
<tr>
<td>Male</td>
<td>0.000 (-)</td>
<td>0.635* (0.560)</td>
<td>1.801 (3.300)</td>
<td>-0.641* (-1.087)</td>
</tr>
<tr>
<td>Number of Vehicles</td>
<td>0.000 (-)</td>
<td>-1.506* (-1.495)</td>
<td>-1.143* (-0.608)</td>
<td>0.184* (0.143)</td>
</tr>
<tr>
<td>Consumer Surplus (utils)</td>
<td>1.709* (1.688)</td>
<td>0.140* (0.098)</td>
<td>0.097* (0.108)</td>
<td>0.364* (0.560)</td>
</tr>
<tr>
<td></td>
<td>Transition Model (Given Class 4 in Wave t-1)</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Alternative Specific Constant</td>
<td>0.000 (-)</td>
<td>1.064* (0.504)</td>
<td>0.636 (123.621)</td>
<td>0.968 (1003.253)</td>
</tr>
<tr>
<td>Household Income (100,000s CLP)</td>
<td>0.000 (-)</td>
<td>-0.370* (-0.712)</td>
<td>-0.060* (-0.001)</td>
<td>0.050* (0.001)</td>
</tr>
<tr>
<td>Male</td>
<td>0.000 (-)</td>
<td>1.84* (1.07)</td>
<td>1.03* (1.10)</td>
<td>0.04* (0.06)</td>
</tr>
<tr>
<td>Number of Vehicles</td>
<td>0.000 (-)</td>
<td>-1.805* (-1.905)</td>
<td>-0.163* (-0.058)</td>
<td>0.142* (0.061)</td>
</tr>
<tr>
<td>Consumer Surplus (utils)</td>
<td>0.088* (0.513)</td>
<td>0.094* (0.501)</td>
<td>0.083* (0.487)</td>
<td>-</td>
</tr>
</tbody>
</table>

- Not applicable; * Insignificant at the 5% level
Class 1 (drivers): This class constitutes 36% of the sample population during wave 1, and the share of the class slowly but steadily increases to 40% by wave 4. Individuals belonging to this class consider all available modes of transport, but 70% of all trips are made by auto. Value of time varies between 0.36$/hr for waiting time and 0.62$/hr for walking time, and the class is completely insensitive to public transport transfers. High-income men with cars are most likely to belong to this class.

Class 2 (bus users): This class constitutes 39% of the sample population during wave 1, and the share of the class steadily decreases to 20% by wave 4. Individuals belonging to this class deterministically choose bus for all their trips. Value of time is low, at approximately 0.07$/hour across different travel time components. Note that even though the class-specific choice model is deterministic, parameters denoting sensitivities to travel times and costs can still be estimated indirectly through the transition model through the construct of consumer surplus. High-income individuals with cars are most likely to belong to this class initially, but they are also most likely to leave this class after the introduction of Transantiago.

Class 3 (bus-metro users): This class constitutes 14% of the sample population during wave 1, and the share of the class steadily increases to 24% by wave 4. Individuals belonging to this class consider the metro, bus and bus-metro alternatives. Value of time varies between 0.09$/hr for in-vehicle time and 0.26$/hr for waiting time. Each public transport transfer is equivalent to 12 minutes of in-vehicle time. Low-income women without access to cars are most likely to belong to this class.

Class 4 (auto-metro users): This class constitutes 11% of the sample population during wave 1, and the share of the class increases marginally to 16% by wave 4. Individuals belonging to this class consider the auto, metro and auto-metro alternatives. Value of time varies between 0.06$/hr for waiting time and 0.12$/hr for walking time, and the class is completely insensitive to public transport transfers. While low-income individuals without access to cars are most likely to belong to this class initially, over time, more high-income individuals with access to cars migrate to this class.

Now that we have estimated our hidden Markov model, we want to explore the power of this model in terms of explaining the evolution of preferences, or modality styles, in response to the introduction of Transantiago. The population distribution of individuals across the four classes for each of the waves, as determined by sample enumeration, is displayed in figure 3.5. It is evident that a shock to the transportation network along the lines of Transantiago did force people to reconsider their modes for travel. The market share of drivers, bus-metro, and auto-metro users has increased after the introduction of Transantiago, while the market share for bus users has drastically decreased. These results are aligned with findings from Section 6 regarding mode share percentages of the different modes across the four waves. We can see that major reductions and increases in shares of modality styles occurred right after Transantiago revolutionized the public transit system. These population changes stabilize over time. It is also evident from the figure that population preferences have in fact changed over time, and in particular after the introduction of Transantiago.
However, the stability in preferences at the population level belies the instability at the individual level. Figure 3.6 illustrates the average transition probabilities between different modality styles across successive time periods. Note that while Figure 3.5 could have been reproduced using a static framework, such as an LCCM, with repeated cross-sectional data (see, for example, Vij et al., 2017), Figure 3.6 could only be produced using a dynamic framework with longitudinal data, such as the HMM proposed here. Interestingly, transition probabilities were not found to differ substantially across time periods, and for this reason, we present average values over all time periods. There are two key trends to note here. First, the construct of habit formation is implicitly captured in the relative magnitude of the transition probabilities. In general, decision-makers are more inclined to remain in the same modality style over time than switch to a different modality style. For three of the four modality styles, the probability of staying in that modality style over successive time periods is found to be greater than half. And second, there is considerable instability in travel mode preferences, despite the relative stability at the population level and the strong influence of habit at the individual level. For example, roughly 30% of bus users and bus-metro users become drivers each time period. Part of this transition could be explained by the introduction of Transantiago, which did make use of the public transport system in a more onerous manner. However, the trend persists beyond wave 2, several months after the introduction of Transantiago, indicating a more general and ongoing shift in preferences towards the car over time, triggered possibly in part by the introduction of Transantiago.
Figure 3.6: Estimated Average Transition Probabilities across Modality Styles over Time
3.8 Policy Analysis
Practitioners and policy analysts are often interested in understanding and predicting broad population trends in travel and activity behavior. Does failure to account for preference dependencies over time impact population estimates? Or is it reasonable to ignore such dependencies when undertaking population-level analysis? We address these questions by comparing aggregate forecasts from the HMM with static frameworks that do not account for preference dependencies over time. The forecasting horizon is limited to three waves post the fourth wave (i.e. waves five, six and seven). We simulate the following two policy scenarios:

1- Increasing household income by 10% at waves five, six and seven respectively.
2- Reducing travel time by 15% for the bus and bus to metro alternatives. This could be brought about by a new transportation policy, dedicated bus lanes for example. This particular shock to the transportation network is assumed to take place between waves four and five.

We compare forecasts from the HMM with latent class choice models (LCCMs). To ensure that the LCCMs and the HMM are as similar as possible, and any potential differences in forecasts cannot be attributed to differences in either observed data or model specification, we use the following procedure. Since an LCCM would typically be estimated using a single cross-section, we estimate two separate LCCMs using data from the first and last wave respectively. Each of the LCCMs comprises four modality styles (preference states), same as our HMM. We constrain the class-specific choice model for each LCCM to be the same as that of the HMM. We only estimate the class membership model parameters, where we formulate class membership as a function of socio-demographic variables, namely income, gender and level of car ownership, and the consumer surplus offered by each class. These are the same variables that are included in the specification of the transition model for the HMM.

Figure 3.7 plots the change in modality styles across waves five, six and seven for the first policy scenario, as predicted by the HMM and the two LCCMs, and figure 3.8 plots the corresponding travel mode shares for the same. As is evident from the figures, even at the population level, there are considerable differences between forecasts from the three models. In general, the LCCM estimated using wave 4 data more closely tracks forecasts from the HMM. Relative to the HMM, the LCCM estimated using wave 4 data under predicts the share of drivers and auto-metro users, and over predicts the share of bus-metro users, whereas the LCCM estimated using wave 1 data under predicts the share of bus-metro users, and over predicts the share of drivers and bus users. These differences translate into similar inconsistencies in travel mode shares. For example, travel mode shares for the pure public transport modes, i.e. bus, metro and bus to metro, during wave 5 are predicted to be 49% by the HMM, 45% by the LCCM estimated using wave 1 data, and 54% by the LCCM estimated using wave 4 data.

Figures 3.9 and 3.10 plot corresponding forecasts for the second policy scenario, as predicted by the HMM and the two LCCMs. Note that the travel mode shares are the same across all three waves, since the change in the transportation system precedes wave 5. Therefore, we show them as a single plot.
Figure 3.7: Share of Individuals in Each Modality Style for Policy Scenario 1, as Predicted by the HMM, the LCCM Estimated Using Wave 1 Data, and the LCCM Estimated Using Wave 4 Data

Figure 3.8: Mode Shares for Policy Scenario 1, as Predicted by the HMM, the LCCM Estimated Using Wave 1 Data, and the LCCM Estimated Using Wave 4 Data
Figure 3.9: Share of Individuals in Each Modality Style for Policy Scenario 2, as Predicted by the HMM, the LCCM Estimated Using Wave 1 Data, and the LCCM Estimated Using Wave 4 Data

Figure 3.10: Mode Shares for Policy Scenario 2, as Predicted by the HMM, the LCCM Estimated Using Wave 1 Data, and the LCCM Estimated Using Wave 4 Data
In terms of modality styles, there are considerable differences between forecasts from the three models, though forecasts from the LCCM estimated using wave 4 data are in closer agreement with those from the HMM. Interestingly, changes in in-vehicle travel times between waves 4 and 5 do not have a significant impact on the likelihood of belonging to a particular modality style over subsequent waves, as predicted by each of the three models, and the population distribution remains largely unchanged across waves 5, 6 and 7. It is important to note that across both scenarios, the predicted share of drivers and bus users has been strictly higher via the LCCM estimated using wave 1 data, compared to the other two models, while the share of bus-metro users has been significantly lower. The reason behind that is the fact that observations pertinent to wave one (before the introduction of Transantiago) constituted a sample of the population that preferred taking the bus or driving to work. Moreover, the market share for the metro alternative was significantly lower during wave one. In addition to that, forecasts from the HMM and LCCM estimated using wave 4 data seem to be more consistent with each other in terms of the evolutionary trends of preferences. However, the share of individuals in the four preference states tends to be different.

In terms of aggregate mode shares, differences across the three models are equally sizeable. For example, travel mode shares for bus are predicted to be 21% by the HMM, 26% by the LCCM estimated using wave 1 data, and 23% by the LCCM estimated using wave 4 data. And similarly, travel mode shares for bus to metro are predicted to be 18% by the HMM, 12% by the LCCM estimated using wave 1 data, and 21% by the LCCM estimated using wave 4 data. As we argued before, relative to the HMM, the LCCM estimated using wave 1 data over predicts mode shares for bus and under predicts mode shares for bus to metro, and the LCCM estimated using wave 4 data over predicts mode shares for bus to metro. These differences are not unexpected. Bus use was at its greatest during the first wave of observation. And subsequent structural changes in the public transportation system, initiated by Transantiago, increased the popularity of bus to metro over the following waves. On one hand, the LCCM estimated using wave 1 data is unable to predict the full extent of changes in behavior in response to these changes in the transportation system. On the other, the LCCM estimated using wave 4 data overstates these changes in behavior, as it does not account for habit formation from preferences and behaviors that precede Transantiago.

3.9 Conclusion

The objective of this study was to develop a methodological framework that can model and forecast the evolution of individual preferences and behaviors over time. Traditionally, discrete choice models have formulated preferences as a function of demographic and situational variables, psychological, sociological and biological constructs, and available alternatives and their attributes. However, the impact of past experiences on present preferences has usually been overlooked.

We developed a hidden Markov model (HMM) of travel mode choice behavior. The hidden states denote travel mode preferences, or modality styles, that differ from one another in terms of the travel modes considered when deciding how to travel, and the relative sensitivity to different level-of-service attributes of the transportation system. The evolutionary path is assumed to be a first-order Markov process, such that an individual’s modality style during a particular time period
depends only on their modality style in the previous time period. Transitions between modality styles over time are assumed additionally to depend on changes in demographic variables and the transportation infrastructure (available travel modes and their attributes). Conditional on the modality styles that an individual has during a particular time period, the individual is assumed to choose that travel mode which offers the greatest utility.

The model framework was empirically evaluated using data from the Santiago Panel. The dataset comprises four waves of one-week pseudo travel diaries each. The first wave was conducted before the introduction of Transantiago, a complete redesign of the public transit system in Santiago, Chile, and the next three waves were conducted after. The dataset offered a unique opportunity to study the impact of a shock to the transportation network on the stability of travel mode preferences over time. The model identified four modality styles in the sample population: drivers, bus users, bus-metro users and auto-metro users. At the population level, the proportion of drivers, auto-metro users, and bus-metro users has increased after the introduction of Transantiago, and the proportion of bus users has drastically decreased. The biggest shift happens between the first and second wave, the same period when Transantiago is introduced. The population distribution is more or less stable across the latter three waves. However, at the individual level, we observe two interesting phenomena. First, habit formation is found to impact transition probabilities across all modality styles. Individuals are more likely to stay in the same modality style over successive time periods than transition to a different modality style. And second, despite both the stability in preferences at the population level and the influence of habit formation at the individual level, nearly 40% of the sample population is found to change modality styles between any two successive waves, reflecting great instability in individual preferences, much after the introduction of Transantiago. These findings hold implications for aggregate forecasts. We simulated two policy scenarios using the HMM, and two latent class choice model (LCCM) framework with comparable specifications, estimated using two separate cross-sections of the Santiago Panel. Relative to the HMM, the first LCCM, estimated using data from before the introduction of Transantiago, under predicts changes in travel mode shares, due to its inability to observe the potential impact of a transformative change such as Transantiago. Relative to the HMM, the second LCCM, estimated using data from after the introduction of Transantiago, over predicts changes in travel mode shares, due to its inability to account for habit formation of preferences and behaviors from before the introduction of Transantiago.

There are two key directions in which future research can build on findings from this study. First, the methodological framework developed here captures preference dependencies across time for the same individual, explicitly accounting for the effect of habit formation on travel behavior. The framework offers the potential to improve the accuracy of the long-range forecasts made from large-scale urban travel demand models. Future research should explore ways in which existing travel demand modeling paradigms can adopt dynamic representations of behavior that capture temporal trends in preferences and behaviors. And second, the framework developed here provides a quantitative basis for modeling and forecasting structural shifts in preferences that are bound to occur in this era of transformative mobility. We observed great flux in individual commute travel mode preferences over time, triggered at least in part by a major redesign of the public transportation system. It would be interesting to see how these findings compare with corresponding changes in preferences across other dimensions of travel behavior, such as car...
ownership and residential location, and in response to other changes in transport policy, infrastructure and services, such as the introduction of congestion charge schemes, the diffusion of alternative-fuel vehicles and the emergence of shared mobility services.

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Chapter 4

Expectation Maximization Algorithm: Derivation and Formulation for Mixture Models and Hidden Markov Models with Logit Kernels

4.1 Introduction

Statistical inference for mixture models and hidden Markov models could be conducted using traditional batch gradient descent algorithms to maximize the likelihood function. However, due to the non-convex nature of the objective function, direct maximization of the likelihood could become difficult and highly unstable. Traditional optimization methods, for example Newton-Raphson, have the following limitations: (1) evaluating the gradient (set of first derivatives) becomes more complicated and requires significantly more time with an increase in the number of parameters; and (2) inversion of the hessian becomes numerically more difficult with the possibility of empirical singularity at some iterations (Train, 2008). Those issues are likely to occur as the number of parameters to be estimated increases and as maximizing the likelihood function becomes more complex and numerically difficult, which is the case with advanced discrete choice models that entail latent variables.

The EM algorithm, first introduced by Dempster et al. (1977), is a statistical learning technique used in models that entail discrete latent variables and use the method of maximum likelihood to estimate parameters (Jordan, 2003). The EM algorithm provides a more efficient approach to deal with the above issues by maximizing a lower bound function of the maximum likelihood (an expectation function), which is computationally much easier to maximize as opposed to the model’s full likelihood function (Train, 2008). The EM algorithm framework comprises the following three steps: (1) writing the complete log-likelihood function assuming the discrete latent variables are in fact observed; (2) evaluating the expectation of all required sufficient statistics conditioned on the observed variables and current estimates of the unknown parameters denoted as the E-step; and (3) maximizing the complete log-likelihood function to update parameter estimates conditioned on the observed variables and expectation of the sufficient statistics denoted as the M-step. The algorithm alternates between the E-step and M-step until the convergence criterion is met. The EM algorithm tends to be more stable than gradient-descent based algorithms when latent variables are involved, and requires fewer iterations to converge by taking advantage of the conditional independence structure of the model framework. As we will see in this chapter, logit kernels will result in closed form gradients that can be analytically evaluated. This is extremely beneficial from an optimization perspective as the optimizer will not have to deal with numerical approximations of the gradient at each iteration, which becomes time consuming with an increase in the number of parameters.

Bhat (1997) and Train (2008) discuss and provide derivations for the EM algorithm in the context of mixture models. They do provide the general guiding steps of the EM algorithm, however in this chapter, we will go into more detail with our derivations of the various steps of the EM
algorithm including the closed form gradients (property of the logit kernels). The motivation here is to dive into the details of the various steps of the EM algorithm to encourage modelers to estimate latent class choice models more efficiently. The major contribution of this chapter is in the case of hidden Markov models with logit kernels. Dynamic discrete choice frameworks that employ hidden Markov models are becoming more popular in the transportation literature. For example, Choudhury et al. (2010), used traditional gradient descent algorithms to maximize the likelihood while Xiong et al. (2015) used Bayesian estimation and Markov Chain Monte Carlo (MCMC) simulation to estimate model parameters. We will provide rigorous derivations of the EM algorithm when dealing with HMMs to highlight its computational efficiency as compared to standard gradient descent algorithms including the closed form gradients. Using such a statistical learning technique i.e. the EM algorithm, model estimation time will be reduced from the order of many hours to minutes.

We are interested in providing the formulation, and derivation of the EM algorithm for both latent class choice models and hidden Markov models with logit kernels, to enable travel demand and behavioral modelers to estimate such advanced models while saving on estimation time. This chapter is organized as follows: Section 2 provides the derivations of the various steps of the EM algorithm in addition to the gradients for all required parameters in the case of mixture models with logit kernels. Section 3 entails the same set of derivations of the EM algorithm and the required gradient vectors in the case of hidden Markov models with logit kernels.

4.2 Mixture Models with Logit Kernels
The proposed framework for modeling and forecasting the adoption and diffusion of new transportation services, which was formulated in chapter two of this dissertation, is displayed in the figure below.

![Figure 4.1: Generalized Technology Adoption Model](image-url)
Based on derivations in chapter two, the marginal probability \( P(y) \) of observing a vector of choices \( y \) for all decision-makers in the sample is:

\[
P(y) = \prod_{n=1}^{N} \sum_{s=1}^{S} P(y_n|q_{ns}) P(q_{ns}|Z_n) = \prod_{n=1}^{N} \sum_{s=1}^{S} P(q_{ns}|Z_n) \prod_{t=1}^{T_n} \prod_{j \in C} P(y_{ntj}|Z_{nt}, X_{ntj}, q_{ns})^{y_{ntj}}
\]

where \( y_{ntj} \) equals one if individual \( n \) during time period \( t \) chose to adopt the new technology \((j=1)\) and zero otherwise, conditional on his/her characteristics during time period \( t \) denoted as \( Z_{nt} \) and attributes of the new technology \((j=1)\) during time period \( t \) denoted as \( X_{ntj} \), and conditional on the decision-maker belonging to latent class \( s \) \((q_{ns} \text{ equals one and zero otherwise})\), \( C \) denotes the choice set i.e. either adopting to the new service or not which is common to all individuals, \( T_n \) is the total number of time periods available for individual \( n \) until he/she adopts, \( Z_n \) denotes the set of socio-demographic variables associated with decision-maker \( n \), \( S \) denotes the total number of distinct latent classes, which is equal to three in our case, and \( N \) represents the total number of individuals in the sample.

### 4.2.1 The EM Formulation

The first step to using the EM algorithm entails writing the complete log-likelihood assuming that the discrete latent variable \((q_{ns})\) is in fact observed. Through the complete log-likelihood formulation, we can uncover the form of the M-step estimates as well as the sufficient statistics required for the E-step. In order to do so, let us express the above likelihood equation in terms of the corresponding logit kernels for the class membership model and class-specific adoption model.

\[
P(y) = \prod_{n=1}^{N} \sum_{s=1}^{S} e^{x'_{ntj} \beta_s} \sum_{s'=1}^{S} e^{x'_{ntj} \beta_{s'}} \prod_{t=1}^{T_n} \prod_{j \in C} \frac{e^{x'_{ntj} \beta_s}}{\sum_{j' \in C} e^{x'_{ntj} \beta_{j'}}} y_{ntj}
\]

where \( x'_{ntj} \) is a row vector that entails attributes of the new technology, cumulative number of adopters of the new technology during time period \((t-1)\), and socio-demographic variables, \( \beta_s \) is a column vector of parameters specific to latent class \( s \), \( z'_{nt} \) is a row vector of socio-economic and demographic variables, and \( \tau_s \) is a column vector of parameters pertinent to latent class \( s \).

In order to simplify notation, \( x'_{ntj} \) in the class-specific adoption model utility specification comprises attributes of the new technology, social influences and socio-demographic variables. We simply aggregated those three exogenous variables into a vector \( x'_{ntj} \). This will make it easier to derive the E-step and M-step equations of the EM algorithm. The same behavioral rationale for each class-specific utility equation still applies as per our previous definition in chapter two.

The above likelihood function could be expressed as follows:

\[
P(y) = \prod_{n=1}^{N} \sum_{s=1}^{S} e^{x'_{nts} \tau} \sum_{s'=1}^{S} e^{x'_{nts} \tau'} \prod_{t=1}^{T_n} \prod_{j \in C} \frac{e^{x'_{ntj} \beta_s}}{\sum_{j' \in C} e^{x'_{ntj} \beta_{j'}}} y_{ntj}
\]
where $z'_{ns}$ is a row vector of socio-economic and demographic variables that are interacted with latent class specific binary variables. This is a preferred specification as it will enable us to estimate one vector of class membership parameters for all latent classes instead of estimating three separate vectors pertinent to each latent class.

Now, assuming that the adoption styles (innovators, imitators and non-adopters) are no longer latent but are in fact observable variables, the complete likelihood $L_C$ can be written as:

$$L_C = \prod_{n=1}^{N} \prod_{s=1}^{S} \left[ \frac{e^{z'_{ns}\tau}}{\sum_{s'=1}^{S} e^{z'_{ns}\tau}} \right] q_{ns} T_n \prod_{n=1}^{N} \prod_{s=1}^{S} \prod_{t=1}^{T_n} \left[ \frac{e^{x'_{ntj}\beta_s}}{\sum_{j' \in C} e^{x'_{ntj}\beta_{s'}}} \right] y_{ntj} q_{ns}$$

The unknown parameter vectors in the above equation are $\{\tau, \beta\}$. Taking the logarithm, it can be seen that the complete log-likelihood function $L_C$ breaks apart quite conveniently into two separate components, each corresponding to the two endogenous variables:

$$L_C = \sum_{n=1}^{N} \sum_{s=1}^{S} q_{ns} \log \left[ \frac{e^{z'_{ns}\tau}}{\sum_{s'=1}^{S} e^{z'_{ns}\tau}} \right] + \sum_{n=1}^{N} \sum_{s=1}^{S} \sum_{t=1}^{T_n} \sum_{j \in C} y_{ntj} q_{ns} \log \left[ \frac{e^{x'_{ntj}\beta_s}}{\sum_{j' \in C} e^{x'_{ntj}\beta_{s'}}} \right]$$

From the above equation, it is evident that $q_{ns}$ is the only sufficient statistic required for estimating all of the unknown parameters. Let us denote $\Phi$ as the vector of unknown parameters to be estimated $= \{\tau, \beta\}$.

### 4.2.2 The E-step

The following section focuses on the derivations pertinent to the E-step, which requires evaluating the expectation of every sufficient statistic. In this case, we will compute the expectation of the latent variable $q_{ns}$ denoted as $E[q_{ns}|y; \Phi]$. The updates for $E[q_{ns}|y; \Phi]$ as given by the E-step in the $(t+1)$ iteration of the EM algorithm will computed as follows:

$$E[q_{ns}|y; \Phi] = P(q_{ns} = 1|y; \Phi) = P(q_{ns} = 1|y_n; \Phi)$$

$$= \frac{P(y_n|q_{ns} = 1; \Phi)P(q_{ns} = 1|\Phi)}{P(y_n|\Phi)} \quad \text{(Bayes Rule)}$$

Then,

$$q_{ns}^{(t+1)} = E[q_{ns}|y; \Phi^{(t)}] = \frac{P(y_n|q_{ns} = 1; \Phi^{(t)})P(q_{ns} = 1|\Phi^{(t)})}{P(y_n|\Phi^{(t)})}$$

where $\Phi^{(t)}$ denotes the parameter updates as given by the M-step in the $t^{th}$ iteration of the EM algorithm.
Now, let’s replace the above probability functions by their respective values:

\[
q_{ns}^{(t+1)} = \frac{\prod_{t=1}^{T_n} \prod_{j \in C} \left[ \frac{e^{x'_{ntj} \beta_s^{(t)}}}{\sum_{j' \in C} e^{x'_{ntj} \beta_s^{(t)}}} \right]^{y_{ntj}} \times \frac{e^{z'_{ns} \tau^{(t)}}}{\sum_{s' = 1}^{S} e^{z'_{ns} \tau^{(t)}}}}{\sum_{s = 1}^{S} \frac{e^{z'_{ns} \tau^{(t)}}}{\sum_{s' = 1}^{S} e^{z'_{ns} \tau^{(t)}}}}
\]

**4.2.3 The M-Step**

Having derived expressions for the updates in the E-step for the sufficient statistic, \(q_{ns}\), we can proceed now to the M-step. In the M-step, the expectation of the sufficient statistic is treated as a true value and the complete log-likelihood is subsequently maximized for the unknown parameters \(\{\tau, \beta\}\). Taking the derivative of the complete log-likelihood function with respect to the unknown parameters, we get the following updates for the M-step:

\[
\beta_s^{(t+1)} = \arg\max_{\beta_s} \sum_{n=1}^{N} \sum_{t=1}^{T_n} \sum_{j \in C} y_{ntj} q_{ns}^{(t+1)} \log \left[ \frac{e^{x'_{ntj} \beta_s}}{\sum_{j' \in C} e^{x'_{ntj} \beta_s}} \right]
\]

\[
\tau^{(t+1)} = \arg\max_{\tau} \sum_{n=1}^{N} \sum_{s=1}^{S} q_{ns}^{(t+1)} \log \left[ \frac{e^{z'_{ns} \tau}}{\sum_{s' = 1}^{S} e^{z'_{ns} \tau}} \right]
\]

Those two equations are both weighted multinomial logit models that can be solved fairly efficiently. The EM algorithm iterates between the E-step and the M-step, until the convergence criterion is satisfied.

**4.2.4 Gradient for Weighted Multinomial Logit Model**

We will focus on the derivation of the gradient for a weighted multinomial logit model, which is required for the estimation of the class membership and class-specific choice model parameters. The log-likelihood function for a weighted multinomial logit model in the case of the class-specific choice model is given by:
\[ L = \sum_{n=1}^{N} \sum_{t=1}^{T_n} \sum_{j \in C} y_{ntj} q_{ns} \log \left( \frac{e^{x'_{ntj} \beta_s}}{\sum_{j' \in C} e^{x'_{ntj'} \beta_s}} \right) \] (refer to above M - step)

Let us define the weight vector, \( w_{ntj} = y_{ntj} q_{ns} \) and \( P_{ntj} = \frac{e^{x'_{ntj} \beta_s}}{\sum_{j' \in C} e^{x'_{ntj'} \beta_s}} \). Then,

\[ L = \sum_{n=1}^{N} \sum_{t=1}^{T_n} \sum_{j \in C} w_{ntj} \log \left( \sum_{j' \in C} e^{x'_{ntj'} \beta_s} \right) - \sum_{n=1}^{N} \sum_{t=1}^{T_n} \sum_{j \in C} w_{ntj} \log \left( \sum_{j' \in C} e^{x'_{ntj'} \beta_s} \right) \]

\[ = \sum_{n=1}^{N} \sum_{t=1}^{T_n} \sum_{j \in C} w_{ntj} x'_{ntj} - \sum_{n=1}^{N} \sum_{t=1}^{T_n} \sum_{j \in C} \sum_{j' \in C} x'_{ntj'} P_{ntj'} \sum_{j' \in C} w_{ntj} \]

Taking the derivative of the log-likelihood with respect to the unknown parameters:

\[ \frac{dL}{d\beta_s} = \sum_{n=1}^{N} \sum_{t=1}^{T_n} \sum_{j \in C} w_{ntj} x'_{ntj} - \sum_{n=1}^{N} \sum_{t=1}^{T_n} \sum_{j \in C} \sum_{j' \in C} x'_{ntj'} P_{ntj'} \sum_{j' \in C} w_{ntj} \]

\[ = \sum_{n=1}^{N} \sum_{t=1}^{T_n} \sum_{j \in C} w_{ntj} x'_{ntj} - \sum_{n=1}^{N} \sum_{t=1}^{T_n} \sum_{j \in C} \sum_{j' \in C} x'_{ntj'} P_{ntj'} \sum_{j' \in C} w_{ntj} \]

Now, when taking derivatives for \( \beta_s \), this implies that we are conditioning on a certain class \( "s" \) such that \( q_{ns} = 1 \), which implies the following:

\[ \sum_{j' \in C} w_{ntj'} = \sum_{j' \in C} y_{ntj'} q_{ns} = 1 \]
Therefore:

\[
\frac{dL}{d\beta_s} = \sum_{n=1}^{N} \sum_{t=1}^{T_n} \sum_{j \in C} [w_{ntj} - P_{ntj}] x'_{ntj}
\]

Now, let us derive the closed form gradient for the class membership model in a similar manner, which again has a weighted multinomial logit structure. The log-likelihood function is given by:

\[
L = \sum_{n=1}^{N} \sum_{s=1}^{S} q_{ns} \log \left[ \frac{e^{z'_{ns}}} {\sum_{s'=1}^{S} e^{z'_{ns}}} \right] \quad \text{(refer to above M - step)}
\]

Let us define \( P_{ns} = \frac{e^{z'_{ns}}}{\sum_{s'=1}^{S} e^{z'_{ns}}' \tau} \) and re-express the log-likelihood function accordingly.

\[
L = \sum_{n=1}^{N} \sum_{s=1}^{S} q_{ns} z'_{ns} \tau - \sum_{n=1}^{N} \sum_{s=1}^{S} q_{ns} \log \left[ \sum_{s'=1}^{S} e^{z'_{ns'} \tau} \right]
\]

Taking the derivative of the log-likelihood with respect to the unknown parameters:

\[
\frac{dL}{d\tau} = \sum_{n=1}^{N} \sum_{s=1}^{S} q_{ns} z'_{ns} - \sum_{n=1}^{N} \sum_{s=1}^{S} q_{ns} \sum_{s'=1}^{S} z'_{ns'} P_{ns'}
\]

\[
= \sum_{n=1}^{N} \sum_{s=1}^{S} q_{ns} z'_{ns} - \sum_{n=1}^{N} \sum_{s=1}^{S} z'_{ns} P_{ns} \quad \text{(since} \sum_{s=1}^{S} q_{ns} = 1)\]

\[
= \sum_{n=1}^{N} \sum_{s=1}^{S} [q_{ns} - P_{ns}] z'_{ns}
\]

We can clearly see that the gradient for weighted multinomial logit models has a closed form, which will in turn be very beneficial from an optimization perspective. This will enable the optimizer to update parameter estimates at a much faster pace rather than having to numerically approximate the gradient, which becomes time consuming with an increase in the number of parameters.
4.3 Hidden Markov Models with Logit Kernels

The proposed framework in chapter three of this dissertation to model and forecast the evolution of individual preferences over time in response to changes in socio-demographic variables and the built environment is displayed in the figure below.

![Figure 4.2: Dynamic Discrete Choice Framework](image)

Based on derivations in chapter three, the marginal probability $P(y_n)$ of observing a sequence of choices $y_n$ for decision-maker $n$ over $T$ waves is expressed as follows:

$$P(y_n) = \sum_{s_1=1}^{S} \sum_{s_2=1}^{S} \ldots \sum_{s_T=1}^{S} \prod_{t=1}^{T} P(y_{nt}|q_{nts_t} = 1) \cdot P(q_{n1s_1} = 1|Z_{n1}) \prod_{t=2}^{T} P(q_{nts_t} = 1|q_{n(t-1)s_{t-1}} = 1)$$

where $(y_{nt}|q_{nts_t} = 1)$ denotes predicting the probability for individual $n$ over wave $t$ making a certain sequence of choices conditional on belonging to modality style $s$ during wave $t$ ($q_{nts_t}$ equals one and zero otherwise), $P(q_{n1s_1} = 1|Z_{n1})$ represents the probability that individual $n$ belongs to modality style $s$ during the first wave conditional on his/her socio-demographic variables during the first wave, $P(q_{nts_t} = 1|q_{n(t-1)s_{t-1}} = 1)$ denotes one entry of the transition probability matrix, which involves predicting the probability that individual $n$ belongs to modality style $s_t$ during wave $t$, conditional on modality style $s_{t-1}$ during the previous wave, and $S$ denotes the total number of modality styles in the sample.
4.3.1 The EM Formulation

Again, as we have seen earlier, the first step of the EM algorithm entails writing the complete log-likelihood. We will express the complete log-likelihood equation in terms of the corresponding logit kernels for the class-specific choice model, initialization model, and transition model. Note that we will restrict the formulation of the transition probability model to entail socio-demographic variables. The EM algorithm won’t be a suitable approach when the transition model is parametrized to reflect changes in the built environment through the consumer surplus. Assuming that the individual modality styles over the waves are no longer latent but are in fact observable variables, the complete likelihood $L_C$ can be written as:

$$L_C = \prod_{n=1}^{N} \prod_{t=1}^{T} \prod_{s=1}^{S} [P(y_{ntkj}|q_{nts} = 1)]^{y_{ntkj}*q_{nts}} \left[ \prod_{n=1}^{N} \prod_{s=1}^{S} [P(q_{n1s} = 1|Z_{n1})]^{q_{n1s}} \right].$$

where $y_{ntkj}$ equals one if decision-maker $n$ over wave $t$ and choice situation $k$ chose alternative $j$ and zero otherwise, $C_{ntkj}$ denotes the choice set available for individual $n$ at wave $t$ and choice situation $k$ conditional on modality style $s$, $K_{nt}$ is the distinct number of choice situations observed for individual $n$ over wave $t$, and $N$ represents the total number of individuals in the sample.

Replacing the probability distributions with their corresponding logit kernels:

$$L_C = \prod_{n=1}^{N} \prod_{t=1}^{T} \prod_{s=1}^{S} \prod_{k=1}^{K_{nt}} e^{x'_{ntkj}\beta_s} \left[ \sum_{j' \in C_{ntkj}} e^{x'_{ntkj'}\beta_s} \right]^{y_{ntkj}*q_{nts}} \prod_{n=1}^{N} \prod_{s=1}^{S} \left[ e^{z'_{n1}s\tau_s} \right]^{q_{n1s}}.$$

where $x'_{ntkj}$ is a row vector of attributes of alternative $j$ during choice situation $k$ over wave $t$ for individual $n$, $\beta_s$ is a column vector of parameters specific to modality style $s$, $z'_{n1}$ is a row vector of socio-economic and demographic variables for individual $n$ during the first wave and $\tau_s$ is the associated column vector of parameter estimates for modality style $s$, $z'_{nt}$ is a row vector of observable socio-economic and demographic characteristics of individual $n$ over wave $t$ and $\gamma_{sr}$ is
a column vector of parameters specific to modality style s at wave t given that the individual belonged to modality style r during wave (t-1).

The above likelihood function could be expressed as follows:

\[
L_C = \prod_{n=1}^{N} \prod_{t=1}^{T} \prod_{s=1}^{S} \prod_{k=1}^{K_{nt}} \prod_{j \in C_{ntk}} \left[ \frac{e^{x'_{ntkj}} \beta_s}{\sum_{j' \in C_{ntk}} e^{x'_{ntkj}} \beta_s} \right] ^ {y_{ntkj}s \cdot q_{nts}} \left[ \sum_{s'=1}^{S} \frac{e^{x'_{nts}} \gamma_r}{e^{x'_{nts}} \gamma_r} \right] ^ {q_{nts} \cdot q_{n(t-1)r}}
\]

where \( z'_{nts} \) is a row vector of socio-economic and demographic variables at wave t that are interacted with modality style specific binary variables.

The unknown parameter vectors in the above equations are \( \{ \beta, \tau, \gamma \} \). Taking the logarithm, it can be seen that the complete log-likelihood function \( L_C \) breaks apart quite conveniently into three separate components:

\[
L_C = \sum_{n=1}^{N} \sum_{t=1}^{T} \sum_{s=1}^{S} \sum_{k=1}^{K_{nt}} \sum_{j \in C_{ntk}} y_{ntkj} q_{nts} \log \left[ \frac{e^{x'_{ntkj}} \beta_s}{\sum_{j' \in C_{ntk}} e^{x'_{ntkj}} \beta_s} \right] + \sum_{n=1}^{N} \sum_{s=1}^{S} q_{nts} \log \left[ \frac{e^{x'_{nts}} \gamma_r}{\sum_{s'=1}^{S} e^{x'_{nts}} \gamma_r} \right]
\]

From the above equation, it is evident that \( q_{nts} \) and \( q_{nts} q_{n(t-1)r} \) are the sufficient statistics required for estimating all of the unknown parameters. Let us denote \( \Phi \) as the vector of unknown parameters to be estimated = \( \{ \beta, \tau, \gamma \} \).

### 4.3.2 The E-step

The following section focuses on the derivations pertinent to the E-step, which requires evaluating the expectation of every sufficient statistic. Let \( \pi_{nts} \) and \( \omega_{nts} \) denote the expectations \( E[q_{nts} | y; \Phi] \) and \( E[q_{nts} q_{n(t-1)r} | y; \Phi] \) respectively. The updates for \( \pi_{nts} \) and \( \omega_{nts} \) as given by
the E-step in the \((t+1)\) iteration of the EM algorithm may be computed using the following expressions:

\[
\pi_{nts}^{(t+1)} = E[q_{nts} \mid \mathbf{y}; \Phi^{(t)}] = P(q_{nts} = 1 \mid \mathbf{y}; \Phi^{(t)})
\]

\[
\omega_{ntsr}^{(t+1)} = E[q_{nts}q_{n(t-1)r} \mid \mathbf{y}; \Phi^{(t)}] = P(q_{nts} = 1, q_{n(t-1)r} = 1 \mid \mathbf{y}; \Phi^{(t)})
\]

where \(\Phi^{(t)}\) denotes the parameter updates as given by the M-step at the \(t^{th}\) iteration of the EM algorithm.

In order to calculate the expectations of those two sufficient statistics, we need to evaluate the posterior probabilities \(P(q_{nts} = 1 \mid \mathbf{y}; \Phi^{(t)})\) and \(P(q_{nts} = 1, q_{n(t-1)r} = 1 \mid \mathbf{y}; \Phi^{(t)})\). To make progress, we should take advantage of conditional independence properties of the graphical model structure of the HMM. The sections below are adapted from Jordan (2003).

Let us define the parameters \(\alpha_{nts}\) and \(\beta_{nts}\) as follows:

\[
\alpha_{nts} = P(y_{n1}, \ldots, y_{nt}, q_{nts} = 1 \mid \Phi)
\]

\[
\beta_{nts} = P(y_{n(t+1)}, \ldots, y_{nT} \mid q_{nts} = 1; \Phi)
\]

where \(\alpha_{nts}\) is the probability of observing a partial sequence of choices \(y_{n1}, \ldots, y_{nt}\) that concludes with individual \(n\) having modality style \(s\) at time \(t\) \((q_{nts} = 1)\), and \(\beta_{nts}\) is the probability of observing a partial sequence of choices \(y_{n(t+1)}, \ldots, y_{nT}\) given that decision-maker \(n\) begins with modality style \(s\) at time \(t\).

We apply Bayes rule to calculate the posterior probability, \(P(q_{nts} = 1 \mid \mathbf{y}_n; \Phi)\), that individual \(n\) over wave \(t\) belongs to modality style \(s\) conditioned on the observed vector of choices \(y_n\) for the individual:

\[
P(q_{nts} = 1 \mid y_n; \Phi) = \frac{P(y_n \mid q_{nts} = 1; \Phi)P(q_{nts} = 1 \mid \Phi)}{P(y_n \mid \Phi)}
\]

\[
= \frac{P(y_{n1}, \ldots, y_{nt}, y_{n(t+1)}, \ldots, y_{nT} \mid q_{nts} = 1; \Phi)P(q_{nts} = 1 \mid \Phi)}{P(y_n \mid \Phi)}
\]

However, the set of choices \(\{y_{n1}, \ldots, y_{nt}\}\) and \(\{y_{n(t+1)}, \ldots, y_{nT}\}\) are assumed to be conditionally independent given that individual \(n\) over wave \(t\) has modality style \(s\). Therefore,
\[ P(q_{nts} = 1|y_n; \Phi) = \frac{P(y_{n1}, \ldots, y_{nt}|q_{nts} = 1; \Phi)P(y_{n(t+1)}, \ldots, y_{nT}|q_{nts} = 1; \Phi)P(q_{nts} = 1|\Phi)}{P(y_n|\Phi)} \]
\[ = \frac{P(y_{n1}, \ldots, y_{nt}, q_{nts} = 1|\Phi)P(y_{n(t+1)}, \ldots, y_{nT}|q_{nts} = 1; \Phi)}{P(y_n|\Phi)} \]
\[ = \frac{\alpha_{nts}\beta_{nts}}{P(y_n|\Phi)} = \pi_{nts} \]

For any \( t \in \{1, \ldots, T\} \), the following identity will hold true:
\[ \alpha_{nts}\beta_{nts} = P(q_{nts} = 1|y_n; \Phi)P(y_n|\Phi) \]

Now, the sum of \( P(q_{nts} = 1|y_n; \Phi) \) over the possible values of \( q_{nts} \) must equal one. Using this property we obtain:
\[ \sum_{s=1}^{S} \alpha_{nts}\beta_{nts} = \sum_{s=1}^{S} P(q_{nts} = 1|y_n; \Phi)P(y_n|\Phi) = P(y_n|\Phi) \]

This implies that we can estimate the likelihood \( P(y_n|\Phi) \) by calculating \( \alpha_{nts} \) and \( \beta_{nts} \) for any wave \( t \) and summing their product. This presents a way to calculate the likelihood function for hidden Markov models. It is evident that our problem of calculating the expectation of the sufficient statistic, \( q_{nts} \), involves calculating the alphas and betas.

From here onwards, for the sake of notational convenience we will not explicitly include \( \Phi \) in any of the expressions, but all the probabilities are conditioned on knowing the vector of parameters \( \Phi \). Also, the indicator value for modality style \( s \) of a certain individual \( n \) at wave \( t \) period will be represented as \( q_{nts} \) instead of \( (q_{nts} = 1) \) for notational convenience. Now, the variable \( \alpha_{nts} \) will be calculated as follows:

\[ \alpha_{nts} = P(y_{n1}, \ldots, y_{nt}, q_{nts}) \]
\[ = P(y_{n1}, \ldots, y_{nt}|q_{nts})P(q_{nts}) \]
\[ = P(y_{n1}, \ldots, y_{n(t-1)}|q_{nts}) P(y_{nt}|q_{nts}) P(q_{nts}) \]
\[ = P(y_{nt}|q_{nts}) P(y_{n1}, \ldots, y_{n(t-1)}, q_{nts}) \]
\[ = P(y_{nt}|q_{nts}) \sum_{s'=1}^{S} P(y_{n1}, \ldots, y_{n(t-1)}, q_{n(t-1)s'}, q_{nts}) \]
\[ = P(y_{nt}|q_{nts}) \sum_{s'=1}^{S} P(y_{n1}, \ldots, y_{n(t-1)}, q_{nts}|q_{n(t-1)s'}) P(q_{n(t-1)s'}) \]
\[ P(\mathbf{y}_{nt}|q_{nts}) \sum_{s'=1}^{S} P(\mathbf{y}_{n1}, \ldots, \mathbf{y}_{n(t-1)}|q_{n(t-1)s'}) P(q_{nts}|q_{n(t-1)s'}) P(q_{n(t-1)s'}) \]

\[ = P(\mathbf{y}_{nt}|q_{nts}) \sum_{s'=1}^{S} P(\mathbf{y}_{n1}, \ldots, \mathbf{y}_{n(t-1)}, q_{n(t-1)s'}) P(q_{nts}|q_{n(t-1)s'}) \]

\[ = P(\mathbf{y}_{nt}|q_{nts}) \sum_{s'=1}^{S} \alpha_{n(t-1)s'} P(q_{nts}|q_{n(t-1)s'}) \]

The algorithm proceeds “forward” in time to compute alphas for all \( t \in \{1, \ldots, T\} \). For the first time period, i.e. \( t=1 \), the algorithm may be initialized as follows:

\[ \alpha_{n1s} = P(\mathbf{y}_{n1}, q_{1s}) = P(\mathbf{y}_{n1}|q_{1s}) P(q_{1s}) \]

The variable \( \beta_{nts} \) may be calculated recursively via a “backward” recursion according to the following set of derivations:

\[ \beta_{n(t-1)s} = P(\mathbf{y}_{nt}, \ldots, \mathbf{y}_{nT}|q_{n(t-1)s}) \]

\[ = \sum_{s'=1}^{S} P(\mathbf{y}_{nt}, \ldots, \mathbf{y}_{nT}, q_{nts'}|q_{n(t-1)s}) \]

\[ = \sum_{s'=1}^{S} P(\mathbf{y}_{nt}, \ldots, q_{n(t-1)s}, q_{nts'}|q_{n(t-1)s}) P(q_{nts'}|q_{n(t-1)s}) \]

\[ = \sum_{s'=1}^{S} P(\mathbf{y}_{nt}|q_{nts'}) P(\mathbf{y}_{n(t+1)}, \ldots, \mathbf{y}_{nT}|q_{nts'}) P(q_{nts'}|q_{n(t-1)s}) \]

\[ = \sum_{s'=1}^{S} P(\mathbf{y}_{nt}|q_{nts'}) \beta_{nts'} P(q_{nts'}|q_{n(t-1)s}) \]

This time the algorithm starts at the final wave \( t = T \) and proceeds backward in time. For \( t = T \), the algorithm cannot use the definition of \( \beta_{nTS} \) since it relies on non-existent \( \mathbf{y}_{n(T+1)} \). However, if we define \( \beta_{nTS} = 1 \) for all \( n \in \{1, \ldots, N\} \) and \( s \in \{1, \ldots, S\} \), then we can apply the above backward recursion equation to show that \( \beta_{n(T-1)s} \) will be calculated correctly as follows:

\[ \beta_{n(T-1)s} = \sum_{s'=1}^{S} P(\mathbf{y}_{nT}|q_{nTS'}) \beta_{nTS'} P(q_{nTS'}|q_{n(T-1)s}) \]
\[
\begin{align*}
\sum_{s' = 1}^{s} P(y_{nT} | q_{ns}) P(q_{ns} | q_{n(T-1)s}) \\
\sum_{s' = 1}^{s} P(y_{nT}, q_{ns'}, q_{n(T-1)s}) P(q_{ns'} | q_{n(T-1)s}) \\
\sum_{s' = 1}^{s} P(y_{nT}, q_{ns'}) = P(y_{nT} | q_{n(T-1)s})
\end{align*}
\]

Therefore, the initialization definition makes sense.

To calculate the expectation of the other sufficient statistic \(q_{nts}q_{n(t-1)r}\), we need to calculate the posterior probability \(P(q_{nts} = 1, q_{n(t-1)r} = 1 | y_n)\), denoted by \(\omega_{nts}r\), as follows:

\[
\omega_{nts}r = P(q_{nts} = 1, q_{n(t-1)r} = 1 | y_n) = \frac{P(y_n, q_{nts}, q_{n(t-1)r}) P(q_{nts} | q_{n(t-1)r}) P(q_{n(t-1)r})}{P(y_n)}
\]

\[
= \frac{P(y_n, q_{nts}, q_{n(t-1)r}) P(y_{nt} | q_{nts}) P(y_{n(t+1)} | q_{nts}) P(q_{nts} | q_{n(t-1)r}) P(q_{n(t-1)r})}{P(y_n)}
\]

\[
= \frac{P(y_n, q_{nts}, q_{n(t-1)r}) P(y_{nt} | q_{nts}) P(y_{n(t+1)} | q_{nts}) P(q_{nts} | q_{n(t-1)r})}{P(y_n)}
\]

\[
= \frac{\alpha_{n(t-1)r} P(y_{nt} | q_{nts}) \beta_{nts} P(q_{nts} | q_{n(t-1)r})}{P(y_n)}
\]

\[
4.3.3 \text{ The M-Step}
\]

Having derived expressions for the updates in the E-step for both sufficient statistics, we can proceed now to the M-step. Taking the derivative of the complete log-likelihood with respect to the unknown parameters, we get the following updates for the M-step:

\[
\beta_s^{(t+1)} = \arg\max_{\beta_s} \sum_{n=1}^{N} \sum_{t=1}^{T} \sum_{k=1}^{K_{nt}} \sum_{j \in C_{nts|s}} y_{ntk} \pi_{nts}^{(t+1)} \log \left[ \frac{e^{x_{ntkj}^{s}} \beta_s}{\sum_{j' \in C_{nts|s}} e^{x_{ntkj'}^{s}} \beta_s} \right]
\]
\[
\tau^{(t+1)} = \arg\max_{\tau} \sum_{n=1}^{N} \sum_{s=1}^{S} \pi_{n1s}^{(t+1)} \log \left[ \frac{e^{x'_{n1s}\tau}}{\sum_{s'=1}^{S} e^{x'_{n1s}\tau}} \right]
\]

\[
y^{(t+1)}_r = \arg\max_{y} \sum_{n=1}^{N} \sum_{t=2}^{T} \sum_{s=1}^{S} \omega_{ntrs}^{(t+1)} \log \left[ \frac{e^{x'_{nts}y}}{\sum_{s'=1}^{S} e^{x'_{nts}s}} \right]
\]

Those three equations are weighted multinomial logit models that can be solved fairly efficiently. The EM algorithm iterates between the E-step and the M-step, until the convergence criterion is satisfied.

4.3.4 Gradient for Weighted Multinomial Logit Model
We will focus on the derivation of the gradient for a weighted multinomial logit model, building off the derivation from the static mixture model (LCCM). The log-likelihood function for a weighted multinomial logit model in the case of the class-specific choice model is given by:

\[
L = \sum_{n=1}^{N} \sum_{t=1}^{T} \sum_{k=1}^{K_{nt}} \sum_{j \in C_{ntk|s}} y_{ntkj} \pi_{nts} \log \left[ \frac{e^{x'_{ntkj}\beta_s}}{\sum_{j' \in C_{ntk|s}} e^{x'_{ntkj}'\beta_s}} \right]
\]

Let us define the weight vector, \(w_{ntkj} = y_{ntkj} \pi_{nts}\) and \(P_{ntkj} = \frac{e^{x'_{ntkj}\beta_s}}{\sum_{j' \in C_{ntk|s}} e^{x'_{ntkj}'\beta_s}}\). Then,

\[
L = \sum_{n=1}^{N} \sum_{t=1}^{T} \sum_{k=1}^{K_{nt}} \sum_{j \in C_{ntk|s}} w_{ntkj} \log \left[ \frac{e^{x'_{ntkj}\beta_s}}{\sum_{j' \in C_{ntk|s}} e^{x'_{ntkj}'\beta_s}} \right]
\]

\[
= \sum_{n=1}^{N} \sum_{t=1}^{T} \sum_{k=1}^{K_{nt}} \sum_{j \in C_{ntk|s}} w_{ntkj} x'_{ntkj} \beta_s - \sum_{n=1}^{N} \sum_{t=1}^{T} \sum_{k=1}^{K_{nt}} \sum_{j \in C_{ntk|s}} \sum_{j' \in C_{ntk|s}} w_{ntkj} x'_{ntkj} P_{ntkj} \sum_{j' \in C_{ntk|s}} e^{x'_{ntkj}' \beta_s}
\]

Taking the derivative of the log-likelihood with respect to the unknown parameters:

\[
\frac{dL}{d\beta_s} = \sum_{n=1}^{N} \sum_{t=1}^{T} \sum_{k=1}^{K_{nt}} \sum_{j \in C_{ntk|s}} w_{ntkj} x'_{ntkj} - \sum_{n=1}^{N} \sum_{t=1}^{T} \sum_{k=1}^{K_{nt}} \sum_{j' \in C_{ntk|s}} x'_{ntkj} P_{ntkj} \sum_{j \in C_{ntk|s}} e^{x'_{ntkj}' \beta_s}
\]

\[
= \sum_{n=1}^{N} \sum_{t=1}^{T} \sum_{k=1}^{K_{nt}} \sum_{j \in C_{ntk|s}} w_{ntkj} x'_{ntkj} - \sum_{n=1}^{N} \sum_{t=1}^{T} \sum_{k=1}^{K_{nt}} \sum_{j' \in C_{ntk|s}} x'_{ntkj} P_{ntkj} \sum_{j \in C_{ntk|s}} w_{ntkj}
\]
\[
\sum_{n=1}^{N} \sum_{t=1}^{T} \sum_{k=1}^{K_{nt}} \sum_{j \in C_{ntkj}} \left[ w_{ntkj} - P_{ntkj} \sum_{j' \in C_{ntkj}} w_{ntkj}' \right] x_{ntkj}'
\]

However, for similar reasons as the class-specific choice model for the latent class choice model, \( \sum_{j' \in C_{ntkj}} w_{ntkj}' = 1. \)

Thus,
\[
\frac{dL}{d\beta_s} = \sum_{n=1}^{N} \sum_{t=1}^{T} \sum_{k=1}^{K_{nt}} \sum_{j \in C_{ntkj}} \left[ w_{ntkj} - P_{ntkj} \right] x_{ntkj}'
\]

Similarly based on the derivations of the above weighted multinomial logit model, the gradients for the remaining parameters are computed as follows:

\[
\frac{dL}{d\tau} = \sum_{n=1}^{N} \sum_{s=1}^{S} \left[ \pi_{n1s} - P_{n1s} \right] z_{n1s}' \text{ where } P_{n1s} = \frac{e^{z_{n1s}' \tau}}{\sum_{s'=1}^{S} e^{z_{n1s}' \tau}}
\]

\[
\frac{dL}{d\gamma_r} = \sum_{n=1}^{N} \sum_{t=2}^{T} \sum_{s=1}^{S} \left[ \omega_{nts} - P_{nts} \right] z_{nts}' \text{ where } P_{nts} = \frac{e^{z_{nts}' \gamma_r}}{\sum_{s'=1}^{S} e^{z_{nts}' \gamma_r}}
\]

Again, we can clearly see that the gradient for weighted multinomial logit models has a closed form, which is the case for all sets of parameters in our HMM. This will be very beneficial from an optimization perspective in reducing computation and estimation time.

### 4.4 Conclusion

Estimating advanced discrete choice models, such as mixture models or hidden Markov models with logit kernels are prone to numerical difficulty when maximizing the likelihood function using tradition gradient descent techniques. The EM algorithm is an alternative procedure for maximizing the likelihood for models that entail discrete latent variables. The EM algorithm is a more stable alternative approach, which involves maximizing functions that are much easier to be maximized as opposed to the model’s full likelihood function. In this chapter, we provide rigorous derivations of the various steps of the EM algorithm for both mixture models and hidden Markov models with logit kernels, in addition to the closed form gradients. Our objective is to enable travel demand and behavioral modelers to estimate such advanced models while saving on computation and estimation time.
Chapter 5

Conclusion

5.1 Summary
We started our discussion in this dissertation by identifying the need for developing quantitative methods to model and predict trends of travel behavior in response to major technological and infrastructural changes. Understanding travel behavior in this era of transformative mobility is key to assessing how policies and investment strategies can transform cities to provide a higher level of connectivity, improve the economic and environmental health for people, attain significant reductions in congestion levels, and encourage multimodality. In addition to that, literature suggests that over time, travel choices, attitudes, and social norms will result in changes in lifestyles and travel behavior. Hence, dynamic modeling of changes in lifestyles and behavior in response to infrastructural and technological investments is central to modeling and influencing trends of travel behavior, and improving long-range forecasting accuracy. Current travel demand models do not reflect such dynamics, which becomes questionable in times such as the present.

In order to account for all of the aforementioned limitations and needs, we develop a disaggregate, dynamic discrete choice framework to model and predict long-range trends of travel behavior to account for upcoming technological and infrastructural changes (see figure 5.1 below). The building blocks of this proposed framework were developed and tested to empirically highlight the value of the framework to transportation policy and practice.

The proposed disaggregate, dynamic discrete choice framework in this dissertation addresses two key limitations of existing travel demand models, specifically:

1- Trends of evolution of preferences, lifestyles and transport modality styles in response to changes in socio-demographic variables and the built environment.
2- Trends of technology and service adoption, in order to gain insight about the projected market shares of upcoming modes of transport.

This dissertation also provides the derivation and formulation of the Expectation Maximization (EM) algorithm in the context of discrete mixture models and hidden Markov models with logit kernels to save on computation and estimation time. Such a statistical technique becomes extremely useful to travel demand and behavioral modelers when estimating advanced models.
The building blocks of the proposed dynamic, disaggregate discrete choice framework were estimated on two different datasets. The first component focuses on estimating a disaggregate technology adoption model with a discrete choice kernel. This component integrates a network effect and latent class choice model to understand and forecast the adoption and diffusion of upcoming modes of transportation (see figure 5.2 below). The second component focuses on estimating hidden Markov models with logit kernels to model and forecast the evolution of preferences, lifestyles and transport modality styles over time in response to changes in socio-demographic variables and the built environment. This component quantifies the evolution of lifestyles and modality styles over time in response to policies and investment strategies (see figure 5.3). The developed methodological framework in this dissertation will in turn project the market share of modes of transportation in a more representative manner in the long run.

Throughout the previous chapters of the dissertation, we provided model estimation results using two datasets to test and demonstrate the use, practicality and methodological robustness of the proposed framework.
Figure 5.2: Generalized Technology Adoption Model

Figure 5.3: Dynamic Discrete Choice Framework
The generalized technology adoption model, which was developed and tested in chapter 2, is rooted in the technology diffusion literature that identifies two distinct types of adopters: innovators and imitators. Our framework builds on the formulation of dynamic latent class choice models, which were integrated with a network effect model. We were interested in developing a network effect model to understand how the size of the network, governed by the new mode of transportation, influences the adoption behavior of the different market segments. A confirmatory approach was adopted to estimating our dynamic latent class choice model based on findings from the technology diffusion literature that focus on defining two distinct types of adopters: innovators/early adopters and imitators. The technology adoption model predicts the probability that a certain individual will adopt the service at a certain time period, and is explained by social influences, network effect, socio-demographics and level-of-service attributes. There are two key contributions in our methodological framework: (1) capturing heterogeneity in the adoption utility among different market segments; and (2) capturing the impact of the spatial/network effect of the new technology on the utility of adoption. The proposed adoption model is powerful in terms of forecasting the number of adopters for different policies and investment strategies into the future.

The dynamic discrete choice model, which was developed and tested in chapter 3, models the evolution of preferences, lifestyles, and transport modality styles over time. The contribution in this chapter is to develop, apply, and test an HMM framework to capture, model and forecast the evolution of individual preferences and behaviors over long-range forecasting horizons. The methodological framework focuses on developing a structural approach for modeling the evolution of preferences over time due to changes in socio-demographic variables and the built environment. The construct of modality styles is used to denote preferences states. It is those modality style preference states that evolve dynamically over time. Model results depict that preference states, denoted by modality styles, did indeed shift and evolve over time as a result of changes in the transportation system. Preferences of individuals have shifted in terms of their choice set consideration and sensitivities to level-of-service attributes. This dynamic choice model entails a richer behavioral dimension and will in turn quantify the influence of policies and investment strategies on the projected market shares of the modes of transport more accurately in the long run.

Both methodological frameworks in this dissertation employ the Expectation Maximization (EM) algorithm for model estimation. The required formulation, derivation, and application of the EM algorithm in the context of discrete mixture models and hidden Markov models with logit kernels to save on computation and estimation time denote the third component of this dissertation, and were presented in chapter 4.
5.2 Research Directions
The proposed dynamic, disaggregate discrete choice framework in this dissertation requires further investigations across multiple dimensions to enhance its empirical flexibility and robustness. That said, future directions pertinent to the proposed framework entail the following:

1- Rigorous data collection in terms of collecting panel data of travel and activity behavior while accounting for the uptake of new modes of transportation such as carsharing and ridesharing. This will enable us to estimate the joint proposed dynamic, disaggregate discrete choice framework (figure 5.1), which is required to understand and predict long-range trend of travel behavior. Estimating the joint framework allows us to model how modality styles can impact adoption styles in order to understand how adoption and diffusion of new technologies and services will be influenced by habits, and lifestyles built around the use of a certain subset of travel modes.

2- The discrete choice framework of adoption and diffusion of new transportation services that was developed in chapter 2 of this dissertation fails to account for the effect of competition between various modes of transport, new technologies and services. Future extensions of this framework will allow us to understand how the diffusion of carsharing and ridesharing services will evolve over time as those new modes compete with each other in terms of capturing ridership. This will improve the accuracy of projected demand and minimize the bound of its confidence interval.

3- The validation of the hidden Markov model presented in chapter 3 of this dissertation has focused merely on statistical and goodness of fit measures: $\hat{\rho}^2$, AIC and BIC. We also rely on examining the behavioral richness that is represented and captured by the model framework. More work needs to be done with respect to model validation, which is more aligned with the field of machine learning. It will be better to have a validation sample of the data (hold-out) whereby we train the model on an estimation dataset and determine model accuracy on the validation dataset. Such an approach was conducted in the adoption and diffusion framework in chapter 2 whereby we generated confidence intervals for predicted demand on a validation dataset and evaluated discrepancies between those confidence intervals and actual demand.

4- Both methodological frameworks of chapters 2 and 4 do not incorporate the effects of social norms, psychometric and psychological constructs of attitudes and perceptions into the decision-making process. In our methodological framework, the impacts of social norms, attitudes and perceptions were confounded with the alternative specific constants of the respective utility equations. For example, it will be important to quantify the effects and shifts in attitudes (e.g. towards/away from auto-orientation, environmental consciousness, etc.) on adoption, travel and activity behavior. When social norms, attitudes and perceptions comprise
a major determinant of adoption, travel and activity behavior, then it is critical that we quantify their effects explicitly. If we don’t, omitted variable bias can become worrisome and the estimated parameters could become inconsistent.

5- This dissertation is rooted in addressing limitations of existing travel demand models in modeling and forecasting the evolution of trends of travel behavior in response to transformative technologies and services. The scope of the proposed methodological framework of chapter 1 could be extended to more medium and long-term dimensions of travel and activity behavior, for example car ownership and residential choice location. Residential choice location decisions and car ownership levels are to be conditioned on modality styles and adoption styles. While such a framework will cater for the dynamic evolution of preferences over time in addition to the adoption and diffusion of new transportation services, it will also capture the influence of adoption styles and modality styles on those long-term decisions. This will allow us to evaluate the impact of policies and investment strategies on several dimensions of the mobility decision bundle. Such a framework will enable us to understand how to: (1) influence trends of travel behavior to be more sustainable and multimodal and more aligned with the envisioned sharing economy future; (2) guide adoption styles to increase the adoption and diffusion of carsharing and ridesharing services; (3) significantly reduce car ownership levels to mitigate congestion and greenhouse gas emissions by effectively nudging and influencing lifestyles; and (4) transform cities in terms of residential choice location by encouraging urban sprawl away from congested cities through influencing preferences and modality styles in the right direction followed by nudging adoption styles to encourage the adoption of ridesharing, carsharing, and autonomous vehicles.
5.3 Conclusion

Travel demand models constitute a critical component in transportation planning and policy. Travel demand models used in practice have shifted over the years to constitute disaggregate models of decision-making as opposed to aggregate models. Current disaggregate activity-based travel demand models entail a sequence of models that tackle different dimensions of the decision-making process at the individual and household levels such as mode choice, residential location, etc. Such models are used to forecast market shares of biking and walking, transit ridership and traffic volumes that are the result of large scale transportation investments and policy decisions.

However, travel demand models currently used in practice lack a methodological framework that is required to model and forecast long-range trends of travel behavior in response to upcoming technologies and services, for example ridesharing, carsharing and autonomous vehicles. Moreover, the range of travel choices will be wider over time, which in turn influences lifestyles and travel behavior. Hence, dynamic modeling of changes in lifestyles and behavior in response to infrastructural and technological investments is central to modeling and influencing trends of travel behavior, improving long-range forecasting accuracy, and guiding transformative mobility towards a more sustainable, equitable and efficient system.

The proposed dynamic, disaggregate discrete choice framework of this dissertation entails advanced models. This however comes at a cost in terms of prolonged computation and estimation times. This dissertation tries to account for this issue by providing the derivation and formulation of the EM algorithm for mixture models and hidden Markov models with logit kernels, which are the building blocks of the generalized dynamic framework. As such, this shall offer a greater potential to understand and predict behavior, improve forecasting accuracy, influence lifestyles and trends of travel behavior to be more sustainable and multimodal, and test behavioral hypotheses. The framework presented in this dissertation is flexible, theoretically grounded, empirically tested and verified, and behaviorally rich.

This dissertation brings together techniques and tools from machine learning, econometrics (particularly discrete choice analysis), and the technology diffusion literature. The disaggregate technology adoption model of chapter 2 is rooted in the diffusion literature and tries to understand the dynamic adoption behavior of the different market segments over time. In addition to that, we blend machine learning methods, and in particular hidden Markov models that are widely used in speech recognition, with discrete choice kernels to model and forecast the evolution of individual preferences and behaviors over long-range forecasting horizons. We believe that attaining accurate long-range forecasts lies in bringing those three worlds together. Behavioral modeling of decision-makers, which is rooted in the discrete choice modeling domain, is a key ingredient in our analysis. We strongly believe that integrating such techniques with machine learning methods, the technology diffusion literature, and statistical learning techniques, in particular the EM algorithm will: (1) enable us to model the complicated decision making process more accurately while saving on computation time; (2) allow for interpretation of model results as desired by policy makers; and (3) add richness to the behavioral process represented by the models.
Trends of travel behavior are evolving as new technologies and services are introduced. Over the coming decades, this evolution could play out in utopian or dystopian scenarios or anywhere in between. The proposed methodological frameworks in this dissertation entail the building blocks to advances in travel demand modeling required to influence trends of travel behavior and guide transformative mobility towards a sustainable, efficient and equitable system. Throughout the dissertation, empirical results are presented to highlight findings and to empirically demonstrate and test the proposed frameworks in the case of transformative mobility.
Bibliography


