#### Université de Montréal Faculté des arts et des sciences

#### Cette thèse intitulée:

## Route choice and traffic equilibrium modeling in multi-modal and activity-based networks

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#### Résumé

Que ce soit pour aller au travail, faire du magasinage ou participer à des activités sociales, la mobilité fait partie intégrante de la vie quotidienne. Nous bénéficions à cet égard d'un nombre grandissant de moyens de transports, ce qui contribue tant à notre qualité de vie qu'au développement économique. Néanmoins, la demande croissante de mobilité, à laquelle s'ajoutent l'expansion urbaine et l'accroissement du parc automobile, a également des répercussions négatives locales et globales, telles que le trafic, les nuisances sonores, et la dégradation de l'environnement. Afin d'atténuer ces effets néfastes, les autorités cherchent à mettre en œuvre des politiques de gestion de la demande avec le meilleur résultat possible pour la société. Pour ce faire, ces dernières ont besoin d'évaluer l'impact de différentes mesures. Cette perspective est ce qui motive le problème de l'analyse et la prédiction du comportement des usagers du système de transport, et plus précisément quand, comment et par quel itinéraire les individus décident de se déplacer.

Cette thèse a pour but de développer et d'appliquer des modèles permettant de prédire les flux de personnes et/ou de véhicules dans des réseaux urbains comportant plusieurs modes de transport. Il importe que de tels modèles soient supportés par des données, génèrent des prédictions exactes, et soient applicables à des réseaux réels. Dans la pratique, le problème de prédiction de flux se résout en deux étapes. La première, l'analyse de choix d'itinéraire, a pour but d'identifier le chemin que prendrait un voyageur dans un réseau pour effectuer un trajet entre un point A et un point B. Pour ce faire, on estime à partir de données les paramètres d'une fonction de coût multi-attribut représentant le comportement des usagers du réseau. La seconde étape est celle de l'affectation de trafic, qui distribue la demande totale dans le réseau de façon à obtenir un équilibre, c.-à-d. un état dans lequel aucun n'utilisateur ne souhaite changer d'itinéraire. La difficulté de cette étape consiste à modéliser la congestion du réseau, qui dépend du choix de route de tous les voyageurs et affecte simultanément la fonction de coût de chacun.

Cette thèse se compose de quatre articles soumis à des journaux internationaux et d'un chapitre additionnel. Dans tous les articles, nous modélisons le choix d'itinéraire d'un individu comme une séquence de choix d'arcs dans le réseau, selon une approche appelée modèle de choix d'itinéraire récursif. Cette méthodologie possède d'avantageuses propriétés, comme un estimateur non biaisé et des procédures d'affectation rapides, en évitant de générer des ensembles de chemins. Néanmoins, l'estimation de tels modèles pose une difficulté additionnelle puisqu'elle nécessite de résoudre un problème de programmation dynamique imbriqué, ce qui explique que cette approche ne soit pas encore largement utilisée dans le domaine de la recherche en transport. Or, l'objectif principal de cette thèse est de répondre des

défis liés à l'application de cette méthodologie à des réseaux multi-modaux. La force de cette thèse consiste en des applications à échelle réelle qui soulèvent des défis computationnels, ainsi que des contributions méthodologiques.

Le premier article est un tutoriel sur l'analyse de choix d'itinéraire à travers les modèles récursifs susmentionnés. Les contributions principales sont de familiariser les chercheur.e.s avec cette méthodologie, de donner une certaine intuition sur les propriétés du modèle, d'illustrer ses avantages sur de petits réseaux, et finalement de placer ce problème dans un contexte plus large en tissant des liens avec des travaux dans les domaines de l'optimisation inverse et de l'apprentissage automatique.

Deux articles et un chapitre additionnel appartiennent à la catégorie de travaux appliquant la méthodologie précédemment décrite sur des réseaux réels, de grande taille et multi-modaux. Ces applications vont au-delà des précédentes études dans ce contexte, qui ont été menées sur des réseaux routiers simples. Premièrement, nous estimons des modèles de choix d'itinéraire récursifs pour les trajets de cyclistes, et nous soulignons certains avantages de cette méthodologie dans le cadre de la prédiction. Nous étendons ensuite ce premier travail afin de traiter le cas d'un réseau de transport public comportant plusieurs modes. Enfin, nous considérons un problème de prédiction de demande plus large, où l'on cherche à prédire simultanément l'enchaînement des trajets quotidiens des voyageurs et leur participation aux activités qui motivent ces déplacements.

Finalement, l'article concluant cette thèse concerne la modélisation d'affectation de trafic. Plus précisément, nous nous intéressons au calcul d'un équilibre dans un réseau où chaque arc peut posséder une capacité finie, ce qui est typiquement le cas des réseaux de transport public. Cet article apporte d'importantes contributions méthodologiques. Nous proposons un modèle markovien d'équilibre de trafic dit stratégique, qui permet d'affecter la demande sur les arcs du réseau sans en excéder la capacité, tout en modélisant comment la probabilité qu'un arc atteigne sa capacité modifie le choix de route des usagers.

**Mots-clés:** Modèles de choix d'itinéraire récursifs, modèle markovien d'équilibre de trafic, estimation par maximum de vraisemblance, programmation dynamique, réseaux multi-modaux.

# Summary

Traveling is an essential part of daily life, whether to attend work, perform social activities, or go shopping among others. We benefit from an increasing range of available transportation services to choose from, which supports economic growth and contributes to our quality of life. Yet the growing demand for travel, combined with urban sprawl and increasing vehicle ownership rates, is also responsible for major local and global externalities, such as degradation of the environment, congestion and noise. In order to mitigate the negative impacts of traveling while weighting benefits to users, transportation planners seek to design policies and improve infrastructure with the best possible outcome for society as a whole. Taking effective actions requires to evaluate the impact of various measures, which necessitates first to understand and predict travel behavior, i.e., how, when and by which route individuals decide to travel.

With this background in mind, this thesis has the objective of developing and applying models to predict flows of persons and/or vehicles in multi-modal transportation networks. It is desirable that such models be data-driven, produce accurate predictions, and be applicable to real networks. In practice, the problem of flow prediction is addressed in two separate steps, and this thesis is concerned with both. The first, route choice analysis, is the problem of identifying the path a traveler would take in a network. This is achieved by estimating from data a parametrized cost function representing travelers' behavior. The second step, namely traffic assignment, aims at distributing all travelers on the network's paths in order to find an equilibrium state, such that no traveler has an interest in changing itinerary. The challenge lies in taking into account the effect of generated congestion, which depends on travelers' route choices while simultaneously impacting their cost of traveling.

This thesis is composed of four articles submitted to international journals and an additional chapter. In all the articles of the thesis, we model an individual's choice of path as a sequence of link choices, using so-called recursive route choice models. This methodology is a state-of-the-art framework which is known to possess the advantage of unbiased parameter estimates and fast assignment procedures, by avoiding to generate choice sets of paths. However, it poses the additional challenge of requiring one to solve embedded dynamic programming problems, and is hence not widely used in the transportation community. This thesis addresses practical and theoretical challenges related to applying this methodological framework to real multi-modal networks. The strength of this thesis consists in large-scale applications which bear computational challenges, as well as some methodological contributions to this modeling framework.

The first article in this thesis is a tutorial on predicting and analyzing path choice behavior using recursive route choice models. The contribution of this article is to familiarize researchers with this methodology, to give intuition on the model properties, to illustrate its advantages through examples, and finally to position this modeling framework within a broader context, by establishing links with recently published work in the inverse optimization and machine learning fields.

Two articles and an additional chapter can be categorized as applications of the methodology to estimate parameters of travel demand models in several large, real, and/or multi-dimensional networks. These applications go beyond previous studies on small physical road networks. First, we estimate recursive models for the route choice of cyclists and we demonstrate some advantages of the recursive models in the context of prediction. We also provide an application to a time-expanded public transportation networks with several modes. Then, we consider a broader travel demand problem, in which decisions regarding daily trips and participation in activities are made jointly. The latter is also modeled with recursive route choice models by considering sequences of activity, destination and mode choices as paths in a so-called supernetwork.

Finally, the subject of the last article in this thesis is traffic assignment. More precisely, we address the problem of computing a traffic equilibrium in networks with strictly limited link capacities, such as public transport networks. This article provides important methodological contributions. We propose a strategic Markovian traffic equilibrium model which assigns flows to networks without exceeding link capacities while realistically modeling how the risk of not being able to access an arc affects route choice behavior.

**Keywords:** Recursive route choice models, Markovian traffic assignment model, maximum likelihood estimation, dynamic programming, multi-modal route choice, activity-based travel demand.

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### List of Abbreviations

**BFGS** Broyden-Fletcher-Goldfarb-Shanno approximation ВННН Berndt-Hall-Hall-Hausman approximation DeCDecomposition method DP Dynamic programming GPS Global positioning system IIA Independence from irrelevant alternatives i.i.d. independent and identically ditributed LS Link size MDP Markov decision process MRL Mixed recursive logit MSA Method of successive averages MTE Markovian traffic equilibrium NRL Nested recursive logit ODOrigin destination PLPath based logit PTPublic transportation RLRecursive logit RPRevealed preferences SPShortest path SQP Single queue processing SSP Stochastic shortest path

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# 1 Introduction

This thesis is concerned with the development and application of models to predict flows of people and/or vehicles in transportation networks. We focus on two interrelated aspects of the problem. First, estimating parameters of cost functions representing the observed behavior of network users with probabilistic demand models; second, assigning travelers to the network's paths using traffic equilibrium models. In this section, we first present the motivation underlying this work. Then, we give an overview of the research context which precedes this thesis. We subsequently lay out the scope and describe the specific objectives we set out to achieve. We conclude this section by providing an overview of the structure of this thesis and its contributions.

#### 1.1 Motivation

Transportation systems are an essential component of the livability of any city. We all travel to go to work, pick up children or perform various activities, whether by necessity or for recreation. Urban transportation systems typically consist of infrastructure, including roads, bridges and railways, but also vehicles, such as buses, trams and cars. The planning and management of transportation systems is the role of central authorities, i.e., public administrations or network operators. These actors can make strategic choices which have a long-term impact on the system, such as enacting regulations and policies, planning investments in facilities, or making decisions regarding the use of existing resources.

In the last decades, most cities have witnessed an increase in road traffic and travel demand. This phenomenon is partly explained by rapid growth rates in vehicle ownership, longer travel distances due to urban sprawl, but also the expansion of the transportation supply which is known to trigger more demand. The

expanded mobility we benefit from contributes to economic growth and quality of life. Yet, the resulting road traffic also has visible and inevitable detrimental effects on society. Air quality degradation, congestion, noise and traffic hazards are local burdens associated to most urban areas. World-wide negative impacts are also felt as CO<sub>2</sub> concentration reaches alarming levels.

Reducing traffic growth and driving individuals towards a more sustainable use of the transportation system is therefore a long-standing objective for our society. Nowadays, people benefit from an increasingly wide range of available services to choose from to perform trips. In addition to the traditional modes consisting of cars, metro lines and buses, emerging bike sharing systems and alternative vehicles at the frontier between public and private modes are changing the way people travel. There exists thus many ways for cities to encourage a shift towards more efficient and sustainable traveling via subsidies, congestion charges, improvement of public transportation and biking facilities or implementation of pilot projects. However, in order to appropriately plan infrastructure and demand management policies, authorities need decision aid tools to forecast the effect of such measures. This requires the development of models which can predict flow patterns resulting from different scenarios and can be used to answer questions such as "What is the impact of improving the capacity of a metro line?" or "What is the effect of building separate bike lanes on specific streets?".

As opposed to goods, transportation of people, on which this thesis focuses, is driven by individual intentions which cannot be controlled by a globally optimized system. Therefore, effectively managing travel demand and traffic flows requires to design the right incentives to encourage behavioral change, informed by knowledge of the mechanisms and trade-offs driving individual decisions. Many dimensions of travel choice, such as why, where, how and when each person chooses to travel, are central to understanding urban flow patterns. Naturally, analyzing this complex system requires answering many overlapping questions. This thesis addresses some of them, and it specifically seeks to understand what path individuals choose to travel between a specific origin and destination in a multi modal urban network, and how these individual choices aggregate to form urban traffic. The overall motivation is to predict network flows, which are the number of pedestrians and/or vehicles present on a given link within a certain time unit. With this background in mind, it is desirable that the models developed and applied in this thesis be

data-driven, have predictive accuracy and be operational for real networks.

#### 1.2 Research context

Consider a network composed of links connecting nodes representing an urban transportation system. The state of such a network at a given time is defined by the flows of persons and/or vehicles on each arc. Network flow patterns are commonly described in the literature as the result of two distinct mechanisms (Sheffi, 1985). On the one hand, individuals choose a path in the network to reach their desired destination so as to minimize their personalized generalized cost. On the other hand, the finite capacity of the network induces congestion which impacts this cost, thus forcing individuals to adapt their path choice in accordance with other users. Over time, the interaction of these competing mechanisms yields a user equilibrium (UE), defined by Wardrop (1952) as a network state in which the journey costs on all routes actually used are equal, and less than those which would be experienced by a single traveler on an unused path.

In practice, distinct bodies of literature address each part of the problem. Travelers' route choice preferences are unknown, but it is generally assumed that the cost of traveling takes a parametric form and depends on several attributes, including travel time and other route characteristics. Uncovering this generalized cost function is part of the demand analysis problem. The discrete choice framework is widely used to estimate models of users' behavior, and it is the most endorsed methodology for the route choice problem in the literature (Ben-Akiva et al., 1984; Frejinger, 2008; Prato, 2009). Such models are calibrated on data which generally consists of observed individual decisions (e.g., GPS traces). Discrete choice models specifically assume that costs are random variables in order to account for the inherent uncertainty and heterogeneity of human behavior. As a result, estimated models identify a choice probability distribution over the network's paths instead of a single best path. There exists different model structures based on hypotheses on the distribution of random terms (e.g., multinomial logit, nested logit, mixed logit). A desirable property of this methodology is its microeconomic foundation (McFadden, 1978), which is suitable for behavioral interpretation of the model and computation of welfare change measures.

The literature on traffic assignment analyses the second part of the problem, which takes as input an origin-destination matrix representing the total demand and a cost function dependent on the amount of flow. Usually, the analysis is restricted to a small time interval under which the travel costs and the demand are considered constant. The aim of traffic assignment models is to compute the equilibrium flows resulting from loading the given demand. Different traffic assignment models exist based on distinct assumptions regarding users' path choice behavior. Initial models (Wardrop, 1952) treated the path choice component deterministically, implicitly implying that individuals behaved identically and with perfect knowledge of costs. The theory underlying stochastic traffic equilibrium models has since then been developed by Daganzo and Sheffi (1977) to overcome limitations of deterministic models, by postulating that users' path choices are governed by a discrete choice model.

The main challenge associated with both route choice and traffic assignment models is the impractically large number of paths in real urban networks. This is why traditionally, modelers first generate plausible sets of routes before modeling how travelers choose between them. There are however drawbacks to assuming that travelers choose among a restricted choice set, discussed in many works: in particular, the resulting parameter estimates may be biased, the predicted flow patterns may be unrealistic, and this imposes a need to perform some beforehand calculations (Frejinger et al., 2009; Bliemer and Bovy, 2008; Akamatsu, 1996). How to circumvent the need for path generation has thus been a central problem in the literature, until recent work (Baillon and Cominetti, 2008; Fosgerau et al., 2013) proposed general recursive models based on links. In these models, Markov decision processes (MDPs) characterize the path choice behavior of travelers, and the obstacle of path enumeration is replaced by the necessity to solve a dynamic programming (DP) problem. The models hence borrow terminology from DP: the concept of state is used to represent the network link (or node) where the traveler finds himself, while an action is a choice of outgoing arc. The forward looking behavior of users is captured by adding the expected minimum cost to destination (value function) to the immediate cost of each arc. Discrete choice models based on this concept have been called recursive route choice models and more generally dynamic discrete choice models. In the traffic assignment literature, the corresponding Markovian traffic equilibrium model (MTE) emerged in parallel, based on an embedded recursive path choice model. This thesis is built on ideas proposed in these initial works and further pursued by Mai (2016a).

#### 1.3 Scope, objectives and challenges

Considerable recent progress has been made to improve recursive route choice and traffic equilibrium models. For example, Mai et al. (2015) proposed an extension of the discrete choice modeling framework of Fosgerau et al. (2013) which allows path costs to be correlated. Oyama and Hato (2017) introduced a discount factor in the model in order to capture more complex decision-making dynamics. Cominetti and Torrico (2016) considered the risk adverse behavior of users in the context of Markovian traffic equilibrium modeling. These improvements are mostly aimed at enhancing the realism of the behavioral assumptions underlying the models. Still, we believe there are presently important incentives to give consideration to more complex network settings.

In previous works (e.g., Fosgerau et al., 2013; Mai et al., 2015), applications of recursive models have been directed at uni-modal networks with deterministic link attributes, aiming at modeling car traffic. In reality, while the car remains the most widely used transportation mode, a non negligible proportion of trips are performed either by bike or public transport, or increasingly by combining distinct modes (Kuhnimhof et al., 2012). Such travel behavior is the key to sustainable mobility. There is thus an increased political and academic interest in better understanding flows of alternative modes and the deciding factors driving their use. It is however non trivial to direct this analysis towards other modes than car. The route choice behavior of cyclist is influenced by considerably more factors than that of car drivers; flows in public transportation networks follow entirely different dynamics because of transfers and limited capacities of transit vehicles.

To capture the complexity of real mobility patterns, and to fulfill the promise of driving individuals towards a more sustainable use of the transportation infrastructures, an integrated approach is necessary. The choices of mode and route, although viewed for the most part as sequential in the demand modeling literature, are in fact interrelated: the number and attractiveness of routes connecting a given origin and destination is likely to influence the mode choice of an individual

traveling between them. In fact, several other aspects of trip making behavior are interdependent. When making trade-offs between one mode or another, individuals consider as well the possibility to reschedule trips, chain trips, or substitute them entirely for in-home time. There are therefore benefits to model jointly not only route and mode choice, but also decisions related to which activities are pursued when, where and for how long, which is the conceptual basis behind activity-based travel demand models.

Interrelated decisions regarding e.g., mode, route, timing and activity participation, can also be represented as a network. Traditionally, a network represents a physical structure (e.g., roads and intersections, or metro lines and stations), but it can also be an abstract representation. Supernetworks, defined by Sheffi (1985) as networks augmented with virtual dummy links to represent multiple choice dimensions, provide an ideal representation to model multi-faceted demand problems as a choice of path. Thus, a link in a supernetwork could represent a specific leg of a trip using a certain mode at a given time. Recursive models can conceptually easily be adapted to such networks and offer great flexibility. Indeed states as well as actions in recursive choice models can be defined as any combination of variables. There are however non trivial challenges associated with modeling complex travel choice situations in such networks.

The overall objective of this thesis is to develop recursive route choice and traffic equilibrium models which are suitable for both real large scale networks and multi-dimensional supernetworks, in order to (i) estimate parameters of travelers' behavior, and (ii) predict equilibrium flows in such networks. Although this thesis does not aim at proposing a solution which addresses all issues simultaneously, it tackles several specific problems within this scope. In the following, we detail the specific objectives of this thesis and the related challenges.

The first and main objective is to propose methodological developments in order to deal with networks which may be dynamic, stochastic and represent combinations of choices. Traveling in real multi-modal networks is subject to sources of uncertainty, related to, e.g., the available capacity of a transit line or its arrival time. Existing recursive route choice models do not allow to take stochastic outcomes into account because they have degenerate state transitions (i.e., the next state is always equal to the chosen link). Incorporating stochastic transitions between states offers the potential for modeling sources of uncertainty, however this is at the cost of

solving more complex DP problems. A second issue occurring in multi-dimensional networks is the question of how to handle correlation between random path costs. Mai et al. (2015) proposed an extension of Fosgerau et al. (2013) to model correlation between physically overlapping paths, yet multiple choice dimensions require more complex correlation structures. Finally, an additional challenge posed by dynamic or multidimensional networks is their large number of state-action pairs, which entails great computational efforts due to the curse of dimensionality.

The second objective of this thesis is to use real networks and revealed preference data to apply the proposed models on a large set of applications. Previous work by Fosgerau et al. (2013) and Mai (2016a) has only been applied on the small road network of Borlänge (about 7000 arcs), and focuses exclusively on the problem of model estimation. We aim at illustrating the applicability of recursive route choice models by estimating parameters of travelers preferences for a large variety of route characteristics and modes. Moreover, we aim at illustrating the benefits of the methodology from a policy analysis perspective by discussing the interpretation of results in depth.

#### 1.4 Thesis outline and contributions

In this thesis we present four published or submitted articles and one additional chapter which was part of research work leading to a related paper (de Freitas et al., 2019). They consist of one tutorial, three application-oriented articles, and a methodological paper. Specific contributions of this thesis can be grouped under three different themes: recursive route choice modeling, estimation of large-scale demand models, and traffic assignment modeling.

Although we do not propose new recursive route choice models, our contribution around the first theme is to render recursive route choice models more accessible to researchers and practitioners. While such models overcome many limitations of their path-based counterparts, they are not yet widely used in the transportation research community, as their advantages are outweighed by the additional complexity introduced by embedded dynamic programming problems. Therefore, we propose a tutorial in Zimmermann and Frejinger (2019) which provides guidance on recursive route choice models, by summarizing the overall advantages of

the methodology and illustrating them on toy examples. The tutorial also positions this work within a broader context by providing links to related work in the machine learning and inverse optimization fields. Secondly, while Fosgerau et al. (2013) focused on model properties related to estimation, in Zimmermann et al. (2017), we set out to illustrate advantages related to prediction. Our contributions are i) deriving the accessibility measure for recursive route choice models and showing that previous results deemed a paradox are in fact a consequence of choice set generation, and ii) illustrating gains in computational time for prediction on real networks.

Under the second theme, the main contribution consists in exhibiting extensive large-scale applications of different recursive route choice models and dealing with associated computational challenges. We consider recursive logit models (RL), but also other choice structures to account for correlation (nested logit, mixed logit). We select appropriate estimation methods to deal with the curse of dimensionality. More specifically, we treat three different applications which are relevant to travel behavior research, for which we provide estimation results and interpretation for policy analysis. In Zimmermann et al. (2017), we analyze the path choice of cyclists from GPS traces in the real network of Eugene, Oregon (40,000 links). In an additional chapter, we extend this analysis to a dynamic multi-modal public transport network consisting of three modes (bus, train, tram) with a case study in Zürich (around 1 million links). Finally, Zimmermann et al. (2018) treats the case of an abstract supernetwork expanded in multiple dimensions (mode, destination, timing, activity) based on travel diary in Stockholm (millions of links).

Finally, regarding the last theme, the principal contribution consists in incorporating sources of uncertainty in Markovian traffic equilibrium models. More specifically, we contribute by considering in Zimmermann et al. (2018) the case of networks with strict capacity limits, which induces uncertainty related to the unknown availability of links. We introduce to this effect a strategic Markovian traffic equilibrium model, which also generalizes previous work on assignment in capacitated networks (Marcotte et al., 2004). Unlike other works which treat capacity limits in an heuristic way by artificially increasing link costs, we model the effect of this uncertainty on user behavior by introducing arc access probabilities in the cost function and supposing users have recourse actions.

Below, we summarize the structure of the thesis. Each chapter contains a

prologue before the manuscript itself, summarizing the relevance of the article within the thesis, stating the author's contributions and the publication details. The chapter outline is the following:

- Chapter 2 (Zimmermann, M., Frejinger, E., submitted to EURO Journal on Transportation and Logistics), is a tutorial on the recursive models for route choice analysis which are at the heart of this thesis.
- Chapter 3 (Zimmermann, M., Mai, T., Frejinger, E., published in Transportation Research Part C), presents recursive models for the choice of route of cyclists estimated on GPS data.
- Chapter 4 (Zimmermann, M., Frejinger, E., Axhausen, K., presented at the IATBR conference), presents a recursive model for the choice of path in public transport networks with train, tram and bus modes.
- Chapter 5 (Zimmermann, M., Blom Västberg, O., Karlström, A., Frejinger, E., published in Transportation Research Part C), presents recursive models for activity-based travel demand accounting for correlation across alternatives.
- Chapter 6 (Zimmermann, M., Frejinger, E., Marcotte, P., under review in Transportation Science) presents a strategic Markovian traffic equilibrium model for networks with strict link capacities.
- Chapter 7 provides a conclusion and outlook.

# A tutorial on recursive models for analyzing and predicting path choice behavior

#### Prologue

#### Context

Route choice models exist in the transportation demand literature since the early works of Ben-Akiva et al. (1984). More recently, there has been progress to overcome a major inconvenient of traditional route choice models, namely the necessity of a choice set generation step preceding the path choice modeling itself. This state of the art framework is known as recursive route choice modeling (Fosgerau et al., 2013).

Nowadays, the majority of applied studies in transport demand modeling adopt traditional path-based models. There is a lack of familiarity in the transportation research community with recursive choice models and related work which has emerged independently in separate research areas, such as inverse optimization and inverse reinforcement learning. These research communities work on similar issues, namely identifying the utility function of a decision maker, and yet keep each other at bay, mainly because of the use of distinct notation and terminology.

#### Contributions

This article is the first tutorial on analyzing and predicting path choice behavior of network users. It ties together different threads of research and establishes links between route choice modeling and related works in different research communities, in particular inverse optimization and inverse reinforcement learning. This tutorial is also specifically addressed at transportation modelers. It highlights shortcomings of path-based models, introduces recursive choice models in a didactic fashion, and illustrates the advantages of the latter through examples.

#### Author contributions

The ideas in this tutorial came both from me and Emma Frejinger. I was responsible for running the numerical experiments and the full redaction of the article, which was revised by Emma Frejinger.

#### **Article Details**

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#### 2.1 Introduction

Road traffic, while essential to the proper functioning of a city, generates a number of nuisances, including pollution, noise, delays and accidents. It is the role of city managers, network administrators and urban planners to attempt to mitigate the negative impact of transportation by planning adequate infrastructure and policies. Most of the traffic is generated by individual travelers who seek to minimize their own travel costs without guidance from a system maximizing the overall welfare. It is thus a necessity to understand how users of the transportation system behave and choose their path in the network in order to provide planners with decision-aid tools to manage it.

This is the main motivation for the introduction of what is known in the transport demand modeling literature as the route choice problem, which seeks to predict and explain the choice of path of travelers in a network. All path choice models are based on the assumption that individuals behave rationally by minimizing a certain cost function. The models' aim is to identify this cost function from a set of observed trajectories, which allows to predict chosen paths for all origin destination pairs.

It is desirable that path choice models satisfy several properties, such as i) scaling with the size of large urban networks in order to be efficiently used for real applications, ii) lending themselves well to behavioral interpretation, in order to, e.g., assess travelers' value of time, and iii) yielding accurate predictions. In the

transportation demand literature, the most common methodology is a probabilistic approach known as discrete choice modeling, which finds its origin in econometrics. It views path choice as a particular demand modeling problem, where the alternatives of the decision maker are the paths in the network. The principal issue with this modeling approach stems from the fact that the number of feasible paths in a real network cannot be enumerated, and we do not observe which paths are actually considered by individuals. As a result, discrete choice models based on paths currently used in the transportation literature may suffer from biased estimates and inaccurate predictions, as well as potentially long computational times.

This work is a tutorial on a modeling framework which in comparison meets the previously enumerated expectations. Dubbed "recursive choice models", this methodology draws its efficiency from modeling the path choice problem as a parametric Markov decision process (MDP) and resorting to dynamic programming to solve its embedded shortest path problem. In this tutorial, we aim at i) facilitating understanding of the recursive model's formulation by drawing links to related work in inverse optimization, and ii) comparing recursive models on the basis of desirable properties with the most well-known approach in the transportation demand literature, i.e., discrete choice models based on paths. We note here that this tutorial is addressed to both transportation demand researchers who are unfamiliar with recursive models, and researchers from the machine learning community who are keen to find out about state-of-the-art methods in the area of transportation science. For this purpose, we use general terminology and speak about path choice instead of route choice in the remaining of this paper.

This tutorial proposes to view this problem from a fresh perspective and makes several contributions. First, we give background and intuition on recursive models' formulation and properties. Indeed, we contextualize discrete choice models as a probabilistic approach for what is in fact an inverse optimization problem. Through a brief overview of that literature, we motivate and throw light on the recursive formulation, which bears similarities to models for inverse reinforcement learning, but is also theoretically equivalent to a discrete choice model based on the set of all feasible paths. Second, we illustrate the advantages of the recursive model, namely consistent estimates and fast predictions, through several examples and discussions related to model estimation and prediction.

The remainder of this paper is organized as follows. In the following section,

we provide a broader context with an overview of inverse shortest path problems. In Section 2.3, we present discrete choice models, which we liken to a probabilistic paradigm for solving inverse optimization problems with noisy data. In particular, we introduce recursive discrete choice models in Section 2.3.2, which provides consistent parameter estimates of the cost function. Section 2.4 provides an illustrative comparison of path choice probabilities under both the recursive model and a path-based discrete choice model. Section 2.5 discusses the issues related to the latter and demonstrates the advantages of recursive models through practical examples of both model estimation and prediction. Finally, Section 5.6 provides an outlook and concludes.

# 2.2 Context: from shortest paths problems to path choice models

In this section, we frame the path choice problem as that of unveiling an unknown cost function from noisy shortest paths observations, which is an inverse optimization problem where the forward (inner) problem is a shortest path. We give some background on the literature on inverse optimization and we situate the problem this tutorial addresses within this context. We illustrate that there is a close connection between stochastic shortest path problems and the inverse problem with noisy data we are interested in. For the sake of clarity we start this section by introducing deterministic and stochastic shortest path problems before describing the related inverse problems.

#### 2.2.1 Shortest path problems

Throughout this section, we consider a simple oriented graph G with a set of nodes  $\mathcal{V}$  and a set of arcs  $\mathcal{A} = \{(i,j) \mid i,j \in \mathcal{V}\}$ . We denote v the nodes in  $\mathcal{V}$  and a the arcs in  $\mathcal{A}$ , which are characterized by a source node  $i_a$  and a tail node  $j_a$ . Arcs (i,j) have an associated cost  $c_{ij}$  given by a function  $c: \mathcal{A} \to \mathbb{R}$ . A path is a sequence of arcs such that the head node of each arc is the tail node of the next.

#### The deterministic shortest path problem

The deterministic shortest path problem (DSP) in the graph G is concerned with finding the path with minimum cost between an origin node and a destination node, where the cost of a path is defined by the sum of its arc costs. More often, methods developed in the literature are designed to solve the shortest path problem between a given origin and all possible destinations, or a given destination and all possible origins.

This combinatorial optimization problem has been amply studied in the literature. Its chief difficulty is the existence of a very large number of feasible paths between each node pair, which precludes proceeding by naive enumeration. The problem could be formulated and solved as a linear program, however more efficient algorithms have been developed, relying on  $dynamic\ programming\ (DP)$ . In general, DP is a methodology to solve optimization problems in dynamic (often discrete time) systems, where a decision (denoted action or control) must be taken in each state in order to minimize future additive costs over a certain time horizon (finite or infinite). The shortest path problem in the graph G can be formulated as a DP problem by considering nodes as states and an arc choice as an action taken in a given state.

The Bellman principle of optimality at the core of deterministic problems states that for an optimal sequence of choices (in this case, arcs along the shortest path), each subsequence is also be optimal. This allows to decompose the problem and formulate a recursive expression for the optimal arc choice at node i as well as the cost C(i) of the shortest path from i to destination node d,

$$C(i) = \begin{cases} 0, & i = d \\ \min_{j \in \mathcal{V}_i^+} \{ c_{ij} + C(j) \}, & \forall i \neq d, i \in \mathcal{V} \end{cases}$$
 (2.1)

where  $V_i^+ = \{ j \in \mathcal{V} \mid (i, j) \in \mathcal{A} \}.$ 

Solving (2.1) is however not straightforward in cyclic graphs. In this case, note that the problem is well-defined only when there are no negative cost cycles, otherwise there would be paths of cost  $-\infty$ . Under this assumption, the shortest path in G contains at most  $|\mathcal{V}| - 1$  arcs. Bellman (1958) shows how to solve the shortest path problem by backward induction as a deterministic finite state finite

horizon optimal control problem. The DP algorithm is

$$C_N(i) = c_{id}, \quad \forall i \in \mathcal{V}_d^-$$
  
 $C_n(i) = \min_{j \in \mathcal{V}_i^+} \{ c_{ij} + C_{n+1}(j) \}, \quad \forall i \in \mathcal{V}, n = 1, ..., N - 1$  (2.2)

where  $V_i^- = \{h \in \mathcal{V} \mid (h, i) \in \mathcal{A}\}$ , and  $N = |\mathcal{V}| - 1$  is the length of the horizon. The value  $C_n(i)$  represents the cost of the shortest path from i to d using at most N - n + 1 arcs, and in this sense is an upper bound on the cost of the shortest path. The cost of the shortest path from i corresponds to  $C_1(i)$ . Note that the value of the shortest paths can also be found by label correction algorithms (see, e.g., Dijkstra, 1959; Floyd, 1962).

#### The stochastic shortest path problem

The stochastic shortest path problem (SSP), as defined by Bertsekas and Tsitsiklis (1991), is an extension of the previous problem which considers a discrete time dynamic system where a decision must be made in each state and causes the system to move stochastically to a new state according to a transition probability distribution. This problem can be analyzed using the framework of Markovian Decision Processes (MDP), formally defined as:

- A set of states S and a set of available actions A(s) for each state  $s \in S$ .
- The cost  $c_{s,a,s'}$  incurred by taking action a in state s and moving to next state s'.
- p(s'|s,a) the transition probability from s to s' when taking action a.

An MDP models problems where an action must be taken in each state, with the aim to minimize expected future discounted costs over a certain horizon. The SSP is a special case of MDP with infinite horizon, no discounting and a cost-free absorbing state d, where  $p(d|d,a) = 1 \,\forall a$ . The SSP is an infinite horizon problem since there is no upper limit on the number of arcs traversed. However, by assumption the absorbing state can be reached with probability 1 in finite time. The optimal solution of the SSP is not a path but a policy, which consists in a probability distribution over all possible actions in each state. When the optimal policy is followed, the path which is actually travelled is random but has minimum expected cost.

This stochastic problem can be solved with DP and the recursion which defines

the optimal expected cost V(s) from any given state s is given by the Bellman equation

$$V(s) = \min_{a \in A(s)} \left[ c_{s,a} + \sum_{s'} p(s'|s, a) V(s') \right], \qquad (2.3)$$

where  $c_{s,a} = \sum_{s'} p(s'|s,a)c_{s,a,s'}$ . V(s) is also known as the value function.

Note that the DSP is a particular degenerate case of the SSP where states s are nodes i of the graph G, action costs are arc costs  $c_{ij}$  and state transitions are deterministic, since the next state is always equal to the chosen successor node. Therefore, it is in fact a deterministic MDP.

This definition of SSPs provided by Bertsekas and Tsitsiklis (1991) is very general. It also encompasses variants of shortest paths problems on random graphs (see, e.g., Polychronopoulos and Tsitsiklis, 1996), where arc costs are modeled as random variables  $\tilde{c}_{ij} = c_{ij} + \varepsilon_{ij}$ , with  $c_{ij}$  the average arc cost and  $\varepsilon_{ij}$  a random error term. Arguably the most interesting variation of the problem is the one where the realization of the arc costs is learned at each intersection as the graph is traversed. Below, we make the additional assumption that  $\varepsilon_{ij}$  are i.i.d. variables. In this case, by defining an action a as an arc (i,j) and a state s as a network node i and a vector  $e_i$  of learned realizations  $e_{ij}$  of the error term for all outgoing arcs from i, (2.3) becomes

$$V(i, e_i) = \min_{j \in \mathcal{V}_i^+} \left[ c_{ij} + e_{ij} + \int V(j, e_j) f(de_j) \right],$$
 (2.4)

where transitions between states are entirely contained by the density  $f(e_j)$ . This specific SSP will be of importance in Section 2.3.2.

#### 2.2.2 Inverse shortest path problems

In shortest path problems it is assumed that the modeler has complete knowledge of the cost function c or its distribution in the previous case, as well as state transitions p. In contrast, inverse shortest path problems study the case where the cost function is unknown and must be inferred with the help of an additional source of information at disposal, in the form of observed optimal paths between some origin-destination (OD) pairs. This class of problems broadly belongs to inverse optimization, an extensively studied problem (see e.g. Ahuja and Orlin, 2001)

where the modeler seeks to infer the objective function (and sometimes the constraints) of a forward (inner) optimization problem based on a sample of optimal solutions.

Motivation for studying inverse problems can be drawn from several types of applications. Burton and Toint (1992) cites possible motivations to examine inverse shortest path problems, one of which is precisely the subject of this tutorial. One may view the underlying optimization problem as a model for rational human decision making and assume that the cost function represents the preferences of users traveling in a network (possibly a parametrized function of certain arc features). In this context, recovering the cost function allows to analyze why individuals choose the observed routes and to gain understanding of network users' behavior. Using the recovered cost function, the inner shortest path problem can be solved and in this sense yield predictions of path choices for unobserved OD pairs.

Related to inverse shortest path problems is the literature on *inverse reinforce-ment learning* (IRL) or imitation learning (Ng et al., 2000; Abbeel and Ng, 2004). The IRL problem is more general than the inverse shortest path, since it considers an underlying optimization problem generally formulated as a infinite horizon MDP. In this context, observations consist of optimal sequences of actions. Nevertheless, models for IRL have also been applied to the problem of recovering the cost function of network users (e.g. Ziebart et al., 2008). Such applications consider specific MDPs where an action is a choice of arc in a network, and the destination is an absorbing state, as in Section 2.2.1. Most applications of IRL on path choice however consider a deterministic MDP (state transitions probabilities are degenerate) in contrast to the more general formulation in Section 2.2.1.

Inverse problems are in general under-determined and may not possess a unique solution. In the inverse shortest path problem and in IRL, there may be an infinite number of ways to define the cost function such that observations form optimal solutions. Different modeling paradigms propose to solve this issue. They may be separated in two categories depending on the assumptions made on the presence of noise in the data, which distinguishes between deterministic and stochastic problems. The former considers that demonstrated behavior is optimal, while the latter makes the hypothesis that observed trajectories deviate from deterministic shortest paths. The second case is often studied when the data collecting process may have induced measurement errors or when the data is generated by a decision

maker who exhibits seemingly inconsistent behavior. In the following sections, we review existing models for the above mentioned inverse problems.

#### Deterministic problems

Burton and Toint (1992) introduced the original deterministic inverse shortest path problem where observed trajectories are assumed to correspond to deterministic shortest paths. They do not assume that the cost function is parametrized by arc features and simply seek the value  $c_{ij}$  associated to each arc (i, j). They propose to provide uniqueness to the inverse problem by seeking the arc costs c that are closest to a given estimation  $\hat{c}$  of costs based on a certain measure of distance, thus minimizing an objective of the form  $||c-\hat{c}||$ . This implies that the modeler has an a priori knowledge of costs, which is reasonable in some applications. Burton and Toint (1992) provide seismic tomography as an example. Seismic waves are known to propagate according to the shortest path along the Earth's crust, but the geological structure of the zone of study is typically not entirely known, although modelers have an estimate. Given measurements of earthquakes' arrival times at different points in the "network", the goal is then to predict movements of future earthquakes by recovering the actual transmission times of seismic waves.

Variants of this problem have been studied by Burton and Toint (1994); Burton et al. (1997), for instance considering the case where arcs costs may be correlated or their values belong to a certain range. In Burton and Toint (1992) and following works, the  $l_2$  norm is selected as a distance measure between initial and modified costs, and yields a quadratic programming formulation. In Zhang et al. (1995), the  $l_1$  norm is assumed so that the problem can be modelled as a linear program and solved using column generation. In all the studies above, the inverse shortest past problem is modeled as a constrained optimization problem, with an exponential number of linear constraints to ensure that each observed path is shortest under the chosen cost function.

Bärmann et al. (2017) provide another example of inverse optimization with an application to learning the travel costs of network users, in particular subject to budget constraints. More precisely, they consider an inverse resource-constrained shortest path problem. Their approach does not recover an exact cost function, but provides a sequence of cost functions  $(c_1, ..., c_T)$  corresponding to each observation t = 1, ..., T, which allows to replicate demonstrated behavior. Their framework

explicitly assumes the optimality of observations in order to infer the objective functions  $c_t$ .

The deterministic problem has also notably been studied under the guise of inverse reinforcement learning in Ratliff et al. (2006), with an application to robot path planning. The objective of their work is to learn a cost function in order to teach a robot to imitate observed trajectories, which are assumed optimal. In contrast to the aforementioned works, no hypothesis is made regarding preliminary arc costs. However, the environment is considered to be described by features, such as elevation, slope or presence of vegetation, and the model seeks to obtain a mapping from features to costs by learning the weights associated to each feature. To obtain uniqueness of the solution, they cast the problem as one of maximum margin planning, i.e., choosing the parameters of the cost function that makes observed trajectories better by a certain margin than any other path, while minimizing the norm of weights. This notion of distance between solutions is defined by a loss function to be determined by the modeler. Under the  $l_2$  norm, this also results in a quadratic programming formulation with a number of constraints that depend on the number of state-action pairs, which consist of node-arc pairs in this context.

#### Stochastic problems

Inverse optimization problems with noisy data have been studied in, e.g., Aswani et al. (2018) or Chan et al. (2018). In addition to non-uniqueness, the problem which typically arises in this situation is that there may not be any non trivial value of arc costs which makes the demonstrated paths optimal solutions of a DSP. If solutions do exist, they may be uninformative, such as the zero cost function. To solve this issue, the previous framework is extended by letting solutions be approximately optimal and measuring the amount of error. Thus, accommodating noise requires to estimate a model for the choice of path which "fits" as closely as possible the observed data with various methods for measuring the fit, or loss, drawing from statistics. The chosen measure for the fit should uniquely define the solution.

Different points of views exist on achieving a good fit in the literature. Approaches grounded in machine learning make no assumptions on the underlying process that generated the data and merely focus on obtaining good predictive power with the simplest possible model while considering a large family of po-

tential functions. In contrast, the statistical inference perspective on the problem considers that there exists an underlying true cost function with a known parametric form. The aim is to obtain parameter estimates that asymptotically converge to the real values, a property known as *consistency*. Several loss functions are conceivable to formulate a minimization problem, and often the choice of loss is directly related to assumptions made on the underlying model.

Examples for the former are the work of Keshavarz et al. (2011), who estimate cost functions in a flow network assuming an affine parametric shape, and the work of Bertsimas et al. (2015), who seek to infer cost functions in a network subject to congestion at equilibrium. The specificity of the latter is that the cost functions are endogenous, i.e., the cost of paths include congestion costs. This makes it an inverse variational inequality problem with noisy data. In both works the proposed method is a heuristic and treats the process that generates the data as a black box. E.g. in Bertsimas et al. (2015), nonparametric cost functions are considered and the problem is formulated as a constraint programming model which balances the objective of minimizing the norm of the cost function against that of maximizing the fit of the data. They follow the approach of measuring the loss of the model by the amount of slack required to accommodate equilibrium constraints, i.e., making observed solutions " $\epsilon$ -optimal".

In contrast, the latter category of models assume that observed behavior deviates randomly from optimality according to a certain known probability distribution. This leads to a different modeling paradigm, in which a random term is added to the true cost function of the inner optimization problem, with the interpretation that each observation corresponds to an instantiation of the cost. This framework, described in, e.g., Nielsen and Jensen (2004) for general inverse problems, has received limited attention in the literature on inverse shortest path problems. One notable exception consists in path choice models based on the discrete choice modeling framework. In the next section, we review the literature surrounding this probabilistic modeling framework, which is at the heart of this tutorial.

#### 2.3 Probabilistic models for path choice

The inverse shortest path problem with noisy data is motivated by the situation of individuals traveling in real networks, where the assumption that a cost function can account for all observed behavior is rarely valid. Probabilistic methods for this noisy problem assume that observed path choices randomly deviate from deterministic shortest paths. In particular, discrete choice models are a particular type of probabilistic models grounded in econometrics, which provides the theoretical basis for behavioral interpretation.

One of the interpretations of the distributional assumption on the data is that travelers act rationally but observe additional factors impacting their path choice which vary among individuals and are unknown to the modeler. These factors are encompassed in a random term  $\varepsilon$  added to the cost function. Discrete choice models assume that the cost function is a parametrized function of several attributes. The only option available to the modeler, who knows the family of distributions for  $\varepsilon$  but does not observe the realization of random terms for a given individual, is to infer the probability that a given path is optimal.

The problem becomes akin to density estimation, i.e., recovering the parameters of a probability distribution over a set of paths. In this context, statistical consistency of the estimator is a desirable property. Yet there are several ways to define a probability distribution over paths, well-known in the discrete choice literature, which do not necessarily yield a consistent estimator. In the following sections, we elaborate on the above statement and describe two distinct discrete choice models for path choice.

Note that discrete choice models employ the terminology of utilities instead of costs and that we uphold this convention in the remainder of this tutorial. This implies a trivial change of the above formulations from minimization to maximization problems and the definition of a utility function v = -c.

#### 2.3.1 Path-based models

Discrete choice models based on paths are the methodology embraced by most works on the topic (Prato, 2009; Frejinger, 2008). They assume that the utility of a path i is a random variable  $u_i = v_i + \mu \varepsilon_i$ , where  $\varepsilon_i$  is a random error term,  $\mu$  is its scale, and the deterministic utility  $v_i$  is parametrized by attributes of the network,

such as travel time. Often the parametrization consists of a linear in parameters formulation of the shape  $v_i = \beta^T x_i$ , where  $\beta$  is a vector of parameters and  $x_i$  is a vector of attribute variables of the path i. Measuring the fit of a discrete choice model to the data naturally leads to selecting the log-likelihood loss, which assesses the plausibility of observing the chosen trajectories  $\{\sigma_n\}_{n=1,\dots,N}$  under the current value of parameters  $\beta$ . Thus the problem is one of maximum likelihood estimation, i.e., finding the set of parameters that minimize the log-likelihood loss.

The difficulty in specifying the probability of a given path is to identify the class of paths over which this probability should be defined. Since the very large number of feasible paths in a real network precludes enumeration, the immediate solution consists in choosing a subset of reasonable paths, assuming that all other paths have a null choice probability. This implies a two-step modeling framework, in which

- 1. Plausible paths are generated between the origin and destination of each observation n by solving versions of the DSP, forming the choice set  $C_n$ ;
- 2. Parameters  $\hat{\beta}$  that maximize the probability  $P(\sigma_n|C_n;\beta)$  of observed paths within the choice set previously defined are estimated via maximum likelihood, i.e., by maximizing  $\mathcal{LL}(\beta)$  defined as

$$\mathcal{LL}(\beta) = \log \prod_{n=1}^{N} P(\sigma_n | C_n; \beta).$$
 (2.5)

The distribution chosen for  $\varepsilon_i$  leads to different forms of discrete choice models with distinct path choice probabilities. The most well-known is the multinomial logit formulation, resulting from the assumption of i.i.d Extreme value type I distributed error terms, also known as the softmax in the machine learning community. Other models exist, such as the probit model. In the logit case, we have

$$P(\sigma_n|C_n;\beta) = \frac{e^{\frac{1}{\mu}v_{\sigma_n}(\beta)}}{\sum_{j\in C_n} e^{\frac{1}{\mu}v_{jn}(\beta)}}.$$
 (2.6)

There exists a vast array of methods to extract plausible paths from the network in order to generate the needed choice sets. Usually, they consists in assuming an a priori cost function and solving variants of the shortest path problem described in Section 2.2.1, until a large enough set of paths is obtained. Problematically,

the preliminary value of costs used to define the probability distribution through the choice set is in general not equivalent to the true value of the utility which is ultimately sought. This discrepancy is what prevents the consistency of the resulting estimates.

Frejinger et al. (2009) designed a method to correct for the induced sampling bias, by adjusting the choice probability  $P(\sigma_n|C_n;\beta)$  of a given path depending on parameter values and the choice set. The adjusted path choice probabilities include a correction term which accounts for the probability  $P(C_n|\sigma_n;\beta)$  that the given choice set was selected under the current parameter values conditionally on the observed choice.

The method proposed by Frejinger et al. (2009) can be understood as assuming that the true distribution is based on the set consisting of all feasible paths, while resorting to sampling paths in order to estimate the parameters of the distribution in practice. The advantage is that it yields consistent parameter estimates. Nevertheless, since there is no means to compute the normalizing constant of the distribution save for the impractical enumeration of all paths, the estimated model still requires to sample choice sets for prediction, an issue we further discuss in Section 2.5.2.

Arguably, since these issues arise from the combinatorial size of the inner problem, one may expect that DP could provide a solution for the inverse problem as well. The literature on IRL supplies such an example with Ziebart et al. (2008), who model the path choice problem as a MDP and estimate a probabilistic model which normalizes over the global set of feasible paths. This is achieved without enumeration nor sampling by viewing the path choice process as a sequence of action choices depending on a current state as in Section 2.2.1. In fact, this methodology is equivalent to the recursive discrete choice model, which has been developed independently and in parallel in the transportation research community. We introduce this model in the following section, which provides a method to consistently estimate parameters of the utility function without resorting to choice sets of paths.

#### 2.3.2 Recursive models

In this section, we introduce the recursive model proposed by Fosgerau et al. (2013) for the choice of path within the discrete choice modeling framework. We

also discuss the link to the IRL model by Ziebart et al. (2008).

#### Path choice as a deterministic MDP

Contrary to the previous section in which the problem is formulated in the high dimensional space of paths, the recursive choice model considers arc-based variables. Its formulation is explicitly based on the framework of Markov Decision Processes used to solve shortest path problems in Section 2.2.1.

In recursive models, network arcs correspond to states, while outgoing links at the head node of the current arc assume the role of available actions. For this purpose, we subsequently denote arcs as either k or a depending on whether they play the role of states or actions, and we denote  $\mathcal{A}(k)$  the set of outgoing arcs from k. Note that it would also be possible to select nodes as states, however the arc-based formulation allows the deterministic utility v(a|k) of an action-state pair to depend on turn angles between two subsequent arcs k and a. The destination is represented by a dummy link d which is an absorbing state of the MDP, where no additional utility is gained. Finally, utilities are undiscounted and the action-state transition function is assumed to be degenerate, since the new state is simply the chosen arc. A path under this framework is a sequence of states  $\{k_0, k_1, ..., k_T\}$ , starting from an origin state  $k_0$  and leading to the absorbing state  $k_T$  representing the destination d.

#### Parametric estimation of MDPs

Under this perspective, the inverse problem of recovering the utility function is a problem of parametric estimation of MDPs, as first described by Rust (1994). As in the previous section, the noise in the data is accounted for by assuming the presence of an i.i.d random error term  $\varepsilon_a$ , added to the utility v(a|k). The utility becomes a random variable  $u(a|k) = v(a|k) + \mu \varepsilon_a$ , where  $\mu$  is the scale of the error term. It is assumed that the individual observes the realizations of the random variables at each step of the process and chooses the best action accordingly. From the point of view of the modeler, the individual's behavior hence consists in solving a stochastic shortest path problem similarly to Section 2.2.1. In this context, the Bellman equation gives the optimal value function when the state consists of an

arc k and realizations  $e_{a \in \mathcal{A}(k)}$ ,

$$V^{d}(k, e_{a}) = \begin{cases} 0, & k = d, \\ \max_{a \in \mathcal{A}(k)} \left( v(a|k) + \mu e_{a} + \int V^{d}(a, e_{a'}) f(de_{a'}) \right), & \forall k \in \mathcal{A}, \end{cases}$$
(2.7)

which is very similar to (2.4). We may however simplify this equation by taking the expectation with respect to  $\varepsilon_a$  of (2.7) and defining the expected value function  $V^d(k) = \int V^d(k, e_a) f(de_a)$  of a state k, which gives

$$V^{d}(k) = \begin{cases} 0, & k = d, \\ E_{\epsilon} \left[ \max_{a \in \mathcal{A}(k)} \left\{ v(a|k) + \mu \epsilon_{a} + V^{d}(a) \right\} \right], & \forall k \in \mathcal{A}. \end{cases}$$
 (2.8)

For simplicity and consistency with terminology in other works (Fosgerau et al., 2013; Mai et al., 2015), we nevertheless refer to (2.8) as the value function in this work.

The modeler does not observe the realized utilities and can only compute the probability that each given action be optimal. According to the modeler, the observed behavior of individuals follows a probability distribution over the set of actions which maximizes the expected utility in (2.8). As in Section 2.3.1, choice probabilities may take several forms depending on the distributional assumption for the error terms  $\epsilon_a$ . Assuming an Extreme value type I probability distribution, the probability of an individual choosing a certain action a conditional on the state k and the destination a is given by the familiar multinomial logit formula:

$$P^{d}(a|k;\beta) = \frac{e^{\frac{1}{\mu}v(a|k;\beta) + V^{d}(a|\beta)}}{\sum_{a' \in A(k)} e^{\frac{1}{\mu}v(a'|k;\beta) + V^{d}(a'|\beta)}}.$$
 (2.9)

Given observations of sequences of actions (i.e., paths), the model can be estimated by maximum likelihood. This requires to define the probability of choosing an observed path, which can be expressed as the product of the corresponding action choice probabilities using (2.9). For an observed path  $\sigma_n = k_0, k_1, ..., k_T$ , the path choice probability is given by

$$P(\sigma_n|\beta) = \prod_{j=0}^{T-1} P^d(k_{j+1}|k_j;\beta),$$
 (2.10)

where d is the link  $k_T$ , which can more simply be expressed as

$$P(\sigma_n|\beta) = \frac{e^{\frac{1}{\mu}v(\sigma_n|\beta)}}{e^{\frac{1}{\mu}V(k_0|\beta)}}$$
(2.11)

where  $v(\sigma_n|\beta)$  is the sum of the link utilities of the path  $\sigma_n$ .

As a result, the likelihood of a set of N path observations  $\{\sigma_n\}_{n=1,\dots,N}$  is defined as

$$\mathcal{L}(\beta) = \prod_{n=1}^{N} P(\sigma_n | \beta) = \prod_{n=1}^{N} \prod_{i=0}^{T_{n-1}} P^d(k_{i+1}^n | k_i^n; \beta).$$
 (2.12)

The expression in (2.12) does not depend on choice sets, in contrast to (2.5). However, the value function which appears in (2.9) must be computed in order to evaluate the likelihood. This suggests resorting to a two-step likelihood maximization algorithm, in which an inner loop solves the SSP and obtains the value function in (2.8) for the current value of parameters  $\beta$ , while an outer loop browses through the values of  $\beta$ . Rust (1994) proposed such a method, denoted the *nested fixed point* algorithm. The resulting parameter estimates are consistent.

The model for IRL proposed in Ziebart et al. (2008) bears another name but is equivalent to a recursive logit model, since they assume a maximum entropy (exponential family) distribution. The only difference lies in the method for estimating the model, as Ziebart et al. (2008) approximate the value function in (2.8), whereas we exemplify in the next section that they can conveniently be solved as a system of linear equations (Fosgerau et al., 2013; Mai et al., 2016).

# 2.4 Illustrative examples

Section 2.3 presented two discrete choice models for the problem of estimating the utility function of travelers in a network: (i) Path-based models, (ii) Recursive models. Although the first is extensively used in practice, the second is superior because of its consistent estimator and accurate predictions without choice set generation.

This section has two purposes. First, we use small illustrative examples on acyclic and cyclic toy networks to provide a clear understanding and intuition of

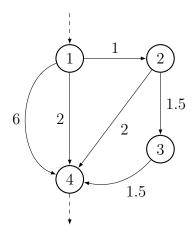


Figure 2.1 – Small network

the recursive model and the value function; second, we compare path probabilities obtained with both model formulations. Although both models can take several forms depending on distributional assumptions on the error terms, the focus of this tutorial is on the logit model. Therefore in the following we refer to the recursive logit as the RL model and the path-based logit as the PL model. We refer the reader to Mai et al. (2015); Mai (2016b) for details regarding the incorporation of complex correlation structures in recursive discrete choice models (e.g., nested logit, mixed logit).

Note that the MATLAB code used for these numerical examples is available online, as well as a tutorial detailing how to use it <sup>1</sup>.

# 2.4.1 An acyclic network

The motivation for this example is to show that it is possible to obtain with the recursive formulation in (2.9) the same choice probabilities on paths as with the PL model in (2.6). For this illustrative purpose, it is meaningful to consider a given specification of the utility function. Hence we assume that path utilities are specified by an additive function of arc length  $L_a$ , such that for each path i we have  $v_i = -L_i$ , where  $L_i$  is the sum of the lengths of arcs contained in path i.

The OD pair considered for the toy network displayed in Figure 2.1 is (1,4). The two dashed arcs represent dummy origin and destination links. There exists 4

<sup>1.</sup> http://intermodal.iro.umontreal.ca/software.html

| Path          | Length | Path probability (PL) | Product of link probabilities (RL) |
|---------------|--------|-----------------------|------------------------------------|
| 1 - 4         | 2      | 0.6572                | 0.6572                             |
| 1 - 4         | 6      | 0.0120                | 0.0120                             |
| 1 - 2 - 4     | 3      | 0.2418                | $0.3307 \cdot 0.7311 = 0.2418$     |
| 1 - 2 - 3 - 4 | 4      | 0.0889                | $0.3307 \cdot 0.2689 = 0.0889$     |

Table 2.1 – Path choice probabilities under both models

| Node | Value function |
|------|----------------|
| 4    | 0              |
| 3    | -1.5000        |
| 2    | -1.6867        |
| 1    | -1.5803        |

Table 2.2 - Value function at each node

possible paths from node 1 to node 4, of respective length 2, 3, 4 and 6. Under the logit model, it is easy to compute the choice probability of the shortest path for this OD pair, which goes directly from node 1 to node 4 with length 2. Assuming that the scale  $\mu$  of the random term for this example is 1, we obtain at the denominator of the logit function in (2.6) the term  $e^{-2}$ , and at the numerator the term  $e^{-2} + e^{-3} + e^{-4} + e^{-6}$ , therefore the choice probability is equal to 0.6572. Table 2.1 displays similarly the choice probability of all other paths.

Let us now suppose that instead of choosing between the possible paths connecting origin and destination, the traveler builds the chosen path along the way through a series of consecutive link choices, as in the RL formulation. In each link choice situation, the alternatives to choose from are the outgoing links at the current node. We denote  $v(a|k) = -L_a$  the utility of links  $a \in \mathcal{A}(k)$  originating from link k. The choice probability of a path under the RL model is then equal to the product of each link choice probability in (2.9).

In order to compute link choice probabilities, we need to compute the value function in (2.7). This equation can be rewritten as the logsum when  $\epsilon_a$  is assumed to be i.i.d. Extreme value type I distributed as in the logit model:

$$V^{d}(k) = \begin{cases} \mu \ln \sum_{a \in A(k)} e^{\frac{1}{\mu}(v(a|k) + V^{d}(a))} , \forall k \in \mathcal{A} \\ 0 , k = d. \end{cases}$$
 (2.13)

Since the specified utility of a link does not depend on the incoming arc, the value

function is identical for all links with the same end node. It is thus more convenient to compute the value function at each of the 4 nodes (the value function at a link is then equivalent to the value function at the end node of that link). Below, we show how to compute the value function in this network and display the value for each node.

In this case, since the network is acyclic, it is possible to compute the value function by backward induction. At the destination node 4, given that there is no utility to be gained, the value function V(4) is zero. Working our way backwards, we compute at node 3 the value function  $V(3) = \ln(e^{-1.5}) = 1.5$ . At node 2, we have  $V(2) = \ln(e^{-2} + e^{-3}) = -2.6867$ . Finally, at node 1 we obtain  $V(1) = \ln(e^{-6} + e^{-2} + e^{-2.6867}) = -1.5803$ . The values for all nodes are summarized in Table 2.2.

Having computed the value function for this network, we may apply (2.9) to this example and we obtain the path probabilities in the last column of Table 2.1. We notice that they are identical to choice probabilities under the PL model. This is due to the property of the RL model of being formally equivalent to a discrete choice model over the full choice set of paths (Fosgerau et al., 2013). Therefore, the PL and the RL models are two strictly equivalent approaches when the set of all possible paths in the network can be enumerated.

# 2.4.2 A cyclic network

Let us now consider a very similar network in Figure 2.2, with an added link between nodes 3 and 1. This network is no longer acyclic, and as a result there is in theory an infinite number of paths between nodes 1 and 4, when accounting for paths with loops.

The first consequence of dealing with a cyclic network is that the value function can no longer be computed by backwards induction starting from destination, since the network admits no topological order. However, the value function is still well defined as the solution of the fixed point problem (2.7) and can be solved either by value iteration or, in the case of the recursive logit, as the solution of a system of linear equations. For the latter, notice that by taking the exponential of (2.13)

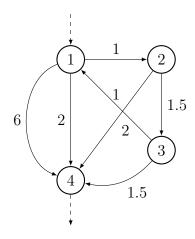


Figure 2.2 – Small cyclic network

and raising to the power  $\frac{1}{\mu}$ , we obtain

$$e^{\frac{1}{\mu}V^{d}(k)} = \begin{cases} \sum_{a \in \mathcal{A}(k)} e^{\frac{1}{\mu}(v(a|k) + V^{d}(a))} & \forall k \in \mathcal{A} \\ 1 & k = d. \end{cases}$$
 (2.14)

This is a linear system of equations if we solve for variable  $z = e^{\frac{1}{\mu}V}$ . Doing so, we obtain the value function in Table 2.3.

As in the previous example, having solved the value function, we can trivially compute the choice probabilities for different paths in this network as product of link choice probabilities. As can be observed, the probabilities of the four paths used in the acyclic example do not sum to 1 anymore (rather to 0.9698), and neither do the probabilities of the additional paths displayed in Table 2.4, which sum to 0.9965. This is because a cyclic network contains an infinite number of possible paths, and the RL model attributes a positive choice probability to each outgoing arc at an intersection. Hence, even paths with multiple cycles have a small probability of being chosen. We notice however that choosing a path with two or more cycles is extremely unlikely, with a probability of 0.0009 according to the model.

This example illustrates that the RL model offers a convenient mathematical formulation for the choice of path in a cyclic network. In comparison, using the PL model for this network raise a well-known challenge. Indeed, the logit formula in (2.6) requires to define a finite choice set of alternative paths for the OD pair. Given

| _ | Node | Value function |
|---|------|----------------|
|   | 4    | 0              |
|   | 3    | -1.1998        |
|   | 2    | -1.5968        |
|   | 1    | -1.5496        |

**Table 2.3** – Value function at each node

| Path              | Length | Product of link choice probabilities                                  |
|-------------------|--------|---|
| 1 - 4             | 2      | 0.6374  |
| 1 - 4             | 6      | 0.0117  |
| 1 - 2 - 4         | 3      | $0.3509 \cdot 0.6682 = 0.2345$  |
| 1 - 2 - 3 - 4     | 4      | $0.3509 \cdot 0.3318 \cdot 0.7407 = 0.0863$                           |
| 1 - 2 - 3 - 1 - 4 | 5.5    | $0.3509 \cdot 0.3318 \cdot 0.2593 \cdot 0.6374 = 0.0192$              |
| 1 - 2 - 3 - 1 - 4 | 9.5    | $0.3509 \cdot 0.3318 \cdot 0.2593 \cdot 0.0117 = 0.0004$              |
| 1-2-3-1-2-4       | 6.5    | $0.3509 \cdot 0.3318 \cdot 0.2593 \cdot 0.3509 \cdot 0.6682 = 0.0071$ |

Table 2.4 – Recursive logit path choice probabilities

that the possible paths cannot be all enumerated in this example, the modeler is compelled to make hypotheses on which subset of paths should have a non zero choice probability. The value of the resulting path choice probabilities will depend the composition of the choice set. In reality, this issue is not necessarily related to cycles only. In large networks, the number of possible acyclic paths may also be too large to enumerate in practice. In the following section, we delve into the issues which may arise from the necessity to generate choice sets to define choice probabilities in path-based models.

# 2.5 An analysis of the advantages of recursive models compared to path-based models

The goal of this section is to highlight the advantages of recursive models and the issues related to path-based models. In this discussion, we use illustrative examples and we focus on two practical purposes of such models; i) estimating parameters from data of observed paths; ii) predicting choices from an estimated model. We focus on logit models for this comparison.

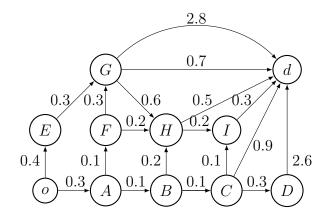


Figure 2.3 – Toy network labeled with link travel times

In practice, the PL model requires to generate choice sets of paths for both purposes. There is an extensive literature on the questions of how to generate choice sets of paths, what characteristics should choice sets observe, and what is the impact of selecting a restricted choice set prior to model estimation and prediction (Bekhor et al., 2006; Prato and Bekhor, 2007; Bovy, 2009; Bliemer and Bovy, 2008). The consensus in that literature is that it is advantageous to explicitly separate the procedures of generating path choice sets and modelling choice. Bekhor and Toledo (2005) argue that predicted paths from link-based models are behaviorally unrealistic as they may contain cycles. Bliemer and Taale (2006) claim that there are computational advantages to choice set generation in large networks.

On the contrary, Horowitz and Louviere (1995) indicate that it is possible to misspecify choice sets with problematic consequences and that choice sets provide no information on preferences besides what is already contained in the utility function, although their study does not investigate path choice. Frejinger et al. (2009), among others, empirically demonstrate that the definition of choice sets may affect parameter estimates. In this section of this tutorial, we offer additional arguments in this sense. We exemplify complications related to choice sets which arise when using path-based models, and we demonstrate that recursive logit models do not display these issues.

| Path $\sigma$ | Nodes                             | $C^1$        | $C^2$        | $C^3$        | $v_{\sigma}$ |
|---------------|-----------------------------------|--------------|--------------|--------------|--------------|
| 1             | 1 - 3 - 4 - 9 - 12 - 13 - 17      | У            | У            | у            | -2.3         |
| 2             | 1 - 3 - 4 - 7 - 10 - 17           | У            | У            | У            | -2.6         |
| 3             | 1 - 3 - 4 - 9 - 10 - 17           | У            | У            | У            | -2.6         |
| 4             | 1 - 3 - 4 - 7 - 10 - 13 - 17      | У            | У            | У            | -2.7         |
| 5             | 1 - 3 - 4 - 9 - 10 - 13 - 17      | У            | У            | У            | -2.7         |
| 6             | 1 - 3 - 6 - 16 - 17               | n            | У            | У            | -3.1         |
| 7             | 1 - 3 - 4 - 9 - 12 - 17           | $\mathbf{n}$ | У            | У            | -3.2         |
| 8             | 1 - 3 - 4 - 7 - 16 - 17           | n            | У            | У            | -3.2         |
| 9             | 1 - 3 - 6 - 16 - 10 - 17          | n            | n            | У            | -4.0         |
| 10            | 1 - 3 - 4 - 7 - 16 - 10 - 17      | $\mathbf{n}$ | $\mathbf{n}$ | У            | -4.1         |
| 11            | 1 - 3 - 6 - 16 - 10 - 13 - 17     | $\mathbf{n}$ | $\mathbf{n}$ | У            | -4.1         |
| 12            | 1 - 3 - 4 - 7 - 16 - 10 - 13 - 17 | $\mathbf{n}$ | $\mathbf{n}$ | У            | -4.2         |
| 13            | 1 - 3 - 4 - 9 - 12 - 15 - 17      | n            | n            | n            | -7.3         |
| 14            | 1 - 3 - 6 - 16 - 17               | $\mathbf{n}$ | $\mathbf{n}$ | $\mathbf{n}$ | -7.3         |
| 15            | 1 - 3 - 4 - 7 - 16 - 17           | n            | n            | n            | -7.4         |

Table 2.5 – Paths contained in each restricted choice set

#### 2.5.1 Example of model estimation

Figure 2.3 displays a network with one OD pair connected by a set of feasible paths  $\mathcal{U}$ . We study estimation results for synthetic data of trajectories on this toy network. This data is generated by simulation assuming that the true utility specification is given by

$$u_a = \beta_T T_a + \beta_{LC} L C_a + \epsilon_a$$

where  $T_a$  is the travel time on arc a, and  $LC_a$  is a constant equal to 1, with  $\beta_T = -2.00$  and  $\beta_{LC} = -0.01$ . Travel time for each link is given in Figure 2.3. The travelers are also assumed to consider every possible path in  $\mathcal{U}$ , such that any trajectory may be observed.

We compare the ability of the PL model versus that of the RL model to recover the true parameter values. To do so, we estimate four path-based models based on different choice sets  $C \subseteq \mathcal{U}$ . Table 2.5 displays the paths contained in each choice set, noting that choice set  $C^4$  contains all 15 paths and is equivalent to  $\mathcal{U}$ . For each observation, the chosen path is added to the choice set if not already present. The last column displays the utility of each path based on the given specification, obtained by summing the link utilities.

Results are shown in Table 2.6. In the cases where the choice set fails to include several relevant alternatives ( $C^1$  and  $C^2$ ), the estimation algorithm for the

| Model     | $eta_T$     | $\beta_{LC}$ |
|-----------|-------------|--------------|
| $PL(C^1)$ | 3.35(0.59)  | -0.64 (0.32) |
| $PL(C^2)$ | 2.00(0.37)  | 0.64(0.10)   |
| $PL(C^3)$ | -2.06(0.17) | -0.14(0.07)  |
| $PL(C^4)$ | -2.15(0.16) | -0.15 (0.07) |
| RL        | -2.15(0.15) | -0.14(0.07)  |

Table 2.6 – Estimation results of different models on synthetic data generated under the assumption that the true choice set is  $\mathcal{U}$ 

PL model does not converge, and the parameter values obtained are significantly different from the true ones. The fact that the algorithm does not converge may seem counter-intuitive at first, but it is in fact due to i) the lack of variance in attributes of the paths in these choice sets, ii) the omission in the choice set of paths 6 to 12, which are chosen relatively often in the data, but only added to C when corresponding to the observed path. As a result, when such paths are present in the choice set, the data reports that they are selected 100% of the time, which cannot be reconciled with the explanatory variables present in the utility specification.

The only case where the PL model recovers the true parameter values based on a restricted choice set is with  $C^3$ , which contains almost the same paths as  $\mathcal{U}$  but for three paths. The estimates have slightly lower variance when all alternatives are included with choice set  $C^4$ , and the RL model obtains equivalent results (the slight difference may be due to different implementations of the optimization algorithm). In accordance with several other studies, we conclude from this experiment that the PL model may not recover the true utility function when the choice set fails to include several relevant alternatives.

Certain studies argue that the assumption that users consider any path in  $\mathcal{U}$  is behaviorally unrealistic, and inquire what would happen if the data reflects instead the possibility that users do restrict their consideration set. In order to shed light on this question, we study a second sample of synthetic data, where observed trajectories include only paths 1 to 12, generated under the assumption that paths 13 to 15 are not considered by travelers due to their highly negative utility.

In Table 2.7, we show the estimation results of the same models on this new data. It shows that although the RL model considers more paths than the true choice set, it still recovers the true parameter values. On the other hand, the

| Model     | $eta_T$      | $\beta_{LC}$ |
|-----------|--------------|--------------|
| $PL(C^1)$ | 3.00 (0.47)  | -0.59 (0.26) |
| $PL(C^2)$ | 3.00(0.49)   | 0.93(0.13)   |
| $PL(C^3)$ | -1.94(0.17)  | -0.07(0.07)  |
| $PL(C^4)$ | -2.04(0.16)  | -0.07 (0.07) |
| RL        | -2.04 (0.15) | -0.07(0.07)  |

Table 2.7 – Estimation results of different models on synthetic data generated under the assumption that the true choice set is  $\mathbb{C}^3$ 

models based on choice sets  $C^1$  and  $C^2$  do not. This second experiment suggests that restricting the choice set without evidence regarding what alternatives are truly considered is potentially harmful, while considering a larger set including "irrelevant" alternatives does not interfere with estimation results in this case.

Finally, we note that Frejinger et al. (2009) provide a method to correct parameter estimates of path-based models. However, while this leads to consistent estimates, there is no method to consistently predict path choice probabilities according to the estimated model. Indeed, as the next examples highlight, predictions vary significantly depending on the definition of the choice set.

# 2.5.2 Examples of prediction

In general, predicting choices from discrete choice models for a certain demand requires knowing the utility function  $v_n$  and choice sets  $C_n$  of the decision makers n, on which the probability distribution depends. This is in theory more complex when the utility function  $v_n$  depends on socio-economic characteristics of individuals n. However, in the following, we make the assumption that the utility function is not individual specific and depends only on attributes of network links.

#### Link flows

Predicting link flows in the network is a typical application of path choice models, of importance in, e.g., stochastic user equilibrium models. Link flows represent the amount of individuals (or other unit) on each arc of the network corresponding to loading a certain OD demand.

Two methods exist to predict expected flows with the RL model, none of which require to enumerate choice sets of paths. The first method consists in sampling paths link by link for each individual using link choice probabilities in (2.9). The second method allows to compute expected link flows without resorting to simulation. According to the Markov property of the model, Baillon and Cominetti (2008) proved that destination-specific link flows  $f^d$  are obtained by solving the linear system

$$(I - P^{d^T})^{-1} f^d = g^d, (2.15)$$

where  $g^d$  is the demand vector from all origins to destination d and  $P^{d^T}$  is the transposed of the matrix of link choice probabilities, where  $P^d_{ka} = P^d(a|k)$ .

In this example, we predict link flows for the network in Figure 2.3, assuming a demand of 100 for the single OD pair and the same utility specification as in section 2.5.1. We compare the link flows predicted by the RL model and the three PL models based on different restricted choice sets  $C^1$ ,  $C^2$  and  $C^3$ . In each case, the expected flow on a given path  $\sigma$  is equal to the fraction of the demand choosing  $\sigma$  according to  $P(\sigma|C_n)$ . We do not consider  $C^4$ , because since  $C^4$  consists of the unrestricted network, the link flows obtained from this model will be identical to those computed from the RL model.

For the RL model, link flows are obtained by solving (2.15). For the PL models, flows on paths are computed from the path choice probabilities  $P(\sigma|C_n)$  for  $C_n = C^1, C^2, C^3$ . Flows on links are then obtained by summing the flows on all paths traversing each link. Table 2.8 displays the amount of flow on each link according to each model. As expected, we observe that the amount of predicted flow varies greatly between path-based models depending on the chosen choice set. When the choice set size increases, predicted flows tend to be closer to the values forecast by the RL model. A particularity of the RL model is that it predicts non-null flow on every link. However, the amount of flow on links 7, 10 and 16, which belong only to paths with very small choice probabilities, is very close to zero.

In reality, it is difficult to judge which model predicts link flows better without being able to compare to observed link counts. However, a crucial remark is that in the absence of any information regarding which paths are truly considered by travelers, the predictions of the PL models are arbitrarily dependent on the choice set. On the other hand, the RL model allows to predict according to the true estimated probability distribution. In addition, the RL model offers the advantage of computing link flows very efficiently, as only one system of equations must be

| Link | Nodes                          | $PL(C^1)$ | $PL(C^2)$ | $PL(C^3)$ | RL    |
|------|--------------------------------|-----------|-----------|-----------|-------|
| 1    | o-E                            | 0.00      | 8.83      | 13.88     | 12.99 |
| 2    | o-A                            | 100.00    | 91.17     | 86.12     | 87.01 |
| 3    | A-F                            | 36.92     | 35.75     | 37.10     | 37.39 |
| 4    | A-B                            | 63.08     | 55.42     | 49.02     | 46.63 |
| 5    | B-C                            | 26.16     | 27.67     | 24.47     | 25.10 |
| 6    | В-Н                            | 36.92     | 27.75     | 24.55     | 24.53 |
| 7    | C-D                            | 0.00      | 0.00      | 0.00      | 0.12  |
| 8    | C- $d$                         | 0.00      | 8.00      | 7.07      | 6.77  |
| 9    | C-I                            | 26.16     | 19.67     | 17.40     | 18.21 |
| 10   | $\mathrm{D}\text{-}\mathrm{d}$ | 0.00      | 0.00      | 0.00      | 0.12  |
| 11   | E- $G$                         | 0.00      | 8.83      | 13.88     | 12.99 |
| 12   | F- $G$                         | 0.00      | 8.00      | 12.55     | 12.86 |
| 13   | F-H                            | 36.92     | 27.75     | 24.55     | 24.53 |
| 14   | G-H                            | 0.00      | 0.00      | 11.54     | 12.04 |
| 15   | G-d1                           | 0.00      | 16.83     | 14.89     | 13.60 |
| 16   | G-d2                           | 0.00      | 0.00      | 0.00      | 0.20  |
| 17   | H-I                            | 35.08     | 26.36     | 28.80     | 30.40 |
| 18   | H-d                            | 38.76     | 29.14     | 31.84     | 30.70 |
| 19   | I-d                            | 61.24     | 46.03     | 46.20     | 48.60 |

Table 2.8 – Link flows according to each model

solved to obtain link flows for all OD pairs with the same destination. On the contrary, the PL models require to define a choice set for each OD pair.

# 2.5.3 Accessibility measures

Accessibility measures are another example of information which can be computed from path choice models. The accessibility is a measure of the overall satisfaction of an individual for the available alternatives, i.e. the existing paths in a network for a given OD pair, and is formally defined as the maximum expected utility of the alternatives. According to the RL model, the accessibility is simply the value function at the origin in (2.13). In path-based models there is no notion of value function, and instead the accessibility depends on the generated choice set,

$$E(\max_{i \in C_n} u_i) = \mu \log \sum_{i \in C_n} e^{\frac{1}{\mu}v_i}.$$
 (2.16)

In the network of this example, accessibility measures are given in Table 2.9. This illustrates that the value of accessibility significantly differs depending on choice set composition, and that as more paths are added to  $C_n$  the value predicted by PL models converges to that predicted by the RL model, as asserted by

$$\begin{array}{c|ccccc} PL(C^1) & PL(C^2) & PL(C^3) & RL \\ \hline -0.9592 & -0.6738 & -0.5512 & -0.5478 \end{array}$$

Table 2.9 – Accessibility measures according to each model

Zimmermann et al. (2017). Obtaining a prediction of accessibility which is independent of choice sets is very useful, as it allows to compare changes in accessibility before and after network improvements (e.g. after links are added) without bias. When path-based models are used, reported accessibility measures may be incoherent, e.g. decreasing after network improvements, an issue dubbed the Valencia paradox in Nassir et al. (2014).

## 2.6 Conclusion

This paper presented a tutorial on analyzing and predicting path choices in a network with recursive discrete choice models. The goal of path choice models is to identify the cost function representing users' behavior, assuming that individuals act rationally by maximizing some kind of objective function when choosing a path in a network. Such models are useful to provide insights into the motivations and preferences of network users and to make aggregate predictions, for instance in the context of traffic equilibrium models.

In this tutorial, we presented the state of the art methodology for this problem, namely recursive discrete choice models. This methodology is superior in many respects to the discrete choice models based on paths extensively used in the transportation demand modeling literature. This tutorial achieved two main contributions, which we describe below.

First, we provided a fresh and broader research context for this problem, which has traditionally been addressed mostly from the angle of econometrics in transportation. Namely, we drew links between discrete choice modeling and related work in inverse optimization and inverse reinforcement learning, which facilitates a greater understanding of the recursive models presented in this work. In particular, we contextualized discrete choice as a method for inverse optimization with noisy

data, and showed that viewing the inner problem as a Markov decision process naturally yields the recursive formulation.

Second, we highlighted the advantages of recursive models through an illustrated comparison with the most widely used method in the literature, i.e., path-based discrete choice models. While we do not aim at discussing the validity of the behavioral assumptions between both models, we illustrated that recursive models display mathematical convenience, by yielding consistent parameter estimates and predicting choices faster without choice set generation.

# Bike route choice modeling using GPS data without choice sets of paths

# Prologue

#### Context

This chapter focuses on the timely topic of sustainable means of transportation by estimating a bike route choice model based on the recursive modeling framework introduced in Chapter 2. Before this article, a majority of existing research on cyclists' route choice behavior was based on stated preference data (i.e., surveys), and the few which made use of revealed trajectories (Broach et al., 2012; Menghini et al., 2010; Hood et al., 2011) worked with path-based models, with known issues. Although recursive discrete choice modeling appears as a suitable candidate for the bike route choice problem, the methodology had previous to this article only been applied to relatively small networks (about 7,000 links) with no more than 3 link attributes.

#### Contributions

This article mostly makes an empirical contribution. We apply the recursive choice modeling framework to GPS-based trajectories of cyclists in the network of Eugene, Oregon (about 40,000 links), and we report estimation results of several models. We analyze the path-choice behavior of cyclists with respect to 14 different network link attributes, provide an interpretation of results as well as a comparison with the literature.

Besides model estimation, this article also addresses the problem of prediction and illustrates that recursive models are in this respect superior to the path-based methodology. First, we provide a comparison of two methods to predict traffic flows in an uncongested network which are compatible with the recursive models, namely simulation and solving a system of linear equations (Baillon and Cominetti, 2008).

Second, we highlight a property of the recursive logit model related to accessibility predictions, which sheds light on a paradox recently observed in the route choice literature by Nassir et al. (2014).

#### Author contributions

The general idea for this paper came from Emma Frejinger. I was responsible for writing the code with initial script and support from Tien Mai, and for running experiments. I took charge of the full redaction of the article, while Emma Frejinger revised the manuscript.

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# 3.1 Introduction

The increasing concern of policy makers for the nuisances generated by motorized travel, including air pollution, urban congestion and energy waste, has triggered the need for research into sustainable means of transportation, such as cycling. Cycling is not a popular option for US households, 92% of which owned a car in 2001 (Pucher and Renne, 2003) and used it as their usual commute mode (Polzin and Chu, 2005). In some European countries, however, cycling levels have increased sharply since 1975, when efforts were first made to accommodate cyclists on the road network, providing evidence of the powerful impact of policy on travel behavior (Pucher and Buehler, 2008). The challenge policy makers face nowadays is providing a safe and convenient cycling environment that will encourage a greater shift to this mode.

The high travel demand and the size constraints on the street network make it difficult for urban planners to create a system adapted to cyclists. In order to determine exactly what facilities are worth investing in, urban planners need to understand the behavior of bike users and gain insight into the trade-offs they make when choosing their route. Indeed, cyclists do not always choose the shortest distance path to go from an origin to a destination, and in fact many other factors play a part. For example, would a cyclist be willing to go far out of their way to avoid a hill, or to use a bike lane?

One way to answer these questions is route choice analysis. Route choice models in a real network deal with identifying the route a traveler would take to go from one location to another. Discrete choice models and revealed preference (RP) data can be used to define a choice probability distribution over paths in a network. Such models have applications on multiple levels. Firstly, the interpretation of model parameters quantifies the trade-offs made by cyclists, which provides helpful guidance for improving network infrastructure. Secondly, link flows predicted by the model are useful to target the network areas most in need of improvement. Thirdly, route choice model output provides bike accessibility prediction to higher-level models, e.g. mode choice.

GPS technology can be used to collect RP data on path choices in real networks. In this case, the raw data is a sequence of GPS coordinates and this data needs to be matched to the network used by the analyst. This may be challenging, in particular if trip start and end coordinates are not identified by the participant, or if the precision of the GPS coordinates is poor. There is a vast literature focusing on various modeling and data processing issues related to GPS data (see for example, Murakami and Wagner, 1999; Wolf et al., 2001; Du and Aultman-Hall, 2007; Bierlaire and Frejinger, 2008; Schuessler and Axhausen, 2009; Bierlaire et al., 2013). This study focuses on bike route choice modeling rather than data processing and the GPS data has already been matched to the network. The observations hence correspond to paths.

In the literature on route choice models based on RP data in a real network, there are two main modeling approaches. The most common approach is path-based, in the sense that the model describes a discrete choice among paths. A well-known issue associated with this framework is that, in a real network, the universal set of all paths is intractable. The other approach, put forward by Fosgerau et al.

(2013), is link-based. In this model, called recursive logit (RL), the choices of itineraries are modeled as a sequence of link choices.

The literature on bike route choice modeling is scarce compared to its car counterpart, and all current models are based on the first approach (e.g. Broach et al., 2012; Hood et al., 2011; Menghini et al., 2010). A shortcoming of these models is that due to the exponential number of paths in the network one has to make assumptions about which paths to consider (i.e. sample a restricted choice set). This sampling process may introduce variability in estimation results, as pointed out by Frejinger et al. (2009). Moreover, it is unknown how to use these models to obtain correct predictions, as further detailed in Section 3.2. Link-based models have the advantage of not requiring any sampling of paths. In fact, it was shown that the RL model is equivalent to a path-based model with unrestricted choice set (Fosgerau et al., 2013).

In this work, we propose a link-based bike route choice model which overcomes these challenges. We adapt to the bike route choice problem the RL model formulated by Fosgerau et al. (2013), based on the assumption of an unrestricted choice set and not requiring any sampling of paths. Unlike previous studies, this work addresses both the issues of estimation and prediction. More precisely, we make the following empirical and theoretical contributions. First, we show how nonlink-additive attributes, such as slope, can be incorporated into the link utilities of the RL model. Second, we provide estimation results based on GPS observations in the network of Eugene, Oregon, which reveal cyclists' preferences and quantifies trade-offs between different network attributes. Third, we provide numerical results which illustrate the advantages of the RL model over path-based models in the context of prediction, in particular regarding gains in computational time. Fourth, we study properties of the RL model and specifically discuss accessibility measures. The analysis illustrates that the paradoxical results reported e.g. by Nassir et al. (2014) obtained when path-based models predict accessibility are due to the necessity to sample paths but can be avoided by the RL model.

The remainder of this paper is structured as follows. In Section 3.2, we start by describing the state of the art in bike route choice modeling and we highlight gaps in previous research. In Section 3.3, we review the RL model and in Section 3.4 we describe the data used for this application. We provide estimation results and discuss their implications in terms of travel behavior in Section 3.5. Then Section

3.6 focuses on prediction of link flows and accessibility. Finally, we conclude in Section 3.7.

# 3.2 Literature review

In this section, we review the path-based modeling approach for the route choice problem and highlight differences with the link-based approach. We then focus specifically on bike route choice modeling and describe previous studies.

#### 3.2.1 Path-based approach to route choice modeling

The path-based models are more commonly used than link-based ones. A wellknown issue associated with these models is that the set of all feasible paths is intractable and the actual choice sets of paths are unknown to the analyst. In fact, in a real-sized network, there is an unlimited number of paths connecting each origin-destination pair if loops are permitted. In order to estimate such a model, a restricted choice set has to be defined for each path observation. They can be generated with some sort of path-generation algorithm, such as link elimination (e.g. Menghini et al., 2010), or route labeling (e.g. Ben-Akiva et al., 1984). This process can lead to two different hypotheses on the choice set. The classic approach hypothesizes that the generated choice sets contain all the paths considered as alternatives by travelers. As argued by Frejinger et al. (2009), the issue with this approach is that parameter estimates may vary significantly with the definition of choice sets. This led Frejinger et al. (2009) to propose a sampling approach. In this approach, all feasible paths connecting an origin-destination pair are assumed to belong to the choice set, denoted as the universal choice set, and the parameter estimates are corrected for the bias induced by sampling a restricted set.

The issue of choice set generation has been mainly discussed in the context of model estimation. However, the intractability of choice sets is also an issue for prediction. Indeed, having access to the estimated path choice probabilities requires to explicitly enumerate the choice set. In the literature, most route choice models follow the classic approach, which counters the problem by assuming that only a subset of alternatives is actually considered as relevant by travelers. The

constructed choice set is assumed to contain all of them. However, as argued by Prato (2009), an objective definition of relevant routes is currently missing. Therefore, the correctness of path choice sets for prediction purposes cannot be ascertained. This is an important issue since predictions vary depending on which paths are assumed to be part of the choice set. When a route choice model is estimated based on the hypothesis of an unrestricted choice set, any feasible path is associated a non-zero choice probability. In this setting it is difficult to use the model to forecast path choices. To the best of our knowledge, the only known method to sample paths according to a given distribution without enumerating the choice set is Metropolis-Hastings sampling of paths (Flötteröd and Bierlaire, 2013). The method only requires to know the distribution up to a multiplicative constant, which obviates the computation of the denominator in the logit function and avoids path enumeration. However, Metropolis-Hastings sampling is time-consuming and may be too costly to use in, for example, traffic simulation models.

### 3.2.2 Bike route choice modeling literature

Until recent years, the literature on bike route choice was exclusively based on stated preference (SP) data. In the simplest case, individuals take part in a survey in which they are asked to evaluate routes based on their main characteristic (e.g. Winters et al., 2011). In other studies like that of Sener et al. (2009), surveys are designed in a way that forces the respondent to make trade-offs between combinations of attributes. Some studies based on SP methods are limited to performing a descriptive analysis without estimating a formal model, while others use multinomial logit or regression analysis methods, including Tilahun et al. (2007), Sener et al. (2009), Hunt and Abraham (2007), and Stinson and Bhat (2003).

Although SP studies can be relatively inexpensively implemented and are able to evaluate alternatives that are not yet available (e.g. nonexistent facilities), they also have a number of well-known shortcomings. The limitations of SP studies arise mostly from the difference between claimed and observed behavior, as described in numerous works, for example by Sener et al. (2009). Indeed, it is difficult for SP studies to put respondents in a setting where they can best reproduce the behavior they exhibit in reality.

RP studies were enabled by the emergence of geographic information systems

(GIS) which gave access to new types of data. Data was then still collected through surveys, but instead of being put in hypothetical choice situations, participants had to recall their actual commuting routes, which were subsequently analyzed with GIS. While providing valid insights, these first attempts to analyze bike route choice based on RP data never resulted in the estimation of a full route choice model, as observed by Broach et al. (2012). In particular, the models lack a comprehensive choice set of paths since the recalled route is compared mostly only to the shortest path (e.g. Harvey et al., 2008). In addition, the models focus on predicting specific aspects of route choice, such as the distance deviation from the shortest path or the presence of bike facilities, but cannot be applied to predict path probabilities for a large set of routes. In other words, they are certainly useful for behavioral analysis, but not for trip distribution in a network.

The first RP study that overcame these various limitations was the work of Menghini et al. (2010). Its main innovation was to exploit automatically processed GPS-based observations. Car route choice models had already been estimated on this kind of data (e.g. Ramming, 2001), since this area of research benefited from a few years' lead in data collecting efforts. However Menghini et al. (2010) were the first to obtain a large scale GPS sample of cyclists trajectories matched to a suitable network and to estimate a complete bike route choice model.

Some other noteworthy studies followed the steps of Menghini et al. (2010), but overall the literature on bike route choice based on RP is still in its early stages compared to its car counterpart. Notably, Hood et al. (2011) extended the Zürich results of Menghini et al. (2010) to the US context, in a study based in San Francisco. Broach et al. (2012) contributed as well to the state of the art by estimating a model comprising a richer set of attributes.

The previously cited works are all based on the hypothesis that choice sets contain the actual paths considered by cyclists. Part of the focus of their study was then on the development of realistic choice set generation methods. A common measure of the adequacy of choice sets is the coverage of observed routes (Ramming, 2001). In other words, path generation algorithms should be able to reproduce the observed routes for a high proportion of origin-destination pairs. However, the network density and the variety of attributes influencing cyclists' choices make this especially difficult for bike networks. As noted by Broach et al. (2012), common algorithms for car routes based on shortest paths are often not directly applicable.

Menghini et al. (2010) developed a choice set generation algorithm for high resolution data (Rieser-Schüssler et al., 2013), deemed suitable for bike networks, and Hood et al. (2011) and Broach et al. (2012) experimented with methods to account for the diversity of attributes. Despite this progress, these studies highlight the challenges raised by the restricted choice set hypothesis, especially for bike route choice. Considered choice sets are rarely observed, thus even the quality measures proposed in the literature have limitations (Frejinger, 2008). Moreover, even based on these criteria the most recent algorithms fail to include all observed alternatives. As pointed out by Horowitz and Louviere (1995), when there exists no observation on choice sets, it is better to rely solely on the utility function to predict choices, which is the assumption of the RL model.

# 3.3 Methodology

In this section, we present the link-based recursive models. We recall the formulation of the RL model and we review subsequent works which relax its IIA property.

# 3.3.1 The recursive logit model

The RL model (Fosgerau et al., 2013) corresponds to a dynamic discrete choice model and the choice of path is formulated as a sequence of link choices. At each node in the network, an individual chooses the utility-maximizing link, where the utility is the sum of the instantaneous link cost, the maximum expected utility to the destination and i.i.d. extreme value type I error terms. Therefore, attributes of the RL model are attributes of the links in the network and they are specified to be link-additive, such that the utility of a path is the sum of the utility of each link in the path.

Formally, the model can be described as follows (Fosgerau et al., 2013). The road network is a directed connected graph  $G = (\mathcal{A}, \mathcal{V})$ , where  $\mathcal{A}$  is the set of links and  $\mathcal{V}$  is the set of nodes. More precisely, a set of absorbing links without successors, corresponding to the observed destinations, is added to  $\mathcal{A}$ . We denote links  $a, k \in \mathcal{A}$ , and the set of outgoing links from k, A(k). Each link pair (k, a)

where  $a \in A(k)$  then has a deterministic utility component v(a|k), based on the attributes x(a|k) of the link pair. In the terminology of dynamic programming, k is a state and a is an action given k, although in this context choosing an action translates simply to choosing the next link in the path.

Consider now an individual n traveling in this network. The instantaneous random utility for the individual n of a link a conditionally on being in state k can then be defined as:

$$u_n(a|k) = v_n(a|k) + \mu \epsilon_n(a), \tag{3.1}$$

where  $\epsilon_n(a)$  are i.i.d extreme value type 1 error terms with zero mean and  $\mu$  is a fixed scale parameter. The full utility of link a conditionally on being in state k is obtained by adding to the instantaneous utility  $u_n(a|k)$  the maximum expected utility to destination d, denoted the value function  $V_n^d(a)$  and defined by the Bellman equation as follows

$$V_n^d(k) = E \left[ \max_{a \in A(k)} \left\{ v_n(a|k) + V_n^d(a) + \mu \epsilon_n(a) \right\} \right].$$
 (3.2)

Therefore, upon observing the random term  $\epsilon_n(a)$ , the individual chooses in A(k) the link a which maximizes  $u_n(a|k) + V_n^d(a)$ .

The probability of choosing a link a given state k conditionally on going to destination d is then given by the multinomial logit model

$$P_n^d(a|k) = \frac{e^{\frac{1}{\mu}v_n(a|k) + V_n^d(a)}}{\sum_{a' \in A(k)} e^{\frac{1}{\mu}v_n(a'|k) + V_n^d(a')}}.$$
(3.3)

In this case the value function is the logsum

$$V_n^d(k) = \mu \ln \sum_{a \in A(k)} e^{\frac{1}{\mu} v_n(a|k) + V_n^d(a)}.$$
 (3.4)

We note that the denominator in (3.3) simplifies to  $e^{\frac{1}{\mu}V_n^d(k)}$ . As a result, the probability of choosing a path  $\sigma = \{k_i\}_{i=0}^l$  where  $k_0$  is the origin and  $k_l = d$ , given

by the product of the link choice probabilities, also has a simple expression:

$$P_n^d(\sigma) = \prod_{i=0}^{l-1} e^{\frac{1}{\mu}(v_n(k_{i+1}|k_i) + V_n^d(k_{i+1}) - V_n^d(k_i))}$$
(3.5)

$$= \frac{e^{\frac{1}{\mu} \sum_{i=0}^{l-1} v_n(k_{i+1}|k_i)}}{e^{\frac{1}{\mu} V_n^d(k_0)}}.$$
 (3.6)

Denoting  $\sum_{i=0}^{l-1} v_n(k_{i+1}|k_i)$  as  $v_n(\sigma)$ , Equation (3.6) can be rewritten as:

$$P_n^d(\sigma) = \frac{e^{\frac{1}{\mu}v_n(\sigma)}}{\sum_{\sigma' \in \mathcal{U}} e^{\frac{1}{\mu}v_n(\sigma')}},\tag{3.7}$$

where  $\mathcal{U}$  is the universal set of all possible paths. Therefore, the RL model is equivalent to a static model of multinomial logit form with an infinite choice set (Fosgerau et al., 2013).

We also note that the hypotheses of the RL model, namely deterministic state transitions and a discount factor equal to one, allow Bellman's equation (3.2) to be rewritten as

$$\mathbf{z} = \mathbf{M}\mathbf{z} + \mathbf{b},\tag{3.8}$$

where  $\mathbf{z}_k = e^{\frac{1}{\mu}V^d(k)}$ ,  $M_{ka} = \delta(a|k)e^{\frac{1}{\mu}v(a|k)}$  and  $b_k = 0$  if  $k \neq d$  and  $b_d = 1$  (Fosgerau et al., 2013). Therefore, the value function for each destination can be obtained by simply solving a system of linear equations.

# 3.3.2 Modeling correlated utilities

When discrete choice models are used to analyze path choice in a network, it is well known that the IIA property may not hold for a given logit specification, e.g., due to overlapping paths in the network (Ben-Akiva and Bierlaire, 2003). Paths sharing links in the network may share unobserved attributes and the route choice model should account for this correlation in order to produce accurate predictions. Several solutions, such as path size logit (Ben-Akiva and Bierlaire, 1999), have been proposed in the literature to model correlated path utilities, as reported by Frejinger and Bierlaire (2007).

Similarly to the path size logit model, Fosgerau et al. (2013) propose a so-called Link Size (LS) attribute that can be used in combination with the RL model. It

heuristically corrects the utility of overlapping paths and relaxes IIA while keeping the logit structure.

Mai et al. (2015) relax the IIA property in the RL model by allowing scale parameters of random terms to be link-specific. The model contains scale parameters  $\mu_k$  for each link  $k \in A$  and the utility function becomes

$$u_n(a|k) = v_n(a|k) + \mu_k \epsilon_n(a). \tag{3.9}$$

The resulting model is called the nested recursive logit (NRL) and it allows path utilities to be correlated in a fashion similar to the nested logit (McFadden, 1978). The path probabilities are in this case defined by

$$P_n^d(\sigma) = \prod_{i=0}^{l-1} e^{\frac{1}{\mu_{k_i}} (v_n(k_{i+1}|k_i) + V_n^d(k_{i+1}) - V_n^d(k_i))}.$$
 (3.10)

The scales  $\mu_k$  are parameters of the model to be estimated, similarly to the parameters  $\beta$  associated with the attributes of the instantaneous utilities. Due to the impossibility to estimate a scale parameter for each link in a real network, it is assumed that scale parameters are a function  $\mu_k(\beta_{\text{scale}})$  of parameters  $\beta_{\text{scale}}$  to be estimated.

There is a trade-off between modeling correlated utilities and being able to estimate the models in a reasonable amount of time. The RL model requires to solve the systems of linear equations in (3.8). Thanks to a decomposition (DeC) method for RL proposed by Mai et al. (2016), it is sufficient to solve one system for all destinations in order to evaluate path choice probabilities. This is not the case for RL with the LS attribute which requires to solve one system per origin-destination pair. The DeC method is not compatible with NRL either. The destination specific value functions corresponding to the NRL model are solutions to a system of non-linear equations. They can be computed by value iteration as described in Mai et al. (2015) which is more time consuming than solving a linear system.

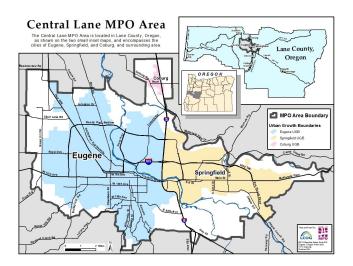


Figure 3.1 – Map of the region of study. Source: www.thempo.org

# 3.4 Data

This study is based on GPS observations of cyclists trajectories in the city of Eugene, Oregon. The data was collected and processed by the Central Lane Metropolitan Planning Organization as part of their ongoing research on bicycle travel behavior in the area. Their goal was to collect the data in an inexpensive manner in terms of time and money, which pointed towards the use of a smartphone application instead of a bicycle-mounted GPS device. This led to the development of the CycleLane smartphone application. CycleLane builds on code provided by the San Francisco County Transportation Authority, who has previously developed a similar application called CycleTracks (see Hood et al., 2011).

Upon downloading the CycleLane application, users are first asked about demographics and cycling frequency. They may then voluntarily record any bike trip they undertake by switching on the application. At the end of a trip, the user fills in the purpose of the trip and the data is automatically sent to the CLMPO.

In total, 648 observations of bike trips were collected from 103 users, after the CLMPO screened observations in order to remove trips not within the region, trips not fully recorded, and duplicate trips. Most users were frequent cyclists (with 55% of the sample riding several times per week or daily). There is also a bias towards males, who represent 74% of participants, and surprisingly towards people older

than 26, who amount to 81%, despite the high number of university students in the region (Roll, 2014).

The observations were matched to the route network of the Eugene Springfield Metropolitan area (Figure 3.1). The network contains 16,352 nodes and 42,384 links. It was enlarged to include not only traditional car routes but also the many minor alleys and multi-use paths bikes may take. The area comprises some 80 miles of off-street bicycle and pedestrian paths and over 140 miles of bike lanes and bike boulevards, according to the CLMPO. As a result, we can analyze preferences towards different types of bike facilities.

Several network characteristics are available to describe the network's links, such as length, average slope and upslope, estimated car traffic volume, one-way restrictions, speed limits, presence of various types of bike facilities, traffic signals, and stop signs. In contrast with previous path-based studies, the data does not need to be processed in order to compute attribute levels of each generated path. In the following section, we describe how to exploit the data in order to meet the RL model's assumptions.

# 3.5 Recursive bike route choice models

In this section, we use the recursive models of Section 3.3 to analyze the data presented in Section 3.4. We present the specification of link utilities, estimation and cross-validation results.

#### 3.5.1 Link utilities

We specify four different models within the recursive framework: the RL model with and without the LS attribute, and the NRL model, also with and without LS attribute.

We start by noting that it is important to define link utilities as functions of link-additive attributes. Indeed, the likelihood function is defined over path observations. In the RL model, the probability of choosing a path is equal to the product of the link choice probabilities, which results in an expression (3.6) that is

based on the sum of link utilities. Link-additive attributes ensure that the sum of link utilities can be interpreted as a path utility.

As a result of the link-additivity assumption, link characteristics such as slope need to be carefully incorporated in the utility function. For example, it is not possible to include slope as a continuous variable, since the average slope of a path consisting of two links is not equal to the added average slopes of each link. In our case, these inherently non-link-additive attributes are slope, traffic volume and presence of bike facilities. The solution we adopt is to specify a dummy variable  $\delta_a$  for each of these attributes and let the dummy variables interact with the link length attribute. On each link a, the variable  $\delta_a$  takes the value 1 if the attribute is present or greater than a chosen threshold in case of continuous attributes, and 0 else. The interaction term is simply the product of the two attribute values. Not only does this specification allow us to include important characteristics in a way that respects link additivity, but the interpretation is also simple and intuitive.

As an illustration, let us assume links are characterized by three attributes, link length, slope, and the presence of a bike lane. Let us also assume a certain threshold above which slope affects utility has been chosen. If we denote  $L_a$  the length of link a,  $\delta_a^S$  and  $\delta_a^B$  the previously introduced dummy variables corresponding to slope and presence of a bike lane respectively,  $\beta_L$  the length parameter, and  $\beta_{L,S}$ ,  $\beta_{L,B}$  the parameters corresponding to the interaction terms, then the deterministic utility component of a link a given a state k would be:

$$\beta_L \cdot L_a + \beta_{L,S} \cdot L_a \cdot \delta_a^S + \beta_{L,B} \cdot L_a \cdot \delta_a^B$$

$$= \underbrace{(\beta_L + \beta_{L,S} \cdot \delta_a^S + \beta_{L,B} \cdot \delta_a^B)}_{\beta_{TL}} L_a.$$

Implied is that length is associated to a total length parameter, referred in this example as  $\beta_{TL}$ , which may take different values across links. For example, for a link a with a slope greater than the chosen threshold and with a bike lane, the variables  $\delta_a^S$  and  $\delta_a^B$  would take the value 1. In this case, the parameters of the interaction terms would add to  $\beta_L$ , and  $\beta_{TL}$  would be equal to  $\beta_L + \beta_{L,S} + \beta_{L,B}$ .

Intuitively, the way individuals perceive length is influenced by other characteristics of the link. In the illustrative example, if  $\beta_{L,B}$  is positive, the fact that there is a bike lane will increase the value of the total parameter  $\beta_{TL}$ , making traveling

a unit of distance on this link less unpleasant for the individual. Similarly, if  $\beta_{L,S}$  is negative, a link with a slope higher than the threshold will cost more per unit of length, making it less attractive. The implied behavior is plausible, as travelers might be willing to cope with negative attributes, but more so for relatively short distances.

We summarize in Table 3.1 the network attributes x(a|k) of each link pair (k,a) included in the deterministic utility specification of all four models. Non-link-additive attributes which are included through the specification of one or several dummy variables are traffic volume, average upslope, and three types of bike facilities. Turn attributes are computed based on link orientation at each node. Obtaining these link pair attributes from the network data is straightforward and does not require extensive computations. This makes the model practical to estimate compared to path-based models which require to compute path attributes for each path in the choice set.

In order to account for the correlation due to overlap between paths, we follow the methodology detailed in Section 3.3.2. In addition to the RL model, we specify a RL model with LS attribute, a NRL model, and a NRL model with LS. The LS attribute is specific to each pair of origin-destination (OD). It represents the expected link flow between each OD and is generated from the RL model with chosen parameter values. The two NRL models include link-specific scale parameters  $\mu_k$  which are a function of a single parameter  $\beta_{\text{scale}}$ .

#### 3.5.2 Estimation results

We first make some remarks regarding the estimation algorithm and computational times. As described in Fosgerau et al. (2013) and Mai et al. (2015), the optimization algorithm is a basic trust-region algorithm which uses the BFGS Hessian approximation for the RL model, and the BHHH approximation for the NRL. The systems of equations in (3.8) are computed using MATLAB's solver for sparse systems. The models are estimated with MATLAB 2016 based on the implementation of Mai et al. (2015). We have used an Intel(R) Xeon(R) X5675 @ 3.07GHz machine. The machine has a multi-core processor but we only used one processor to estimate the models. As expected, the computational time required to estimate

<sup>1.</sup> Code distributed on github: https://github.com/maitien86/RecursiveLogit.Bike

| Attribute                                 | Description  |
|---|--|
| Length                                    | Link length (1/1000 feet)  |
| Link Constant                             | A constant equal to one for each link intended to penalize paths with many crossings.            |
| Length · Upslope                          | Interaction between link length and average upslope $> 4\%$ .                                    |
| Length · Medium Traffic                   | Interaction between link length and medium traffic volume (between 8000 and 20000 vehicles/day). |
| $Length \cdot Heavy \ Traffic$            | Interaction between link length and heavy traffic volume (greater than 20000 vehicles/day).      |
| $Length \cdot RMUP$                       | Interaction between link length and regional multi-use path.                                     |
| Length · Bike Boulevard                   | Interaction between link length and bike boulevard.  |
| $Length \cdot Bike Lane$                  | Interaction between link length and bike lane.   |
| Bridge                                    | Presence of bridge   |
| $Bridge \cdot Bike Fac$                   | Interaction between presence of bridge and bike facilities.                                      |
| No Turn                                   | Straight direction of travel (no turn $\pm 5^{\circ}$ )  |
| No Turn $\cdot$ Crossroad                 | Straight direction of travel at a crossroad  |
| Left Turn · Crossroad ·                   | Left turn through medium traffic at crossroad without traffic sig-                               |
| Medium Traffic                            | nal (at an angle between 60° and 179°)   |
| Left Turn $\cdot$ Crossroad $\cdot$ Heavy | Left turn through heavy traffic at crossroad without traffic signal                              |
| Traffic                                   | (at an angle between $60^{\circ}$ and $179^{\circ}$ ).   |

**Table 3.1** – Description of attribute variables

the NRL models (about 15 days) is much greater than that of the RL models (1h without LS using the decomposition method, and 43h with LS).

Tables 3.2 and 3.3 display the estimation results for all four model structures and for the chosen utility specification. All parameter estimates are significantly different from zero and have their expected sign. The models with the LS attribute have a significantly better in-sample fit than those without, and the NRL model has a significantly better in-sample fit than the RL model. With the LS attribute, the NRL model is the best of all four, but without it is outperformed by the RL model with LS. The ratio between parameter estimates remain similar for the RL and NRL models. Therefore, the interpretation of parameters is consistent with all models considered. In the following discussion, we focus on the estimates of the RL model without LS.

Consistent with the expectation that cyclists are highly put off by long distances, the link length parameter assumes a negative value. This was found to be the attribute dominating the choices of cyclists by Menghini et al. (2010) and an important factor in virtually all bike route choice research. However, as described in Section 3.5.1, this parameter represents only part of a total length parameter, the magnitude of which varies across links depending on other relevant characteristics influencing length perception.

| Model  |             | RL             |        |             | RL-LS          |        |
|--|-------------|----------------|--------|-------------|----------------|--------|
| Attribute  | $\hat{eta}$ | $\hat{\sigma}$ | t-test | $\hat{eta}$ | $\hat{\sigma}$ | t-test |
| Length   | -2.25       | 0.13           | -17.31 | -2.28       | 0.14           | -16.28 |
| Link Constant                                      | -1.61       | 0.02           | -80.50 | -1.60       | 0.02           | -80.00 |
| Length · Upslope                                   | -3.24       | 0.55           | -5.89  | -3.15       | 0.50           | -6.30  |
| Length · Medium Traffic                            | -0.81       | 0.08           | -10.13 | -0.82       | 0.08           | -10.25 |
| Length · Heavy Traffic                             | -1.01       | 0.10           | -10.10 | -1.02       | 0.08           | -12.75 |
| Length · Bike Boulevard                            | 0.74        | 0.08           | 9.25   | 0.76        | 0.07           | 10.86  |
| $Length \cdot RMUP$                                | 1.80        | 0.07           | 25.71  | 1.81        | 0.07           | 25.86  |
| Length $\cdot$ Bike Lane                           | 0.92        | 0.06           | 15.33  | 0.87        | 0.06           | 14.50  |
| Bridge   | -5.41       | 0.97           | -5.58  | -4.56       | 1.00           | -4.56  |
| Bridge · Bike Fac.                                 | 2.83        | 0.52           | 5.44   | 1.99        | 0.56           | 3.56   |
| No Turn  | 1.37        | 0.03           | 45.67  | 1.33        | 0.03           | 44.33  |
| No Turn $\cdot$ Crossroad                          | -0.28       | 0.03           | -9.33  | -0.29       | 0.03           | -9.67  |
| Left Turn $\cdot$ Crossroad $\cdot$ Medium Traffic | -0.28       | 0.09           | 3.11   | -0.33       | 0.09           | 3.67   |
| Left Turn $\cdot$ Crossroad $\cdot$ Heavy Traffic  | -1.84       | 0.33           | -5.58  | -1.86       | 0.34           | -5.47  |
| Link Size  | _           | _              | _      | -0.24       | 0.03           | -8.00  |
| Log likelihood at $\hat{\beta}$                    | -12383      |                |        | -12202      |                |        |

Table 3.2 – Estimation results: RL model

| Model  |             | NRL            |        |             | NRL-LS         |        |  |
|--|-------------|----------------|--------|-------------|----------------|--------|--|
| Attribute  | $\hat{eta}$ | $\hat{\sigma}$ | t-test | $\hat{eta}$ | $\hat{\sigma}$ | t-test |  |
| Length   | -1.48       | 0.14           | -10.57 | -1.54       | 0.17           | -9.06  |  |
| Link Constant                                      | -1.07       | 0.05           | -21.40 | -1.09       | 0.06           | -18.17 |  |
| Length · Upslope                                   | -2.97       | 0.55           | -5.40  | -3.05       | 0.55           | -5.55  |  |
| Length · Medium Traffic                            | -0.53       | 0.07           | -7.57  | -0.59       | 0.08           | -7.38  |  |
| Length · Heavy Traffic                             | -0.66       | 0.08           | -8.25  | -0.70       | 0.08           | -8.75  |  |
| Length · Bike Boulevard                            | 0.51        | 0.06           | 8.50   | 0.46        | 0.06           | 7.67   |  |
| $\operatorname{Length} \cdot \operatorname{RMUP}$  | 1.15        | 0.09           | 12.78  | 1.18        | 0.10           | 11.80  |  |
| Length · Bike Lane                                 | 0.62        | 0.06           | 10.33  | 0.60        | 0.06           | 10.00  |  |
| Bridge   | -2.83       | 0.56           | -5.05  | -2.08       | 0.47           | -4.43  |  |
| Bridge · Bike Fac.                                 | 0.86        | 0.29           | 2.97   | 0.19        | 0.33           | -0.58  |  |
| No Turn  | 0.89        | 0.05           | 17.80  | 0.88        | 0.06           | 14.67  |  |
| No Turn $\cdot$ Crossroad                          | -0.14       | 0.02           | -7.00  | -0.15       | 0.02           | -7.50  |  |
| Left Turn $\cdot$ Crossroad $\cdot$ Medium Traffic | -0.05       | 0.05           | 1.00   | 0.03        | 0.05           | 0.60   |  |
| Left Turn · Crossroad · Heavy Traffic              | -1.56       | 0.40           | -3.90  | -1.28       | 0.27           | -4.74  |  |
| Scale  | -0.11       | 0.01           | -11.00 | -0.11       | 0.02           | -5.50  |  |
| Link Size  | _           | _              | _      | -0.16       | 0.02           | -8.00  |  |
| Log likelihood at $\hat{\beta}$                    | -12325      |                |        | -12143      |                |        |  |

 ${\bf Table~3.3}-{\rm Estimation~results:~NRL~model}$ 

Characteristics related to slope were included in the form of a dummy variable interacting with link length. We chose a threshold of an average link upslope higher than 4%. The negative value of the slope parameter, about 1.5 times that of the length parameter, shows that a large upslope considerably increases the magnitude of the total length parameter. We tested a higher threshold of 6% in addition to a 4-6% threshold, but the difference between the estimates was not significant. A 2-4% threshold was also investigated but the estimate was not significantly different from 0. The most similar findings are those of Broach et al. (2012) whom included as an attribute the proportion of route length within three categories of average slope (2-4%, 4-6%, 6% and more). They found this specification to perform better than the most common alternatives, such as maximum or average slope of the path, found in Hood et al. (2011) and Menghini et al. (2010).

Traffic volumes also affect the way cyclists perceive distances, but less so than slope. Medium (between 8000 and 20000 vehicles/day) and heavy (more than 20000 vehicles/day) traffic are both associated with negative parameters, however, not significantly different. While the value of the total length parameter is -2.25 on a segment with low traffic, assuming no other link characteristics contribute to its value, it becomes -3.06 on a segment with medium traffic volume (and similarly -3.26 with heavy traffic volume). Thus the model did not identify a significant difference between medium and heavy traffic. The ratio between both values indicates that cycling 1 mile surrounded by heavy traffic would be perceived equivalent to cycling 1.45 miles on a low traffic road.

Bike facilities are all associated with a positively signed parameter, indicating that cyclists are willing to travel greater distances to use them. The regional multiuse path is the bike facility with the largest parameter value. Bike lanes and bike boulevards both have a significantly smaller parameter estimate, consistently with the results of Broach et al. (2012). On a segment with a bike facility, the value of the total length parameter increases and is equal to -1.51 if the facility is a bike boulevard, -1.33 for a bike lane and -0.45 for a regional multi-use path. Thus, traveling on a street with a bike boulevard is equivalent to a reduction in distance of 33%. This becomes a reduction of 41% for the bike lane and of 80% for the regional multi-use path. The value placed on separate multi-use paths is surprisingly high, and suggests that cyclists are willing to travel on roads more than 4 times longer to use them. This result may be due to the relatively small number of observations

available, many of which use regional multi-use paths. We also note that the bike lane parameter is of a similar magnitude as the ones for traffic volume, which have an opposite sign. This suggests that the presence of a bike lane counterbalances the negative impact of heavy traffic on the utility of a road, however it has no residual value. This last observation supports the conclusions of Broach et al. (2012), who also stated that bike lanes are no more and no less attractive than a basic low traffic street.

A bridge is in general an unattractive feature of a path for a cyclist, as the negative value of the estimate shows. However, if the bridge has a separated bike facility, the positive value associated to the bike facility in that case outweighs the negative one, and the sum of both parameters is not significantly different from zero, meaning that in this case bridges are not penalized compared to other links. The link constant parameter has a negative sign, meaning that paths with many crossings are less attractive to cyclists.

The coefficient associated to a straight direction of travel is significantly positive, probably because many turns may cause detours or result in an intricate path. Cyclists thus have a preference for simple routes. However, the model suggests that at a crossroad (instead of another type of intersection with fewer outgoing links) the incentive for going straight is slightly lowered. In this specification, left and right turns at crossroads do not contribute to the utility, while being still less attractive relative to a straight route. We expect in contrast difficult left turns which cause delays to be especially inconvenient to cyclists. The model shows indeed that left turns through heavy traffic at crossroads without signals are greatly penalized. Cyclists are also sensitive to left turns through medium traffic, but less so.

#### 3.5.3 Cross-validation

In this section, we compare the out-of-sample fit of the four models with a cross-validation approach, in order to check for overfitting. The observations are repeatedly and randomly split into a training set (80% of all observations) and a test set (20%), until 20 different training sets and matching test sets have been generated. The performance of the models is evaluated by computing the log-likelihood loss on the test sets, after having estimated the models on the training

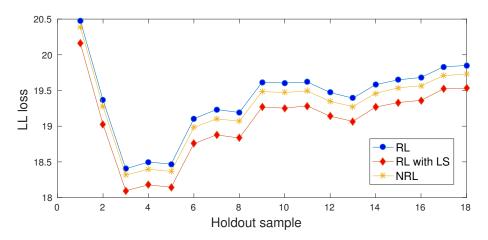


Figure 3.2 – Moving average of  $err_i$  across samples i = 1, ..., 18

sets. The log-likelihood loss of sample i is defined as:

$$err_i = -\frac{1}{|S_i|} \sum_{\sigma \in S_i} \ln P(\sigma, \hat{\beta}_i),$$

where  $S_i$  denotes test set i, and  $\hat{\beta}_i$  the vector of estimated parameters on training set i. Thus, the lowest the loss is, the best a model performs.

We performed the cross-validation on all four models. However, there were too few observations in the training set for the estimation algorithm of the NRL model with LS to converge and it was excluded from the comparison. The estimation algorithm for the NRL model also did not converge for two training sets, therefore we compare the RL, the RL with LS and the NRL on the 18 remaining sample sets. Figure 5.5 plots the moving average of  $err_i$  across sample sets i=1,...,18. The cross-validation is in line with in-sample fit and confirms that the RL model with LS performs best of the three models, followed by the NRL model, and that the RL model has the highest log-likelihood loss.

# 3.6 Prediction

In this section, we extend the analysis beyond the interpretation of model parameters. We address the general issue of applying bike route choice models for prediction. In a policy analysis perspective, important applications of the model are i) predicting link-level bike volume and ii) measuring cyclist specific accessibility.

We aim with this section to contrast the path-based approach to prediction with that of the link-based RL model. In both cases, we review the prediction methods provided by all models. We enlighten the methodological issues associated with path-based models, then explain how the RL model overcomes them. For link flows, we provide in addition numerical results which highlight the potential gains of time associated to the RL model.

#### 3.6.1 Link flows

We start by stating that in the following, the methods we discuss are based on the assumption of an uncongested network. This means that route choice probabilities are independent of the amount of flow on each link, which is reasonable in the case of many bike networks, in particular in North America. Link-level traffic volume is predicted from route choice models by distributing a given travel demand between each OD pair on the network. We assume that an OD matrix characterizing this demand exists. The recursive models offer two ways to distribute demand in the network according to an estimated model: by simulation or by computing link flows as solutions to systems of linear equations. Both ways make use of destination specific link choice probabilities  $P^d(a|k; \widehat{\beta})$  given by (3.3) but with the parameter estimates  $\widehat{\beta}$ . We denote  $\mathbf{P}^d$  the matrix with elements  $P^d(a|k; \widehat{\beta})$ .

The first way of distributing demand consists of simulating path choices for each origin destination pair by sampling from  $\mathbf{P}^d$ . There are different simulation methods available with different computational cost. For the sake of illustration, we use a simple approach in this paper that consists of drawing the same number r of paths for each OD pair. The path choice probabilities are known for each of these paths (3.6) and we normalize them so that the sum over the r simulated paths for each OD equals one. We then distribute the demand given by the OD matrix according to the path probabilities. While this simulation approach may at a first glance seem similar to the classic way of distributing demand according

to a path-based model, there is an important difference. Path-based models make use of choice sets that are arbitrarily generated while the recursive model allows to simulate according to the estimated model  $\mathbf{P}^d$  without generating any choice sets.

The second way to distribute demand in the network is grounded in the link-based structure of the RL model and was proposed by Baillon and Cominetti (2008). It allows to compute link flows without resorting to simulation. The method consists in solving a system of linear equations for each destination d in the network, and to sum the resulting link flows over all destinations. Let us denote the demand originating from each link a to destination link d as the vector  $\mathbf{G}^d$ , the vector of destination-specific link flows as  $\mathbf{F}^d$ . Then, the vector of expected link flows  $\mathbf{F}^d$  is obtained by solving

$$(\mathbf{I} - \mathbf{P}^{dT})\mathbf{F}^d = \mathbf{G}^d, \tag{3.11}$$

and the vector of link flows  $\mathbf{F}$  resulting from demand with multiple destinations is equal to  $\mathbf{F} = \sum_d \mathbf{F}^d$ .

To the best of our knowledge, this second method has not been used with an estimated model and a real network before. In the following we compare predictions generated with both methods. The objective is to assess the potential gain in computational time of avoiding simulation.

We applied both method to predict link flows in the Eugene bike network with the RL model. Since we assumed an uncongested network, we did not iterate to find a traffic equilibrium condition. The flows were predicted for a given demand matrix consisting of 666 origins and destinations in the Eugene bike network which was obtained from a mode choice model. Figure 3.3 plots the amount of flow on each link according to each prediction method. The figure indicates that both methods yield very similar results, even with a relatively small number of paths sampled in the choice set. The average flow on each link amounts to 55.36 according to the solution of (3.11). The average difference of flow on each link when comparing these results with simulated link flows is 3.03 when 10 draws are used, and 2.95 when 20 draws are used. We conclude that it would take a very large number of draws for the simulated flows to converge to the solution of the system of equations, nevertheless the difference is very small. Furthermore, we note that the average difference is inflated by a few links with a very large amount of flow, while for the great majority of links this difference is comprised in the [-4; 4] interval and close to 0, as seen in Figure 3.4.

A difference between both methods is that solving the linear system of equations assumes that there is a non-zero probability of flow on each link. As a result, the amount of flow on each link is strictly positive (although negligible for many links). On the contrary, when link flows are simulated, there is only flow on links of paths that were sampled. When 10 draws were used, we found that 30,205 links out of 43,050 had non-zero flow, and this became 31,039 when 20 draws were used. On the other hand, by solving the system of equations, we obtain slightly higher flows: 27,077 links have a flow higher than 1, while this amounts to 25,583 (25,760) links for simulation with 10 (20) draws.

In terms of computational time, solving the system of linear equations for all destinations requires 6 minutes, while simulating link flows via sampling took about 25 hours for r=10, and about 70 hours for r=20 (non-parallelized MATLAB code). Even though the code has not been optimized for simulation, the results illustrate the potential gain associated with solving systems of linear equations as opposed to simulation. Moreover, this approach has the advantage of producing deterministic link flows and hence overcomes the issues associated with simulation bias.

# 3.6.2 Accessibility measure

Accessibility is a widely studied notion in transportation, and in this context it can be defined as information evaluating the attractiveness of a network (regardless of activity participation, which is encompassed in a more general definition, e.g. Bhat et al., 2000). Accessibility measures are useful in travel demand modeling, as they provide input to higher-level models, such as mode choice, household location choice or car ownership models. These measures are often OD-specific, in which case they characterize the level of service of a network when traveling from an origin O to a destination D.

In particular, bike accessibility encapsulates information regarding the suitability of the network for cycling, and has been also denoted bikeability in other works (Lowry et al., 2012). According to Hood et al. (2011), current bike accessibility measures used in higher-level models are more predictive of automobile travel than cycling, while Mesbah and Nassir (2014) asserts that traditional measures are only based on shortest path computations between OD pairs and thus unsuitable for

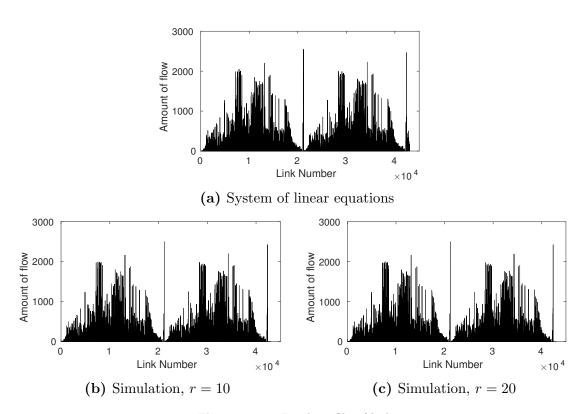


Figure 3.3 – Load profile of links

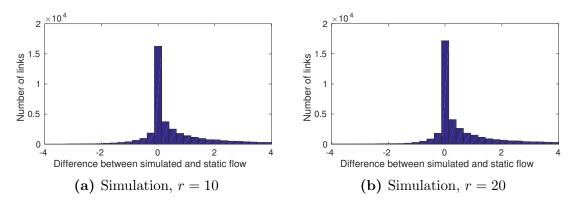


Figure 3.4 – Histogram of link flow difference

bike accessibility. As a result, recent works now recognize the importance of improving two aspects of bike accessibility measurement, first to incorporate route choice preferences of cyclists, and secondly to capture the diversity of suboptimal available routes instead of the utility of the single best path.

Deriving an accessibility measure from a bike route choice model appropriately

fits these two purposes and was recently investigated by Nassir et al. (2014). This idea is not new and originates from the general concept of deriving an accessibility measure from a random utility model, introduced by Ben-Akiva and Lerman (1979). They defined accessibility as the logsum

$$E(\max_{i \in C_n} u_i) = \mu \log \sum_{i \in C_n} e^{\frac{1}{\mu} v_i}.$$
 (3.12)

This measure guarantees that accessibility does not decrease if the systematic utility of any alternative in the choice set increases, as proven by Ben-Akiva and Lerman (1979). In other words, if an alternative becomes more attractive, for example, as a result of infrastructure enhancements, the accessibility measure mirrors this improvement.

However, with a route choice random utility model based on paths, we argue that this important property no longer holds due to the intractable nature of the choice set  $C_n$  in (3.12). Whether it is assumed that the true choice set consists of all feasible paths or that only a subset of alternatives are in fact considered does not affect the prediction method. In each case, it becomes necessary to define a restricted set of paths in order to evaluate Equation (3.12). Similarly to the link flow problem, in the absence of a clear methodology any choice set could be selected and the ensuing accessibility measures vary.

It is straightforward to explain why this implies that the property of monotonicity with respect to the systematic utility no longer holds. Indeed, the sampled choice set  $C_n$  in (3.12) needs to be updated after network changes in order to account for potential newly attractive paths that were not previously generated. Paths that were sampled in the first choice set may not appear in the second one. However if accessibility after network changes is computed based on a different choice set  $\tilde{C}_n$ , there is no basis for comparison. As such there can be no guarantee of monotonicity. This has given rise to what Nassir et al. (2014) denote the Valencia paradox. This paradox was observed when the predicted accessibility counter-intuitively decreased for some origin-destination pairs after network improvements and is tangible proof of the problematic consequences of this limitation.

In essence, we argue that this paradox is an artifact inherent to path-based models and arises from the necessity to explicitly generate a restricted choice set for prediction. The RL model allows to predict accessibility according to the true model with the hypothesis of an unrestricted choice set. The ensuing measure prevents paradoxical predictions. In order to illustrate this assertion, we first derive the accessibility measure resulting from the RL model.

In the RL model, the accessibility of an origin-destination pair as defined previously by the logsum formula is simply equivalent to the value function to destination d at the origin link k (Fosgerau et al., 2013):

$$V^{d}(k) = E\left[\max_{a \in A(k)} \left(v(a|k) + V^{d}(a) + \mu\epsilon(a)\right)\right] = \mu \ln \sum_{a \in A(k)} e^{\frac{1}{\mu}(v(a|k) + V^{d}(a))}.$$
 (3.13)

The value function from an origin to a destination encompasses the expected maximum utility of all paths connecting them. This becomes clear when recalling that the RL model is equivalent to a path-based multinomial logit model over the set of all possible paths (see Section 3.3). This property is what allows the value function to be rewritten in an equivalent non-recursive form:

$$V^{d}(k) = \mu \ln \sum_{\sigma \in \mathcal{U}} e^{\frac{1}{\mu}v(\sigma)}$$
(3.14)

where  $\mathcal{U}$  is the set of all paths between origin k and destination d, and  $v(\sigma)$  is the deterministic utility component of path  $\sigma$ . It is then apparent that the value functions of the RL model are of the form in (3.12), and consequently they retain the property of monotonicity with respect to the deterministic part of utilities. The fundamental point here is that, to the difference of path-based models, the value functions of the RL model can be conveniently computed by solving systems of linear equations and do not rely on enumerating the set  $\mathcal{U}$ .

Naturally, accessibility in (3.14) could also be approximated with Monte Carlo techniques by generating a subset of paths  $C_n$  from  $\mathcal{U}$ , just as link flows may be predicted by sampling from the true model. Intuitively, as more paths are sampled and added to  $C_n$ , the value obtained converges towards an asymptotic value which is given by the value function. Finally, this means that path-based models can only provide an approximation of accessibility based on the entire network. Whether it is judicious from a behavioral perspective to assume that any feasible path should enter the choice set is yet another much-debated question. Nevertheless, this work, along with others (e.g. Horowitz and Louviere, 1995), provide evidence that for mathematical reasons, it is pragmatic to do so.

# 3.7 Conclusion

We outlined the development of several versions of a bike route choice model based on the recursive logit framework of Fosgerau et al. (2013), with and without relaxing the IIA property through nesting, as proposed by Mai et al. (2015). We estimated the models on 648 GPS-based observations of paths collected in Eugene, Oregon, and matched to a network of 16'352 nodes and 42'384 links. Our utility specification successfully incorporates fundamental attributes impacting cyclists' route choice while respecting link additivity. To do so, we let inherently non-link additives such as slope interact with link length.

Estimation results emphasize the sensibility of cyclists to distance, traffic volume, slope, crossings and presence of bike facilities. The preferred facilities are separate multi-use paths, followed by bike lanes and then by bike boulevards. Our results confirm the findings of previous studies, in particular the strong preference for separate paths and the small residual value of bike lanes after compensating the negative effect of high traffic volumes, as highlighted by Broach et al. (2012). Our model did not identify as many distinct categories of slope or traffic volume as the one of Broach et al. (2012), distinguishing only between average slope above or below 4%, and traffic volume above or below 8000 vehicles per day.

The RL model is fast to estimate when applying the decomposition method of Mai et al. (2016). However, the method is not applicable when including a link size attribute or when relaxing the IIA property via nesting. Since models accounting for correlated utilities performed better than the simple RL models, a trade-off has to be made between accuracy and computational time.

In addition to analyzing cyclists' route choice preferences, this paper makes valuable contributions, both theoretical and empirical, in the field of prediction. We experimented two methods to predict traffic flows, simulation and solving a system of linear equations (Baillon and Cominetti, 2008). We find that solving the system requires shorter computational time than sampling paths while resulting in similar link flows. We also highlighted a theoretical property of the RL model, namely that its value function corresponds to the accessibility measure obtained asymptotically from a path-based model, if the sampled choice set grows towards including all paths. The implication of this result is that the RL model yields an accessibility measure which is monotonous with respect to deterministic utilities,

and can be consistently incorporated in higher-level models, such as mode choice models. Thus, the result discussed at length in Nassir et al. (2014) and dubbed a paradox is an artifact of the hypothesis of a restricted choice set.

# Multi-modal route choice modeling in a dynamic schedule-based transit network

# Prologue

#### Context

The previous chapter applied the recursive logit framework to GPS-based trajectories of cyclists. This short chapter is an extension of the previous work to model path choice behavior for public transportation (PT) modes. The additional challenge posed by transit networks is that individuals may transfer between different lines of public transport services, the availability of which depends on time. In general, studies on transit path choice may make the assumption that transit lines run according to a given schedule for the day, or assume a constant headway across time. In this work, we have available data on the exact schedule of the full transit network of the city of Zürich, therefore we chose the schedule-based approach.

#### Article Details

This work was jointly performed with Emma Frejinger and Kay Axhausen, and presented at the 15th International Conference on Travel Behavior Research, Santa Barbara, California, July 15-20, 2018.

#### Related Work

A related article was published as:

De Freitas, L. M., Becker, H., Zimmermann, M., Axhausen, K. W. (2019). Modelling intermodal travel in Switzerland: A recursive logit approach. Transportation Research Part A: Policy and Practice, 119, 200-213.

In that paper, the "frequency-based" approach is used to model transit route choice, i.e., a constant headway is assumed. This allows to consider only a static version of the PT network, thus limiting the size of the problem. On the other hand, information on trade-offs made by individuals regarding the waiting/transfer times of different itineraries is less precise, as the actual wait depends on the time at which the trip is made.

#### 4.1 Introduction

Route choice behavior has predominantly been analyzed from the angle of a single mode, most often the car. Considering route choice in the broader context of multi-modal networks yet opens the way to more complex policy analysis and wider applications. In particular, multi-modal traffic assignment models (Lo et al., 2004) and advanced traveler information systems (Zhang et al., 2011) can analyze the effect of fares on congestion or answer routing queries involving several modes. Their mechanisms rely on sound knowledge of traveler's preferences for attributes of multi-modal trips, such as travel time, waiting time or number of transfers.

On many levels, the behavior of travelers in multi-modal networks is more complex to model than that of car drivers. Traditional models of route choice analysis in traffic networks are not directly applicable in this context. To represent a multi-modal trip as a path, it is necessary to combine the networks of available modes via transfer, waiting and/or access links into a so-called supernetwork (Sheffi, 1985). An additional difficulty is the limited availability of public transport services. Indeed transit lines are subject to a frequency or a schedule, which imposes constraints on the route choice and calls for an appropriate treatment of time. To get around this problem, some studies have attempted to simplify the network representation or the level of detail, focusing on schematic networks (e.g. Raveau et al., 2011). Another challenge is related to the definition of alternatives to the observed path. Not only is it more complex to generate realistic path alternatives in a multi-modal network, but there may be a bias in parameter estimates induced by the selection of a restricted choice set (Frejinger et al., 2009).

This paper tackles these challenges by applying the recursive logit to model the choice of transit modes and route in a real network. The model is based on the assumption of a full available schedule. The approach presents numerous advantages. First, route choice preferences can be consistently estimated without generating choice sets of paths. Second, the model can be used to predict fast and accurately path choices in real network by sampling from estimated link choice probabilities. Although the network is much larger than previous applications of the RL model with over 1 million links, we obtain reasonable computational times. Third, the approach allows to include all transit services without restriction in one large-scale network, providing the possibility to estimate realistic rates of substitution between different attributes.

## 4.2 Literature review

There is a large body of literature which reports route choice preferences of travelers in a multi-modal network, most of which are based on stated preference (SP) data (e.g. Vrtic et al., 2010; Arentze and Molin, 2013; Fosgerau et al., 2007). Such studies are simpler to implement as the modeler can entirely define the choice situation and its alternatives according to convenience. However SP data has notable disadvantages, in particular the potential disparity between answers given to hypothetical choice situations and behavior exhibited in reality. In addition, although such studies can provide an interpretation of estimated parameters in terms of policy implications, the models cannot directly be applied to predict route choices in a real network.

Route choice models based on revealed preference (RP) data are congruent with observed behavior in actual choice situations, but face other challenges. The modeler must define a restricted set of path choice alternatives for each observation, as the many possibilities to connect an origin-destination pair are too numerous to enumerate in a real network. In multi-modal networks, there is not only a large number of paths confined to each single mode, but also nearly unlimited transfer possibilities as well as different runs of parallel lines, resulting in a very large number of alternatives. Most studies avoid dealing with the full inherent complexity of the problem. For example, Bovy and Hoogendoorn-Lanser (2005) consider a multi-modal interurban corridor between two Dutch cities which is a schematic network of small size, where some modes only serve as access or egress

modes to train. Raveau et al. (2011) restricts the number of modes by considering only the Santiago metro network, a schematic public transport network with no time dimension.

While other studies examine larger and more realistic networks with several modes (e.g. Eluru et al., 2012; Anderson et al., 2014, in Montreal and Copenhagen respectively), there also exists limitations regarding how the issue of choice sets is addressed. In Eluru et al. (2012) the observed trip is compared only with few alternatives (between one and six) generated via Google Maps. Anderson et al. (2014) and Bovy and Hoogendoorn-Lanser (2005) generate more alternatives using respectively doubly stochastic and constraint enumeration algorithms, however treat the generated choice sets as the actual alternatives. This implies that the validity of estimation results is questionable due to the bias induced by choice set selection (Frejinger et al., 2009). Finally we also note that there is ongoing research from Montini et al. (2016) to estimate mode and route choice models from a sample of GPS traces collected in Zürich.

The current study fills a gap in the literature by estimating a multimodal transit route choice model with unrestricted choice sets based on RP data collected in a complex network. The approach has the advantage of yielding consistent estimates and can also be used for prediction in a real network without generating choice sets of paths.

# 4.3 Model

We assume that the transit system can be described by a static and deterministic network representing the transit lines of each mode, and a timetable which lists the arrival and departure time of each run at each station for a whole day. The complete set of available transit services can be represented as a time-expanded network  $G = (\mathcal{A}, \mathcal{V})$  in which each node  $v \in \mathcal{V}$  corresponds to a transit stop location l and a time t, and links move through time and/or space. Links belong to one of the following categories:

**Transit arc:** The arc corresponds to an in-vehicle trip on a transit line (e.g. a bus or a metro line) between two consecutive stations at a specific time.

Waiting arc: The arc corresponds to waiting at the same station for the arrival of another vehicle.

Walking arc: The arc corresponds to a walking trip between two geographically close stations.

Contrarily to other time-expanded networks (e.g. Hamdouch and Lawphongpanich, 2008), we do not discretize the day into equally spaced points in time. Instead, time is continuous and the nodes of the static network are expanded according to the schedule. In other words, the nodes v = (l, t) in the time-expanded network are defined only for times t corresponding to the arrival or departure of a transit line. This network representation is similar to what has been called a diachronic graph in the literature (Nuzzolo et al., 2012) and it is at the core of several assignment models.

The network must be extended to include absorbing links without successors to represent destinations. In the model, we assume that travelers have a fixed departure time and must arrive to the destination stop l within a certain time interval T. To represent the destination of an individual traveling in this network, we must define absorbing links outgoing from node (l,t) for all valid times t within the time window T for arrival. Thus in this model the destination of an individual n is represented as a set of absorbing links  $D_n$ .

The RL model can be used for the multimodal transit route choice problem by defining states and actions as links  $k, a \in \mathcal{A}$  in the dynamic network previously defined. From a state k, the traveler reaches the next state by choosing an action a in the set of outgoing links A(k) in order to maximize instantaneous link utility  $u(a|k) = v(a|k) + \mu \epsilon(a)$  and expected maximum utility to destination  $V_n(a)$ , which is the solution of a dynamic programming problem given by the Bellman equation. The value function  $V_n$  is defined for the set of links  $D_n$  corresponding to the arrival stop and time window of individual n and is given as follows

$$V_n(k) = \begin{cases} \mu \ln \sum_{a \in A(k)} e^{\frac{1}{\mu} v_n(a|k) + V_n(a)} & \forall k \in \mathcal{A} \\ 0 & \forall k \in D_n \end{cases}$$
(4.1)

The random terms  $\epsilon(a)$  are assumed i.i.d. Gumbel with scale parameter  $\mu$ , resulting in the multinomial logit model's conditional probability of choosing action

a in state k:

$$P_n(a|k) = \frac{e^{u_n(a|k) + V_n(a)}}{\sum_{a' \in A(k)} e^{u_n(a'|k) + V_n(a')}}$$
(4.2)

The model can be estimated using an approach similar to the nested fixed point algorithm and link choice probabilities in (5.3) can be used to predict path choices link by link without generating any choice sets.

#### 4.4 Data

We use a real network in the city of Zürich and we estimate the model based on GPS trajectories of travelers collected in that network by Montini et al. (2013). There are 5'276 stop locations, 724 transit lines and 40'031 runs over a day, for which the exact arrival and departure time at each station along the line is known. Some lines have very frequent services while others are only available at sparse times. Each transit lines corresponds to one of the 6 available modes (bus, train, tram, boat, taxi, cable car). Representing the transit service for one day with a time-expanded network requires over one million links.

We have 302 observations of trips in the transit network. The observations are described as a sequence of stops, line IDs, and a departure time. Since we do not have access to arrival and departure time at each stop, we reconstruct the trip assuming that the first available vehicle matching the observed stops was taken (i.e. individuals did not wait for a subsequent run of the same line). This is a realistic assumption if the observed trips did not take place in a congested network. We obtain a sequence of transit, waiting and/or transfer links in the time-expanded network.

# 4.5 Results

We note that link utilities in the RL model must be defined as a function of additive link attributes (Fosgerau et al., 2013). Therefore, dummy variables for link

| Model   | RL          |        |
|---|-------------|--------|
| Link attribute                                | $\hat{eta}$ | t-test |
| In-vehicle time [1/1000s]                     | -12.57      | -5.66  |
| Waiting time $[1/1000s]$                      | -8.57       | -9.82  |
| Transfer dummy                                | -5.67       | -5.84  |
| Link constant                                 | -0.10       | -4.16  |
| Tram dummy $\cdot$ in-vehicle time [1/1000s]  | -6.24       | -3.42  |
| Bus dummy $\cdot$ in-vehicle time $[1/1000s]$ | -11.91      | -5.41  |
| Log likelihood at $\hat{\beta}$               | -783.87     |        |

**Table 4.1** – Estimation results

types cannot be directly incorporated in the utility function, since their sum over links in a path cannot be interpreted as a measure of path utility. As an example, the number of tram links contained in a given path is not representative of how much the tram was used, since some links have longer travel time than others. Thus in this model we interact dummy variables for the mode of a link with the travel time of that link.

We retain a model specification with 6 attributes, consisting of the in-vehicle time, the waiting time, a dummy for a transfer between two stations, a link constant, and the in-vehicle time attribute interacted with a dummy for the tram and bus modes. Table 4.1 displays the estimations results of the chosen utility specification. Following Zimmermann et al. (2017), we note that we may interpret the results as letting the value of the travel time coefficient depend on the mode. Indeed, by adding the in-vehicle time coefficient with each interaction coefficient, we obtain that the value of travel time is -18.81 on a tram and -24.48 on a bus. We note that the observed trips only used the tram, bus and train modes, thus the travel time coefficient on a train would be -12.57.

The model is expensive to estimate, since the state space is large and the value function needs to be solved for each individual. In order to speed up computational time, the value functions are only solved for a subset of links in the time-dependent network. More precisely, for an individual n with observed departure time  $t_o$  and latest possible arrival time  $t_d$ , we only compute the value function for links (l,t) with  $t \in [t_o, t_d]$ . As a result, the linear systems which need to be solved to obtain  $V_n$  for each observation n have a maximum size of 255,369 for this dataset. The total estimation time is then less than a day.

# Capturing correlation with a mixed recursive logit model for activity-travel scheduling

# Prologue

#### Context

Compared to the previous chapters, where the recursive choice modeling framework was applied in physical transportation networks, we consider in this article a much larger and abstract supernetwork. As in Chapter 4, the network is expanded in time; however it considers other additional dimensions, in order to link individuals' choice of daily trips to their intentions of pursuing out of home activities. In the literature on so-called activity-based travel demand modeling, representing the decision of what activities and travels to schedule during a day as path choice in a supernetwork is a relatively novel perspective, first conceptualized by Karlström (2005). Blom Västberg et al. (2016) provided the first implementation of such a model, and this chapter introduces an extension of the latter which improves the model's predictions by capturing correlation across alternatives.

#### Contributions

The contribution of this article is mostly empirical. This paper is the first publication to apply the recursive choice modeling framework to model jointly the interrelated decisions which compose the activity-scheduling problem, i.e., choice of mode, destination, departure time and activity participation. The article shows that it is possible to capture complex correlation patterns across multi-dimensional alternatives and to estimate the model in reasonable time despite its complex structure and the large network size.

#### **Article Details**

This work was presented at the Joint International Meeting of the Canadian Operational Research Society (CORS) and the Institute for Operations Research and the Management Sciences (INFORMS), and resulted in a paper published in Transportation Research Part C:

Capturing correlation with a mixed recursive logit model for activity-travel scheduling. Maëlle Zimmermann, Oskar Blom Västberg, Emma Frejinger, Anders Karlström. *Transportation Research Part C: Emerging Technologies*, 93, pp. 273-291.

#### Author contributions

The initial work on which this article is based was performed by Oscar Blom Västberg and Anders Karlström. The idea of relaxing the model's IIA property was Anders Karlström's. The subsequent experiments were performed by me with the collaboration of Oscar Blom Västberg, and the writing of the article is my own.

# 5.1 Introduction

Activity-based travel demand analysis consists in jointly modeling choices concerning transportation and activity participation, based on the assumption that individuals undertake trips with the intention to pursue activities. At the core of activity-based modeling is the idea that trips result from scheduling decisions within a continuous time interval: individuals dispose of a limited amount of time (often, a day) to allocate to activities and subsequent trips (Pinjari and Bhat, 2011).

Activity-based travel demand has been the subject of various studies, attempting to predict choices primarily from utility maximization econometric models (Habib, 2011) or using rule-based computational process models (e.g. Miller and Roorda, 2003; Arentze and Timmermans, 2004). Most approaches require to define utility functions, and the purpose of such studies varies between estimating parameters of a choice model and developing mechanisms for prediction. The challenge

all models yet face is how to represent the immense number of possibilities to plan a day. As seen in e.g. Bowman and Ben-Akiva (2001), Bhat et al. (2004), or Cirillo and Axhausen (2010), a common approach is to decompose daily activity-travel patterns into multinomial logit or nested logit layers, where each layer represents the choice of a specific facet of the pattern, such as number and structure of tours, tour mode and stop location. The main criticism of these models is the lack of integrity among some of their choice dimensions, typically the independence of secondary tours in Bowman and Ben-Akiva (2001), which results in an unrealistic representation of time, or the restriction to a-priory defined patterns criticized by Karlström (2005).

Overall, most models fail to fully represent activity-travel patterns and to consider all components of individuals' decisions in an integrated fashion. A different approach has this potential and consists in associating activity-travel patterns to paths in a dynamic network describing the state of the individual at different time steps, also referred to as a multi-state network in other works (e.g. Liao et al., 2013; Liao, 2016). Several variants of such networks are conceivable, such as the activity network described in Danalet (2015). The core idea is that a link in such a network represents a choice alternative across several dimensions, such as activity type, location and transport mode. While network representations are promising, to the best of our knowledge most previous works have focused on deriving optimal paths from predefined utility functions and have not addressed the problem of estimating a probabilistic choice model.

Karlström (2005) shows how dynamic discrete choice theory allows to formulate such a model, where the choice of activity-travel pattern corresponds to a choice of path in an appropriate network. In the framework, individuals make a sequence of simultaneous choices of activity type, duration, mode of transport and location, taking into consideration both the instantaneous utility of their actions (dependent on previous actions through the current state) and the expected maximum future utility. Implementing and estimating a full-sized version of the model proved to be a computational challenge and only achieved recently by Blom Västberg et al. (2016). The resulting model has the advantage of integrating all components of an activity-travel pattern in one choice of path while avoiding restrictive assumptions on choice sets. It is also straightforward to use for prediction as paths can be simply sampled from the model using estimated link choice probabilities. This paper builds

on this work and the modeling framework is further detailed in Section 5.2.2.

Although the approach (Blom Västberg et al., 2016) has gained attention from the state of practice (see e.g. Jonsson et al., 2014), the model still suffers from major limitations. In particular, the earlier work is rather restrictive as the model retains the property of independence from irrelevant alternatives (IIA). This assumes the absence of any common unobserved factors across alternatives, which may be an unrealistic hypothesis in this setting, as suggested by Mai et al. (2015). A growing body of literature (Bhat, 1998; Hess et al., 2007) has signaled the need to capture correlation in unobserved factors in order to be accurately used for policy evaluation, especially in a multi-dimensional setting with a large choice space. Our contribution consists in overcoming the identified limitations by proposing a flexible approach to relax the independence of error terms over alternatives which can be implemented on a real size application, and showing that predictive accuracy is improved.

In this paper, we propose a mixed recursive logit model which meets these expectations. The method is appropriate to accommodate correlation across alternatives in different dimensions and across repeated link choices. The challenge to estimate such a model is that due to the combinatorial explosion of the number of possible states and actions, approaches similar to Rust's nested fixed point algorithm are too computationally expensive to apply here. We propose to estimate the model via sampling of alternatives, applying recent results by Guevara and Ben-Akiva (2013) which show that mixed logit models can be consistently estimated using sampled choice sets. The key advantage is that the recursive formulation allows to use the model for prediction without sampling any choice sets of paths. The methodology is illustrated with an application based on travel diary data, and we provide an extensive empirical analysis of the results.

This paper is structured as follows. Section 5.2.1 reviews the literature, focusing first on activity-based modeling, while Section 5.2.2 details the modeling framework of Blom Västberg et al. (2016) upon which we build in Section 5.3 by relaxing the IIA property. In Section 5.4, we present extensive numerical results based on a travel survey conducted in Stockholm. In addition to estimation results, we present in Section 5.5 i) an empirical analysis of activity-travel patterns in predicted activity schedules and ii) illustrate substitution patterns iii) a cross-validation study. Finally, we conclude in Section 5.6.

# 5.2 Literature review

In this section, we first give an overview of activity-based travel demand modeling approaches and in particular identify how sources of correlations are specified in existing models. In a second part, we describe formally the approach based on the recursive logit (RL) model formulated by Blom Västberg et al. (2016) on which we base our work. Then we provide some background on existing extensions of the RL model which relax the IIA property for other applications.

#### 5.2.1 Activity-based models in the literature

Activity-based models emerged as an alternative to traditional four-step models with the prospect of overcoming their most fundamental limitations. As argued by Rasouli and Timmermans (2014), the most prominent criticisms surrounding these models are related to lack of integrity and assumption of independence of the four steps. Among the promises of activity-based modeling is an integrated framework which would enable the appraisal of a wider set of policies. As a result, applications of activity-based models to policy analysis have since been studied for an increasingly large variety of transport policies such as peak period tolls (Dong et al., 2006), land-use policies (Shiftan, 2008), parking policies (Habib et al., 2012) and congestion pricing schemes (Vovsha et al., 2006).

There are several approaches to activity-based modeling, which are neither exhaustive nor exclusive. It is however common in the literature to group models into one of two approaches: econometric models based on utility maximization, and rule-based computational process models. We narrow down this review to models based on the concept of random utility, which are the focus of this paper. Such models assume that individuals choose between a large but limited number of activity-travel patterns alternatives in order to maximize the utility derived from the choice.

An inherent problem is the combinatorial nature of the choice space, arising from the multiplicity of choice dimensions involved in the modeling of activity-based travel demand: activity participation, timing, location and transport mode. Not only is there in theory an intractable number of ways to schedule activities and travel over a day, but given the multidimensional nature of the choice context, the many alternatives in the choice set naturally share observed and unobserved

characteristics. As argued in other works (e.g. Bhat, 1998), the IIA property resulting from logit assumptions is untenable in such circumstances and the question of how to accommodate correlation of error terms across alternatives must be addressed. Simple nesting is not sufficient to fully capture perceptual correlation among alternatives, since the choice of schedule represents choices along multiple dimensions at the same time. Most works in the literature address the issue by defining a hierarchy in the decision process. The chosen decomposition structure and hierarchy reflect assumptions about the relationships among choice components and determine the correlation pattern between alternative schedules. As a result, in most model systems found in the literature, the choice of a whole schedule is decomposed into sequential nested or multinomial logit models linked through conditionality and expected utility.

In the following, we review recent activity-based modeling systems and their treatment of correlation between utilities of alternatives. A prime example of the hierarchical layers approach is the daily activity schedule model proposed by Bowman and Ben-Akiva (2001). In order to reach a manageable size of alternatives, the model relies on the concept of home-based tours to decompose the choice of activity-travel pattern. This model served as groundwork for several further developments and proposed an over-arching choice among predefined daily tour patterns. The alternatives are thus defined by a certain number of primary and secondary tour in an upper nest. Four submodels are concerned with the choice of departure time, mode and destination for both types of tour. The model is a sequentially estimated nested logit system with five layers.

Several models developed for planning agencies follow the concepts proposed in Bowman and Ben-Akiva (2001), such as the San Francisco (Jonnalagadda et al., 2001) and the Sacramento DaySim (Bradley et al., 2010) models, however differences exist in the ordering of the levels of nesting. In Bowman and Ben-Akiva (2001), there is a nest around the overarching daily pattern which conditions lower dimensions, and the joint choice of mode and destination is conditioned by time of day decisions. In DaySim, the hierarchy includes more layers and the model has a nested structure which sequentially predicts tour destination, tour main mode and departure time. In Jonnalagadda et al. (2001), there is a nested structure with a mode choice nest under destination choice.

Deciding which multi-level structure to impose is complex and requires empir-

ical analysis, which is why several studies focus exclusively on a restricted subset of dimensions. Hess et al. (2007) discuss the ordering of nesting along the time and mode dimensions. Other works have developed models that do not impose a hierarchy and can accommodate correlation across several dimensions, applying approaches such as cross-nested models or error components. Examples exist for the joint mode and time of day choice (Hess et al., 2007; Bhat, 1998; De Jong et al., 2003), or the joint activity and time of day choice (Wang, 1996). Few works attempt to model interdependencies across more than 2 dimensions, to the notable exception of Yang et al. (2013) who models joint choice of mode, time of day and residential location. In each of these studies, the models relax the independence of error terms over joint alternatives by creating nests in each dimension. Such models dealing with only a partial facet of the daily activity schedule are promising, but usually too complex to be integrated in a complete activity-based travel model.

We note that in addition to the nesting of choice dimensions, it is necessary to model correlation across alternatives within each level. In the case of a hierarchical nesting structure, the marginal submodels may thus be also formulated as nested logit models. For example in the model of Bowman and Ben-Akiva (2001), the first tier concerned with the choice of overall daily pattern is itself a nested logit model with a nest around all patterns involving out of home travel (as opposed to the alternative of staying at home all day). In Bradley et al. (2010), the location choice model for work tour has a nest around all non-usual work locations nested together under the conditioning choice between usual and non-usual. In addition, the tour-level main mode choice model is also a nested logit with the upper level grouping similar mode alternatives such as walk and bike. In De Jong et al. (2003), the model accommodates correlation within time of day alternatives, assuming that consecutive time periods likely have common unobserved effects. There also exists studies dealing with location choice which accommodate correlation across alternatives due to common unobserved spatial elements (Bhat and Guo, 2004), but to the best of our knowledge, such approaches have not been incorporated in full-scale activity-based demand models due to their complexity.

To summarize, most full-scale activity-based modeling approaches consist of a system with a hierarchical structure which decomposes the choice of schedule from activity pattern to trips, relying on deep nested models. A criticism of these models is that they need to make some simplifications in the definition and construction of

tours in order to limit the number of alternatives (Miller et al., 2005). Furthermore, choices made in the context of activity-based modeling are very interrelated and it is difficult to define a nesting hierarchy which corresponds to actual behavior. The chosen structure imposes particular substitution patterns and cannot let data analysis reveal what patterns occur. In addition, models with multi-level nested structures are often complex to estimate, as noted by Pinjari et al. (2011).

## 5.2.2 Recursive logit for activity-based modeling

The approach of Karlström (2005) and Blom Västberg et al. (2016) possesses a key advantage over the state of the art by integrating all components of an activity pattern into one choice of path while avoiding restrictive assumptions on choice sets through a recursive logit formulation.

#### Activity network

In this approach, the feasible activity schedules of an individual are represented as paths in a directed connected graph  $G = (\mathcal{A}, \mathcal{V})$  called activity network, where  $\mathcal{A}$  is the set of links and  $\mathcal{V}$  the set of nodes. Nodes in the network are states in the terminology of dynamic programming, providing information regarding the current time of the day, activity and location of the individual among other variables. Time is discretized in time steps of one minute. Figure 5.1 presents a simplified illustration of such an activity network where each node corresponds to a (time, location, activity) triplet. A link between two nodes in the network is an action that an individual can take in a given state, combining the choice of transport mode, next activity and location, and resulting in a new state. The chosen mode and destination are associated with a travel time discretized in minutes which determines the time of the resulting next state. Note that for the sake of convenience, the mode choice of each action is not identified in Figure 5.1. The chosen activity is initially conducted for 10 minutes and duration can be extended in the next action choice. The choice to continue an activity corresponds to the horizontal links in the figure. Note that since travel times are not a multiple of ten minutes, individuals may arrive at work at e.g. 8.06. Individual time and space constraints limit available actions. For example, work may have a fixed location and duration as illustrated by the figure. Each path in this network consists of a sequence of such actions,

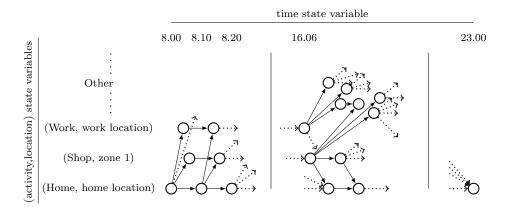


Figure 5.1 – Illustration of an activity network

starting at home in the morning and ending back home in the evening. Thus, a path can be interpreted as a daily schedule of trips and activities.

#### Modeling framework

The modeling framework is based on the RL model formulated by Fosgerau et al. (2013). Each node in the activity network is a state  $x_t$  and each link between two states  $x_t$  and  $x_{t+1}$  is an action  $a_t$  for time step t = 1, ..., T. We denote  $A(x_t)$  the set of feasible actions in state  $x_t$ . An activity schedule is represented as a sequence of actions  $\mathbf{a} = (a_0, ..., a_{T-1})$  corresponding to a sequence of states  $(x_1, ..., x_T)$ , such that  $a_t \in A(x_t)$  and  $x_{t+1}$  is given deterministically by  $a_t$ . The state variables are further detailed in Section 5.4.2. In order to find a utility maximizing path, individuals choose at each time t the action  $a_t \in A(x_t)$  that maximizes the sum of the instantaneous utility of the outgoing link  $u(a_t|x_t) = v(a_t|x_t) + \mu \epsilon(a_t)$  and the expected maximum downstream utility given recursively by the Bellman equation

$$V(x_t) = E\left(\max_{a_t \in A(x_t)} \{v(a_t|x_t) + \mu \epsilon(a_t) + V(x_{t+1})\}\right),$$
 (5.1)

where  $\epsilon(a_t)$  are independent and identically distributed (i.i.d.) extreme value error terms with zero mean. For simplicity, we omit individual subscripts in this section.

Using this assumption on error terms, the value function in (5.1) can be written as

$$V(x_t) = \mu \log \left( \sum_{a_t \in A(x_t)} e^{\frac{1}{\mu}(v(a_t|x_t) + V(x_{t+1}))} \right).$$
 (5.2)

The conditional probability for individual n of choosing action  $a_t$  in state  $x_t$  is given by the multinomial logit model:

$$P_n(a_t|x_t) = \frac{e^{v_n(a_t|x_t) + V_n(x_{t+1})}}{\sum_{k_t \in A(x_t)} e^{v_n(k_t|x_t) + V_n(x_{t+1})}}.$$
 (5.3)

Using (5.1) and (5.3), this probability simplifies to

$$P_n(a_t|x_t) = e^{v_n(a_t|x_t) + V_n(x_{t+1}) - V_n(x_t)}. (5.4)$$

This formulation has many benefits, discussed at length in other works (e.g. Fosgerau et al., 2013). In particular, the model can be straightforwardly used for prediction once it has been estimated, by simulating choices from the Markov chain transition probabilities in (5.3). Log-sums for policy assessment can be easily obtained for the full day from the value function in (5.2), and can be used to analyze how accessibility changes over time and space (see e.g. Jonsson et al., 2014). Also, since decisions are carried out sequentially in time, it allows agents to reschedule in case of unexpected events. However, the major limitation of the model is that it exhibits the IIA property, since it is in fact equivalent to a multinomial logit model over sequences of actions. Indeed, the probability of choosing a sequence of actions  $\mathbf{a} = \{a_t\}_{t=0}^{T-1}$  conditionally on the initial state  $x_0$  is given by (Fosgerau et al., 2013)

$$P_{n}(\boldsymbol{a}|x_{0}) = \prod_{t=0}^{T-1} e^{v_{n}(a_{t}|x_{t}) + V_{n}(x_{t+1}) - V_{n}(x_{t})}$$

$$= \frac{e^{v_{n}(\boldsymbol{a}|x_{0})}}{e^{V_{n}(x_{0})}},$$
(5.5)

$$=\frac{e^{v_n(\boldsymbol{a}|x_0)}}{e^{V_n(x_0)}},\tag{5.6}$$

where  $v_n(\boldsymbol{a}|x_0)$  is the deterministic path utility, equal to  $\sum_{t=0}^{T-1} v_n(a_t|x_t)$ .

A consequence of the IIA property is that the model is limited to proportional substitution patterns between alternatives. As documented by a large body of literature, the model's predictions may therefore be significantly biased when evaluating responses to transportation control measures, which compromises the overall goal of policy sensitivity, one of the main motivations behind the development of activity-based models.

Another concern is that the model cannot accommodate any correlation over action choices made throughout the day by the same individual. Several studies have found that patterns of repeated behavior empirically observed in travel diary data (see e.g. Schlich and Axhausen, 2003) could be accounted for by incorporating heterogeneity in preferences. For example, Cherchi and Cirillo (2008) demonstrate that integrating correlation across tours performed on the same day by the same individual significantly improved predictions. Capturing such tendencies would prove especially relevant if the current model was extended over periods of several days.

Combining the promising above framework for the choice of activity schedule with a flexible approach to capture correlation of unobserved factors across time and alternatives can potentially improve the prediction accuracy and consequently achieve a more realistic modeling of activity-based travel behavior.

# 5.2.3 Extensions of recursive logit models in the literature

In the context of route choice, several studies have relaxed the IIA property of the RL model. In Mai et al. (2015), Mai et al. (2016), Mai (2016b) and Zimmermann et al. (2017) recursive models are introduced covering nested logit, MEV and mixed logit versions of the RL model as well as an application to route choice for cyclists. There also exists a deterministic attribute called link size (LS), which is a deterministic correction for utilities of overlapping paths, thus not relaxing the IIA property of the logit model.

The nested recursive logit (NRL) proposed by Mai et al. (2015) is an extension of the RL model which allows error terms to be correlated by having link-specific scale parameters. This is the first proposed method to relax the IIA property of the RL model while allowing estimation without sampling choice sets. The systems of equations characterizing the value function are however non-linear and thus more difficult to solve, which makes the model cumbersome to use in practice for large-scale networks, even sparse ones.

Mai (2016b) subsequently proposed a more general method to deal with cor-

relation, in which the choice at each stage may be any member of the network multivariate extreme value model. The resulting recursive cross-nested (RCNL) model is more flexible but comes at the price of added complexity. In this case, Bellman's equation cannot be solved as a system of linear equations and requires defining a contraction mapping and performing contraction iterations.

Mai et al. (2016) also proposed a mixed recursive logit (MRL) model. In this case, Bellman's equation can be solved as a system of linear equations, but the log-likelihood must be numerically evaluated by Monte Carlo simulation. Several specifications of mixed logit were tested. One specification included a random travel time parameter, while another was based on Frejinger and Bierlaire (2007)'s subnetwork components approach. In the latter, four subnetworks components were defined, allowing non-overlapping paths to be correlated according to shared subnetwork components.

All models were illustrated on the small network of Borlänge containing 7,459 links, with the exception of the NRL which was applied on a bike network of 40,000 links (in Zimmermann et al., 2017). Numerical results showed that extensions of the RL model which relax the IIA property systematically have a better prediction performance. Nevertheless, all models do so with a large increase in computational time. Mai (2016a) reports that while the RL model with link size can be estimated in 8 hours on the Borlänge network, the NRL extension requires 30 hours, the RCNL 3 days, and the MRL 3 to 5 days.

In this paper, we consider a network considerably larger than state of the art applications. This gives rise to major computational challenges, which we describe further in the next section.

# 5.3 Methodology

In this section, we propose a mixed recursive logit approach to account for correlation of error terms between alternatives and between repeated link choices in the activity-based model described in Section 5.2.2. We illustrate our approach by categorizing the obtainable correlation patterns, and subsequently explain how we address the main challenge of model estimation.

#### 5.3.1 Challenges

While extensions of the RL model described in Section 5.2.3 accommodate to some extent correlation of path utilities in a route choice context, they have limitations in terms of applicability to the activity scheduling context. The main challenges consist in proposing a method that can scale with a real size application, is consistent with the interpretation of paths as activity schedules, and can be estimated within reasonable time.

The first challenge is related to the size of the problem we model. In Fosgerau et al. (2013), Mai et al. (2015) and Mai et al. (2016), the RL model and extensions are estimated with the nested fixed point algorithm. This method consists in a nested subroutine which computes value functions for the current trial value of the parameters within a non linear optimization algorithm maximizing the log-likelihood function. Thus at each iteration, value functions and their gradients need to be solved for each state and each individual (if link utilities include individual-specific attributes). Although this is not necessarily the case in route choice, we note that the activity network is on the contrary defined for each individual with specific space-time constraints. As each observation contains the choice of path of a different individual, this algorithm takes a time that grows with the number of observations, the number of parameters in the model and the number of links in network.

In route choice modeling, the number of attributes included in a model rarely exceeds 15. On the other hand, in activity-travel modeling, the number of estimated parameters can easily reach 40 (Blom Västberg et al., 2016) or up to 70 (Bowman and Ben-Akiva, 2001). When applying the NRL model on a bike network comprising 40,000 links and 15 attributes, Zimmermann et al. (2017) state that estimation takes around two weeks. If we estimate in contrast the size of the activity network, we observe that it is around 10,000 times bigger. Considering a real application with 1,000 locations, 8 activities and 4 modes, in a single state there are 32,000 outgoing links, as opposed to 2 or 3 in a physical road network. Note that this is an approximation to provide an order of magnitude, since all modes or activities may not be available in all states or for all individuals. Given that locations are both actions and states in the framework, the total number of links would be at least 32,000,000. Moreover, time is also a state variable, and although approximations allow to consider only a discrete number of points (as

explained in Section 5.4.2), there remains at least 60 time points when considering the length of a typical work day. The scale of the activity network can thus reach 1,920,000,000 links. This means that previous works on relaxing the IIA property described in Section 5.2.3 cannot be directly applied here.

The second concern arises from the fact that path choice in a real network or in an activity network are choices of a different nature, because the second involves multiple choice dimensions. In a route choice context, the IIA property is violated by the overlapping of links, since paths are perceived to be correlated when comprised of a same portion of the road network. In activity path choice however, perceived correlation between alternatives does not necessarily emerge from physical overlap, due to the fact that the network is dynamic and paths have a time dimension. Rather, paths which correspond to schedules with identical choices in one or several of the dimensions would be regarded as correlated. For example, two paths defining two identical sequences of activities and trips, to the difference that one starts 1 hour later than the other, might actually overlap little in the network but would most likely have shared unobserved characteristics from the common mode, activity and destination choices. The time dimension also indicates that there is probably shared unobserved effects across link choices. Indeed, each link choice situation in the activity network consists of a joint choice of activity, location and mode among similar alternatives, made by the same individual only in a different state. We also note that in contrast to a simple choice of outgoing road segment, the choice of link in the activity network represents in itself a joint decision, which also involves interdependencies between components which must be addressed.

# 5.3.2 Mixed recursive logit for activity-travel choices

In this section, we propose a mixed recursive logit framework which relaxes the IIA property such that utilities of activity paths that share common unobserved effects are correlated through an error component approach. We introduce error components in the link utilities  $u(a_t|x_t)$  in the RL model. In the following, we describe how the proposed framework allows both link and path utilities in the activity network to exhibit correlated error terms.

In the activity-based model, link choice situations correspond to a joint choice

of activity p, location l and mode m, as described in Section 5.4.2. For the sake of illustration, we develop this framework in the context of mode choice. We note that it is possible to accommodate correlation across multiple choice dimensions, and following Bhat (1998) we explain how.

Let  $u(a_t|x_t)$  be the instantaneous utility associated with action  $a_t = (p, l, m)$  corresponding to activity p, location l and mode m, depending on current state  $x_t$ . For notational simplicity we omit an index for individuals. We assume that  $u(a_t|x_t)$  is the sum of a deterministic term  $v(a_t|x_t)$ , and a random term  $\zeta_m(a_t) = \nu' z_m + \epsilon(a_t)$ , where  $\epsilon(a_t)$  is an i.i.d extreme value distributed error term,  $\nu$  is a random vector and  $z_m$  is a vector of dummy variables indicating mode choice. Each component of  $z_m$  is associated to a travel mode  $m' \in \{1, ..., M\}$ , and  $z_{m'} = 1$  if and only if m = m'. The random vector  $\nu$  has dimension M and zero mean, and is normally distributed with variance covariance matrix  $\Sigma$ . It is possible to specify  $\Sigma$  to be diagonal, with coefficient  $\sigma_{m'}^2$  on row m', such that the components of  $\nu$  are independently distributed, but it is also possible to incorporate covariance parameters  $\sigma_{m,m'}$  between modes m and m'. Thus,  $\epsilon(a_t)$  is the i.i.d component of the error term, while  $\nu' z_m$  represents the heteroscedastic component, which is correlated across link alternatives sharing the same mode.

Mixed logit models have an advantage over nested logit models in the case of multidimensional joint choices, such as the joint choice of mode, activity and location in the context of activity-based modeling: while in a bi-dimensional setting the nested logit model requires to define a hierarchy and can only accommodate shared unobserved attributes in the upper dimension (Bhat, 1998), the mixed logit can incorporate correlation of unobserved effects across alternatives along all dimensions. In order to do so, it suffices to also introduce error components in the activity and/or locations dimensions. As an example, we may define  $\eta$  and  $y_k$  in a manner similar to  $\nu$  and  $z_m$ , but in the context of another choice dimension with alternatives  $k \in \{1, ..., K\}$ . The error term would then be  $\zeta_{mk}(a_t) = \nu' z_m + \eta' y_k + \epsilon(a_t)$ and the random vector  $[\nu; \eta]$  of dimension M + K would be normally distributed with variance covariance matrix  $\Sigma$ . Note that in case of dimensions with many alternatives, such as location choice, it is possible to limit the number of random parameters by aggregating contiguous locations and letting each error component correspond to a larger spatial unit. We refer the reader to Bhat and Guo (2004) for more details on the treatment of spatial correlation with an error components approach.

We note that the error component model is equivalent and may be more easily understood as a random parameter specification. As outlined by e.g. Train (2003), mixed logit models may either be derived from the need to accommodate flexible substitution patterns across alternatives or the concept of allowing taste parameters to vary randomly within the population. Indeed, under the second interpretation the proposed formulation is equivalent to having normally distributed random parameter vector  $\beta_m \sim N(\bar{\beta}_m, \Sigma)$  associated to dummy attribute  $z_m$ . The above-mentioned vector  $\nu_n$  then corresponds to the individual deviation from the mean of realization  $\beta_{m,n} = \bar{\beta}_m + \nu_n$ .

#### 5.3.3 Mixing specifications

The mixed logit model with error components offers a great deal of flexibility in terms of achievable correlation patterns. In the following, we provide guidance on the specification of error components.

The model allows to relax the IIA property in a link choice situation, where the individual faces numerous combinations of activity, location and mode alternatives. Defining a diagonal variance covariance matrix for error components in the mode choice dimension only results in partitioning the link alternatives into non-overlapping nests in a fashion similar to the nested logit, where two actions with the same mode choice share unobserved attributes. Including off-diagonal parameters  $\sigma_{m,m'}$  between two distinct modes m, m' allows to model more complex correlation patterns, where similar modes have common unobserved effects.

Estimating a diagonal variance covariance matrix for error components in multiple choice dimensions results in an intricate correlation structure, where each action or link belongs to several nests, as the modeler may for instance specify nests for specific modes and others for activities. Interaction between dimensions may be incorporated through off-diagonal estimates. For instance, we may include a term  $\sigma_{m,p}$  identifying the dependency between a mode m and an activity p within an action. Thus the model is flexible and it is up to the modeler to control the modeling complexity through the number of estimated variance covariance parameters.

The mixed recursive logit framework relaxes not only the IIA property over link choice situations, but also over paths. The utility of an activity path a =

 $(a_0, ..., a_{T-1})$ , denoted  $u(\boldsymbol{a}|x_0)$ , is given by  $\sum_{t=0}^{T-1} v(a_t|x_t) + \zeta(a_t)$ , to which an i.i.d extreme value distributed error term  $\epsilon$  is added. Thus, the random utility of path  $\boldsymbol{a}$  contains the term  $\sum_{t=0}^{T-1} \zeta(a_t)$ , which generates a covariance across alternatives containing similar action choices shifted by a time interval (such as schedules with the same mode choices at different times of day, or schedules containing the same activities). We further exemplify the resulting correlation structure over paths in Section 5.3.4.

Finally, specifying random components is also appropriate to deal with potential correlation across repeated link choices by the same individual. For instance, it is likely that unobserved sources of utility that impact mode choice at a specific time remain present throughout the day. By ensuring that the same draw of the random vector  $\beta_n = \bar{\beta} + \nu_n$  is used for all choices of an individual n, correlated error terms between successive actions using the same mode arise from the common effect of the  $\nu'_n z_m$ .

# 5.3.4 Illustrative example

The following example illustrates how the mixed recursive model allows to incorporate common error terms between schedules that share a common characteristic, without necessarily overlapping in the network, as in Frejinger and Bierlaire (2007)'s subnetwork component approach. In order to build such intuition, we study the example in Figure 5.2: we consider four activity schedules  $a_1$ ,  $a_2$ ,  $a_3$ ,  $a_4$ . The first two schedules consist in making a round trip to spend 8 hours at work and spending the remaining time home. The last two include a social activity after the round trip to work. Schedules  $a_1$ ,  $a_2$  and  $a_4$  contain trips to and from work by car, while in  $a_3$  all trips are performed by public transport, which takes 10 minutes longer. The departure to work in schedule  $a_2$  is delayed by 10 minutes. We note that all paths have a large amount of overlap, corresponding to the time spent at the work and home locations. Nevertheless, this overlap is the result of space time constraints in the activity scheduling choice (work takes place at a fixed location and has a mandatory duration) and characterizes all feasible alternatives. Instead, perceptual correlation among schedules is attributed to the shared unobserved attributes corresponding to the common mode in  $a_1$ ,  $a_2$  and  $a_4$ , as well as the common additional activity in  $a_3$  and  $a_4$ .

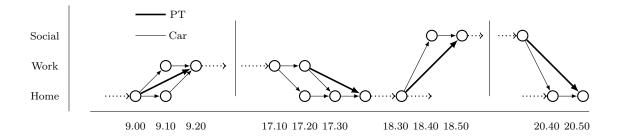


Figure 5.2 – Illustration of 4 paths in the activity network

In order to capture this correlation, we define error components for the car mode, the PT mode, and the social activity and specify a diagonal variance covariance matrix. This is equivalent to letting alternative specific constants for modes  $ASC_{car}$ ,  $ASC_{PT}$  and constant for starting a social activity  $c_{social}$  be randomly distributed with mean vector  $(\bar{\beta}_{car}, \bar{\beta}_{PT}, \bar{\beta}_{social})$  with a variance covariance matrix of random coefficients defined as

$$\Sigma = \begin{pmatrix} \sigma_{car}^2 & 0 & 0\\ 0 & \sigma_{PT}^2 & 0\\ 0 & 0 & \sigma_{social}^2 \end{pmatrix}.$$
 (5.7)

We now compare link and path utilities for the four schedules with the mixed logit specification described above. Let state x correspond to being home at 9:00 and let us consider the choice of subsequent actions. Let  $a_1$  represent the choice of traveling to work by car, and  $a_2$  traveling to work by public transport. The deterministic utilities of respective actions are

$$v_n(a_1|x) = \beta^T X_n(a_1|x) + ASC_{car,n} = \beta^T X_n(a_1|x) + \bar{\beta}_{car} + \nu_{car,n},$$
  
$$v_n(a_2|x) = \beta^T X_n(a_2|x) + ASC_{PT,n} = \beta^T X_n(a_1|x) + \bar{\beta}_{PT} + \nu_{PT,n},$$

where  $X_n(a|x)$  are the other attribute variables of action a dependent on state x.

Since the utility of a schedule is equal to the sum of the utilities of its consecutive actions, and each schedule contains two trips, the random path utilities for this

example are

$$u_{n}(\boldsymbol{a}_{1}|x_{0}) = \beta^{T} X_{n}(\boldsymbol{a}_{1}|x_{0}) + 2\bar{\beta}_{car} + 2\nu_{car,n} + \epsilon_{n},$$

$$u_{n}(\boldsymbol{a}_{2}|x_{0}) = \beta^{T} X_{n}(\boldsymbol{a}_{2}|x_{0}) + 2\bar{\beta}_{car} + 2\nu_{car,n} + \epsilon_{n},$$

$$u_{n}(\boldsymbol{a}_{3}|x_{0}) = \beta^{T} X_{n}(\boldsymbol{a}_{3}|x_{0}) + 4\bar{\beta}_{PT} + 4\nu_{PT,n} + \bar{\beta}_{social} + \nu_{social,n} + \epsilon_{n},$$

$$u_{n}(\boldsymbol{a}_{3}|x_{0}) = \beta^{T} X_{n}(\boldsymbol{a}_{3}|x_{0}) + 4\bar{\beta}_{car} + 4\nu_{car,n} + \bar{\beta}_{social} + \nu_{social,n} + \epsilon_{n},$$

where  $\nu_n$  is a draw from  $N(0, \Sigma)$ .

In this example, schedules  $a_1$  and  $a_2$  obtain correlated utilities resulting from the common component  $2\nu_{car,n}$  in their error terms. Indeed for each choice of action a corresponding to a car trip in the sequence, the component  $\nu_{car,n}$  appears in the utility of the schedule. The variance-covariance matrix M of the error terms of the four alternatives in this example is

$$M = \begin{pmatrix} 4\sigma_{car}^2 & 4\sigma_{car}^2 & 0 & 8\sigma_{car}^2 \\ 4\sigma_{car}^2 & 4\sigma_{car}^2 & 0 & 8\sigma_{car}^2 \\ 8\sigma_{car}^2 & 0 & 16\sigma_{PT}^2 + \sigma_{social}^2 & \sigma_{social}^2 \\ 8\sigma_{car}^2 & 0 & \sigma_{social}^2 & 16\sigma_{car}^2 + \sigma_{social}^2 \end{pmatrix}.$$

# 5.3.5 Maximum likelihood estimation with sampling of alternatives

The nested fixed point algorithm, in which an inner dynamic programming algorithm solves value functions while an outer algorithm updates parameter values, is not the only possible estimation technique for the RL model. The alternative method we present here consists in using sampling of alternatives. Although Fosgerau et al. (2013) described this technique for the RL model, it has not been used before in conjunction with a mixed logit extension. Guevara and Ben-Akiva (2013) however proved that sampling of alternatives yields consistent estimated for logit mixture models although the estimates loose efficiency. In the following, we recall their results and adapt them to the path choice problem formulated as a mixed RL model.

In the following, we define  $\theta$  as the parameters of the mixing distribition  $f(\beta|\theta)$ . More precisely, in this case  $\theta$  represents the mean and standard deviation of the normal distribution of  $\beta$ . The choice probability of a path  $\boldsymbol{a}$  conditional on a sampled choice set  $\tilde{C}_n$  parameters  $\theta$  is given by

$$P_n(\boldsymbol{a}|\tilde{C}_n,\theta) = \int \left(\frac{q(\tilde{C}_n|\beta)}{q(\tilde{C}_n|\theta)}\right) \frac{e^{u(\boldsymbol{a}|\beta) + \log(q_n(\tilde{C}_n|\boldsymbol{a}))}}{\sum_{j \in \tilde{C}_n} e^{u(j|\beta) + \log(q_n(\tilde{C}_n|j))}} f(\beta|\theta) d\beta.$$
 (5.8)

Defining  $W_n$  as  $\frac{q(\tilde{C}_n|\beta)}{q(\tilde{C}_n|\theta)}$ , the log-likelihood function of a set of N observations of paths  $\{a\}_{n=1...N}$  in the mixed RL model therefore corresponds to

$$\mathcal{L} = \sum_{n=1}^{N} \log \int W_n \frac{e^{u(\boldsymbol{a}_n|\beta) + \log(q_n(\tilde{C}_n|\boldsymbol{a}_n))}}{\sum_{\boldsymbol{a} \in \tilde{C}_n} e^{u(\boldsymbol{a}|\beta) + \log(q_n(\tilde{C}_n|\boldsymbol{a}))}} f(\beta|\theta) d\beta.$$
 (5.9)

However, (5.9) is not adapted to the problem of using sampling of alternatives for logit mixture models since the term  $W_n$  still depends on the unknown full choice set  $C_n$ 

$$W_n = \frac{\sum_{\boldsymbol{a} \in \tilde{C}_n} P_n(\boldsymbol{a}|\beta, C_n) q(\tilde{C}_n|\boldsymbol{a})}{\sum_{\boldsymbol{a} \in \tilde{C}_n} P_n(\boldsymbol{a}|\theta, C_n) q(\tilde{C}_n|\boldsymbol{a})}.$$
 (5.10)

We use the approximation  $W_n = 1$  proposed by Guevara and Ben-Akiva (2013), resulting from approximating the probability  $P_n(\boldsymbol{a}|\beta, C_n)$  with the probability  $P_n(\boldsymbol{a}|\theta, C_n)$ ; in other words approximating the choice probability given a specific  $\beta$  by the mixed logit probability given the set of parameters  $\theta$  of the mixture distribution. Thus the log-likelihood becomes

$$\mathcal{L} = \sum_{n=1}^{N} \log \int \frac{e^{u(\boldsymbol{a}_n|\boldsymbol{\beta}) + \log(q_n(\tilde{C}_n|\boldsymbol{a}_n))}}{\sum_{\boldsymbol{a} \in \tilde{C}_n} e^{u(\boldsymbol{a}|\boldsymbol{\beta}) + \log(q_n(\tilde{C}_n|\boldsymbol{a}))}} f(\boldsymbol{\beta}|\boldsymbol{\theta}) d\boldsymbol{\beta}.$$
 (5.11)

The true value of the log-likelihood in (5.11) needs to be approximated via Monte Carlo or quasi-Monte Carlo simulation, as described by, e.g., Revelt and Train (1998). Formally, the method to approximate the choice probabilities of a mixed logit model consists in averaging the value of the integrand over discrete points  $\beta_r$ . The values  $\beta_r$  may be randomly chosen from the distribution  $f(\beta|\theta)$  or chosen cleverly to be evenly spaced on the integration domain. The resulting pseudo log-likelihood  $\mathcal{SL}$  for the proposed model is

$$\mathcal{SL} = \sum_{n=1}^{N} \log \left\{ \frac{1}{R} \sum_{r=1}^{R} \frac{e^{u(\boldsymbol{a}_{n}|\beta_{r}) + \log(q_{n}(\tilde{C}_{n}|\boldsymbol{a}_{n}))}}{\sum_{\boldsymbol{a} \in \tilde{C}_{n}} e^{u(\boldsymbol{a}|\beta_{r}) + \log(q_{n}(\tilde{C}_{n}|\boldsymbol{a}))}} \right\}.$$
 (5.12)

For a proof that the maximization of the pseudo log-likelihood defined in (5.12) yields consistent estimators of the model's parameters, we refer the reader to Guevara and Ben-Akiva (2013).

There exists a vast literature on Monte Carlo and quasi-Monte Carlo simulation methods, for example Bhat (2001), Bhat (2003) and Bastin et al. (2006). In this paper, the draws  $\beta_r$  are constructed using quasi-random Halton sequences. Although there are other approaches, this method was chosen because of its conceptual simplicity and the low number of integration dimensions we face in the application.

One of the advantages of the recursive logit formulation is that the model is straightforward to use for prediction, as path choices can be simulated link by link using equation (5.3) sequentially. It is important to note that estimating the model via sampling of alternatives does not invalidate such advantages with respect to prediction. Equation (5.3) can still be used to sample paths in short computational time once the model is estimated. In the mixed recursive logit, simulating path choices can be performed in the same way as in the RL model, to the difference that several draws of  $\beta$  must be used. Finally, generating choice sets  $\tilde{C}_n$  for estimation is also very simple. Instead of using an arbitrary path generation algorithm, we can simulating paths from the RL model also using (5.3) with some initial parameter values.

# 5.4 Application

We apply the modeling framework presented in Section 5.3 to analyze activity-travel demand in Stockholm from a 2004 travel survey. We compare estimation results of both RL and mixed RL specifications.

#### 5.4.1 Data

The models are estimated on data from the Stockholm travel survey from 2004, in which individuals were asked to describe their full travel diary between 6am and 11pm for one day. The dataset was restricted to individuals who go to work, return home at the end of the day, and have work schedules not starting earlier than 6am or ending later than 8pm. In addition only individuals who use the car for either all or no trip of a tour are kept in the dataset. This leaves 3,150 observations of individual activity schedules for the current analysis.

For each trip, the data reports (a) the start time, (b) the arrival time (c) the mode of transport used (d) the activity pursued at destination (e) the location of the activity (f) the duration of the activity.

Socio-demographic characteristics of the individual are reported in the survey and Table 5.1 summarizes the socio-demographics characteristics of the data. In particular, for each individual, the survey indicates level of income, gender, work and home locations, whether the work schedule is fixed or flexible and the number of working hours, whether the individual owns a car or public transport card and whether the individual has children. We note that there are several methods to include socio-demographic variables in the model. One option is to specify such variables as attributes in the utility function, another is to make use of them in the choice set definition. In this paper, we do both. First, socio-demographic variables are used to restrict the choice set at specific times and thus impose temporal-spatial constraints on the schedule. For example, household information is used to determine whether picking up children is a mandatory activity to be performed on that day, and information on the flexibility of an individual's work schedule limits the potential starting times for the work day. Second, we also incorporate socio-demographic variables in the utilities, which we describe in Section 5.4.3.

#### 5.4.2 States and actions

The state space is key to ensuring a certain level of consistency among the diverse components of the activity-travel pattern. In the choice of daily schedule, there may be interdependencies between the different trips, tours and activities initiated by an individual during the day. Such effects can be conveniently modeled using conditionality, when one choice is model conditionally upon a known

| Age<br>(years) | [%]  | Income<br>(SEK) | [%]  | Household          | [%]  | Working<br>hours | [%]  |
|----------------|------|-----------------|------|--------------------|------|------------------|------|
| 12-18          | 1.9  | 0-15000         | 1.8  | Single             | 28.2 | < 6              | 5.0  |
| 19-24          | 1.6  | 15001 - 25000   | 15.1 | Couple             | 30.1 | 6-8              | 21.2 |
| 25-39          | 31.3 | 25001-40000     | 24.3 | Single w.<br>child | 2.6  | 8-10             | 66.0 |
| 40-64          | 63.8 | 40001-55000     | 44.1 | Couple w.          | 39.2 | > 10             | 7.8  |
| > 64           | 1.3  | > 55000         | 14.7 |                    |      |                  |      |

| Gender | [%]  | Owns car | [%]  | Owns PT<br>card | [%] |
|--------|------|----------|------|-----------------|-----|
| Female | 58.4 | Yes      | 20.9 | Yes             | 42  |
| Male   | 42.6 | No       | 79.1 | No              | 58  |

Table 5.1 – Socio-demographic characteristics in the data

previous choice. Hence, an outcome can be explained not only by attributes of the alternatives but by variables indicating other choices. In order to model such dependencies, the model needs to keep track of past decisions made earlier in the day through state variables. Following Blom Västberg et al. (2016), we assume that a state  $x_t$  in the activity network consists of the following variables:

| Time $t \in$                | Current time of day, discretized in time steps of one              |
|-----------------------------|--|
| [5am,11pm]                  | minute.  |
| Location $l \in L$          | Current location, one of the 1240 zones in the region of           |
|                             | Stockholm.   |
| Activity $p \in P$          | Current activity type. The possible types are social,              |
|                             | recreational, shop small, shop medium, shop large,                 |
|                             | home, work and escort children.                                    |
| Errand indicator            | Discrete state variable keeping track of the number of             |
| $e \in \{0, 1, 2, 3\}$      | finished mandatory activities, such as picking up chil-            |
|                             | dren.  |
| Car availability            | Dummy variable for car availability. The individual has            |
| $\delta_{car} \in \{0, 1\}$ | to travel with the car if $\delta_{car} = 1$ and he is out of home |
|                             | (meaning that he used the car on a previous trip away              |
|                             | from home), and cannot travel with car if $\delta_{car} = 0$ .     |

The state space contains current location and activity, which allows to establish a relationship with the next activity and location, since the individual can choose to continue the activity for another time period. More precisely, in each state  $x_t$  the individual can choose between continuing the same activity or changing it, which implies traveling (possibly within the same zone). In either case, an action  $a_t$  consists of any feasible combination of activity p, location l and transport mode m.

Activity  $p \in P$  New activity (possibly unchanged). Location  $l \in L$  New location (possibly unchanged). Mode  $m \in M$  Transport mode for trip. Car, Public Transport, Walk and Bike are the available modes of transportation. If no trip takes place, the mode of the action is "no mode".

Activity duration is discretized in time steps of 10 minutes. This means that decisions to continue or change the current activity are taken every 10 minutes. Since travel times are not divisible by this time step length, the state variable for time is discretized in smaller time steps of one minute. The number of states for which the value function in (5.1) can be computed is however limited by computational time. The value is hence only computed in a restricted number of states corresponding to 10-minute time steps, and is interpolated in states between these points, as explained by Blom Västberg et al. (2016).

Space-time constraints can be incorporated either by restricting the state space, or a state specific actions choice set. For instance, some activities such as work have a time constraint, e.g. arriving at 8am. To ensure that individuals go to work, the value function of explicitly forbidden states at 8am is set to  $-\infty$ . The choice set at times before 8am is then restricted to actions that do not lead to an implicitly infeasible state. Such states may be trivially found recursively, as the value function of preceding states will also be set to  $-\infty$  if there are no actions leading to a admissible state. As another example of constraint, an individual who does not own a car will be prevented from doing any car trips by fixing  $\delta_{car} = 0$ . For more details on time-space constraints, see Blom Västberg et al. (2016).

# 5.4.3 Utility specifications

The utility is specified as follows. For an individual n, the deterministic utility  $v_n(a_t|x_t)$  of an action  $a_t = (p', l', m)$  given a state  $x_t = (t, l, p, e, \delta_{car})$  is the sum of

the (dis)utility of traveling to the chosen destination l' with the chosen mode m, and the utility of participating in the chosen activity p'. Both depend on the current time of the day and location given by the state  $x_t$ . More precisely, the utility of traveling with mode m for individual n can then be written as  $v_{n,m}(l,l',t)$ , as it is dependent on the individual n, the origin l, destination l', time of day t and mode m. For each mode it is specified as:

$$v_{n,car}(l,l',t) = ASC_{car} + \theta_{t,car}T_{car}(l',l,t) + \theta_{c}C_{car}(l',l,t)$$

$$v_{n,PT}(l,l',t) = ASC_{PT} + \theta_{t,PT}T_{PT}(l',l,t) + \theta_{wait,PT}T_{wait,PT}(l',l,t)$$

$$+ \theta_{c}C_{PT}(l',l,t)$$

$$v_{n,bike}(l,l',t) = ASC_{bike} + \theta_{t,bike}T_{bike}(l',l,t)$$

$$v_{n,walk}(l,l',t) = ASC_{walk} + \theta_{t,walk}T_{walk}(l',l,t) + \theta_{samezone}\delta_{samezone}$$

where  $ASC_m$  represents the constant associated to choosing mode m,  $T_m(l, l', t)$  and  $C_m(l, l', t)$  denote the travel time and cost of going from origin l to destination l' with mode m at time t. The variable  $T_{wait,PT}$  is the waiting time when using public transport. We also incorporate socio-demographic variables in the specification by introducing additional constants and time parameters which depend on individual characteristics, such as gender and age. These parameters are listed in Table 5.2.

Starting a new activity p at time  $t' = t + T_m(l, l', t)$  is associated to a time-of-day dependent constant  $c_p(t')$  for starting the activity, and a duration and time-of-day dependent utility  $v_{n,p}(t', \Delta_{t_p})$ . Choosing to continue with the same activity for another time step is only associated to the duration utility  $v_{n,p}(t', \Delta_{t_p})$ , to ensure that individuals have an incentive to continue with the current activity. The utility is given by time-of-day varying parameters  $\theta_{p,T_k}$  and  $c_{p,T_k}$  specified on discrete time steps  $T_k$ . For example, the work activity has time-of-day specific constants  $c_{\text{work},T_k}$  for  $T_k \in \{6\text{AM}, 7\text{AM}, 8\text{AM}, 9\text{AM}, 10\text{AM}\}$ , as shown in Table 5.3. On the other hand, starting other activities p has a time independent constant  $c_p$  in order to limit the number of parameters in the model. The marginal utility v(p,t) of activity participation at time t is then given by linear interpolation of  $\theta_{p,T_k}$  between the closest discrete points  $T_j, T_{j+1}$  where  $t \in (T_j, T_{j+1})$ , and the utility  $v_{n,p}(t, \Delta_{t_p})$  of an activity episode of duration  $\Delta_{t_p}$  at time t is defined as the integral  $\int_t^{t+\Delta_{t_p}} v(p,\tau) d\tau$ . Note that we also include constants  $c_p$  for starting activities dependent on sociodemographic characteristics, in particular age and having children. All parameters

related to activity choice are listed in Table 5.3.

A utility associated with choosing a location l is defined by size parameters  $\theta_{p,LSM}$  and  $\gamma_{p,s}$  representing the number of available opportunities for each activity p at that location. This utility is given by

$$v_{n,p}(l) = \theta_{p,LSM} \log \left( \sum_{s=1}^{S_p} x_{p,l,s} e^{\gamma_{p,s}} \right)$$

where  $S_p$  is the number of size variables for activity p, and the size variables  $x_{p,l,s}$  may be for instance the number of employees in a specific sector at location l. Table 5.4 gives the complete list of the variables included in the location choice utility.

#### 5.4.4 Correlation structure

Although the mixed logit approach is flexible for reasons discussed in Section 5.3, for the sake of illustration we choose to incorporate in this specification shared unobserved attributes along the mode dimension. Thus, we let alternative specific constants associated to the mode choice dummy vector  $z_m$  be randomly distributed. More specifically, the parameter vector  $(ASC_{car}, ASC_{PT}, ASC_{walk}, ASC_{bike})$  is randomly distributed with mean vector  $(\bar{\beta}_{car}, \bar{\beta}_{PT}, \bar{\beta}_{walk}, \bar{\beta}_{bike})$  and a variance covariance matrix defined as

$$\Sigma = \begin{pmatrix} \sigma_{car}^2 & 0 & 0 & 0\\ 0 & \sigma_{PT}^2 & \sigma_{walk,PT} & 0\\ 0 & \sigma_{walk,PT} & \sigma_{walk}^2 & 0\\ 0 & 0 & 0 & 0 \end{pmatrix}.$$
 (5.13)

We also test a specification in which parameters  $ASC_{car}$ ,  $ASC_{PT}$  and  $ASC_{walk}$  are specified as independent random parameters following a distribution  $N(\bar{\beta}_{car}, \sigma_{car}^2)$ ,  $N(\bar{\beta}_{PT}, \sigma_{PT}^2)$  and  $N(\bar{\beta}_{walk}, \sigma_{walk}^2)$  respectively.

# 5.4.5 State space augmentation

Augmenting the state space allows to take into account more linkages and interdependencies between successive activity/travel choices. It is however not trivial as it results in an increased computational time required to compute value functions and therefore estimate the model. In this application, we exemplify how to capture trip chaining tendencies, in particular the consistency of mode choices within a tour. We present the models both with and without state space augmentation for the sake of comparison.

The augmented state space we consider includes an additional variable  $\delta_{bike}$  indicating whether the bike mode was chosen on the first trip of the current tour away from home.

Bike tour  $\delta_{bike} \in$  Dummy variable indicating whether the chosen mode on  $\{0,1\}$  the first trip of the current tour away from home was the bike.

With this specification we aim to capture the fact that people who use the bike to travel away from home have an incentive to bring the bike home, although this behavior is not systematic. We therefore modify in consequence the utility of traveling by introducing additional ASCs conditional on  $\delta_{bike}$ :

| $ASC_{bike} \delta_{bike} $       | An alternative specific constant for bike conditional on   |
|-----------------------------------|--|
|                                   | bike being the first chosen mode of the tour.              |
| $\mathrm{ASC}_{PT} \delta_{bike}$ | An alternative specific constant for public transport con- |
|                                   | ditional on bike being the first chosen mode of the tour.  |
| $ASC_{walk} \delta_{bike}$        | An alternative specific constant for walk conditional on   |
|                                   | bike being the first chosen mode of the tour.              |

In the utility of traveling with a given mode m the term  $ASC_m$  is replaced with  $ASC_m + ASC_m |\delta_{bike} \cdot \delta_{bike}$ . This means that when  $\delta_{bike} = 0$ , the utility is unchanged, but when the bike was used on the first trip away from home, the additional term  $ASC_m |\delta_{bike}|$  is added to the utility associated to each mode. We emphasize here the difference with the state variable  $\delta_{car}$ . If an individual used the car on a trip away from home, all subsequent trips within that tour must be made by car. On the other hand, the state variable  $\delta_{bike}$  is not used to enforce that all subsequent trips are made with bike, but merely to serve as an explanatory variable for future mode choices within that tour.

#### 5.4.6 Estimation results

Five model specifications are estimated following the procedure described in Section 5.3.5. Four models correspond to the standard multinomial logit (MNL) and the simple mixed logit structure, with and without augmenting the state space. The last model is the more complex mixed logit model with covariance parameter  $\sigma_{walk,PT}$  and an augmented state space. In the models with the mixed logit specification, we computed the simulated log likelihood (5.12) using 500 Halton draws. The choice sets were sampled with initial parameter values given by the model previously estimated in Blom Västberg et al. (2016). For each choice set, we sample 600 alternatives and add the observed alternative. A correction term is then added to the utility as described in Frejinger et al. (2009).

We display estimation results in Tables 5.2, 5.3 and 5.4. Almost all parameters are significant and have the expected sign. We have fixed certain parameters to zero, as well as certain size parameters  $\gamma_{p,s}$  which enter the utility as an exponent  $e^{\gamma_{p,s}}$  to -100. Note that in both cases this means that the associated variables have no impact on the utility function.

We focus our analysis on mode-related parameters. In the mixed logit specifications, the estimated standard deviation of the random ASC for the car, walk and public transport modes are significantly different from zero. Their large values indicate that the data displays heterogeneity in mode preference. However, in the mixed logit models with state space augmentation and bike dummy, the standard deviation of the public transport random parameter is not anymore significantly different from zero. This could mean that the coefficient  $\text{ASC}_{PT}|\delta_{\text{bike}}$  captures some of the variation in preference for that mode. In the model with covariance between the walk and PT constants, the parameter  $\sigma_{walk,PT}$  is negative, indicating that a strong preference for one of these modes implies a weaker preference for the other. It is likely that since individuals tend to have a single mode of predilection, covariance parameters estimated between any other two modes would be also negative.

In the models with state space augmentation, all conditional ASCs are negative except for  $ASC_{bike}|\delta_{bike}$  which is positive, consistently with expectation. If  $\delta_{bike}$  takes the value 1, the value of both ASCs are added for each mode. Consequently, if the bike was used on the first trip of a tour, the utility of choosing another mode decreases while the utility of choosing to travel by bike again increases. We note

that the magnitude of  $ASC_{bike}|\delta_{bike}$  is small enough to ensure that the total Bike ASC remains negative once both terms are added.

Socio-demographic attributes such as being female and aged above 24 have a significant impact on the choice of traveling by bike or car, although not in all models. Women are more sensitive to longer bike trips, yet tend to choose the bike mode more often and the car mode less. It is interesting that while socio-demographic help capture some of the variance in individual preferences, the standard deviation of mode ASCs is still significant.

The in-sample fit of the mixed logit models can be compared to that of the MNL models through the likelihood ratio test. The log-likelihood values reported in Table 5.2 show that the model with the best in-sample fit is the mixed logit model with covariance parameter and augmented state space. The statistic of the likelihood ratio test when comparing this model to each of the other shows that the increase in goodness of fit is significant.

Finally we make some comments about the computational time. We need about half an hour to estimate the models with the MNL specification, while estimation takes 3 hours for the mixed logit model when the pseudo log-likelihood is computed with 500 draws on a Intel(R) Core(TM) i7-6820HQ CPU @ 2.70GHZ.

|                                   | M        | NL     |                 | MNL<br>bike du | mmy        | Mixed        |             | Mixed<br>bike du | mmy       | Mixed<br>bike<br>covariar | dummy   |
|-----------------------------------|----------|--------|-----------------|----------------|------------|--------------|-------------|------------------|-----------|---------------------------|---------|
| Parameter                         |          | Est.   | t-test          | Est.           | t-test     | Est.         | t-test      | Est.             | t-test    | Est.                      | t-test  |
| Constants for choosin             | a a spec | ific n | node of tras    | nsport on      | a trip     |              |             |                  |           |                           |         |
| Car ASC                           | _ 1      | .498   | -22.897         | -2.532         | -24.588    | -2.756       | -19.745     | -2.746           | -23.832   | -2.743                    | -23.564 |
| 001 1100                          | $\sigma$ | 0      |                 | 0              |            | 1.228        | 13.523      | 0.869            | 15.305    | 0.873                     | 15.165  |
| PT ASC                            | _        | .691   | -36.802         | -3.502         | -37.620    | -4.231       | -25.391     | -3.568           | -36.895   | -3.637                    | -36.683 |
| 111100                            | $\sigma$ | 0      | -               | 0.002          | -          | 0.969        | 9.096       | 0.006            | 0.394     | 0.002                     | 0.244   |
| Walk ASC                          | _        | 708    | -15.651         | -1.648         | -16.185    | -2.142       | -15.772     | -2.009           | -16.818   | -2.013                    | -17.155 |
| ,, am 1100                        | $\sigma$ | 0      | -               | 0              | -          | 1.147        | 15.414      | -0.898           | -14.026   | -0.901                    | -14.539 |
| Bike ASC                          |          | .267   | -14.968         | -7.176         | -21.820    | -4.337       | -19.126     | -7.231           | -21.348   | -7.220                    | -21.348 |
| $\sigma_{ m Walk-PT}$             |          | 0      | -               | 0              | -          | 0            | -           | 0                | -         | 0.257                     | 5.781   |
| Additional constants f            | or choos | sing o | specific m      | node cond      | itional on | bike being   | the first t | rip on the       | tour      |                           |         |
| Bike ASC   $\delta_{\text{bike}}$ |          | 0      | _               | 5.120          | 17.521     | 0            | _           | 4.364            | 13.924    | 4.362                     | 13.949  |
| PT ASC   $\delta_{\rm bike}$      |          | 0      | _               | -2.031         | -6.692     | 0            | _           | -2.593           | -7.937    | -2.581                    | -7.846  |
| Walk ASC   $\delta_{\rm bike}$    |          | 0      | _               | -0.975         | -3.608     | 0            | _           | -1.500           | -6.018    | -1.635                    | -6.582  |
| Additional constants f            | or choo: | sing o | specific m      | $node\ cond$   | itional on | socio- $dem$ | ographics   | $or\ same\ z$    | one trips |                           |         |
| Walk ASC   same zone              | -0       | .598   | -4.517          | -0.640         | -5.162     | -0.572       | -4.865      | -0.540           | -4.854    | -0.558                    | -4.949  |
| Bike ASC   Female                 |          | 143    | 0.574           | 0.455          | 2.922      | 0.326        | 1.263       | 0.415            | 2.414     | 0.431                     | 2.513   |
| Car ASC   Female                  |          | 290    | -6.173          | -0.255         | -5.955     | -0.424       | -5.473      | -0.359           | -6.235    | -0.355                    | -6.134  |
| Parameters for travel             | time, co | st (c  | $ar \ and \ PT$ | ) and wai      | t time (PT | )            |             |                  |           |                           |         |
| Cost                              | -0       | .017   | -6.207          | -0.018         | -6.954     | -0.002       | -0.262      | -0.019           | -5.553    | -0.017                    | -5.417  |
| Car Time                          |          | .080   | -18.688         | -0.079         | -19.730    | -0.111       | -14.281     | -0.082           | -17.711   | -0.085                    | -17.226 |
| PT Time                           |          | .040   | -5.485          | -0.044         | -6.613     | -0.081       | -7.906      | -0.059           | -7.386    | -0.060                    | -7.495  |
| PT Wait Time                      |          | .008   | 0.853           | 0.010          | 1.178      | 0.048        | 3.836       | 0.023            | 2.375     | 0.025                     | 2.504   |
| Walk Time                         |          | .050   | -23.171         | -0.049         | -24.691    | -0.055       | -23.755     | -0.051           | -25.588   | -0.052                    | -25.702 |
| Bike Time                         |          | .050   | -9.336          | -0.035         | -7.957     | -0.057       | -8.416      | -0.041           | -8.230    | -0.042                    | -8.190  |
| Bike Time   age $\geq 24$         |          | .016   | -1.499          | -0.008         | -2.072     | -0.017       | -1.562      | -0.008           | -1.556    | -0.009                    | -1.835  |
| Bike Time   Female                | -0       | .024   | -3.067          | -0.026         | -3.867     | -0.030       | -3.186      | -0.025           | -3.532    | -0.026                    | -3.634  |
| Log-likelihood                    | -23      | 8671   |                 | -22091         |            | -22564       |             | -21865           |           | -21855                    |         |

 ${\bf Table~5.2}-{\rm Estimation~results~for~parameters~related~to~the~utility~of~a~specific~mode~choice~and~log-likelihood~for~respective~models$ 

|                              | MNL        |              | MNL<br>bike du | mmy           | Mixed      |          | Mixed<br>bike du | mmy      | Mixed<br>bike<br>covaria | dummy  |
|------------------------------|------------|--------------|----------------|---------------|------------|----------|------------------|----------|--------------------------|--------|
| Parameter                    | Est.       | t-test       | Est.           | t-test        | Est.       | t-test   | Est.             | t-test   | Est.                     | t-tes  |
| Utility to arrive at work a  | t specific | time, linea  | ır between     | n $paramete$  | rs         |          |                  |          |                          |        |
| Work ASC 6AM                 | 0.946      | 2.512        | 1.045          | 2.772         | 1.575      | 3.850    | 1.457            | 3.711    | 1.491                    | 3.778  |
| Work ASC 7AM                 | 0.506      | 2.751        | 0.507          | 2.796         | 0.674      | 3.372    | 0.648            | 3.377    | 0.677                    | 3.51   |
| Work ASC 8AM                 | 0          | _            | 0              | _             | 0          | _        | 0                | _        | 0                        |        |
| Work ASC 9AM                 | -1.310     | -8.144       | -1.273         | -8.099        | -1.494     | -8.344   | -1.422           | -8.383   | -1.450                   | -8.46  |
| Work ASC 10AM                | -5.092     | -13.627      | -5.008         | -13.637       | -5.573     | -12.854  | -5.344           | -13.364  | -5.416                   | -13.27 |
| Constants for starting act   | ivities    |              |                |               |            |          |                  |          |                          |        |
| Home ASC                     | 0          | _            | 0              | _             | 0          | _        | 0                | _        | 0                        |        |
| Shop ASC                     | -6.767     | -41.591      | -6.769         | -42.708       | -6.658     | -37.692  | -6.643           | -39.807  | -6.595                   | -39.25 |
| Social ASC                   | -9.046     | -46.112      | -9.091         | -48.419       | -8.935     | -45.025  | -8.946           | -47.059  | -8.901                   | -46.55 |
| Recreative ASC               | -7.723     | -51.624      | -7.737         | -53.690       | -7.645     | -47.022  | -7.652           | -50.457  | -7.608                   | -49.78 |
| Other ASC                    | -7.191     | -48.493      | -7.191         | -50.119       | -7.121     | -47.839  | -7.107           | -49.839  | -7.056                   | -49.24 |
| Additional constants for st  | tarting ac | tivities des | pendent o      | on socio-de   | mographi   | cs       |                  |          |                          |        |
| Shop ASC   children          | -0.171     | -1.786       | -0.197         | -2.206        | -0.229     | -2.199   | -0.240           | -2.504   | -0.243                   | -2.53  |
| Freetime ASC   age < 30      | 0.211      | 1.649        | 0.235          | 1.895         | 0.161      | 1.190    | 0.162            | 1.324    | 0.170                    | 1.38   |
| Freetime ASC   age $\geq 60$ | -0.471     | -3.308       | -0.444         | -3.243        | -0.438     | -2.814   | -0.412           | -2.861   | -0.407                   | -2.86  |
| Trip ASC   Own Car           | 0.081      | 1.348        | 0.085          | 1.552         | -0.198     | -2.675   | -0.104           | -1.679   | -0.115                   | -1.86  |
| Utility per minute of activ  | ity partic | ipation      |                |               |            |          |                  |          |                          |        |
| Shop Time                    | -0.021     | -14.137      | -0.021         | -14.131       | -0.021     | -13.299  | -0.021           | -13.919  | -0.021                   | -13.93 |
| Social Time                  | -0.000     | -0.066       | -0.000         | -0.133        | -0.000     | -0.089   | -0.000           | -0.213   | -0.000                   | -0.19  |
| Recreative Time              | 0          | _            | 0              | _             | 0          | _        | 0                | _        | 0                        |        |
| Other Time                   | -0.009     | -6.108       | -0.009         | -6.436        | -0.008     | -5.919   | -0.008           | -6.424   | -0.008                   | -6.39  |
| Freetime Time   children     | -0.003     | -3.511       | -0.003         | -3.488        | -0.004     | -3.989   | -0.003           | -3.963   | -0.003                   | -3.97  |
| Utility per minute of time   | spent at   | home, mar    | rginal util    | lity is lined | ır betweer | the time | periods s        | pecified |                          |        |
| Home Time 6AM                | 0.042      | 8.397        | 0.044          | 8.971         | 0.047      | 8.173    | 0.047            | 8.850    | 0.048                    | 8.81   |
| Home Time 7AM                | 0.040      | 11.688       | 0.039          | 11.864        | 0.043      | 11.607   | 0.041            | 11.781   | 0.042                    | 11.95  |
| Home Time 8AM                | 0.019      | 6.006        | 0.018          | 5.977         | 0.020      | 5.783    | 0.020            | 6.092    | 0.021                    | 6.20   |
| Home Time 9AM                | 0.016      | 3.260        | 0.015          | 3.080         | 0.019      | 3.450    | 0.017            | 3.323    | 0.018                    | 3.40   |
| Home Time 1PM                | -0.012     | -10.839      | -0.012         | -11.317       | -0.013     | -11.721  | -0.012           | -11.776  | -0.012                   | -11.63 |
| Home Time 5PM                | 0.003      | 3.503        | 0.003          | 3.326         | 0.002      | 2.065    | 0.002            | 2.696    | 0.003                    | 2.87   |
| Home Time 7PM                | 0.002      | 2.529        | 0.002          | 2.352         | 0.001      | 1.427    | 0.001            | 1.614    | 0.002                    | 1.66   |
| Home Time 9PM                | 0.018      | 12.858       | 0.018          | 13.482        | 0.019      | 12.761   | 0.019            | 13.298   | 0.018                    | 13.24  |

 $\textbf{Table 5.3} - \text{Estimation results for parameters related to the utility obtained when starting a new activity or performing an activity for a certain amount of time \\$ 

|                |                            | MNL         |                     | MNL<br>bike du         | ımmy                         | Mixed                           |                         | Mixed<br>bike dummy                 |        | Mixed<br>bike<br>covaria | dummy  |
|----------------|----------------------------|-------------|---------------------|------------------------|------------------------------|---------------------------------|-------------------------|-------------------------------------|--------|--------------------------|--------|
| Paramete       | r                          | Est.        | t-test              | Est.                   | t-test                       | Est.                            | t-test                  | Est.                                | t-test | Est.                     | t-test |
| Log-sum        | parameters for size attrib | butes. En   | ters utilit         | $y \ as \ \theta_{LS}$ | M Size $in$                  | $\theta_{LSM~Siz}$              | $e \cdot \log \sum_{s}$ | $e^{\gamma_s} \cdot N_{s,location}$ |        |                          |        |
| Social LS      | M Size                     | 0.017       | 1.964               | 0.017                  | 2.001                        | 0.020                           | 1.528                   | 0.020                               | 1.619  | 0.020                    | 1.611  |
| Recreative     | e LSM Size                 | 0.057       | 1.766               | 0.060                  | 1.871                        | 0.081                           | 2.158                   | 0.078                               | 2.160  | 0.080                    | 2.178  |
| Other LSM Size |                            | 0.318       | 5.663               | 0.309                  | 5.828                        | 0.357                           | 6.240                   | 0.343                               | 6.375  | 0.348                    | 6.449  |
| Shop LSM       | I Size                     | 0.485       | 33.491              | 0.484                  | 33.392                       | 0.487                           | 14.299                  | 0.486                               | 17.289 | 0.487                    | 17.227 |
| Paramete       | rs for size attributes. Er | nters utili | ty as $\gamma_i$ is | $\theta_{LSM}$ S       | $_{ize} \cdot \log \sum_{i}$ | $_{s}e^{\gamma_{s}}\cdot N_{s}$ | s, location             |                                     |        |                          |        |
| Rec.           | Population                 | -100        | _                   | -100                   | _                            | -100                            | _                       | -100                                | _      | -100                     | _      |
|                | No Employed Rec.           | 5.907       | 9.819               | 5.809                  | 9.154                        | 6.154                           | 11.715                  | 6.028                               | 10.881 | 6.030                    | 10.999 |
| Other          | No Employed OE             | -100        | -                   | -100                   | -                            | -100                            | -                       | -100                                | -      | -100                     | -      |
| Shop           | Population                 | -100        | -                   | -100                   | -                            | -100                            | -                       | -100                                | -      | -100                     | -      |
|                | No Employed Shop           | 3.585       | 13.587              | 3.611                  | 13.798                       | 3.685                           | 12.754                  | 3.663                               | 13.259 | 3.682                    | 13.279 |
| Social         | Population                 | -100        | _                   | -100                   | _                            | -100                            | _                       | -100                                | _      | -100                     | _      |

 $\textbf{Table 5.4} - \text{Estimation results for size parameters related to the number of opportunities for a specific activity in a specific location and added to the utility of starting an activity$ 

# 5.5 In-sample fit and predictions

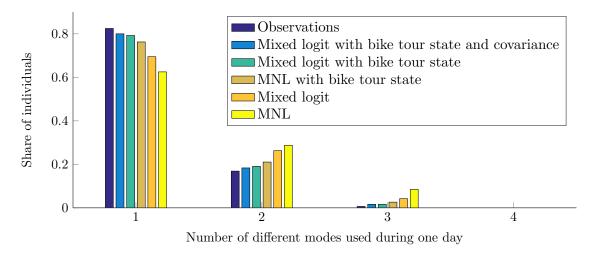
In this section, we present in-sample and out-of-sample prediction results. Given the multiple dimensions of the choice model, it would be possible to present various kinds of analyses, but for the sake of conciseness we focus here on aspects of the model dealing with correlation of activity schedules with respect to mode choice. Therefore in this section we provide an empirical analysis of correlation and substitution patterns in predicted activity schedules, and then present a cross-validation study.

#### 5.5.1 In-sample fit

In this section, we compare some characteristics of the observed choices with model predictions. This experiment aims to empirically verify whether the estimated models reproduce well the patterns observed in the data, in particular the consistency in mode preference over time. We compare the observed activity schedules of the 3,150 individuals with the set of predicted schedules from each model, on the basis of certain aggregate characteristics related to mode choice.

This is an in-sample experiment, since we apply models estimated on the whole data to predict chosen alternatives for the same data set. The pertinence of an in-sample experiment may be unclear, since simple logit models which include a constant for each alternative should in theory reproduce the observed shares of alternatives in the estimation sample (e.g. Train, 1986). However, in the RL model, mode-related constants correspond to alternatives in a link choice situation. When considering the utility of a whole schedule, the constants of each link in the path are added. Alternatives corresponding to the same combination of modes may have a different overall constant once link-specific constants are added, for example if the number of trips differ. Thus some aggregate characteristics over paths, such as mode shares, are inaccurate in the RL model.

We first briefly explain how to predict from the models. For each individual, a set of S=1000 choices of schedules is simulated from each estimated model using (5.3) sequentially. For the mixed logit recursive model, the method is in theory more complex since the true value of the parameters for each individual is unknown. Only the mean and variance of the parameters at the population level are estimated, hence the individual link choice probabilities take the form of an integral which must



**Figure 5.3** – Number of different modes used during a day: histogram of observed and simulated schedules for all models

be approximated by drawing several  $\beta_r$  from the estimated mixing distribution. For the sake of reducing computational time, we resort to a simplification and only use one draw from the mixing distribution for each individual. However, since we analyze prediction results aggregated over the N=3150 individuals, we believe the simplification to be reasonable.

In Figure 5.3, we analyze the number of distinct transport modes used in a day through a histogram. The share of individuals who used 1, 2, 3 or all 4 modes according to their observed schedule is reported. We compare with the predicted number of individuals in each category, computed as an average over the  $N \cdot S = 3150 \cdot 1000$  sampled schedules. Figure 5.3 shows that according to observations, individuals use on average 1 or 2 modes of transportation, but very rarely choose to use 3 or all 4 modes (Car, Public Transport, Walk and Bike). This reflects the fact that people have a preference for a certain mode, and that they tend to choose repeatedly this mode to travel throughout the day. According to Figure 5.3, the basic MNL model however predicts that individuals use on average a higher number of distinct travel modes within a day than what is observed. The mixed logit models empirically display a slightly better fit than the models with the MNL specification and may capture some of the correlation over time of unobserved factors in mode preference. However, the models with augmented state space including additional ASCs are the ones which fit best the patterns displayed in the observations.

Figure 5.4 gives more details on the predicted mode shares over the full day. It reports the share for the main possible combinations of modes in the daily chain of trips. The figure compares the mode shares of the daily chain observed in the 3,150 activity schedules reported by the individuals, and the predicted mode shares from each model. We observe in Figure 5.4 that mode shares are predicted incorrectly by the original model. The number of people traveling with 2 or 3 different modes over the day tends to be overestimated. In particular, the user share of the combination of modes "PT + Bike" and "Walk + Bike" shown in Figure 5.4 are not accurately predicted. As expected, we observe that including additional constants conditional on the new state variable improves the mode share predictions, although the shares of "PT" and "PT + Walk" are still flawed. We note that augmenting further the state space to include dummy variables for these modes could adjust the shares. On the other hand, the mixed logit makes no improvement of the predictions of the MNL in this case.

This empirical analysis shows that augmenting the state space and estimating additional constants improves the in-sample fit and corrects aggregate shares. This is an expected result, since ASCs capture the mean effect of the unobserved factors for each alternative. Furthermore, it has been observed by Train (1986) that including ASCs can mitigate inaccuracies due to the logit model's IIA property, by explicitly incorporating in the utility the source of the correlation in error terms. The risk is that including too many constants may lead to an overspecification of the model, an issue discussed by Bierlaire et al. (1997). For this reason, we investigate out-of-sample predictions in Section 5.5.3.

Finally, this analysis demonstrates that the mixed logit model is not an effective method to correct mode shares, although it yields slightly better predictions than the MNL model. Nevertheless, it has been observed that violating the logit assumptions has less impact when the goal is to estimate average preferences rather than forecasting substitution patterns, according to Train (2003). This is why we also investigate in the following section the substitution patterns of both the mixed and MNL models.

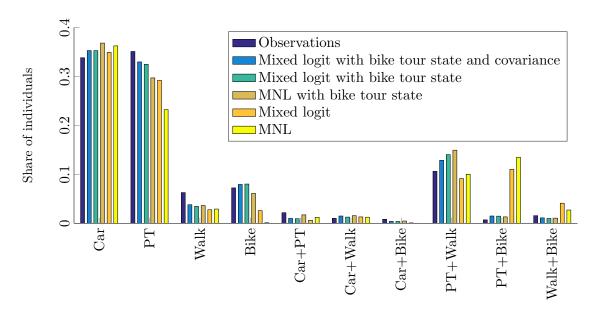


Figure 5.4 – Histogram of the combinations of modes used during one day.

#### 5.5.2 Substitution patterns

The aim of relaxing the IIA property is to suitably model substitution patterns and hence improve predictions. Indeed, the model must be able to predict accurately how choice probabilities will vary in a given scenario. For example, transport demand models can be used to assess how people react to policy or infrastructure changes. Problematically, the IIA property exhibited by the MNL model implies that when the utility of an alternative changes, the choice probabilities of all other alternatives vary in the same proportion. As a result, the restricted substitution patterns of the MNL model may yield inaccurate predictions when assessing scenarios.

In this section, we illustrate how the mixed logit specification accommodates more flexible substitution patterns in the choice of daily schedule. We give the example of a typical scenario forecast experiment for transport demand models, a congestion charge on the price of public transport at specific times. We design the experiment for an individual who has flexible working hours and whose reported schedule features public transport trips. Then we analyze how the choice probabilities of the individual change after the price increase.

Since the RL model has the property of not requiring to sample any choice set in order to compute choice probabilities, we do not need to assume a restricted choice set for the purpose of the experiment. Instead, the choice set we consider is the universal set of all feasible activity schedules for the individual, and the choice probability of each alternative before and after the congestion charge can be computed as a product of link choice probabilities.

The time period during which we apply the price increase is evening peak hour, more specifically between 17:00 and 19:00. While the choice probabilities of all feasible schedules are altered in the price increase scenario, we illustrate the result of the experiment only with a limited number of alternatives, described in Table 5.5. We choose to display alternatives among the set of feasible activity schedules which exhibit relevant characteristics. For each alternative, the change in choice probability after the price increase (in %) is displayed according to three models (MNL model with and without bike tour state variable, and the mixed logit model with bike tour state variable and covariance).

The first alternative in Table 5.5 is the observed alternative, which uses public transport during the peak hour period. Its choice probability has approximately a 100% decrease after the price increase according to the models. The remaining alternatives are chosen not to use public transport at these times and their utility is unchanged. We expect in contrast their choice probability to increase. The exact trips performed in each activity schedule with their chosen mode are listed in the first column of Table 5.5. We note that the listed times correspond to the start and end of each performed activity, and travel takes place between activities. The results confirm that the IIA property holds in the models with the MNL specification (with and without bike tour state variable), as the choice probabilities for alternatives 2 to 8 rise in approximately the same proportion (a 35% and 27% increase respectively). Admittedly, not all alternatives increase by exactly the same percentage, however this is simply due to a small approximation of the model. The value function is only solved for a discrete number of states corresponding to 10minute intervals and the model interpolates its value between these points. As a result, the value functions in (5.6) do not exactly cancel out and the model is close to but not formally equivalent to a MNL.

For the mixed logit model, the choice probabilities were computed with 500 Halton draws. The results reported in Table 5.5 show that the change in probability is no longer proportional, as the mixed logit specification creates nests for all alternatives using the same mode. Thus, schedules where all trips are performed

with another mode (e.g. alternative 8) have a 34% increase, less than schedules where public transport is used but departure time is shifted forward to avoid peak hour (such as alternatives 2 and 7). Indeed, the choice probability of the latter increases by as much as 41%. In alternative 3, where the morning trip is still performed with public transport, but the mode is changed to bike in the afternoon, the increase in probability takes an intermediate value of 36%. In addition, since the model features a negative covariance between the walk and public transport modes, alternatives which perform walk trips have a smaller increase in choice probability: between 18% and 28% depending on the number of walk trips.

The substitution patterns of the mixed logit specification are consistent with the assumption that individuals are more likely to substitute their chosen alternative with one that uses the same mode when facing transportation control measures. Accommodating this flexibility in substitution patterns is a necessity that has been empirically verified by numerous studies, e.g. Bhat (1998), Yang et al. (2013) or De Jong et al. (2003). All found that after a price increase on the observed travel mode, individuals are willing to shift departure time to some extent in order to maintain their mode choice. Naturally, substitutability may also exist in other choice dimensions than travel mode, typically activity or location.

|               | Alteri         | natives      |                       | MNL      | Change in choice MNL with $\delta_{bike}$ | probability (%) Mixed logit with $\delta_{bike}$ |
|---------------|----------------|--------------|-----------------------|----------|---|--|
| Alterna       | ative 1        |              |                       | -100.00  | -100.00                                   | -100.00  |
| 5:00          | 8:30           | Home         | РТ                    | 200.00   | 100.00                                    | 100.00   |
| 8:44          | 17:10          | Work         | PT                    |          |   |  |
| 17:33         | 23:00          | Home         |                       |          |   |  |
| Alterna       | ative 2        |              |                       | +35.05   | +27.65                                    | +39.03   |
| 5:00          | 7:40           | Home         | PT                    |          |   |  |
| 7:54          | 16:20          | Work         | PT                    |          |   |  |
| 16:43         | 23:00          | Home         |                       |          |   |  |
| Alterna       |                |              |                       | +35.00   | +27.51                                    | +36.73   |
| 5:00          | 8:30           | Home         | PT                    |          |   |  |
| 8:44          | 17:10          | Work         | $\operatorname{Bike}$ |          |   |  |
| 17:33         | 23:00          | Home         |                       |          |   |  |
| Alterna       |                |              |                       | +35.00   | +27.51                                    | +28.87   |
| 5:00          | 8:30           | Home         | PT                    |          |   |  |
| 8:44          | 17:10          | Work         | Walk                  |          |   |  |
| 18:18         | 23:00          | Home         |                       |          |   |  |
| Alterna       |                | ***          | *** 11                | +34.92   | +27.44                                    | +21.46   |
| 5:00          | 7:40           | Home         | Walk                  |          |   |  |
| 8:40          | 16:20          | Work         | Walk                  |          |   |  |
| 18:15         | 23:00          | Home         |                       | . 0.4.70 | . 25 20                                   | . 10.00  |
| Alterna       |                | тт           | DIT                   | +34.79   | +27.29                                    | +18.83   |
| 5:00          | 7:50           | Home         | PT                    |          |   |  |
| 8:04          | 16:30          | Work         | Walk                  |          |   |  |
| 17:38         | 18:28          | Home         | Walk                  |          |   |  |
| 18:50 $19:42$ | 19:20<br>23:00 | Shop<br>Home | Walk                  |          |   |  |
| Alterna       |                | Home         |                       | +35.04   | +27.61                                    | +41.18   |
| 5:00          | 7:00           | Home         | PT                    | +55.04   | $\pm 21.01$                               | T41.10   |
| 7:14          | 15:40          | Work         | PT                    |          |   |  |
| 16:10         | 16:30          | Other        | PT                    |          |   |  |
| 16.10 $16:44$ | 23:00          | Home         | 1 1                   |          |   |  |
| Alterna       |                | 1101110      |                       | +34.79   | +27.30                                    | +34.24   |
| 5:00          | 8:10           | Home         | Bike                  | 101.10   | 121.00                                    | 101.21   |
| 8:26          | 16:50          | Work         | Bike                  |          |   |  |
| 17:20         | 23:00          | Home         | 21110                 |          |   |  |

**Table 5.5** – Change in choice probability of alternatives after price increase

#### 5.5.3 Cross-validation

In this section, we assess the out-of-sample prediction accuracy of the four models estimated in Section 5.4.6 with a cross-validation approach. While Section 5.5.1 focused on comparing aggregate measures from the predicted patterns, the aim of this analysis is to compare the predictive accuracy of the models based on the log probability associated to each observed pattern.

The observations are randomly split into a training set (1700 observations) and a validation set with the remaining observations. We generate 13 different pairs

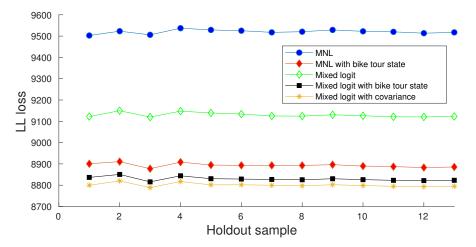


Figure 5.5 – Moving average of log-likelihood loss across sample sets

of training sets and matching validation sets. The performance of the models is evaluated by computing the log-likelihood loss for each validation set, after having estimated the models on the corresponding training set. The log-likelihood loss of validation set i is denoted as

$$err_i = -\frac{1}{|T_i|} \sum_{\sigma \in T_i} \ln P(\sigma, \hat{\beta}_i)$$

where  $T_i$  denotes validation set i, and  $\hat{\beta}_i$  the vector of estimated parameters on matching training set i.

We compute the moving average of  $err_i$  across validation sets i = 1, ..., 13 as follows:

$$\overline{err}_p = \frac{1}{p} \sum_{i=1}^p err_i \quad \forall 1 \le p \le 13.$$

Then the values of the average loss  $\overline{err}_p$  are plotted in Figure 5.5. The model which performs best in terms of out-of-sample fit is the mixed logit model with bike tour state variable. This confirms that relaxing the IIA property via the mixed logit while capturing effects of consistent preference for mode over time with additional constants allows to improve prediction performance.

# 5.6 Conclusion

This work follows the approach of modeling participation in trips and activities as a choice of path in an activity network, where a path represents a sequence of activity episodes over a day. Detailed facets of activity schedules such as locations and transport modes are also included. This view of activity-based modeling is emerging in the literature and a recursive logit model was formulated and estimated by Blom Västberg et al. (2016). In this paper, we build on this methodology and we relax the IIA property by allowing paths utilities to be correlated. The contributions of this paper are: 1) combining sophisticated methods to accommodate significant correlation patterns, while estimating the model within reasonable time on a real-size application 2) showing that predictions are better than the state of the art and analyzing in detail the effects of relaxing the IIA property on predicted activity schedules and substitution patterns.

In order to relax the IIA property of the recursive logit model of Fosgerau et al. (2013), we formulate a mixed recursive logit model. We base the estimation method on sampled choice sets by applying the results of Guevara and Ben-Akiva (2013) on sampling of alternatives in logit mixture models. We argue that this combination of methods in the context of recursive models is new in the literature and provides a suitable approach to the challenges raised in this paper. First, this combination of methods is adapted to address the curse of dimensionality inherent to the problem. The large size and density of the activity network (induced by the extensive number of actions to choose from) makes previous works relaxing IIA in recursive models computationally too expensive to apply here. However, the methods proposed in this paper allow to estimate in reasonable time a model with correlation in error terms. Secondly, the mixed logit explicitly accounts for correlation of unobserved factors across both time and alternatives, which suits well the interpretation of paths as activity schedules in this application.

We provide numerical results and an extensive analysis of the predictive power of the model and its ability to account for correlation. We show that the mixed RL model has a better out-of-sample fit than the model which does not relax the IIA property. Moreover, the mixed RL model accommodates flexible substitution patterns which are in line with what is expected according to previous studies.

Future work can be dedicated to extending the time-span of the model to several

days. Indeed, several activities need not be performed on a daily basis, and it is plausible that individuals consider a planning horizon longer than a day. Existing data on multiple days travel diaries (e.g. Schlich and Axhausen, 2003) could be used to estimate the model. In this case, the mixed logit would be appropriate to model habit persistence over several days, since preferences for modes and/or activities would be heterogeneous between individuals but constant over the planning horizon. Further work on the performance of sampling of alternatives for mixed logit models with panel data would then be required. In addition, future work could focus on applying the proposed travel demand model in conjunction with a Dynamic Traffic Equilibrium (DTA) model, assuming that travel times in the model are no longer exogenous but a function of link flows. Network representations such as the one presented here offer a promising framework to integrate traffic equilibrium models within the activity-based modeling paradigm, as seen in e.g. Ma and Lebacque (2013) and Liu et al. (2015).

# A strategic Markovian traffic equilibrium model for capacitated networks

# Prologue

#### Context

The previous chapters focused mainly on the problem of estimating choice models of travel demand. We also discussed prediction in Chapter 3, where we forecast flows of cyclists in the Eugene network from the estimated route choice model and the total demand given by an origin-destination matrix. Given that cycling levels are usually too low to generate congestion, predicting flows in this case only requires a network loading procedure (i.e., distributing the OD demand on the network's paths according to the fixed estimated costs). However, in the presence of congestion, it is generally assumed that path costs depend on the number of travelers on them. Traffic equilibrium models are used to predict network flow patterns in this context. In this chapter, we focus on the specific case of networks where the amount of flow on links may not exceed a certain capacity. While there is some literature on capacity-constrained traffic assignment, existing approaches either smooth capacity limits or fail to realistically model how user behavior adapts to them.

#### Contributions

The core methodological contribution of this article is to propose a unified modeling framework to model static traffic assignment on networks with strict capacities on links. The strength of the proposed model is to incorporate two sources of stochasticity, stemming respectively from the users' imperfect knowledge regarding link costs (represented as a recursive discrete choice model) as well as the probability of not accessing overcrowded links. The latter is the result of a queuing mechanism at each node which loads capacitated arcs. The resulting model builds

on both the Markovian traffic equilibrium model of Baillon and Cominetti (2008) and the strategic flow model of traffic assignment proposed by Marcotte et al. (2004), and provides a simple and realistic model of how the risk that an arc reaches its capacity affects user behavior strategically.

#### Author contributions

The general idea for this paper came from Emma Frejinger and Patrice Marcotte. The specific research ideas (i.e. the mathematical modeling) came from me. Writing the code, running the experiments and redacting the article was carried out by me, while Emma Frejinger and Patrice Marcotte revised the manuscript.

#### **Article Details**

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# 6.1 Introduction

Traffic equilibrium models are fundamental tools for the design and planning of transportation networks as well as the analysis of their performance. The traffic assignment problem consists in predicting arc flows over a network, given the known travel demand for each origin-destination (OD) pair. Flows are then determined by the interaction of two mechanisms, users' travel decisions and congestion (Sheffi, 1985). Users' route choice preferences are incorporated in a generalized travel cost function that individual travelers aim to minimize, a primary component of which being travel time. Congestion is generally modeled by letting travel impedance functions depend on the usage of the network. As path costs increase with the amount of flow, travelers are induced to reroute on cheaper, less congested paths. The equilibrium assignment of travelers to routes is thus the result of a fixed point problem which is usually solved in an iterative manner. However, the classical

equilibrium principles do not hold any more when side constraints, such as arc capacities, are entered into the model. A solution to that issue, proposed in Marcotte et al. (2004) is to embed within the users' objective function the probability that a link be unavailable, thus introducing a stochastic element that induces strategic behavior.

The main contribution of this paper is to propose a unified model which encompasses two sources of stochasticity by incorporating both unobserved elements and the risk of failure to access an arc in the cost of travel. To do so, we build on existing static traffic assignment models in the following ways. We adopt the framework of Markovian traffic equilibrium introduced by Baillon and Cominetti (2008), where route choice is the outcome of a sequential process of selection of arcs governed by arc choice probabilities (as in Fosgerau et al., 2013). Our model however adds to the latter by proposing a solution to handle rigid arc capacities. More specifically, we embed the concept of strategies governing travelers' movements under capacity constraints in a Markovian traffic equilibrium setting. The key paradigm is to draw a parallel between route choice with recourse actions, according to which travelers readjust their path when reaching a saturated arc, and route choice behavior under imperfect information, similarly to Polychronopoulos and Tsitsiklis (1996). In order to deal with partial information, we expand the state space of the Markov Chain in Baillon and Cominetti (2008), such that a state encompasses two variables: an arc and an information set. The latter enumerates available arcs. User path choice behavior is then characterized by sequences of local arc choices depending on the current state and the destination. To the difference of Unnikrishnan and Waller (2009), who also model user equilibrium with recourse based on realized network states, the probability that a user finds themselves in a given state is flow-dependent. In fact, these probabilities are obtained from a network loading algorithm and are akin to access probabilities in Marcotte et al. (2004), while at the same time representing action-state transition probabilities in the context of Markovian Decision Processes (MDPs). Thus our model borrows algorithms emulating the queuing process to access capacitated arcs from Marcotte et al. (2004). However, it also generalizes the former by proposing a formulation for both deterministic and stochastic user equilibrium, while replacing the formulation using hyperpaths with a simple arc-based model. As in Marcotte et al. (2004), we restrict the model to the case of acyclic network.

The rest of the paper is structured as follows. Section 6.2 presents traffic assignment models and their underlying assumptions, helping to situate the two models on which this work is based, which we describe in detail in Section 6.3. We then introduce the proposed strategic Markovian traffic equilibrium model in Section 6.4. In Section 6.5, we describe algorithms related to those found in Marcotte et al. (2004) to compute availability probabilities from choice probabilities, to compute best response choice probability functions, and to determine an equilibrium. The strategic Markovian traffic equilibrium model is then illustrated on a small network in Section 6.6. We then show in Section 6.7 the amenability of our approach to medium and large size networks, respectively corresponding to a simplified version of the Sioux Falls network, and the time-expanded Springfield transit network. Finally, in the concluding Section 6.8, we provide a discussion on extending the model to cyclic networks.

# 6.2 Review on traffic assignment models

Traffic assignment models aim at predicting flow patterns in a network, under the assumption that travelers minimize some generalized cost, which itself may (or not) depend on flow volumes along the links (or paths) of the network. The equilibrium is thus the result of the interaction between demand and supply. The first and simplest traffic assignment model formulated under these hypotheses is credited to Wardrop (1952), who posed the so-called user equilibrium principle. This states that, at equilibrium, all users are assigned to paths with minimum current cost, which implies that the cost of any unused path is greater or equal to the common cost of paths with positive flow. Beckmann et al. (1956) were the first to translate Wardrop's first principle of optimality into a convex mathematical program in order to obtain fast solution algorithms. A sufficient condition for this reformulation to hold is that the function describing arc costs as a function of the total flow be separable. When this is not the case, the equilibrium problem is usually formulated as a variational inequality or a nonlinear complementarity problem (Dafermos, 1980), which are both a restatement of Wardrop's user equilibrium principle. This basic model has been extensively studied, with proofs of uniqueness and existence of the solution being developed, as well as efficient algorithms to reach it (Patriksson, 2004).

Several traffic equilibrium models extending Beckmann et al. (1956) were developed based on different assumptions regarding user behavior and congestion. In general, hypotheses can be formulated concerning (i) the knowledge that users have of the network and (ii) the effect of congestion on the network's performance. We explain below how relaxing the basic assumptions in each direction led to different model developments.

The basic user equilibrium framework implies that users are able to minimize costs based on perfect knowledge, and thus behave identically. This assumption is however counter-intuitive and assignment models based on it are known to exhibit unrealistic sensitivity to small changes in the network, as asserted by Dial (1971). Distinguishing between perceived and actual travel cost allows to account for users' lack of awareness, preference heterogeneity in the population, or the modeler's failure to identify all attributes of the cost function, and offers a more realistic modeling of route choice behavior. This spurred the development of another class of models based on stochastic user equilibrium conditions, which generalizes the previous (deterministic) user equilibrium condition by introducing a source of uncertainty in the model through random perceived costs. The equilibrium condition for this class of models is that no user can unilaterally improve his/her perceived travel time by changing routes (Daganzo and Sheffi, 1977). This implies that travelers are distributed among several paths, according to the probability that each path is perceived to be the shortest, and the travel cost on all used paths is no longer equal. As with the deterministic case, a characterization of the equilibrium as the solution of a minimization problem has been proposed (Sheffi, 1985), provided that costs be a separable function of flows.

Link performance functions must be defined specifically by the modeler, but under Beckmann et al. (1956)'s formulation, they are assumed to be positive, increasing, and separable, meaning that a link cost depends on the amount of flow on that link only. A lot of research has however dealt with extensions of the traffic equilibrium model's travel cost function (e.g., Larsson and Patriksson, 1999). Such modifications allow to describe more realistic traffic conditions, such as interaction between flows or traffic flow restrictions, the consequence being that the classical Wardrop characterization as an optimization problem usually does not hold in part

because the required cost functions are then non-separable, asymmetric and typically non integrable. For instance, Nagurney (2013) dedicated a large amount of work on more general model formulations, often involving variational inequalities, more adapted to characterize real-world congestion effects. A typical extension consists in relaxing the hypothesis that links may carry an unlimited amount of flow, thus associating a finite capacity to links.

The problem of finite arc capacities has especially been studied in the context of transit assignment, where generalized networks include links representing public transport lines between consecutive stops, which are assigned a capacity and travel cost. The effect of congestion is then different than that in a vehicular road network, as in-vehicle travel times are typically not affected by the number of users. Instead, crowded transit vehicles may no longer be boarded once they are full, creating inherent uncertainty due to the potential unavailability of some network arcs. Incidentally, transit is not the only setting where studying restricted capacity on arcs may be helpful, see, e.g., the context of freight flows (Guélat et al., 1990).

In the context of capacity constraints, the classical Wardrop principle, which does not hold any more, must be adapted. One approach is through the use of asymptotic travel cost functions, meaning that as flow reaches capacity the cost goes to infinity. This solution allows to keep the convex optimization model structure, but has been criticized for entailing numerical difficulties as well as yielding unrealistic travel costs at equilibrium (Boyce et al., 1981; Larsson and Patriksson, 1995). Another solution is to add a well-defined extra cost interpreted as a queuing delay to saturated arcs, leading to a so-called generalized Wardrop equilibrium, as in, e.g., Larsson and Patriksson (1995) or Nie et al. (2004). In both cases, the mechanism which increases travel costs as a result of capacity limits is somewhat implicit and not based on sound behavioral arguments. Indeed, while flow constraints are respected, the equilibrium does not make much sense, since users do not account for the risk to fail to access an arc in their path choice. Therefore, a third approach to capacities was proposed by Marcotte et al. (2004), which we describe below.

The fundamental notion in Marcotte et al. (2004) is the concept of strategy. Originally, this concept was introduced in transit assignment modeling to describe user behavior under uncertain outcomes. A strategy specifies for each node in the network a set of desired outgoing links, but the exact physical itinerary on which

the user following the strategy travels depends on the realization of the random variables contained in the problem. In Spiess and Florian (1989), strategies are used to characterize user itinerary choice with respect to random arrivals of vehicles from several attractive lines. Marcotte et al. (2004) adapted the concept of strategy to relate it to the uncertainty induced by limits on available capacity, as we further explain in Section 6.3. This led to a theoretically appealing equilibrium model where user behavior is characterized by strategies with recourse. The model does not yield flows that may exceed arc capacities, in contrast to, e.g., De Cea and Fernández (1993), and may be applied not only to transit but generally to any acyclic network with capacities.

Strategies exist in an exponential number for each OD pair, as do paths in a network. The optimization problem in Marcotte et al. (2004) is thus formulated in a high dimensional space, which impedes its resolution. While there exists efficient algorithms which circumvent the path enumeration problem (e.g., Dial, 1971), they resort to restricting the routes which can be used by travelers. The drawbacks of relying on path-based variables have also been abundantly emphasized in other works of the user equilibrium and route choice modeling literature (Fosgerau et al., 2013; Wie et al., 2002; Dial, 2006). A different approach was first provided by Akamatsu (1996) in the context of stochastic user equilibrium, as an alternative to Dial (1971)'s well known logit assignment model, which assigns travelers to paths under logit choice probability assumptions. The primary insight of the work of Akamatsu (1996) is to consider path choice probabilities as products of sequential link choice probabilities, obviating explicit path variables. The link choice probability matrix is equivalent to the state transition probabilities of a Markov chain on the network's arcs with an absorbing state corresponding to the destination. Baillon and Cominetti (2008) extended this earlier work by introducing the more comprehensive Markovian traffic equilibrium (MTE) model for the congested case with general probability distributions. Their work established the existence and uniqueness of an equilibrium in the case of flow dependent arc costs, and showed that the approach conveniently circumvents traditional path enumeration issues and facilitates the operationalization of the model to large-scale networks. While this avenue is promising, it has nevertheless not been formally extended to the case of networks with rigid arc capacities.

### 6.3 Two subsumed models

In this section, we introduce the models of Marcotte et al. (2004) and Baillon and Cominetti (2008), on which we build in Section 6.4. Both models deal with traffic equilibrium under entirely different assumptions regarding user behavior and congestion. To describe each work, we assume some standard notation, i.e., the network is represented by a graph  $G = (\mathcal{V}, \mathcal{A})$  with node set  $\mathcal{V}$  and arc set  $\mathcal{A}$ , and each arc  $a \in \mathcal{A}$  possesses a cost  $c_a$  and possibly a finite capacity  $u_a$ . We denote by  $\mathcal{A}_i^+$  the set of outgoing arcs from node  $i \in \mathcal{V}$ .

#### 6.3.1 A strategic flow model of traffic assignment

In the model of Marcotte et al. (2004), it is assumed that users have a perfect knowledge of arc costs, which casts the model within the deterministic user equilibrium framework. Regarding congestion, the model assumes that there exist strict capacity constraints on some of the network's arcs. Thus each arc  $a \in \mathcal{A}$  is associated to a cost  $c_a$  and possibly a finite capacity  $u_a$ . Finally, the network is assumed to be acyclic.

The model provides an entirely different approach to capacities than previous related works. Their solution consists in adopting strategies to describe user behavior, expanding a concept which was first introduced by Spiess and Florian (1989) for transit networks. In this case, users do not aim at minimizing path costs given by the sum of arc costs, but rather strategic costs.

The general idea of a strategy is to model complex decision making under uncertainty in the network service, providing travelers with the opportunity to readjust or refine their path choice as information on the network is gained. In this model, a strategy defines for each node a set of outgoing links ranked by order of preference, thus providing a recourse in case the preferred options have reached capacity. Users choose a strategy in advance, but do not know on which path they will eventually travel.

The inherent uncertainty induced by limited arc availability is encompassed into so-called *access probabilities*, which are conceptually similar to diversion probabilities or failure to board probabilities in some transit assignment models (Kurauchi et al., 2003). They allow the model to strictly enforce capacity constraints. Individuals' travel decisions take into account the randomness embedded into access

probabilities, and consequently users are assumed to minimize the *expected* cost of each strategy s denoted  $C_s$ . This cost can be defined as the weighted sum of path costs by path access probabilities. Extending Wardop's principle to capacitated networks, Marcotte et al. (2004) state that a *strategic equilibrium* occurs when all users are assigned to strategies of minimum expected cost.

The complexity lies in the fact that the cost mapping C is not available in closed form as a function of strategic flows x. Pricing out strategies requires to obtain first the access probabilities  $\pi(x)$  corresponding to the current distribution of users into strategies. It also depends on additional assumptions of the model, namely on the queuing mechanism at each node. Marcotte et al. (2004) rely on two algorithms to compute the expected price of strategies. Access probabilities naturally induces nonlinearity and asymmetry in the cost mapping C, and Marcotte et al. (2004) show that it is not integrable, which prevents it from being reformulated as a standard optimization problem. Thus the equilibrium problem is expressed by the variational inequality

$$\langle C(x), x - y \rangle \le 0, \quad \forall x \in X,$$

where X is the set of feasible strategic flows.

# 6.3.2 A Markovian traffic equilibrium model

The underlying assumption in the model of Baillon and Cominetti (2008) is that travelers do not have perfect knowledge of arc costs, which are thus modeled as random variables representing how individuals perceive cost. In addition to being random variables, costs are also assumed to be flow-dependent to account for congestion.

Under these assumptions, the MTE model falls within the scope of stochastic user equilibrium. Perceived cost is defined as  $\tilde{c}_a = c_a + \epsilon_a$ , where  $c_a$  is the real arc cost and  $\epsilon_a$  is an error term with zero mean. The model considers general distributions for the error term, however its application has been largely restricted to the logit case. Congestion is accounted for by letting the mean cost  $c_a$  be a function of the flow  $f_a$  on the arc through known volume-delay functions.

What distinguishes Baillon and Cominetti (2008) from other stochastic equilibrium models is that the approach is formulated in terms of arc-based variables,

relying on dynamic programming. Travelers' choice of path obeys a sequential process in which a discrete choice model at each node i describes the choice probabilities  $P_{ij}^d$  of outgoing links  $(i,j) \in \mathcal{A}_i^+$  depending on the desired destination d. The arc-based formulation requires to define the notion of perceived cost to destination d from the source node of a given arc a, denoted  $\tilde{w}_a^d = w_a^d + \epsilon_a$ . The cost to destination  $w_a^d$  is the sum of the arc cost  $c_a$  and a destination specific value function defined recursively following Bellman equation of dynamic programming, i.e.

$$w_a^d = c_a + \varphi_{j_a}^d(w^d),$$

where

$$\varphi_i^d(w^d) = E\left(\min_{a \in \mathcal{A}_i^+} w_a^d + \epsilon_a\right).$$

Thus the value function  $\varphi_i^d(w^d)$  represents the expected minimum cost to go to destination d from a node i in the network.

The model assumes that at a node i, individuals traveling towards d observe  $\tilde{w}_a^d$  for all outgoing arcs  $a \in \mathcal{A}_i^+$  and choose the link with the smallest perceived cost to destination. When the variance of error terms is null, individuals choose identically, while they are distributed according to link choice probabilities  $P_{ij}^d$  otherwise. In fact, the MTE model encompasses both the deterministic and stochastic user equilibrium case under the same formulation, and the former is a specific case of the latter. Although the MTE model could be expressed as a variational inequality, it admits a characterization as a convex minimization problem, assuming that congestion functions be integrable.

It is worth mentioning that the formulation in terms of link variables possesses interesting properties. In particular, the link choice probability matrix  $P^d$  may be regarded as the transition probability matrix of an underlying Markov chain where states are network links, meaning that expected arc flows can be easily computed by matrix operations as the expected state visitation frequencies.

Finally, we note that Baillon and Cominetti (2008) mention the possibility of extending the model to networks with arc capacities  $u_a$  by considering bounded volume-delay functions. However, doing so simply heuristically bounds predicted flows without providing a realistic model of how the risk that an arc becomes

inaccessible affects behavior strategically. Moreover, the solution obtained does not satisfy Wardrop's equilibrium conditions.

# 6.4 Strategic Markovian traffic equilibrium model

In this section, we propose a strategic Markovian traffic equilibrium model for capacitated networks that subsumes the principal advantages of both previously described models. It incorporates two sources of stochasticity in user route choice behavior, induced by variations in cost perception and the risk associated with the failure to access an arc. We propose a model formulation in which the deterministic user equilibrium (i.e., arc cost is identical across users) is a specific case of the stochastic user equilibrium. While we do not propose a characterization as a convex minimization problem and we restrict our model to the logit case, we retain the main advantages of the MTE framework. For the sake of clarity, we first describe the deterministic user equilibrium in Subsection 6.4.2 before deriving the more general model in Subsection 6.4.3.

# 6.4.1 Notation and assumptions

We consider a directed acyclic connected graph  $G = (\mathcal{A}, \mathcal{V})$ , where  $\mathcal{A}$  is the set of arcs, or links, and  $\mathcal{V}$  is the set of nodes. Links are denoted  $a = (i_a, j_a)$  and  $\mathcal{A}_i^+$  is the set of outgoing links from node  $i \in \mathcal{V}$ . We assume that every link a has a strict capacity  $u_a$  and an associated generalized cost  $c_a$ . We add absorbing links without successors to each destination node and call  $\mathcal{D}$  this set of destination links. We let  $g^d$  characterize the vector of demand from each node to a destination  $d \in \mathcal{D}$ .

We review below the assumptions made throughout the paper. First, as in Marcotte et al. (2004) and Unnikrishnan and Waller (2009), we assume that the network is acyclic. While this is a strong assumption, we believe it is suitable for several applications of interest which possess time-expanded networks, as we illustrate in numerical experiments in Section 6.7. Adapting the algorithms proposed in this paper for cyclic networks is not trivial, and we discuss the issue in more detail in Section 6.8. Second, we also assume that the network has sufficient capacity to

accommodate the whole demand. In particular, we assume that the subset of the network consisting of uncapacitated arcs is strongly connected, i.e., there exists an uncapacitated path between each pair of nodes in the network. This assumption can be satisfied by creating direct artificial arcs with high cost between nodes and destinations when necessary, which can be interpreted as walking arcs.

Users traveling in this network aim at finding the shortest path to their destination  $d \in \mathcal{D}$ . However, because of limited network capacity, some arcs may be saturated and thus inaccessible depending on route choices made by other travelers. Similarly to Marcotte et al. (2004), we assume a realistic modeling of user behavior in this context, dictating that travel decisions be strategic and include recourse actions, consisting of a set of subpaths in an order of preference, should a link in the preferred itinerary turn out to be unavailable. In addition, we make the hypothesis that travelers do not know in advance what arc will prove to be available, and only observe the outcome when reaching the source node of each arc. Under these assumptions, the problem bears similarities to the stochastic shortest path problem in a probabilistic network studied in, e.g., Andreatta and Romeo (1988). As observed in Polychronopoulos and Tsitsiklis (1996), stochastic programming with recourse can be viewed as a stochastic control problem with imperfect information, and may be solved with dynamic programming methodology. Namely, instead of defining recourse actions, user behavior may equivalently be characterized by an optimal policy given the current state, where the state indicates the realization of the random variables. Below, we explain how we formulate the model following this paradigm.

We assume that the set of available outgoing arcs from node i is a random subset of  $\mathcal{A}_i^+$ , and define the random vector  $X_i$ , which indicates whether each outgoing arc is accessible and may take values in  $\Omega_i = \{0,1\}^{|\mathcal{A}_i^+|}$ . Consequently, we define a state  $s = (i, x_i)$  as a set of two variables, i.e., a node i and a realization  $x_i$  of random vector  $X_i$ . The set of states at node i is denoted  $\mathcal{S}_i$ , while the set of all possible states is denoted  $\mathcal{S}$ . A policy, or action, is then a choice of outgoing arc among the set  $\mathcal{A}(s)$  containing the  $N_s$  available links at the current state  $s = (i, x_i)$ , as illustrated by Figure 6.1. Since we assume that there always exists at least one uncapacitated outgoing link, there is no state in which no link is available. For an unvisited node i, the random vector  $X_i$  follows the discrete availability probability distribution  $\pi_i$ , with support on  $\{0,1\}^{|\mathcal{A}_i^+|}$ . Upon arrival at node i, the user learns

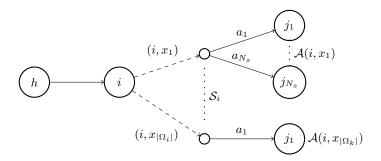


Figure 6.1 – Illustration of state expansion

the realization of  $X_i$ . Therefore, travelers choose their paths sequentially in a dynamic fashion, choosing in each state an action that leads stochastically to a new state.

Travelers' route choice behavior is characterized by choice probabilities, which describe in what proportion individuals choose each action conditionally on the state and the destination. In particular, let  $P_{s,ij}^d$  represent the proportion of individuals traveling to  $d \in \mathcal{D}$  who choose action  $(i,j) \in \mathcal{A}(s)$  in state  $s \in \mathcal{S}$ . We then denote  $\mathbf{P} = \{P_{s,ij}^d\}_{d \in \mathcal{D}, s \in \mathcal{S}, (i,j) \in \mathcal{A}(s)}$  the vector of choice probabilities. The role of availability probabilities  $\boldsymbol{\pi} = \{\pi_{i,s}\}_{i \in \mathcal{V}, s \in \mathcal{S}_i}$  is analog to that of state transition probabilities conditional on choices in a MDP. Given a state  $s_t = (i, x_i)$  and an action  $a_t = (i, j) \in \mathcal{A}(s_t)$ , the probability  $\Pr(s_{t+1}|s_t, a_t)$  of reaching the new state  $s_{t+1} = (j, x_j)$  is given by the distribution  $\pi_j$  of random vector  $X_j$ . In other words, the new state consists of the head node of the chosen available link and a realization of the availability random vector at that node. We can here draw a parallel with the model of Baillon and Cominetti (2008), where the choice of outgoing link may also be viewed as a choice of action leading to a new state. While in Baillon and Cominetti (2008) the new state is given with certainty once the action is selected, and is equal to the chosen link, we obtain a more complex model with non degenerate action-state transition probabilities. Therefore, in a capacitated network, passengers' motions are directed by an underlying Markov chain dependent on both choice and availability probabilities.

The probability of accessing an arc naturally depends on the choices of all other users of the network. Hence, availability probabilities  $\pi$  actually depend on both capacities and choice probabilities P through a loading process similar to the one

found in Marcotte et al. (2004), which we further explain in Section 6.5.

We observe that the probability vector  $\mathbf{P}$  has a close tie to the strategic flow vector in the model of Marcotte et al. (2004), since both specify the distribution of travelers between different travel strategies or policies. The major difference in this work is that we model behavior using local choices at each node instead of a choice of strategy for the entire itinerary. Also, in Marcotte et al. (2004), the model requires one strategic flow vector per OD pair, while  $\mathbf{P}$  in our arc-based model works implicitly with all strategies but is only destination specific. In addition, the framework we propose lends itself to model both deterministic and stochastic equilibrium. Indeed, although  $\mathbf{P}$  is dubbed a vector of choice probabilities, it may be degenerate as exemplified in Section 6.4.2. We summarize below the notation used throughout the paper:

```
set of arcs
\mathcal{A}
\mathcal{V}
              set of nodes
\mathcal{D}
             set of dummy destination links
\mathcal{A}_{i}^{+}
              set of outgoing arcs from node i
\mathcal{S}
              set of states
\mathcal{A}(s)
              set of available outgoing arcs in state s = (i, x_i)
X_i
              random vector indicating available outgoing arcs from i
q^d
              demand vector to destination d
              cost on arc a
V^d(i,x_i)
              minimum expected cost to destination from state (i, x_i) to
              destination d
w_a^d
              expected cost of arc a with regard to destination d
              capacity on arc a
u_a
f_a^d
              expected arc flow on a to destination d
              availability distribution of random vector X_i
\pi_i
              link choice probabilities from state s to destination d
```

# 6.4.2 Deterministic user equilibrium

In this section, we focus on the deterministic user equilibrium case, assuming that individuals have perfect knowledge of arc costs  $c_a$ . We emphasize that perfect knowledge does not refer to availability of outgoing arcs, which we still assume to be unknown for downstream parts of the network.

As in Baillon and Cominetti (2008), in each state  $s = (i, x_i)$  individuals minimize the expected cost to destination of actions  $a \in \mathcal{A}(s)$  corresponding to available outgoing links, where the stochasticity is induced by availability probabilities  $\pi$ . This quantity  $w_a^d$  is the sum of two terms, the link cost  $c_a$  associated to the action, and the minimum expected cost to destination  $V^d(j, x_j)$  from the future state  $(j, x_j)$ , weighted by the probability distribution  $\pi_j$  of reaching each possible state conditional on the action:

$$w_a^d = c_a + E_{x_{j_a} \sim \pi_{j_a}} V^d(j_a, x_{j_a}).$$
(6.1)

The minimum expected cost of traveling to destination d from state  $(i, x_i)$  is denoted the value function and defined recursively by the Bellman equation:

$$V^{d}(i, x_{i}) = \min_{a \in \mathcal{A}(i, x_{i})} \left\{ c_{a} + E_{x_{j_{a}} \sim \pi_{j_{a}}} V^{d}(j_{a}, x_{j_{a}}) \right\}.$$
 (6.2)

Note that costs  $\boldsymbol{w} = \{w_{s,a}^d\}_{d \in \mathcal{D}, s \in \mathcal{S}, a \in \mathcal{A}(s)}$  explicitly depend on access probabilities  $\boldsymbol{\pi}$ , which themselves depend on users' choices  $\boldsymbol{P}$  through a loading mechanism which mirrors the queuing mechanism taking place to access each capacitated link.

An equilibrium is reached when, in each possible state, no user can reduce its expected cost to destination by modifying his/her action choice. Hence, for each state  $s = (i, x_i) \in \mathcal{S}$  and destination  $d \in D$ , all available actions  $a \in \mathcal{A}(s)$  which have a non null choice probability  $P_{s,a}^d$  must have the same expected cost  $w_{s,a}^d$ . If a single action possesses the minimum cost, the probabilities are degenerate. Note that in the deterministic case, the vector  $\mathbf{P}$  is equivalent to splitting proportions in other works (Boyles et al., 2015).

Let us define the set of feasible choice probability vectors

$$\mathcal{P} = \left( \mathbf{P} \in \mathbb{R}_{+}^{|\mathcal{D}| \sum_{s \in \mathcal{S}} |\mathcal{A}(s)|} : \sum_{(i,j) \in \mathcal{A}(s)} P_{s,ij}^{d} = 1 \quad \forall d \in \mathcal{D}, \forall s \in \mathcal{S} \right).$$
 (6.3)

The equilibrium probabilities  $P^*$  must then satisfy the variational inequality

$$\langle \boldsymbol{w}(\boldsymbol{P}^*), \boldsymbol{P}^* - \boldsymbol{P} \rangle \le 0 \quad \forall \boldsymbol{P} \in \mathcal{P}.$$
 (6.4)

Alternatively, the problem may be formulated as the nonlinear complementarity

problem:

$$P_{s,ij}^*(w_{s,ij} - V_s) = 0 \quad \forall s \in \mathcal{S}, (i,j) \in \mathcal{A}(s), \tag{6.5}$$

$$P_{s,ij}^* \ge 0 \quad \forall s \in \mathcal{S}, (i,j) \in \mathcal{A}(s).$$
 (6.6)

#### 6.4.3 Stochastic user equilibrium

In this section, we propose an extension where perception of travel costs  $c_a$  varies across the population. We model perceived arc costs as random variables  $\tilde{c}_a = c_a + \mu \epsilon_a$ , letting the measured arc cost be disrupted by an error term with  $E(\epsilon_a) = 0$ . This source of randomness can be interpreted as users not being capable of perfect discrimination, or the modeler failing to properly identify and measure the cost function.

Under these assumptions, the expected cost of an action a to reach destination d also becomes a random variable  $\widetilde{w}_a^d$ , which is the sum of both the error term  $\epsilon_a$  and the term  $w_a^d$ :

$$\widetilde{w}_a^d = w_a^d + \mu \epsilon_a. \tag{6.7}$$

On the other hand, the cost  $w_a^d$  is still

$$w_a^d = c_a + E_{x_{j_a} \sim \pi_{j_a}} V^d(j_a, x_{j_a}), \tag{6.8}$$

however  $V^d(j_a, x_{j_a})$  is now the *expected* value function. Therefore, according to the Bellman equation, we have

$$V^{d}(i, x_i) = E_{\epsilon_a} \left[ \min_{a \in \mathcal{A}(i, x_i)} \left\{ c_a + E_{x_{j_a} \sim \pi_{j_a}} V^{d}(j_a, x_{j_a}) + \mu \epsilon_a \right\} \right].$$
 (6.9)

In particular, we assume that  $\epsilon_a$  is an Extreme Value Type I distributed error term. Then, (6.9) can be rewritten as the following so-called logsum:

$$V^{d}(i, x_{i}) = \mu \ln \left( \sum_{a \in \mathcal{A}(i, x_{i})} e^{\frac{1}{\mu} \left( c_{a} + E_{x_{j_{a}} \sim \pi_{j_{a}}} V^{d}(j_{a}, x_{j_{a}}) \right)} \right).$$
 (6.10)

Following the notation introduced in the previous section, we can formulate the equilibrium problem as a similar variational inequality. We define  $\bar{w}_{s,a}^d$  as the sum  $w_{s,a}^d + \mu \ln(P_{s,a}^d)$ . Then for each destination the equilibrium choice probabilities  $P_{s,a}^*$ 

are the solution of

$$\langle \bar{\boldsymbol{w}}(\boldsymbol{P}^*), \boldsymbol{P}^* - \boldsymbol{P} \rangle \le 0 \quad \forall \boldsymbol{P} \in \mathcal{P}.$$
 (6.11)

Equivalently, the nonlinear complementarity problem becomes

$$P_{s,ij}^* \left[ \bar{w}_{s,ij} - V_s \right] = 0 \quad \forall s \in \mathcal{S}, (i,j) \in \mathcal{A}(s), \tag{6.12}$$

$$P_{s,ij}^* \ge 0 \quad \forall s \in \mathcal{S}, (i,j) \in \mathcal{A}(s).$$
 (6.13)

In this case all available outgoing arcs have some positive flow since probabilities  $P_{s,ij}^d$  are non null for all available actions  $(i,j) \in \mathcal{A}(s)$ . Thus we note that at equilibrium  $V_s^d$  is equal to  $\bar{w}_{s,ij}^d$  for all arcs  $(i,j) \in \mathcal{A}(s)$ .

### 6.5 Algorithmic framework

In this section, we discuss the existence of solutions to the proposed equilibrium models and propose an algorithmic framework to compute a solution. Applying these models to networks with general topologies is not straightforward, and the case of cyclic networks is more complex. In the following, we focus on the case where the network admits a topological ordering and prove the existence of an equilibrium solution in this context. We present three algorithms which are jointly required to solve the problem. The first is a network loading algorithm to recover arc flows f and availability probabilities  $\pi$  from choice probabilities P. The second is an algorithm to compute the best response choice probabilities corresponding to a given network loading. Finally, the third is an iterative outer algorithm for determining an equilibrium solution, which is a heuristic since the cost function lacks favorable properties (e.g., monotonicity). In Section 6.8, we provide a general discussion regarding how the algorithms in this paper could be adapted to consider general cyclic networks.

#### 6.5.1 Network loading

We start by stating the flow conservation equations for the capacitated network. For each link  $(i, j) \in \mathcal{A}_i^+$ , the incoming flow and demand en route to d at node i is split between the outgoing links according to the choice probabilities  $P_{s,ij}^d$  weighted by the availability probability  $\pi_{i,s}$  of each state  $s \in S_i$ . This gives

$$f_{ij}^{d} = \sum_{s \in \mathcal{S}_{i}} \pi_{i,s} P_{s,ij}^{d} \left( g_{i}^{d} + \sum_{(h,i) \in \mathcal{A}_{i}^{-}} f_{hi}^{d} \right), \quad \forall (i,j) \in \mathcal{A}, \forall d \in \mathcal{D}.$$
 (6.14)

For destination links  $d \in \mathcal{D}$ , we have a flow equivalent to the total demand

$$f_d^d = \sum_{i \in \mathcal{V}} g_i^d, \quad \forall d \in \mathcal{D}. \tag{6.15}$$

Each intersection corresponds to one of the two following cases. If there is no outgoing capacitated link, the availability probabilities are degenerate. The only possible state corresponds to all outgoing links being available. In this case the incoming flow is simply split according to the ratios given by P at that state. On the other hand, if there is at least one capacitated outgoing link, a loading mechanism at that node emulates the queuing process taking place when users attempt to access outgoing arcs. The latter yields the availability probability of each state and computes the corresponding outgoing flows.

#### Treatment of capacitated intersections

We make the following assumptions regarding this loading mechanism at capacitated intersections:

- Users of an arc which terminates at the current node have equal access priority.
- The queuing discipline implemented is the single queue processing (SQP) described in Marcotte et al. (2004), corresponding to users being randomly and uniformly distributed in a single queue.

These assumptions uniquely determine the availability probabilities corresponding to a total incoming flow at a given node. To illustrate this loading process, we consider the intersection in Figure 6.2 with a single node i possessing two capacitated outgoing links. In this example, the demand originating from i plus the flow arriving to i from previous arcs represents the total incoming flow and amounts to 30. Table 6.1 gives the choice probabilities for each possible state at node i. While there is a single destination in this example, this process generalizes to destination-

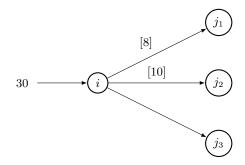


Figure 6.2 – Loading example

specific incoming flows and is described in detail in Algorithm 1.

At the first iteration, users are assigned to links assuming that the initial state is (1,1,1). Links fill up at a rate proportional to the ratio between capacity and the number of individuals who want to access the link. In this case, since 10 and 20 users wish to access  $j_1$  and  $j_2$  respectively according to the choice probabilities given in Table 6.1, the ratios are 8/10 and 10/20. Therefore, having the smallest ratio, the arc leading to  $j_2$  is the one to reach capacity first. At this point, half the users have been assigned, therefore the probability of a user reaching the state  $s_1 = (1, 1, 1)$ , corresponding to all links being available, is 1/2. The 15 users that have not been assigned and are in the remaining of the queue behave conditionally to state  $s_2 = (1, 0, 1)$ . Before performing the next iteration, the capacity of remaining arcs is replaced by the residual capacity, which is obtained by removing the number of users who have successfully accessed the arc. Now, all 15 users want to access  $j_1$ . Since the residual capacity is 3, the ratio is 1/5. Therefore, the probability that a user reaching the tail node finds themselves in state  $s_2 = (1,0,1)$  is equal to  $1/2 \cdot 1/5 = 1/10$ . The remaining users follow the behavior dictated by state  $s_3 = (0,0,1)$  and are all able to access the arc leading to  $j_3$ . We conclude that the probability of state  $s_3 = (0, 0, 1)$  is 4/10.

#### Network loading algorithm

In this section, we seek to find the solution to the system of flow conservation equations (6.14) and (6.15). If the network is acyclic, it possesses a topological ordering of nodes. Then, the assumption that the subnetwork consisting of uncapacitated arcs is strongly connected is sufficient to guarantee that there exists a

| State     | $j_1$ | $j_2$ | $j_3$ |
|-----------|-------|-------|-------|
| (1, 1, 1) | 1/3   | 2/3   | 0     |
| (0, 1, 1) | 0     | 1     | 0     |
| (1,0,1)   | 1     | 0     | 0     |
| (0,0,1)   | 0     | 0     | 1     |

**Table 6.1** – Probability of users choosing each outgoing link in each possible state for the loading example

finite solution to the system. This solution can be constructed by pushing flows forwards with (6.14) in topological order of the nodes, and calling Algorithm 1 when a considered intersection has capacitated outgoing links. This process is summarized by Algorithm 2. As analyzed by Marcotte et al. (2004), each node is visited exactly once, and at least one outgoing arc reaches capacity at each step of the while loop in Algorithm 1, which is therefore executed at most  $|\mathcal{A}_i^+|$  times. Hence, computational time is equal to  $\sum_{i \in \mathcal{V}} |\mathcal{A}_i^+| = |\mathcal{A}|$ .

#### 6.5.2 Solving value functions

This section aims at proposing an algorithm to compute the best response choice probabilities  $\bar{P}$  (not to be mistaken for an equilibrium solution) after the loading of choice probabilities P. Best response choice probabilities characterize the behavior of individuals corresponding to updated expected travel costs after the network loading. Therefore, at the heart of the algorithm lies the computation of the value functions defined in equations (6.2) and (6.10) in the deterministic and stochastic cases respectively. Note that  $\pi$  is fixed in both equations, and obtained from the network loading phase. In the former case, (6.2) forms a system of piecewise linear equations. On the other hand, the logit model combined with the expectation over  $\pi$  gives rise to non-linearities in (6.10).

In an acyclic network, since there exists a topological ordering of the nodes, it is possible to simply compute the value functions by backwards induction in inverse topological order using (6.2) and (6.10) for the deterministic and stochastic models respectively, as in Algorithm 3. Existence and uniqueness of the solution is then trivially established.

Computing a best response policy is simple once the value function V is solved

and the costs  $\boldsymbol{w}$  are updated accordingly. In the deterministic case, the optimal action  $\alpha^d(s)$  for an individual in state  $s=(i,x_i)$  going to destination d consists in choosing arc  $a \in \mathcal{A}(s)$  such that

$$\alpha^d(s) = \arg\min_{a \in \mathcal{A}(s)} \left\{ w_a^d \right\}. \tag{6.16}$$

and a best response choice probability vector  $\vec{P}$  can be obtained by letting all users choose the best action in each state, or split in equal proportions when several actions attain the optimal cost:

$$\bar{P}_{s,a}^{d} = \frac{I\{\alpha^{d}(s) = a\}}{\sum_{a' \in \mathcal{A}_{i}(k)} I\{\alpha^{d}(s) = a'\}}, \quad \forall d \in \mathcal{D}, s \in \mathcal{S}, a \in \mathcal{A}(s).$$
 (6.17)

In the stochastic case, the optimal action  $\alpha^d(s)$  for an individual in state s traveling to d is

$$\alpha^{d}(s) = \arg\min_{a \in \mathcal{A}(s)} \left\{ w_a^d + \mu \epsilon(a) \right\}. \tag{6.18}$$

Thus each arc a is associated to a probability of being the best action in each state, and the best response choice probabilities  $\bar{P}$  distribute the demand on available outgoing arcs according to this probability function, such that

$$\bar{P}_{s,a}^d = E_{\epsilon_a} \left[ I\{\alpha^d(s) = a\} \right], \quad \forall d \in \mathcal{D}, s \in \mathcal{S}, a \in \mathcal{A}(s)$$
 (6.19)

which, in the case of extreme value type I error terms, is equivalent to a multinomial logit

$$\bar{P}_{s,a}^{d} = \frac{e^{\frac{1}{\mu}\left(w_{a}^{d}\right)}}{\sum_{a' \in A(s)} e^{\frac{1}{\mu}\left(w_{a'}^{d}\right)}}, \quad \forall d \in \mathcal{D}, s \in \mathcal{S}, a \in \mathcal{A}(s).$$

$$(6.20)$$

#### 6.5.3 Heuristic solution algorithm

Finding an equilibrium solution comes down to solving (6.4) or (6.11) depending on whether a deterministic or stochastic choice model is considered. In the following, we discuss properties of these variational inequalities and propose a heuristic to find an equilibrium solution.

In order to ensure the existence of a solution, it suffices that the set  $\mathcal{P}$  be compact and the cost mapping w(P) continuous. We can affirm that the set  $\mathcal{P}$  in

(6.3) is indeed compact. Furthermore, under the SQP rule for accessing capacitated arcs, the mapping  $\boldsymbol{w}(\boldsymbol{P})$  is continuously dependent on availability probabilities  $\boldsymbol{\pi}$ , which are continuous functions of choice probabilities  $\boldsymbol{P}$ . In the stochastic case,  $\bar{\boldsymbol{w}}(\boldsymbol{P})$  contains in addition the term  $\mu \ln(\boldsymbol{P})$ , which is a continuous function of  $\boldsymbol{P}$  as well. Therefore, there exists at least one fixed point solution to each variational inequality. However, we cannot prove the uniqueness of the solution, since the mapping  $\boldsymbol{w}(\boldsymbol{P})$  lacks the property of monotonicity (see Marcotte et al., 2004, for a counterexample).

To solve the problem, we propose a method of successive averages (MSA) which iteratively loads the network, solves the value function, updates the cost mapping, computes best response choice probabilities and finally updates P by taking a convex combination of the current and best response choice probabilities. This is a heuristic solution algorithm, since the non monotonicity of the cost function w(P) does not guarantee the convergence of the method to an equilibrium point. Nevertheless, as we numerically demonstrate in the following sections, the method is well-behaved. Algorithm 4 describes the MSA using a relevant stopping criterion. We propose the choice of  $\theta_n = 1/(n+1)$  for the value of the step size.

The gap between a vector P and an optimal solution can be measured at a more or less aggregate level. We may define the gap associated to a specific state s and destination d as

$$g(P_s^d) = \max_{R \in \mathcal{P}} \langle w_s^d, P_s^d - R_s^d \rangle,$$

and its scaled version as

$$g_R(P_s^d) = \frac{g(P_s^d)}{\langle w_s^d, P_s^d \rangle}.$$

The aggregate relative gap  $g_R(P^d)$  for a destination  $d \in \mathcal{D}$  is a weighted average of the state specific relative gaps by the flow on each state, i.e.,

$$g_R(P^d) = \sum_{s \in \mathcal{S}} p_s^d g_R(P_s^d),$$

where the weights  $p_s^d$  are given by  $\frac{f_s^d}{\sum_{s \in \mathcal{S}} f_s^d}$ . Note in addition that we exclude from the sum all states where only one outgoing arc is available, since the gap in such states is trivially null.

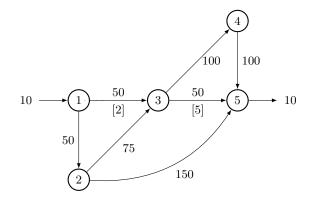


Figure 6.3 – Small capacitated network

| State ID | Node | Availability outgoing links | of |
|----------|------|-----------------------------|----|
| 1        | 1    | (1,1)                       |    |
| 2        | 1    | (1,0)                       |    |
| 3        | 2    | (1,1)                       |    |
| 4        | 3    | (1,1)                       |    |
| 5        | 3    | (1,0)                       |    |
| 6        | 4    | (1)                         |    |
| 7        | 5    | (1)                         |    |

Table 6.2 – Possible states in the example

Finally the aggregate relative gap  $g_R(\mathbf{P})$  for all destinations is given by

$$g_R(\mathbf{P}) = \sum_{d \in \mathcal{D}} q^d g_R(P^d),$$

where the weights  $q^d$  correspond to the proportion of the total demand associated to destination d. While the gap measure  $g_R(\mathbf{P})$  is used as a stopping criterion for Algorithm 4, it remains interesting to analyze the gap at a more disaggregate level, since there may be considerable variance in the state specific gaps.

# 6.6 An illustrative example

Let us consider the network in Figure 6.3, in which each link a is associated with a cost  $c_a$  and possibly a capacity  $u_a$  (bracketed number) as illustrated. The

| State | 1 | 2    | 3    | 4    | 5    |
|-------|---|------|------|------|------|
| 1     | - | 0.50 | 0.50 | -    | -    |
| 2     | - | 1.00 | -    | -    | -    |
| 3     | - | -    | 0.75 | -    | 0.25 |
| 4     | - | -    | -    | -    | 1.00 |
| 5     | - | -    | -    | 1.00 | -    |
| 6     | - | -    | -    | -    | 1.00 |
| 7     | - | -    | -    | -    | 1.00 |

 ${\bf Table~6.3}-{\bf Initial~choice~probability~of~each~available~outgoing~node~in~each~state}$ 

| Strategies | 1      | 2   | 3      | 4   | 5 |
|------------|--------|-----|--------|-----|---|
| $s_1$      | [3, 2] | [3] | [5, 4] | [5] | - |
| $s_2$      | [3, 2] | [5] | [5, 4] | [5] | - |
| $s_3$      | [2]    | [3] | [5, 4] | [5] | - |

Table 6.4 – A set of strategies (Marcotte et al., 2004) for the small network

demand between origin node 1 and destination node 5 is set to 10 units. Since we only consider one destination, we omit the destination index d in the following.

Since there is at most one outgoing arc with limited capacity, each network node corresponds to at most two possible states. The 7 possible states for a user traveling in this network are listed in Table 6.2. In addition, since there are at most two outgoing links per node, in any state where an outgoing link has reached its capacity, the only remaining choice is the other available link.

In the following, we compare the deterministic and stochastic strategic MTE models to the model in Marcotte et al. (2004). We also analyze the performance of the algorithm proposed in Section 6.5.3. We choose initial choice probabilities  $\boldsymbol{P}$  described in Table 6.3.

In their work, Marcotte et al. (2004) consider strategies represented as vectors of size equal to the number of network nodes, prescribing for each an ordered list of successor nodes. Three examples of such strategies are displayed in Table 6.4. For instance, a user following strategy  $s_1$  would choose node 3 from node 1 if the link is available, and node 2 otherwise. Other columns describe the preferences from other nodes. There exists many such strategies, and their number grows exponentially with the size of the network.

Choice probabilities P in this work can be matched to strategic flows x as

| State | 1 | 2    | 3    | 4    | 5    |
|-------|---|------|------|------|------|
| 1     | - | 0.00 | 1.00 | -    | -    |
| 2     | - | 1.00 | -    | -    | -    |
| 3     | - | -    | 0.50 | -    | 0.50 |
| 4     | - | -    | -    | 0.00 | 1.00 |
| 5     | - | -    | -    | 1.00 | -    |
| 6     | - | -    | -    | -    | 1.00 |
| 7     | - | -    | -    | -    | 1.00 |

 ${\bf Table~6.5}-{\bf Equilibrium~choice~probability~of~each~available~outgoing~node~in~each~state}$ 

defined in Marcotte et al. (2004). For instance, the link choice probabilities characterized by the initial  $\mathbf{P}$  are equivalent to a flow on strategies given by  $x = (\frac{1}{4}, \frac{1}{4}, \frac{1}{2})$ , when restricting the number of possible strategies to the three displayed in Table 6.4.

At equilibrium, Marcotte et al. (2004) state that demand is equally split between strategies  $s_1$  and  $s_2$ , of equal expected cost 185, and receiving each 5 units of flow. In other words, the optimal flow on strategies is  $x^* = (\frac{1}{2}, \frac{1}{2}, 0)$ . Both strategies differ only at node 2, where  $s_1$  selects node 3 and  $s_2$  node 5. We can find an equivalent deterministic equilibrium  $P^*$  in the space of choice probabilities, given by Table 6.5, as incoming flow splits in equal proportion between both outgoing arcs from node 2.

#### 6.6.1 Deterministic assignment

Table 6.6 displays the relevant values of P for successive iterations of the algorithm. In particular we look at specific components of P and w corresponding to states 1 and 3, since the other components of P are already at equilibrium. Finally, the last columns displays aggregate and state-specific relative gap values.

The algorithm converges towards the solution  $P^*$  given above, which is equivalent to the equilibrium solution found in Marcotte et al. (2004). In general, we observe that the gap at specific states exceeds the aggregate gap, which is 0.01% after 1000 iterations. This is because the latter is lowered by taking into account some states where the gap is null.

In Marcotte et al. (2004), all used strategies have the same expected cost at equilibrium. Similarly, we observe here that all chosen actions at a given state have the same expected cost. When an equilibrium is reached, both outgoing links in

|        |           | Choice pr | obabilitie | S         |           | Costs     |           |           |        | Gap (%)    |            |              |
|--------|-----------|-----------|------------|-----------|-----------|-----------|-----------|-----------|--------|------------|------------|--------------|
| # Iter | $P_{1,2}$ | $P_{1,3}$ | $P_{3,3}$  | $P_{3,5}$ | $w_{1,2}$ | $w_{1,3}$ | $w_{3,4}$ | $w_{3,5}$ | $V_1$  | $g_R(P_1)$ | $g_R(P_3)$ | $g_R({m P})$ |
| 0      | 0.5000    | 0.5000    | 0.7500     | 0.2500    | 200.00    | 156.25    | 181.25    | 150.00    | 182.50 | 12.28      | 13.51      | 9.25         |
| 1      | 0.2500    | 0.7500    | 0.3750     | 0.6250    | 175.00    | 100.00    | 125.00    | 150.00    | 155.00 | 15.79      | 11.11      | 8.36         |
| $^2$   | 0.1667    | 0.8333    | 0.5833     | 0.4167    | 200.00    | 137.50    | 162.50    | 150.00    | 185.00 | 7.04       | 4.64       | 3.51         |
| 3      | 0.1250    | 0.8750    | 0.4375     | 0.5625    | 188.64    | 113.64    | 138.64    | 150.00    | 171.49 | 7.62       | 4.41       | 3.45         |
| 4      | 0.1000    | 0.9000    | 0.5500     | 0.4500    | 200.00    | 132.81    | 157.81    | 150.00    | 185.07 | 4.82       | 2.78       | 2.17         |
| 5      | 0.0833    | 0.9167    | 0.4583     | 0.5417    | 192.65    | 117.65    | 142.65    | 150.00    | 176.28 | 5.04       | 2.72       | 2.16         |
| 10     | 0.0455    | 0.9545    | 0.5227     | 0.4773    | 200.00    | 128.68    | 153.68    | 150.00    | 185.06 | 2.46       | 1.26       | 1.01         |
| 20     | 0.0238    | 0.9762    | 0.5119     | 0.4881    | 200.00    | 126.95    | 151.95    | 150.00    | 185.03 | 1.35       | 0.66       | 0.54         |
| 50     | 0.0098    | 0.9902    | 0.5049     | 0.4951    | 200.00    | 125.81    | 150.81    | 150.00    | 185.02 | 0.57       | 0.27       | 0.22         |
| 100    | 0.0050    | 0.9950    | 0.5025     | 0.4975    | 200.00    | 125.41    | 150.41    | 150.00    | 185.01 | 0.29       | 0.14       | 0.11         |
| 200    | 0.0025    | 0.9975    | 0.5012     | 0.4988    | 200.00    | 125.21    | 150.21    | 150.00    | 185.00 | 0.15       | 0.07       | 0.06         |
| 500    | 0.0010    | 0.9990    | 0.5005     | 0.4995    | 200.00    | 125.08    | 150.08    | 150.00    | 185.00 | 0.06       | 0.03       | 0.02         |
| 1000   | 0.0005    | 0.9995    | 0.5002     | 0.4998    | 200.00    | 125.04    | 150.04    | 150.00    | 185.00 | 0.03       | 0.01       | 0.01         |

Table 6.6 – Iterations of the deterministic assignment algorithm

state 3 have a cost of 150, while in state 1 the only chosen outgoing link has a cost of 125, which is less than the cost of the other link. Note that the expected cost of the best strategy for the OD pair is equivalent to the value function V at the origin state s=1, as it represents the minimum expected cost to reach destination. As expected, the latter indeed converges to 185.

#### 6.6.2 Stochastic assignment

We next apply the stochastic version of the algorithm, assuming that arc costs are random and given by  $c_a + \mu \epsilon_a$ . Table 6.7 gives the choice probabilities  $\boldsymbol{P}$  and value function  $\boldsymbol{V}$  at origin state after 1000 iterations for different values of the scale parameter  $\mu$ .

As expected, when  $\mu$  is small, the assignment is close to a deterministic one and the equilibrium choice probabilities are close to the values in Table 6.6. On the other hand, when  $\mu$  becomes very large, we observe that the choice of arc is close to a random draw. From arc 2, the flow splits between arcs 4 and arcs 5 in proportion  $\frac{2}{3}$  and  $\frac{1}{3}$  respectively. This is because there are two paths to the destination from arc 4, and only one from arc 5. Similarly from arc 1, choice probabilities converge towards  $\frac{3}{5}$  and  $\frac{2}{5}$  respectively. The expected minimum cost given by  $\boldsymbol{V}$  at the origin state is close to 185 when the value of  $\mu$  is small, and decreases as  $\mu$  tends to infinity and the magnitude of the error term becomes large. Intuitively, the large variance among perceived costs decreases the expected value of the minimum cost.

| $\mu$  | $P_{1,2}$ | $P_{1,3}$ | $P_{3,3}$ | $P_{3,5}$ | $V_1$     |
|--------|-----------|-----------|-----------|-----------|-----------|
| 0.5    | 0.0005    | 0.9995    | 0.5000    | 0.5000    | 184.72    |
| 1      | 0.0005    | 0.9995    | 0.5000    | 0.5000    | 184.44    |
| 5      | 0.0005    | 0.9995    | 0.5000    | 0.5000    | 182.22    |
| 10     | 0.0016    | 0.9984    | 0.5000    | 0.5000    | 179.43    |
| 20     | 0.0454    | 0.9546    | 0.5003    | 0.4997    | 173.12    |
| 30     | 0.1406    | 0.8594    | 0.5035    | 0.4965    | 165.28    |
| 50     | 0.2996    | 0.7004    | 0.5224    | 0.4776    | 145.83    |
| 100    | 0.4495    | 0.5505    | 0.5789    | 0.4211    | 84.41     |
| 1000   | 0.5857    | 0.4143    | 0.6561    | 0.3439    | -1125.60  |
| _10000 | 0.5985    | 0.4015    | 0.6656    | 0.3344    | -13309.00 |

**Table 6.7** – Choice probabilities P and expected minimum cost at origin state  $V_1$  for different values of  $\mu$  after 1000 iterations (common step size)

|        |           | Choice pr | obabilities | 3         |                 | Costs           |                 |                 |        | Gap (%)    |            |                   |  |
|--------|-----------|-----------|-------------|-----------|-----------------|-----------------|-----------------|-----------------|--------|------------|------------|-------------------|--|
| # Iter | $P_{1,2}$ | $P_{1,3}$ | $P_{3,3}$   | $P_{3,5}$ | $\bar{w}_{1,2}$ | $\bar{w}_{1,3}$ | $\bar{w}_{3,4}$ | $\bar{w}_{3,5}$ | $V_1$  | $g_R(P_1)$ | $g_R(P_3)$ | $g_R(\mathbf{P})$ |  |
| 0      | 0.5000    | 0.5000    | 0.7500      | 0.2500    | 199.65          | 155.90          | 181.11          | 149.31          | 182.50 | 12.30      | 13.77      | 9.38              |  |
| 1      | 0.2500    | 0.7500    | 0.3750      | 0.6250    | 174.31          | 99.86           | 124.51          | 149.77          | 155.00 | 15.71      | 11.25      | 8.42              |  |
| $^2$   | 0.1667    | 0.8333    | 0.5833      | 0.4167    | 199.10          | 137.41          | 162.23          | 149.56          | 185.00 | 6.96       | 4.71       | 3.53              |  |
| 3      | 0.1250    | 0.8750    | 0.4375      | 0.5625    | 187.60          | 113.57          | 138.22          | 149.71          | 171.49 | 7.53       | 4.47       | 3.46              |  |
| 4      | 0.1000    | 0.9000    | 0.5500      | 0.4500    | 198.85          | 132.76          | 157.51          | 149.60          | 185.07 | 4.74       | 2.83       | 2.18              |  |
| 5      | 0.0833    | 0.9167    | 0.4583      | 0.5417    | 191.40          | 117.60          | 142.26          | 149.69          | 176.28 | 4.97       | 2.75       | 2.17              |  |
| 10     | 0.0455    | 0.9545    | 0.5227      | 0.4773    | 198.45          | 128.65          | 153.35          | 149.63          | 185.06 | 2.41       | 1.28       | 1.01              |  |
| 20     | 0.0238    | 0.9762    | 0.5116      | 0.4884    | 198.12          | 126.89          | 151.57          | 149.64          | 185.02 | 1.32       | 0.63       | 0.51              |  |
| 50     | 0.0098    | 0.9902    | 0.5002      | 0.4998    | 197.36          | 125.03          | 149.69          | 149.65          | 184.60 | 0.56       | 0.00       | 0.08              |  |
| 100    | 0.0050    | 0.9950    | 0.5000      | 0.5000    | 197.00          | 125.00          | 149.65          | 149.65          | 184.65 | 0.28       | 0.00       | 0.04              |  |
| 200    | 0.0025    | 0.9975    | 0.5000      | 0.5000    | 196.66          | 125.00          | 149.65          | 149.65          | 184.69 | 0.14       | 0.00       | 0.02              |  |
| 500    | 0.0010    | 0.9990    | 0.5000      | 0.5000    | 196.20          | 125.00          | 149.65          | 149.65          | 184.71 | 0.00       | 0.00       | 0.01              |  |
| 1000   | 0.0005    | 0.9995    | 0.5000      | 0.5000    | 195.85          | 125.00          | 149.65          | 149.65          | 184.72 | 0.00       | 0.00       | 0.00              |  |

Table 6.8 – Iterations of the stochastic assignment algorithm for  $\mu=0.5$ 

In Table 6.8, we look in detail at the iterations of the algorithm for  $\mu = 0.5$ . We observe that the gap converges to zero faster than in the deterministic case.

| OD pair | Notation | Demand | Destination index |
|---------|----------|--------|-------------------|
| (1,24)  | OD1      | 35     | $d_1$             |
| (1,22)  | OD2      | 25     | $d_2$             |
| (7,24)  | OD3      | 20     | $d_1$             |
| (7,22)  | OD4      | 20     | $d_2$             |

**Table 6.9** – OD pairs for Sioux Falls network

## 6.7 Numerical experiments

In the following we present two applications of the model. The first one is a simplified and acyclic version of the Sioux Falls network, also used as a numerical example in Marcotte et al. (2004). The network is more complex than the illustrative example, but small enough to analyze in detail the solution of the assignment. The second one is a larger scale experiment involving a time-expanded transit network of over 2000 links.

#### 6.7.1 Sioux Falls network

The network is depicted in Figure 6.4 and contains 24 nodes and 41 links. It has up to 4 outgoing arcs per node, up to three of which may have a limited capacity. In total there are 14 capacitated arcs. We consider four OD pairs with demand described in Table 6.9.

We first solve the deterministic equilibrium. Table 6.10 displays the value function  $V^d$  at origin for each OD pair at equilibrium. The values can be interpreted as the expected minimum cost to travel between each OD pair, and they are close to the minimum strategic costs found in Marcotte et al. (2004). The aggregate relative gap is well below 1%, at around 0.03%.

In contrast with Marcotte et al. (2004), it is not possible to analyze the number of different strategies used at equilibrium, since we cannot recover strategic flows from arc flows. Instead, we may observe for how many couples (s, d) there exist two different outgoing arcs in  $\mathcal{A}(s)$  with non null choice probabilities  $P_{s,a}^d$ . Therefore in Table 6.11, we display the nodes for which there exists outgoing links with equal expected minimum cost, and display the value of corresponding choice probabilities in the state where both links are available. We also analyze the specific relative gap at the corresponding states. In all cases the value is small, illustrating that the

| Expe   | Gap (%) |        |       |                      |
|--------|---------|--------|-------|----------------------|
| OD1    | OD2     | OD3    | OD4   | $g_R(m{P})$          |
| 120.00 | 139.94  | 112.97 | 99.97 | $2.97 \cdot 10^{-2}$ |

**Table 6.10** - Expected minimum cost of OD pairs after 1000 iterations of the deterministic assignment algorithm

| Destination | Node                   | Tail node of outgoing links          | $\operatorname*{Costs}_{w_{s,a}^{d}}$                   |  |  | obabilities $d_{s,a}$                          | $\operatorname{Gap}(\%) \\ g_R(P_s^d)$   |
|-------------|------------------------|--------------------------------------|---|--|--|--|--|
| 24          | 3<br>19                | 4,12<br>20,22                        | 110.0122<br>54.6733                                     | 110.0000<br>55.0000                                      | 0.3263<br>0.9222                               | 0.6737<br>0.0778                               | $3.61 \cdot 10^{-3} \\ 9.92 \cdot 10^{-2}$   |
| 22          | 1<br>7<br>3<br>4<br>10 | 2,3<br>8,18<br>4,12<br>5,11<br>11,17 | 139.9361<br>99.9748<br>129.9361<br>119.9392<br>119.9322 | 139.9748<br>100.0000<br>130.0000<br>119.9322<br>119.4173 | 0.9980<br>0.7176<br>0.8812<br>0.4880<br>0.2834 | 0.0020<br>0.2824<br>0.1188<br>0.5120<br>0.7166 | $5.52 \cdot 10^{-5}$ $7.12 \cdot 10^{-3}$ $5.84 \cdot 10^{-3}$ $2.87 \cdot 10^{-3}$ $1.20 \cdot 10^{-1}$ |

Table 6.11 – Outgoing links with equal strategic cost for each destination after 1000 iterations

aggregate gap value does not conceal large variance.

We then apply the stochastic user equilibrium algorithm on the network for several values of  $\mu$ . From the data diplayed in Table 6.12, we observe that for  $\mu = 0.5$  the expected minimum costs obtained are close to the deterministic solution, while they decrease as  $\mu$  increases.

|       | Expe   | Gap (%) |        |       |                      |
|-------|--------|---------|--------|-------|----------------------|
| $\mu$ | OD1    | OD2     | OD3    | OD4   | $g_R(m{P})$          |
| 0.5   | 119.74 | 138.92  | 114.72 | 99.61 | $2.15 \cdot 10^{-2}$ |
| 5     | 116.83 | 131.42  | 113.00 | 96.23 | $6.26 \cdot 10^{-3}$ |
| 10    | 112.00 | 119.25  | 107.38 | 88.50 | $7.99 \cdot 10^{-2}$ |
| 20    | 95.57  | 106.02  | 94.11  | 80.25 | $9.10 \cdot 10^{-3}$ |

Table 6.12 – Expected minimum cost of OD pairs after 1000 iterations of the stochastic assignment algorithm with different values of  $\mu$ 

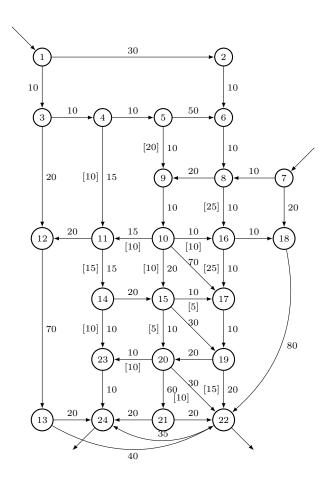


Figure 6.4 – Sioux Falls network

#### 6.7.2 Springfield network

The Springfield network is a 5-zone network that was developed as a generic example for the fast trips Dynamic Transit Passenger Assignment tool (Khani, 2013). The network is composed of three transit lines, as displayed in Figure 6.5, several walking links and a transfer link between transit stops  $B_2$  and  $R_2$ . The train line going through stops  $R_1$ ,  $R_2$  and  $R_3$  has a capacity of 16 units, and the two bus lines have a capacity of 10.

In this example, we apply the strategic Markovian traffic equilibrium model to the time-expanded version of the Springfield network. The transit schedule is given between 3PM and 6PM and there are 152 runs of the transit lines. Demand starts at 3:15 PM, ends at 5:15 PM and is characterized by a trip every ten seconds between two of the five possible zones. Each trip has a latest desired arrival time of 30 minutes after departure time.

We create an acyclic time-space network based on the static bidirectional network in Figure 6.5 and the given schedule. To do so, we build four types of arcs: transit arcs, corresponding to each run of a transit line between two consecutive stops; transfer arcs, connecting two transit stops (here  $B_2$  and  $R_2$ ); walking arcs, between zones and accessible transit stops; waiting arcs, connecting the same zone or transit stop between two consecutive discrete points in time. Transfer and walking arcs are created not at regular time intervals but rather for each arrival or departure of a transit line at the stop. Thus time in this approach is discretized according to the transit schedule. We assume that the capacity of waiting, transfer and walking arcs is infinite.

Artificial origin and destination links are also created to match the dynamic OD information. For each trip in the OD table, an origin link is created at the origin zone, so as to be connected with the first walking arc to leave the zone from the stated departure time. Similarly, a destination link without successor is added at the arrival zone and is connected to the link arriving at the zone at a time closest to the latest desired arrival time. We ensure that the time interval between earliest possible departure and latest possible arrival is at least 30 minutes. Note that origin and destination links are also connected to waiting arcs. Therefore, the demand may leave and arrive at any time between the stated departure time and latest possible arrival time, and use waiting arcs in between. The total number of arcs in the time-expanded network is 2961.

The cost of transit, transfer and walking arcs displayed in Figure 6.5 correspond to the travel time in minutes between nodes. The cost of waiting arcs is equal to the waiting time, which can be inferred from the time index at the nodes of the time-expanded network. However, the cost of waiting arcs at origin and destination zones is upper bounded by a small value (20 seconds). Thus the cost provides individuals with an incentive to arrive earlier at destination if possible and spend less time traveling.

We assume that passengers are loaded randomly at each node. It is usual in dynamic transit assignment to make more complex assumptions, typically that passengers arriving first at a node are loaded before those arriving at a later time step. However, since boarding priorities and first-come first-serve loading is beyond the scope of this paper, we illustrate the model on this example with the assumptions described in Section 6.5.1.

We compute the deterministic and stochastic user equilibrium. We set  $\mu$  to the intermediate value of 5 for the stochastic case. Table 6.13 shows the value of the aggregate gap for iterations of the deterministic and stochastic algorithms. We observe that the algorithm follows the typical slow convergence rate where the gap is roughly halved when the number of iterations double.

While the aggregate gap shows that choice probabilities globally tend towards the equilibrium solution, it is not the only way to investigate the gap. For instance, Table 6.14 displays disaggregate values of the gap for specific destinations and states. In particular, for each destination d, we compare two different gap functions, i.e., the maximum relative gap across all states  $\max_s g_R(P_s^d)$ , and the average of  $g_R(P_s^d)$  over all states. We then show the lowest, highest and average values of these measures across all destinations after 1000 iterations. For the worse destination and state, there is still an 7.60% and 11.34% relative gap for the deterministic and stochastic model respectively. Although it is unnecessarily demanding to require the gap to reach a very low value in all states, this shows that there may be significant variance in the gap across the network.

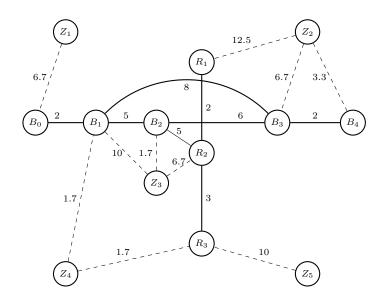


Figure 6.5 – Springfield network

|        | Gap (%)              |                      |  |
|--------|----------------------|----------------------|--|
| # Iter | Deterministic        | Stochastic           |  |
| 0      | 1.70                 | 2524.00              |  |
| 1      | 1.77                 | 31.61                |  |
| 2      | 1.62                 | 9.54                 |  |
| 3      | 1.42                 | $9.43 \cdot 10^{-1}$ |  |
| 4      | 1.29                 | $7.40 \cdot 10^{-1}$ |  |
| 5      | 1.14                 | $5.83 \cdot 10^{-1}$ |  |
| 10     | $7.30 \cdot 10^{-1}$ | $2.85 \cdot 10^{-1}$ |  |
| 20     | $4.44 \cdot 10^{-1}$ | $1.19 \cdot 10^{-1}$ |  |
| 50     | $1.94 \cdot 10^{-1}$ | $3.49 \cdot 10^{-2}$ |  |
| 100    | $1.07 \cdot 10^{-1}$ | $2.93 \cdot 10^{-2}$ |  |
| 200    | $5.63 \cdot 10^{-2}$ | $1.73 \cdot 10^{-2}$ |  |

 ${\bf Table~6.13-Values~of~aggregate~gap~at~iterations~of~the~deterministic~and~stochastic~assignment~algorithm}$ 

|                             | Maximum state specific gap (%)             |  |   |
|-----------------------------|--|--|---|
| Assignment                  | $\min_d \max_s g_R(P_s^d)$                 | $\max_d \max_s g_R(P_s^d)$                 | $\operatorname{mean}_d \operatorname{max}_s g_R(P_s^d)$                 |
| Deterministic<br>Stochastic | $2.92 \cdot 10^{-2} \\ 6.98 \cdot 10^{-4}$ | 7.60<br>11.34                              | $0.33 \\ 0.44$  |
|                             | Average state specific gap (%)             |  |   |
| Assignment                  | $\min_d \operatorname{mean}_s g_R(P_s^d)$  | $\max_d \operatorname{mean}_s g_R(P_s^d)$  | $\operatorname{mean}_d \operatorname{mean}_s g_R(P_s^d)$                |
| Deterministic<br>Stochastic | $6.93 \cdot 10^{-4} \\ 7.45 \cdot 10^{-6}$ | $1.69 \cdot 10^{-2} \\ 7.83 \cdot 10^{-2}$ | $\begin{array}{c} 8.38 \cdot 10^{-3} \\ 3.28 \cdot 10^{-3} \end{array}$ |

**Table 6.14** – Different gap values after 1000 iterations for both the deterministic and stochastic assignment algorithm

#### 6.8 Discussion

We presented a strategic Markovian traffic equilibrium model for capacitated networks, which provides a framework to compute both deterministic and stochastic user equilibrium. The model builds on the work of Baillon and Cominetti (2008) on Markovian traffic equilibrium by considering travel cost functions which instead of bounding flows through exogenous volume-delay functions incorporate the risk of failing to board an arc, thereby allowing users to behave strategically with respect to the stochasticity induced by limits on capacity. The model possesses a travel cost function which explicitly derives delay from an emulation of the queuing process to access capacitated arcs. In that respect, the model is also an extension of the work of Marcotte et al. (2004), who first proposed the concept of strategic equilibrium in the context of deterministic arc costs.

Both approaches are relatively disconnected in the literature, and our contribution consists in merging both models, through the main idea of connecting the concept of strategies (or "hyperpaths") to MDPs with stochastic state transitions. The resulting model has the advantage of incorporating two sources of stochasticity in user route choice behavior, induced by variations in cost perception and the risk associated with the failure to access an arc. Through its arc-based formulation, the model is tractable, requires neither path or hyperpath enumeration nor storage of path-based variables, and can capture strategic user behavior with recourse using relatively few parameters.

The main restriction of this paper is related to the assumption of acyclic net-

works which underlies several models related to ours (Marcotte et al., 2004; Unnikrishnan and Waller, 2009; Wong, 1999). Some issues require careful consideration when extending the proposed framework to cyclic networks. The core of the challenge revolves around the two inner algorithms proposed in Section 6.5, which aim to find a fixed point solution to the flow conservation equations and the value function respectively defined in this work. In the absence of a topological ordering of nodes, these procedures need to be updated in order to iteratively construct a solution. One straightforward method would consist of fixed point iterations measuring the amount of imbalance between left-hand side and right-hand side of the equation at each node, and treating nodes with the largest imbalance first until the maximum error reaches a certain threshold. The open questions are then (i) under which conditions there exists a unique solution to both equations in this context, and (ii) whether the proposed algorithms can be proven to converge to it.

A critical issue is that there may be no finite solution to the flow conservation equations for some choice probability vectors. Infinite arc flows are known to occur in models which allows cyclic behavior if traveling is not sufficiently costly, resulting in a share of the demand never reaching the destination (see, e.g., Akamatsu, 1996). In a network with limited capacity, this outcome is yet more difficult to prevent. Intuitively, it happens when a too large proportion of users seeks to gain access to capacitated arcs and fails to consider uncapacitated options as a recourse, an issue well-documented in Boyles et al. (2015) in the context of a parking search equilibrium model. They defined the notion of strong feasibility in order to characterize choice probability vectors ensuring finite arc flows. In the context of our modeling framework, we identify two practical issues compromising the existence of finite arc flows throughout iterations of MSA, namely, (i) the set of strongly feasible choice probability vectors may not be compact, i.e., the linear combination of two strongly feasible solutions performed by MSA may deviate from strong feasibility, and (ii) the best response choice probabilities may actually not be strongly feasible. An example of the latter is when a proportion of flow which is denied access to a cheap outgoing arc makes cycles to revisit the node in question. While such behavior may seem contradictory, it is an inherent feature of the model. Indeed observing the availability state of an arc does not affect travelers' choice probabilities at other intersections (which depend on expected costs computed at the previous iteration).

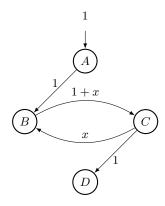


Figure 6.6 – Non uniqueness of arc flows

Besides existence is the question of uniqueness. Considering the example in Figure 6.6 where link C-D is assumed to have capacity 1 and one unit of demand travels between OD pair A-D, we observe that there is not always a unique finite solution to flow conservation equations. Indeed, any value of x produces valid arc flows with a probability 1/(1+x) to access arc C-D, although x=0 is logical. Therefore, future work considering cyclic networks may require to introduce a notion of minimal feasible flows in order to characterize natural solutions to flow conservation equations. If a unique solution can be defined, converging to it might be more difficult in the case of multiple destinations. A loading algorithm for cyclic networks must be careful that the order in which nodes are visited still allows destinations to compete fairly for available capacity. This may require designing more complex algorithms which load capacitated links step by step, inspired from dynamic traffic assignment.

Regarding the solution to Bellman's equation, existence and uniqueness is also not trivial to establish. Proofs of existence and uniqueness of a solution in the literature do not apply when future costs are not discounted. This issue has been discussed in several works, in particular in Fosgerau et al. (2013), Baillon and Cominetti (2008) and Arıkan and Ahipasaoglu (2017), who stated that the existence of a solution depends in particular on the balance between the number of paths in the network and the magnitude of arc costs. If a solution exists, value iterations should converge, however further numerical experiments are required to determine the efficiency of the algorithm on cyclic networks.

#### Algorithm 1 Capload

```
1: procedure CAPLOAD(\boldsymbol{\pi}, \boldsymbol{P}, \boldsymbol{g}, \boldsymbol{f}, i)
             Initialization:
 2:
            \zeta_i^d \leftarrow g_i^d + \sum_{(h,i) \in \mathcal{A}_i^-} f_{hi}^d
 3:
                                                                                                        ▶ Initial incoming demand
             x_i \leftarrow \{1\}^{\mathcal{A}_i^+}
                                                                                  ▷ Initial availability: all arcs available
 4:
             \pi_{i,x} \leftarrow 1 \text{ if } x = x_i, 0 \ \forall x \in X_i \neq x_i
                                                                                           ▶ Initial availability distributions
 5:
            for (i,j) \in \mathcal{A}_i^+ do
 6:
                   f_{ij}^d \leftarrow 0
 7:
                                                                                                                ▶ Initial outgoing flow
                                                                                                                         ▶ Initial capacity
 8:
                   v_{ij} \leftarrow u_{ij}
             end for
 9:
10:
             while not stop do
                   \begin{array}{ccc} \mathbf{for} \ (i,j) \in \mathcal{A}_i^+ \ \mathbf{do} \\ \tilde{f}_{ij}^d \leftarrow P_{(i,x_i),j}^d \zeta_i^d & \forall d \in \mathcal{D} \end{array}
11:
                                                                                                                        ▷ Distribute flows
12:
                         \tilde{f}_{ij} \leftarrow \sum_{d \in \mathcal{D}} \tilde{f}_{ij}^d
13:
                   end for
14:
                   \beta \leftarrow \min\{1, \min_{(i,j) \in \mathcal{A}_{\cdot}^{+}} \{v_{ij}/\tilde{f}_{ij}\}\}
15:
                   for (i,j) \in \mathcal{A}_i^+ do
16:
                  v_{ij} \leftarrow v_{ij} - \beta \tilde{f}_{ij}
f_{ij}^d \leftarrow f_{ij}^d + \beta \tilde{f}_{ij}^d \quad \forall d \in \mathcal{D}
end for
                                                                                                    ▶ Update residual capacities
17:
                                                                                                            ▶ Update outgoing flows
18:
19:
                   if \beta < 1 then
20:
                                                                                         ▷ Save probability of current state
21:
                          p \leftarrow \pi_{i,x_i}
                                                                                    ▶ Update probability of current state
22:
                          \pi_{i,x_i} \leftarrow \beta p
                         b = \arg\min_{(i,j)\in\mathcal{A}^+} \{u_{ij}/\tilde{f}_{ij}\}
                                                                                                                   ▶ New saturated arc
23:
                          x_i(b) \leftarrow 0
                                                                                                  \triangleright Update availability of b at i
24:
                         \pi_{i,x_i} \leftarrow (1 - \beta)p
\zeta_i^d \leftarrow (1 - \beta)\zeta_i^d \quad \forall d \in \mathcal{D}
                                                                                         ▶ Update probability of new state
25:
                                                                                            ▶ Update residual incoming flow
26:
27:
28:
                          stop
29:
                   end if
             end while
30:
             return \{f_{ij}^d\}_{(i,j)\in\mathcal{A}_i^+}, \{\pi_i, x\}_{x\in X_i}
31:
32: end procedure
```

#### Algorithm 2 Load acyclic network

```
1: procedure LOADNETWORK(u, P, g)
 2:
           Initialization:
 3:
           for i \in \mathcal{V} do
                 x_i \leftarrow \{1\}^{\mathcal{A}_i^+}
 4:
                                                                        ▶ Initial availability: all arcs available
                 \pi_{i,x} \leftarrow 1 \text{ if } x = x_i, 0 \ \forall x \in X_i \neq x_i
                                                                                ▶ Initial availability distributions
 5:
           end for
 6:
           while Not all nodes visited do
 7:
                 i \leftarrow \text{next node in topological order}
 8:
                 if u_{ij} = \infty \quad \forall (i,j) \in \mathcal{A}_i^+ then
 9:
                       Uncapacitated intersection:
10:
                      for (i, j) \in \mathcal{A}_i^+ do
11:
                            f_{ij}^d \leftarrow P_{(i,x_i),j}^d \left( g_i^d + \sum_{(h,i) \in \mathcal{A}_i^-} f_{hi}^d \right) \quad \forall d \in \mathcal{D} \quad \triangleright \text{ Distribute flows}
12:
13:
                 else
14:
15:
                       Capacitated intersection:
                      \{f_{ij}^d\}_{(i,j)\in\mathcal{A}_i^+}, \{\pi_i,x\}_{x\in X_i} \leftarrow \mathrm{Capload}(\boldsymbol{u},\boldsymbol{P},\boldsymbol{g},\boldsymbol{f},i)
16:
                 end if
17:
           end while
18:
           return f, \pi
19:
20: end procedure
```

#### Algorithm 3 Solve value function in acyclic networks

```
1: procedure SOLVEVALUEFUNCTION(\pi, \mu)

2: Initialization:

3: V^d(i, x_i) \leftarrow 0 \quad \forall d \in \mathcal{D}, i \in \mathcal{V}, x_i \in \Omega_i

4: for all nodes i in inverse topological order do

5: V^d(i, x_i) \leftarrow \text{RHS } (6.2) \text{ or } (6.10) \quad \forall d \in D, x_i \in \Omega_i

6: end for

7: return V

8: end procedure
```

#### Algorithm 4 Method of successive averages

```
1: procedure MSA(\boldsymbol{P}, \boldsymbol{u}, \boldsymbol{g}, \mu, \epsilon)
           Initialization:
 2:
           n = 1
 3:
           while g_R(\mathbf{P}) > \epsilon do
 4:
                 oldsymbol{f}, oldsymbol{\pi} \leftarrow 	ext{LoadNetwork}(oldsymbol{u}, oldsymbol{P}, oldsymbol{g})
 5:
                 V \leftarrow \text{SolveValueFunction}(\pi, \mu)
 6:
                Update \boldsymbol{w} from (6.1)
 7:
                Compute optimal \bar{P} from (6.17) or (6.20)
 8:
                m{P} \leftarrow m{P} + 	heta_n (ar{m{P}} - m{P})
 9:
                 n \leftarrow n+1
10:
           end while
11:
12: end procedure
```

# Conclusion and outlook

This thesis presented four articles addressing a number of issues related to estimating models of travel demand behavior and predicting flows in transportation networks. The first article is a tutorial on a state-of-the-art modeling framework to analyze and predict the path choice behavior of network users, called recursive route choice modeling, initially introduced by Fosgerau et al. (2013). Two articles and an additional chapter can be categorized as applications of the latter modeling framework to various problems of travel demand estimation, by framing them as path choice in a supernetwork. Finally, the last article is a methodological contribution to the field of traffic equilibrium modeling using a recursive approach.

The common thread to all the papers in this thesis is the methodology at their core, namely recursive models of route choice behavior. This thesis pursues the development and application of this methodology in the direction of modeling more complex choice situations (involving several transportation modes, but also other choice dimensions) and network settings (considering limited capacity of links). Notwithstanding their similarities, each paper addresses specific issues related to the over arching theme of multi-modal networks. Below, we review in detail the contributions of each article.

### 7.1 Synthesis of work

Chapter 2 begins the thesis with a tutorial on recursive route choice models. This work introduces the modeling framework in a didactic fashion, while taking a new perspective on this research topic. We present the problem of route choice analysis as one of inverse optimization with noisy data, which allows to establish links between recursive route choice models (traditionally viewed as probabilistic

demand models in the transportation research community), and works in inverse reinforcement learning and inverse optimization. We gain from this perspective some intuition behind the biases of path-based discrete choice models and the advantage of the recursive counterpart; we illustrate the latter with toy examples. The following chapters offer practical examples of the applicability of this methodological framework.

In Chapter 3, we focus on cyclists' route choice behavior, while in Chapter 4 we consider the more complex case of public transportation networks involving several modes (bus, tram, train). The findings in both these chapters are very relevant for policy analysis and practice. While predicting bike flows in urban networks does not necessitate to apply traffic assignment procedures, as it can usually be assumed that there is no congestion on cycling lanes, it requires to consider a large set of built environment attributes, such as slope or presence of bike facilities. The utility specification we propose in Chapter 3 allows to precisely evaluate behavioral trade-offs, such as what detours are cyclists willing to make to avoid heavy traffic volumes or high slopes. In Chapter 4, we perform a similar analysis with respect to attributes of transit trips, such as transfers and in-vehicle time for different modes. We note here that this analysis is pursued at the scale of a full multi-modal network combining both transit, bike and walk arcs in de Freitas et al. (2019).

In contrast to de Freitas et al. (2019), the transit network in Chapter 4 is time-expanded. While greatly increasing its size, it allows to model decisions of timing of trips, which are intrinsically linked to the choice of route when available itineraries depend on a schedule. Understanding timing decisions is also crucial for policy analysis, as several policies attempt to alleviate congestion by inciting travelers to reschedule their trips before or after peak hours. The activity-based approach to travel demand argues further that timing and mode choices of trips are in fact part of an interrelated set of decisions including also what out-of-home activity to perform, where and for how long. In Chapter 5, we follow this avenue of research and consider an even larger supernetwork, expanded in time and other dimensions. We specifically tackle the issues of correlation across alternatives and model estimation in presence of the curse of dimensionality. Our results are important for policy analysis as well, in particular allowing for correctly predicting how individuals substitute their chosen alternative for a different one in scenario evaluations.

The previously mentioned chapters focused primarily on the demand estimation problem and the behavioral interpretation of results. However, route choice models are also powerful tools in order to predict network flows, and, when congestion is present, can be incorporated in a model of traffic assignment. A recursive link-based model of traffic assignment (the so-called Markovian traffic equilibrium model) was proposed by Baillon and Cominetti (2008). In Chapter 6, we address a main limitation of the MTE model: when networks links have strict capacities, which may typically but not exclusively occur in public transportation networks, the classical equilibrium principle does not hold anymore. We propose a strategic Markovian traffic equilibrium model which assigns flows to networks without exceeding link capacities while realistically modeling how the risk of not being able to access an arc affects route choice behavior.

#### 7.2 Limitations and outlook

While this thesis makes progress in the direction of traffic modeling in large scale multi-modal networks, it has its limitations. Ideally, the goal of future research would be to accurately and efficiently predict traffic flow patterns at the scale of a city, accounting for intermodal trip making and linking travel decisions to activity scheduling ones. This would require to predict first daily activity-travel patterns for the total population, then route choices for each mode and time-dependent OD pair, and finally iterating while updating utilities until the model converges. In a large city where a multi-modal network may reach millions of links, such a task is not computationally feasible while retaining so many choice dimensions. Nevertheless, one may imagine a number of directions for further research which may help nearing this goal.

One of the key challenges when estimating recursive route choice problems is to solve the embedded dynamic programming problem. Acyclic graphs, such as time-expanded networks, allow by their structure to solve a simple backwards induction problem to obtain the value function. Nevertheless, real-life cyclic networks, which may already be of considerable size before any time expansion, still pose a challenge. By considering a large finite horizon instead of an infinite horizon problem (essentially reducing the amount of cycles an individual may make in the

network), similarly to Ziebart et al. (2008), one could obtain value function approximations which could significantly reduce the computational time for large cyclic networks. In addition, the literature on reinforcement learning also provides a variety of methods specifically designed to approximate value functions in large state spaces. It remains to investigate whether the maximum likelihood estimation algorithm would then become unstable and perform poorly, and whether value function approximations would need to be combined with other estimation algorithms. It could be worthwhile (to speed up estimation) to consider machine learning inspired optimization algorithms, such as the Stochastic Newton method (Lederrey et al., 2018), which keeps second order information but provides faster convergence by computing the Hessian on a limited number of observations.

In this thesis, the calibration of individuals' path choice preferences and the computation of a traffic assignment are modeled as two separate steps. One future research objective would be to solve jointly the demand estimation and the traffic assignment problem, i.e., estimating path choice preference parameters assuming that observations correspond to a network equilibrium. There is relatively little literature on this topic, aside from Bertsimas et al. (2015) and Aguirregabiria and Mira (2010). This would be of interest in cities where it is difficult to observe trajectories without the presence of congestion. In particular, it could be interesting to apply the path choice model underlying the traffic assignment model of Chapter 6, which describes behavior under stochastic outcomes, to estimate models of path choice in congested public transport networks.

Finally, the model developed in Chapter 6 has the potential to lend itself to various other applications. Adapting the algorithms proposed in this chapter to deal with general network topologies, including cyclic networks, would open the door to many possibilities. In the perspective of emerging integrated transportation systems, there are now unexpected ways in which capacity limits play a role in network flows. For instance, electric vehicles might need to recharge at stations with limited space at some point during their daily journey. Under a different definition of the state space and an appropriate network representation, the model could express strategic driving behavior in such circumstances. Addressing the issues discussed in detail in the conclusion of Chapter 6 would therefore represent an interesting research direction, and could as well widen the scope of applications of this work.

# A List of articles published or submitted during the thesis

**Zimmermann, M.**, Mai, T., Frejinger, E. (2017). Bike route choice modeling using GPS data without choice sets of paths. Transportation Research Part C: Emerging Technologies, 75, 183-196.

**Zimmermann, M.**, Västberg, O. B., Frejinger, E., Karlström, A. (2018). Capturing correlation with a mixed recursive logit model for activity-travel scheduling. Transportation Research Part C: Emerging Technologies, 93, 273-291.

De Freitas, L. M., Becker, H., **Zimmermann, M.**, Axhausen, K. W. (2019). Modelling intermodal travel in Switzerland: A recursive logit approach. Transportation Research Part A: Policy and Practice, 119, 200-213.

**Zimmermann, M.**, Frejinger, E., Marcotte, P. (2019). A strategic Markovian traffic equilibrium model for capacitated networks. Under revisions in: Transportation Science.

**Zimmermann, M.**, Frejinger, E. (2019). A tutorial on recursive models for analyzing and predicting path choice behavior. Submitted to: EURO Journal on Transportation and Logistics.

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