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OASIS: An integrated optimisation framework for activity scheduling

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Abstract

Activity-based models offer the potential for a far deeper understanding of daily mobility behaviour than trip-based models. Based on the fundamental assumption that travel demand is derived from the need to do activities, they are flexible tools that aim to put individuals and multidimensional interactions at the centre of the analysis.

Due to their complexity and combinatorial nature, activity-based models used in research and practice have often relied on assumptions, predefined rules and modelling structures, which tend to oversimplify the scheduling process and limit the behavioural accuracy of the outputs. Specifically, the sequential approach used to model activity-travel decisions coupled with arbitrary model specifications and parameters significantly hinder the potential of these models. In this thesis, we introduce OASIS (Optimisation-based Activity Scheduling with Integrated Simultaneous choice dimensions), an integrated framework to simulate activity schedules for given individuals based on utility maximisation under time and space constraints. In OASIS, all choice dimensions (activity participation, location, start time, duration and transportation mode) are considered simultaneously into a single optimisation problem. The fundamental behavioural principle behind our approach is that individuals schedule their day to maximise their overall derived utility from the activities they complete, according to their individual needs, constraints, and preferences. Constraints are a critical component in explaining activity-travel behaviour and are explicitly accounted for in OASIS. By combining multiple choices into a single optimisation problem, and considering both the influence of constraints and preferences, our framework can capture trade-offs between scheduling decisions (e.g. spending less time in an activity to ensure enough time for another one or choosing locations where multiple activities can be performed).

We present a methodology to estimate the parameters of the schedule utility function from historical data to generate realistic and consistent daily mobility schedules. The estimation process has two main elements: (i) choice set generation, using the Metropolis-Hasting algorithm, and (ii) estimation of the maximum likelihood estimators of the parameters. We test our approach by estimating parameters of multiple utility specifications for a sample of individuals. The results demonstrate the ability of the new framework to simulate realistic distributions of activity schedules and estimate stable and significant parameters from historic data consistent with behavioural theory.

As the initial analyses of the framework were conducted considering only one day of activities, we extend the single-day framework to include intrapersonal interactions influencing longer-term decisions. We adapt the OASIS simulation module considering that individuals maximise the total utility of their schedules over multiple days (e.g. week), and formulate new decision variables and constraints to capture multiday dynamics (e.g. activity frequency). An empirical investigation shows that the new formulation reflects the observed schedules better than when the intrapersonal interactions are not included.

Finally, we present two successful practical implementations of OASIS, showcasing its versatility and potential for contributions in different research domains.

Keywords: activity-based modelling, scheduling, mixed-integer optimisation, choice set generation, parameter estimation, intrapersonal interactions

Résumé

Les modèles de chaînes d'activité permettent une compréhension plus approfondie du comportement en matière de mobilité que les modèles classiques, basés sur les déplacements. Partant de l'hypothèse fondamentale que la demande de déplacements est dérivée du besoin de faire des activités, ce sont des outils flexibles qui visent à placer les individus et leurs interactions multidimensionnelles au cœur de l'analyse.

En raison de leur complexité et de leur nature combinatoire, les modèles d'activités utilisés dans la recherche comme dans la pratique reposent souvent sur des hypothèses, des règles prédéfinies et des structures de modélisation qui tendent à simplifier à outrance le processus de planification. Ainsi, la précision comportementale des résultats est limitée. Plus précisément, l'approche la plus courante pour modéliser les décisions relatives aux activités et aux déplacements est séquentielle, et associée à des spécifications et des paramètres arbitraires, ce qui entrave considérablement le potentiel de ces modèles.

Dans cette thèse, nous présentons OASIS (Optimisation-based Activity Scheduling with Integrated Simultaneous choice dimensions), un cadre de simulation holistique de programmes d'activités pour des individus donnés, basé sur la maximisation de l'utilité sous contraintes de temps et d'espace. Dans OASIS, toutes les dimensions impliquées dans le choix d'un programme (participation aux activités, lieu, horaire, durée et mode de transport. . .) sont prises en compte simultanément au sein d'un seul problème d'optimisation. Le principe comportemental à la base de notre approche est celui de la maximisation d'utilité : les individus planifient leur journée de manière à maximiser l'utilité globale dérivée des activités qu'ils accomplissent, et cette utilité est définie en fonction de leurs besoins, contraintes et préférences. Les contraintes sont une composante essentielle pour expliquer le choix d'activités et déplacements, et elles sont prises en compte explicitement dans OASIS. En combinant plusieurs choix en un seul problème d'optimisation, et en tenant compte des influences des contraintes et des préférences individuelles, notre modèle est en mesure de refléter les compromis nécessaires entre plusieurs dimensions de choix (par exemple, consacrer moins de temps à une activité en faveur d'une autre, ou choisir des lieux où plusieurs activités peuvent être coordonnées).

Dans un deuxième temps, nous présentons une méthodologie permettant d'estimer les paramètres de la fonction d'utilité à partir de données historiques, afin de générer des programmes de mobilité quotidiens réalistes et cohérents. Le processus d'estimation comporte deux éléments principaux : (i) la génération d'un ensemble d'alternatives de choix, en utilisant l'algorithme de Metropolis–Hasting, et (ii) la dérivation des estimateurs du maximum de vraisemblance des paramètres. Nous testons notre approche en estimant les paramètres de plusieurs formes d'utilité pour un échantillon donné d'individus. Les résultats démontrent qu'avec cette méthode, le modèle est en mesure de simuler des distributions réalistes de programmes d'activité et à estimer des paramètres stables et significatifs à partir de données historiques. Leurs valeurs sont entre autres cohérentes avec les théories de comportement en mobilité.

Les premières analyses du cadre ont été menées en tenant compte d'une seule journée d'activités. Nous étendons donc le cadre à plusieurs jours d'analyse, en incluant les dynamiques intrapersonnelles qui influencent les décisions à long terme. Nous adaptons le module de simulation d'OASIS en considérant que les individus maximisent l'utilité totale de leurs emplois du temps sur plusieurs jours (une semaine, par exemple), et nous formulons de nouvelles variables de décision, contraintes, et influences journalières (par exemple la fréquence des activités). Une étude empirique montre que la nouvelle formulation reflète mieux les programmes observés que le cas où les interactions intrapersonnelles ne sont pas prises en compte.

Pour finir, nous mettons en évidence le succès de deux applications pratiques d'OASIS, qui illustrent sa polyvalence et son potentiel de contribution dans différents domaines de recherche.

Mots-clés : modèles de chaînes d'activité, planification d'emploi du temps, optimisation mixte en nombres entiers, génération d'ensemble d'alternatives de choix, estimation de paramètres, interactions intrapersonnelles

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Acronyms

ABM Activity-based model.

ABS Agent-Based Simulator.

CP Constraint Programming.

HAPP Household Activity Pattern Problem.

ICT Information and communication technology.

IIA Independance from Irrelevant Alternatives.

KS Kolmogorov-Smirnov.

MCMC Markov Chain Monte-Carlo.

MDCEV Multiple Discrete-Continuous Extreme Value.

MH Metropolis-Hastings.

MIP Mixed Integer Programming.

MNL Multinomial Logit.

MOBIS Mobility Behaviour in Switzerland.

MTMC Swiss Mobility and Transport Microcensus.

OASIS Optimisation-based Activity Scheduling with Integrated Simultaneous choice dimensions.

OPTIMS Optimisation of individual mobility plans to simulate future travel in Switzerland.

PT Public Transportation.

SBB Swiss Federal Railways.

Table of Notations

Notation	Description
A	Set of activities.
B	Cost budget.
C_n	Universal choice set of agent n.
G_a	Group of duplicate activities, such that $G_a \subset A$.
L	Set of locations.
M	Set of modes.
P_{in}	Choice probability for individual n and alternative i.
S	Activity schedule.
T	Time horizon/budget.
U	Random utility function.
V	Deterministic utility.
Ω	Set of MH operators.
$\tilde{C}_n$	Sampled choice set of agent n, such that $\tilde{C}_n \subset C_n$.
ℓ	A location, such that $\ell \in L$.
γ_a	Activity-specific constant for activity a.
$\kappa(\ell_a, \ell_b, m)$	Travel cost between locations of activities a and b, using mode m.
$\mathcal{L}$	Likelihood function.
μ_a	Indicator for mandatory activity.
ω_a	Indicator variable for participation to activity a.
$\rho(\ell_a, \ell_b, m)$	Travel time between locations of activities a and b, using mode m.
τ_a^{*+}	Preferred duration for activity a, upper bound.
τ_a^{*-}	Preferred duration for activity a, lower bound.
τ_a	Duration of activity a.
θ_X^a	Penalty for activity a and schedule deviation X.
ε	Error term.
ζ_a^{*+}	Feasible time window for activity a, upper bound.

Notation	Description
ζ_a^{*-}	Feasible time window for activity a, lower bound.
a	An activity, such that $a \in A$.
c_a	Cost of participation to activity a.
m	A mode of transport, such that $m \in M$.
n	An agent.
x_a^{*+}	Preferred start time for activity a, upper bound.
x_a^{*-}	Preferred start time for activity a, lower bound.
x_a	Start time of activity a.
z_{ab}	Indicator variable of succession between activities a and b.

Chapter 1

Introduction

1.1 Context and motivation

Trip-based models have been, for decades, the traditional approach to forecast travel demand. In trip-based analyses, trip purpose, origins, and destinations are usually predicted independently, then paired and assigned to the transport network in subsequent steps. As the interrelations between these choices are not considered, trip-based models are limited when aiding decision-makers to manage existing networks (Castiglione et al., 2014) or prepare to accommodate new mobility paradigms (e.g. mobility as a service).

In response to the lack of flexibility and behavioural realism of the trip-based approach, the activity-based stream of transport research has emerged in the 1970s (e.g. Adler and Ben-Akiva, 1979). Specifically, activity-based models (ABM)[1] aim to solve the following shortcomings of traditional analyses (Vovsha et al., 2005; Castiglione et al., 2014): (i) trips are the unit of analysis and are assumed independent, meaning that correlations between different trips made by the same individual are not accounted for properly within the model, (ii) models tend to suffer from biases due to unrealistic aggregations in time and space, as well as at the level of the population, (iii) space and time constraints are usually not included.

Based on the early works of Hägerstraand (1970) and Chapin (1974), activity-based models consider the fundamental assumption that the need to do activities drives the travel demand in space and time. Mobility is modelled as a multidimensional

[1]To avoid confusion with agent-based models, we use the acronym ABM for activity-based models, and refer to agent-based simulators as ABS.

system rather than a set of discrete observations. Therefore, ABM focus on overall behavioural patterns: decisions are analysed at the level of the household as opposed to independent individuals, and dependencies between events are taken into account (Timmermans, 2003; Pas, 1985). Thus, mobility behaviour is understood in a broader social and environmental context, shaped by inter- and intra-personal interactions. In short, ABM can paint a holistic picture of mobility behaviour.

Two major streams of research can be mentioned: (i) *utility-based models* rely on the assumption that individuals choose their activity schedule to maximise the utility (or satisfaction) they gain from it. These models, such as Bowman and Ben-Akiva (2001); Adler and Ben-Akiva (1979), extend the traditional trip analysis by considering chains of trips (or tours). Mobility behaviour is modelled as a result of discrete choices, usually treated sequentially, and solved with econometric methods like advanced discrete choice models (Bowman and Ben-Akiva, 2001; Wang and Timmermans, 2000; Nurul Habib and Miller, 2009) or with micro-simulations (e.g. Recker et al., 1986; Ettema et al., 2000; Bhat et al., 2004; Pendyala et al., 2005). (ii) *rule-based or computational process models* refute the assumption that decision-makers seek the optimal solution and argue that they consider context-dependent heuristics (Timmermans, 2003). Arentze and Timmermans (2000); Golledge et al. (1994) are examples of rule-based models.

The earliest functional utility-based models are sequential models such as the logit model for household daily travel patterns developed by Adler and Ben-Akiva (1979), which assumes that households choose from a set of possible daily patterns and use a logit model to compute the choice probabilities for each alternative. It was followed by the disaggregate travel demand model developed by Bowman and Ben-Akiva (2001) that models a series of sequential decisions to generate an activity pattern and tours for the day. Sequential modelling is also commonly found in activity-based microsimulators, e.g., STARCHILD (Recker and Root, 1981; Recker et al., 1986), TRANSIMS, Axhausen (1990), (Smith et al., 1995), ALBATROSS (Ettema et al., 2000), FAMOS (Pendyala et al., 2005), mobiTopp (Mallig et al., 2013), MATSim (Axhausen et al., 2016).

Estimating the choices in a sequence allows for simple, clearly defined modelling assumptions. Still, it limits the ability of the framework to capture trade-offs that individuals could make between different choice dimensions. For instance, STARCHILD offers a robust solution to generate the planned set of activities from a larger group of possibilities — or the "opportunity set" (Recker et al., 1986) — but this plan cannot be revised in later stages of the scheduling process (e.g. adding/dropping activities, increasing/decreasing time). Another limitation is the deterministic aspect of the generated alternatives, which relies on a complete enumeration of the choice set, followed by reducing the solution space using decision rules.

More recent works have focused on joint estimation of mobility choices, with a more explicit integration of emerging behaviour in the scheduling process. For instance, Nurul Habib and Miller (2009) use a utility-based approach to model the generation of activities. In this case, a utility function is defined for an agenda (a set of activities to be scheduled) aiming to capture the trade-off between planned and unplanned activities. Bhat et al. (2004) (see also Bhat, 2005, 2018) propose a discrete-continuous approach to model time allocation with the Multiple Discrete-Continuous Extreme Value (MDCEV) model, where multiple choice dimensions are simultaneously considered. Similarly, Ettema et al. (2007) formulate an error-component discrete choice model to jointly estimate duration, time-of-day preference and effect of schedule delays on the utility function of the alternatives.

The simultaneous approach provides greater flexibility than the sequential models that have been presented – however, these examples model only a specific aspect or step of the activity scheduling process but not the entire decision pipeline. Indeed, activity-based models (particularly simultaneous models) are dimensionally cursed and can quickly become intractable with increasing complexity (e.g., interactions between decisions, persons, days, etc.), thus compromising their practicality and ability to produce results. For this reason, most operational models fall back upon simplifying assumptions and heuristics to be functional. As pointed out by multiple authors, (e.g. Axhausen, 2000; Recker, 2001), this means that the current state-of-the-art does not yet fully meet expectations.

Reviewing the literature and operational models, and more specifically, their limitations, two main questions arise:

(i) How can we model the decision-making process involved in every mobility choice as accurately as possible, accounting for every internal (preferences, habits) or external (physical, social and cultural environments) pressure?

(ii) How can we make use of minimal knowledge of these dimensions to infer the parameters quantifying the behaviour of each individual?

The answer to these questions, or the ideal activity-based framework, may include the following modelling features:

- **Simultaneous estimation of choices**: the scheduling choices (activity type, time expenditure, mode, location...) are estimated jointly, which increases the ability of the model to deal with interactions and correlations,
- **Activity participation**: The model includes the choice of participating in a set of possible activities, as opposed to only scheduling a pre-defined set of activities,
- **Explicit modelling of behaviour**: behavioural elements influencing the scheduling choices (e.g. preferences, flexibility, satiation) are explicitly modelled, and their effect can be quantified and interpreted,
- **Social system**: The model includes the impact of social interactions at the level of the household or larger circles,
- **Resource availability**: resources such as mobility tools (private vehicles, public transport subscriptions, etc.) or income are included in the model and impact the availability of certain alternatives to the decision-makers;
- **Scheduling trade-offs**: The model can capture trade-offs in schedule timings (i.e. compromises on timings, for example, to accommodate more or longer activities), participation in activities, location, mode and route choices.

OASIS (Optimisation-based Activity Scheduling with Integrated Simultaneous choice dimensions) is the product of our research effort to provide this complete tool for transport planners, practitioners and researchers – with high levels of flexibility, practicality and theoretical soundness. The framework's development, from the theoretical concept to its practical applications, is documented in this thesis.

1.2 Main objectives

In this thesis, we formalise, implement and test an integrated activity-based simulation framework based on first behavioural principles. In OASIS, the scheduling process is defined as an optimisation model, subject to spatio-temporal constraints.

We assume that when individuals decide about their activity and travel schedules, they are often more driven by constraints than preferences. For example, they might be constrained by strict working hours or limited in their choice of destinations by the availability of a specific mode of transportation. As suggested by Recker (2001), a mathematical optimisation approach is the most straightforward way to model this behaviour. In addition, simulation allows us to deal with complex random distributions in the activity-travel context.

Through the development of this framework, we provide solutions to common limitations in the activity-based literature: interactions of multiple activity-travel dimensions within a single analysis, consistent estimation of parameters, and integration of complex intrapersonal dynamics.

The main contributions of this research can be summarised as follows:

1. **Simultaneous modelling of multiple activity-travel choice dimensions:** Departing from the prevalent paradigm of sequential modelling, we introduce a new approach to model individual activity scheduling where the activity-travel choice dimensions (activity participation, activity location, start time, duration, and travel characteristics to the next activity) are considered simultaneously. The advantage of a simultaneous estimation instead of sequential is that the interactions between the choice dimensions are not limited to a predefined order or hierarchy established based on the modeller's expert knowledge (or lack thereof). This implies that all types of trade-offs are allowed, making the framework both behaviourally realistic and flexible enough to be used in various contexts.

2. **Combination of utility-based and rule-based paradigms:** The framework combines the advantages of both approaches with a simulation component based on random utility maximisation theory and context-dependent rules expressed as model constraints. We can, therefore, provide a rigorous methodology founded on econometric principles and theories while explic-

itly guiding the simulation towards solutions abiding with context- and individual-specific constraints.

3. **Sampling of unchosen alternatives based on Metropolis-Hastings algorithm:** The derivation of the likelihood function for estimating the parameters requires enumerating all alternatives in the choice set. Enumeration is incredibly challenging in the activity-travel context because of the combinatorial nature of the solution space. Traditionally, the choice set is either considered given or requires rules (often based on expert knowledge) to be defined. We propose a general methodology to generate a finite sample of alternatives for each individual. This methodology is based on the Metropolis-Hastings (MH) algorithm, strategically exploring the solution space to form choice sets that are informative and varied enough to obtain robust and consistent parameter estimates.

4. **Activity-based parameter estimation based on maximum likelihood estimation:** We provide estimates of activity-based parameters (e.g., penalties for schedule deviations) for different utility function specifications. This is an essential achievement in the activity-based field, where models are challenging to estimate, and parameter values are not always calibrated to specific datasets. In this thesis, we also investigate how changes in utility specification impact the resulting simulations and what they imply in terms of activity-travel behaviour.

1.3 Outline

The rest of this thesis is laid out as follows:

Chapter 2 introduces the main OASIS framework and defines the fundamental concepts and assumptions of our methodology. More specifically, the simulation component of the framework, based on mixed-integer optimisation, is formalised. We illustrate how the framework works by applying a simplified instance (with arbitrary parameters) on a few individuals of the Swiss Mobility and Transport Microcensus (BfS and ARE, 2017). This chapter is based on the following publication:

> Pougala, J., Hillel, T., and Bierlaire, M. (2022a). Capturing trade-offs between daily scheduling choices. *Journal of Choice Modelling*, 43:100354 DOI: 10.1016/j.jocm.2022.100354

Chapter 3 adresses the issue of parameter estimation for ABM. We formalise the estimation procedure based on maximum likelihood estimation on a sample of alternatives, where this sample is obtained with Metropolis-Hastings sampling. We estimate and test different utility specifications for OASIS and compare them to utility specifications from the literature (e.g. MATSim). This chapter is based upon the following publication:

> Pougala, J., Hillel, T., and Bierlaire, M. (2023c). OASIS: Optimisation-based Activity Scheduling with Integrated Simultaneous choice dimensions. *Transportation Research Part C: Emerging Technologies*, 155:104291 DOI: 10.1016/j.trc.2023.104291

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> Pougala, J., Hillel, T., and Bierlaire, M. (2022b). Parameter estimation for activity-based models. In *Proceedings of the 22nd Swiss Transport Research Conference*, Ascona, Switzerland

Chapter 4 explores the extension of OASIS from a single-day to a multiday framework. We discuss the changes in assumptions, model requirements and specification. We test a simplified version of the multiday framework on an individual from the Mobility Behaviour in Switzerland dataset (Molloy et al., 2022). This chapter is based on the following conference proceedings:

> Pougala, J., Hillel, T., and Bierlaire, M. (2023a). From one-day to multiday activity scheduling: extending the OASIS framework. In *Proceedings of the 23rd Swiss Transport Research Conference (STRC)*, Ascona, Switzerland

Chapter 5 presents practical applications of OASIS to real-life research projects conducted in collaboration with academic and industrial partners. Each project has contributed to developing an operational version of the framework.

Chapter 6 concludes the thesis with a summary of the contributions and a presentation of future research directions.

Chapter 2

Capturing trade-offs between daily scheduling choices

This chapter is based on the following publication:

Pougala, J., Hillel, T., and Bierlaire, M. (2022a). Capturing trade-offs between daily scheduling choices. *Journal of Choice Modelling*, 43:100354 DOI: 10.1016/j.jocm.2022.100354

The candidate has performed this work under the supervision of Prof. Michel Bierlaire and Dr. Tim Hillel.

2.1 Introduction

The scheduling of daily activities is a complex process that combines multiple choices, including deciding which activities to perform in a day and the timings, location, and mode of travel for each performed activity. These choices are not made independently. Instead, peoples' realised schedules result from a series of interconnected, unobserved (and possibly unconscious) dynamics, reasoning, and trade-offs. For example, an individual might leave work earlier than usual on days they need to pick up their children from school or skip a regular exercise session entirely due to a high workload. Being "in a rush", having "plenty of time" or being able to "squeeze in" additional activities in otherwise packed schedules are universal experiences that illustrate the trade-offs we evaluate when scheduling our days.

The daily scheduling process is a critical component of ABM of transport demand, which assume that demand for transportation can be derived from the needs of individuals to perform activities (Bowman and Ben-Akiva, 2001) and that this need is influenced by space and time constraints (Chapin, 1974; Hägerstraand, 1970).

Two major modelling paradigms can be considered: rule-based and econometric models. Rule-based, or computational process, models (e.g. Golledge et al., 1994; Timmermans, 2003; Arentze and Timmermans, 2000) use decision rules to derive feasible solutions. This makes them easier to implement in practice, but the rules are hard-coded and often arbitrary, which limits their generalisation. On the other hand, econometric models postulate that scheduling can be explained with econometric processes such as random utility maximisation. As such, econometric ABM do not typically model behaviour explicitly but consider it a consequence of maximising utility. The different choice dimensions in an econometric model are often modelled sequentially (e.g. Adler and Ben-Akiva, 1979; Bowman and Ben-Akiva, 2001; Recker et al., 1986; Hilgert et al., 2017; Bradley and Bowman, 2008), where each decision is modelled as dependent on all previous choices in the sequence. The modeller decides the decision order; therefore, it may not reflect that of the decision-maker, which may be recursive and not sequential. Other econometric models solve this issue by considering some or all of the choice dimensions jointly (e.g. Ettema et al., 2007; Nurul Habib, 2018; Charypar and Nagel, 2005), but full integration of trade-offs between these choices has not yet been achieved.

This chapter introduces a new approach to modelling individual activity scheduling based on mixed-integer optimisation. The key advantage of our system is that the different modelling dimensions (activity participation, activity location, activity schedule, activity duration, and transportation mode choice to travel to the next activity) are considered jointly in a single optimisation problem. This allows the framework to capture the trade-offs individuals evaluate when scheduling their daily activities. These trade-offs could include changing the duration of an activity to leave more time for others, choosing a specific location for an activity to minimise travel time, or prioritising certain activities over others. Furthermore, our approach can generate an empirical distribution of individual schedules from which different daily schedules can be drawn stochastically for simulation. Finally, the framework is built on first behavioural principles of random utility theory and can be generalised to complex mobility situations.

Our framework focuses explicitly on activity scheduling and travel planning. It does not cover other stages in operational models, such as activity generation and dynamic planning (e.g. schedule updates due to unplanned events). We define a mixed integer optimisation problem subject to time and cost budget constraints to model the trade-offs occurring during the scheduling process. We integrate explicitly the following choice dimensions: (i) activity participation, (ii) timings (i.e. start time and duration), (iii) activity sequencing, (iv) location, (v) and mode of transportation. These choices are each subject to their own set of constraints and requirements (for example, choosing a mode requires its availability to the individual) but are interrelated. Specifically, we include the influence of both observable (e.g. technical constraints) and unobservable (e.g. personality) factors.

2.2 Scope

The framework developed in this thesis is OASIS (Optimisation-based Activity Scheduling with Integrated Simultaneous choice dimensions): a flexible activity-based model able to accommodate the requirements and context-specific constraints of different application domains and thus provide tailored behavioural insights.

OASIS, as presented in this chapter, is intended to be integrated into a broader activity-based modelling process. Figure 2.1 illustrates the framework pipeline, starting from a modelling component to estimate the parameters of the utility functions optimised within the simulation framework. The resulting schedules are used to derive indicators for the analysis of transport behaviour, which can serve as input for agent-based microsimulators (e.g. Manser et al., 2022).

In this initial chapter, we focus only on the simulation aspect of the problem. As such, the parameters used in the model are considered given. They can be imported from literature or calibrated from data. A parameter estimation methodology is conceptualised in Chapter 3.

The rest of the chapter is laid out as follows. Section 2.3 briefly reviews the relevant literature, emphasising utility-based models and simulators. The framework is detailed in Section 2.4, with an overview of the model's key components and the simulation methodology. We illustrate the framework's operation, flexibility, and realism on the Swiss Mobility and Transport Microcensus (MTMC) (BfS and ARE, 2017) in Section 2.5. This investigation aims to demonstrate that the framework can produce sensible results, which can later be included in an activity-based estimation of transport demand.

Finally, we conclude with a discussion on current and future challenges.

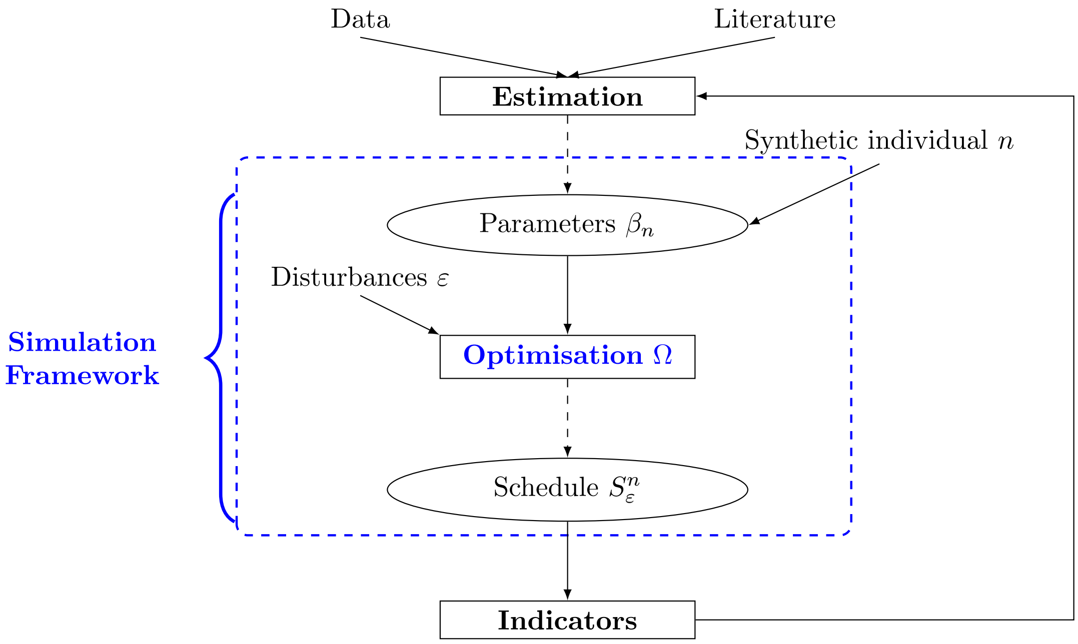


Figure 2.1: Activity-based process including the simulation framework. Dashed arrows represent inputs, while solid arrows represent outputs.

2.3 Relevant literature

ABM originally emerged in the 1970s as a response to the shortcomings of traditional 4-step models (Vovsha et al., 2005; Castiglione et al., 2014), namely: (i) trips are the unit of analysis and are assumed independent, meaning that correlations between different trips made by the same individual are not accounted for properly within the model; (ii) models tend to suffer from biases due to unrealistic aggregations in time, space, and within the population and (iii) space and time constraints are usually not included.

The early works of Hägerstraand (1970) and Chapin (1974) established the fundamental assumption of ABM that the need to do activities drives the travel demand in space and time. Consequently, mobility is modelled as a multidimensional system rather than a set of discrete observations. Unlike traditional trip-based models, ABM focus on overall behavioural patterns: decisions are analysed at the level of the household as opposed to seemingly independent individuals, and dependencies between events are taken into account (Timmermans, 2003; Pas, 1985). Specifically, modellers are interested in the link between activities and travel, often considered within a given timeframe. Typically, a single day is used as the unit of analysis. The resulting goal of studies in the literature is to replicate as accurately as possible the interactions and considerations involved in the development of a daily schedule by an individual.

While the scheduling process is central to activity-based research, there is no clear consensus on the representation and modelling of the daily scheduling process in utility-based frameworks. Typically, individuals are assumed to schedule activities by maximising the utility they can expect to gain. The timeframe is often introduced as a time budget that constrains the overall time expenditure. The scheduling decisions can be modelled as discrete choices: sequential discrete choice models consider a series of choices done consecutively with varying amounts of feedback between each step. On the other hand, joint models also integrate correlations between each aspect of the scheduling decision by evaluating them simultaneously. Other models do not consider the choice fully discrete but a hybrid consumption of discrete and continuous "goods". Furthermore, time trade-offs between activities are not always clearly defined. It is common in the econometric representation of ABM to treat time as a finite good to be consumed. In this context, a marginal change in time is defined as a derivative of the utility function. English (2020) argues that this representation is problematic, as the marginal change in time cannot be interpreted as such. It depends on both the time change and the time replaced.

The earliest functional utility-based models are sequential models such as the logit model for household daily travel patterns developed by Adler and Ben-Akiva (1979), which assumes that households choose from a set of possible daily patterns. It was followed by the disaggregate travel demand model developed by Bowman and Ben-Akiva (2001) that models a series of sequential decisions to generate an activity pattern and tours for the day. These decisions are: (i) the choice of activity pattern (staying at home or travelling), (ii) the primary tour time of day, (iii) the primary tour destination and mode, (iv) the secondary tours' times of day, destination and modes. The choice of activity pattern is modelled using a nested logit model, the tour times of day are generated using a logit model, and the destination and mode with a logit model with alternative sampling. A set of rules defines a hierarchy among activities (primary vs. secondary). The models developed by Adler and Ben-Akiva; Bowman and Ben-Akiva are travel-centric:

while both assume an interdependence among choices, they mainly focus on trip characteristics (e.g. tour frequency, number of stops, mode choice...). Behavioural mechanisms explaining the actual choice of activities and their sequence are examined less closely. In the context of these models, activity schedules and emerging behaviour are implicit and rather consequential to the predicted travel decisions.

Sequential estimation remains popular in the literature, especially for microsimulators (e.g. Recker et al., 1986; Pendyala et al., 2005; Smith et al., 1995; Ettema et al., 2000; Feil, 2010; Axhausen et al., 2016). STARCHILD (Recker and Root, 1981; Recker et al., 1986), is one of the first of many operational microsimulators. STARCHILD models activity-travel decisions as a sequence of five stages (household interactions and individual activity programs, scheduling, recognition of activity patterns, specification of the choice set, and choice model for the activity pattern) to simulate the choice of a daily activity schedule, including planned and unplanned activities, and interactions with household members. Specifically, the scheduling model takes the program (set of planned activities and their spatio-temporal characteristics) as input and generates different combinations of this plan. The resulting set of schedules is evaluated against feasibility constraints and then used as input for a multi-objective optimisation model that simulates the choice set of an individual. Estimating the choices in a sequence allows for simple, clearly defined modelling assumptions. Still, it limits the ability of the framework to capture trade-offs that individuals could make between different choice dimensions. For instance, STARCHILD offers a robust solution to generate the planned set of activities from a more extensive set of possibilities — or the "opportunity set" (Recker et al., 1986) One limitation is the deterministic aspect of the generated alternatives, which relies on a complete enumeration of the choice set and reducing the solution space using decision rules.

These limitations have motivated the development of Household Activity Pattern Problem (HAPP) (Recker, 1995). The HAPP is a variant of the pick-up and delivery problem with time windows (PUDPTW) in operations research (OR), adapted to optimise the utility function of a household that needs to schedule a predefined agenda of activities with given vehicles and destinations. Activities are "picked up" by a household member at a specific location and "delivered" on the return home. The daily schedule is therefore represented as interrelated paths (between vehicles and household members) in time and space. The objective function is the aggregated travel disutility for the household. The constraints are those of a standard PUDPTW, with variables translated to the activity-based context, with additional budget constraints. Recker (1995) have demonstrated with the HAPP that mathematical optimisation programs used in OR have great potential when applied to (utility-based) ABM, as they can efficiently deal with multiple dimensions and associated decisions. We can mention that in this particular formulation of the problem, the focus is on scheduling as a time and resource allocation task – as every activity from the predefined set must be carried out by one of the members of the household (interchangeably only if there exist no constraint on which member must perform the activity). In this sense, *participation* to an activity is not interpreted as the decision of individuals within their household but as an assignment to one of its members. Therefore, with this formulation, it is challenging to understand trade-offs between multiple decisions or interpret individual behaviour beyond sensitivity to travel time.

More recent works have also focused on joint estimation of mobility choices, with a more explicit integration of emerging behaviour in the scheduling process. For instance, Nurul Habib and Miller (2009) use a utility-based approach to model the generation of activities (i.e. which activities are considered in the first place). In this case, the utility function is defined for an agenda (a set of activities to be scheduled) aiming to capture the trade-off between planned and unplanned activities. The choice probabilities are estimated with the Kuhn-Tucker optimality conditions instead of discrete choice models. The resulting agenda is then used as input for a discrete-continuous scheduling model that predicts the choice of activity (discrete choice) and the time expenditure for the chosen activity (continuous choice) sequentially (Nurul Habib, 2011). This theoretical framework is the foundation of CUSTOM, a utility-based scheduling model of workers' daily activities (Nurul Habib, 2018), simulating the discrete choice of performing an out-of-home activity or staying at home all day, and in the former case, the choice of start time of the first trip. The framework goes through multiple "scheduling cycles" to model activity-travel decisions such as the choice of activity type, duration, mode and location for every activity to be scheduled — subject to a time budget. Each scheduling cycle modifies the remaining time budget, which generates a Potential Path Area of feasible locations and modes available for the next activity. The authors model trade-offs between activity cycles and scheduling decisions by assuming that the expected utility of the type and location choice of the following activity impacts the utility of the current cycle. The process is, therefore, not fully simultaneous: the scheduling cycles are evaluated in a series, with each episode influencing and being influenced by the following. This approach provides greater flexibility than strictly sequential models. Still, it limits the ability of the model to capture more complex interactions (e.g. influences of multiple activities).

The discrete-continuous representation of activity schedules has been investigated extensively by Bhat et al. (2004) (see also Bhat, 2005, 2018). In their MDCEV model, the scheduling process is modelled as a combination of a discrete choice (activity participation) and continuous choice (activity duration). Behaviour is explicitly considered with a non-linear utility function and satiation effects (decreasing marginal utility). The discrete-continuous approaches are flexible solutions that consider multiple choice dimensions simultaneously. However, they become limited when integrating time-of-day decisions, which are heavily influenced by external factors (e.g. shop opening times, working hours, commitments, etc.). To address this issue, Palma et al. (2021) propose to modify the MDCEV formulation to estimate the durations of activity episodes instead of activity types by considering a maximum number of episodes per activity and including a polynomial penalty and a satiation parameter in the utility function of each activity. This approach allows the capture of trade-offs between activities - but is limited to the choice of activity participation and duration and, therefore, needs to be combined with a scheduling model to be used in an activity-based context.

Joint estimation of multiple choice dimensions, including time-of-day, has been explored in other works. Ettema et al. (2007) formulate an error-component discrete choice model to jointly estimate duration, time-of-day preference and effect of schedule delays on the utility function of the alternatives. They consider that individuals maximise the sum of the utility gained from travelling and performing the activities. The latter comprises three elements: a time-of-day dependent utility, a duration utility, and a schedule delay utility dependent on the start time. Their model can thus accommodate more explicitly the discontinuities in utility introduced by these external constraints and preferences. However, it mainly focuses on time allocation for a given set of activities, and schedule dynamics linked to activity participation (e.g. dropping an activity if the timings are not convenient for the individual) cannot easily be considered.

Several key features appear in the reviewed methodologies and operational models. We recall (and extend) the list of ideal characteristics of an ABM, which contribute to the behavioural realism of the approach (Section 1.1):

1. Simultaneous estimation of choices: the scheduling choice (activity type,

time expenditure, mode, location...) are estimated jointly, which increases the ability of the model to deal with interactions and correlations;

2. Activity participation: the model includes the choice of participating in a set of possible activities, as opposed to only scheduling a pre-defined set of activities;

3. Continuous time representation: time is modelled as continuous or with fine granularity in order to obtain schedules rich enough for a variety of applications;

4. Explicit modelling of behaviour: behavioural elements influencing the scheduling choices (e.g. preferences, flexibility, satiation, etc.) are explicitly modelled, and their effect can be easily interpreted;

5. Social system: the model includes the impact of social interactions at the level of the household or larger circles;

6. Resource availability: resources such as mobility tools (private vehicles, public transport subscriptions, etc.) or income are included in the model and impact the availability of certain alternatives to the decision-makers;

7. Scheduling trade-offs: The model can capture trade-offs in schedule timings (i.e. compromises on timings, for example, to accommodate more or longer activities), participation in activities, location, mode and route choices.

Table 2.1 maps the discussed methods with these components, highlighting our research's contribution. In the table, X is used to identify a feature available in the corresponding model. (X) is used for our methodology and defines features that have not yet been implemented in the initial state of the framework as described in this thesis but are feasible extensions (as detailed in Section 2.4.4).

Reliable estimation and simulation of activity-travel behaviour requires a framework that includes every choice about the activity-travel behaviour (participation, scheduling, destination and mode of transportation) and can deal with their correlations. This procedure is individual-specific, with parameters and error terms of the utility function to be distributed across the population. Still, the optimisation can be performed at higher dimensions by integrating household dynamics. The model should provide enough flexibility to accommodate different cases and constraints and be easily used with or as input for powerful tools

Table 2.1: Modelling features of utility-based models

Models	**Features**						
	Joint estimation	Participation	Continuous time	Explicit behaviour	Social system	Resources	Trade-offs
Recker et al. (1986)		X			X	X	
Recker (1995)	X		X		X	X	
Miller and Roorda (2003)					X		
Bhat et al. (2004)	X		X	X	X		
Ettema et al. (2007)	X	X	X	X			
Nurul Habib (2018)	X	X	X	X	X	X	
Palma et al. (2021)		X	X	X			X
OASIS	X	X	X	X	(X)	(X)	X

such as agent-based models or traffic simulators.

In this chapter, we lay the foundation of the OASIS framework, with the development of the core optimisation-based simulation of the scheduling process. We focus on the modelling of single-day scheduling. Several authors have pointed out that this ignores day-to-day correlations and dynamics (e.g. Arentze et al., 2011b). We discuss extensions to multiday dynamics in Chapter 4.

2.4 Modelling framework

OASIS simulates the choice of a valid schedule for a given time horizon (typically a day, though it could be any period) made by a single individual called the agent. The central theory behind our approach is that individuals schedule their day to maximise their overall derived utility from the activities they complete, according to their individual needs, constraints and preferences. Therefore, we define a general utility function that captures the derived utility from an individual completing a considered activity. The form of the utility function is flexible. It can include (but is not limited to) features capturing the individual's behaviour related to the given activity and the related trip(s). Additional factors influencing the scheduling process (e.g. interactions with other agents, routine effects..., etc.) can be included in the utility function, with a specification to be defined according to the desired trade-off between model realism and computational accuracy. In this chapter, we consider a utility function that includes the following variables: (i) the preference towards *participating* in that the type of activity, (ii) the desired and scheduled *duration* of the activity, (iii) the desired and scheduled *start time* of the activity, (iv) the flexibility of the individual towards *schedule deviation* in start-time (early/late) and duration (long/short) for the activity, (v) the *cost* of participating in the activity, and (vi) the required *travel time* and *travel cost* to arrive at the activity location from the previous location.

We then define a mixed-integer optimisation problem for each individual, which maximises the sum of the utilities of each completed activity in a schedule over a fixed time horizon. This optimisation problem can, therefore, capture the *trade-offs* between scheduling decisions for multiple activities, such as how spending longer in one activity will reduce the time availability for other activities or how the order of activities changes the travel times. The overall framework takes as input a set of *considered activities*, with associated locations and travel modes, and uses this to define a distribution over possible schedules, from which likely scheduling choices can be stochastically drawn.

In this section, we introduce the modelling elements of the proposed framework. No index is associated with the agent in the following analysis to clarify the notations.

Time can be either continuous or discrete. The time horizon starts at $t = 0$ and finishes at $t = T$. Space is characterised by a discrete and finite list of L locations indexed by ℓ. The location ℓ_0 is called "home" and is assumed to be the agent's location at time $t = 0$ and time $t = T$. As well as a fixed time horizon, the agent is assumed to have a maximum daily budget of B to cover the costs of activity participation and travel.

The agent considers M transportation modes, indexed by m. The travel time between an origin ℓ_o and a destination ℓ_d using mode m is denoted $\rho(\ell_o, \ell_d, m)$ and is exogenous. If ℓ_d cannot be reached from ℓ_o using mode m, then $\rho(\ell_o, \ell_d, m) = +\infty$. Similarly, the travel cost between locations, which is also exogenous, is denoted as $\kappa(\ell_o, \ell_d, m)$.

The agent considers a set of A activities indexed by a. Each activity a is associated with:

- a list L_a of possible locations where the activity could be performed,
- an indicator μ_a that is 1 if the activity is mandatory and 0 if it is optional,
- a time interval when the agent prefers to start the activity[1]: $[x_a^-, x_a^+]$, where $x_a^- \leq x_a^+$,
- a minimum duration $\tau_a^{\min}$,
- a range of desired durations $[\tau_a^-, \tau_a^+]$, where $\tau_a^{\min} \leq \tau_a^- \leq \tau_a^+$,
- a cost c_a for participating in the activity.

Each relevant pair activity/location is associated with a feasible time interval $[\gamma_{a\ell}^-, \gamma_{a\ell}^+]$. It stipulates that the activity can take place only during that time

[1]Note that the assumption that a unique time interval captures preferences in starting time and duration is mathematically convenient but may not be realistic. For instance, a student may prefer to sit an exam either early in the morning or late in the afternoon. In that case, it would be modelled using two different activities.

interval. For example, shopping can typically only happen during the opening hours of the selected shop. Note that the agent may consider a location for an activity even if there is no overlap between $[\gamma^-_{a\ell}, \gamma^+_{a\ell}]$ and $[x^-_a, x^+_a]$. While the former represents a hard constraint, the latter represents a preference.

2.4.1 Valid schedules

Given the above information, the agent considers valid schedules. A schedule is the outcome of the agent's decisions with respect to activity participation, activity location, activity scheduling, and transportation mode choice. More specifically, a schedule S is a sequence of activities $a \in A$, starting with a dummy activity $a =$"dawn", and finishing with a dummy activity $a =$"dusk", both of which take place at home. Their respective utility is set to 0. Each activity $a \in A \setminus$ dawn, dusk is associated with an actual location ℓ_a, an actual starting time x_a and an actual duration τ_a. Except for the last activity "dusk", a trip is performed immediately after each scheduled activity a, using an actual mode of transportation m_a. Note that if the next activity occurs at the same location, the duration of the trip is zero, and the previous mode of transportation does not change.

A schedule is *valid* if

- it spans the whole time horizon, that is, if

$$\tau_{\text{dawn}} + \tau_{\text{dusk}} + \sum_{a,b \in A} \big(\tau_a + \rho(\ell_a, \ell_{a+1}, m_a)\big) = T, \tag{2.1}$$

- it does not exceed the maximum budget, that is, if

$$\sum_{a,b \in A} (c_a + \kappa(\ell_a, \ell_b, m_a)) \leq B, \tag{2.2}$$

- each activity b starts when the trip following the previous activity a is finished, that is

$$x_b = x_a + \tau_a + \rho(\ell_a, \ell_b, m_a), \tag{2.3}$$

- the duration of each activity is valid, that is, if

$$\tau_a \geq \tau_a^{\min} > 0 \tag{2.4}$$

- only one activity from a set of considered duplicates (i.e. same activity with different associated locations or modes) is included in the schedule.

Further constraints on valid schedules can be included to ensure consistent behaviour. Regarding mode choice, we constrain the choice of mode of travel from the location of activity a to activity $a+1$ to a set of feasible modes given the previous mode choices. For example, suppose a traveller takes public transport to work in the morning. In that case, her private car is no longer available to be chosen for other trips until she returns home, when her car will be available again. This behaviour can be generalised to all private vehicles.

2.4.2 Preferences

The agent is assumed to be rational and to select the preferred schedule among all possible valid schedules. The preferences of the agent are captured by a utility function U_S associated with each schedule S.

From the analyst's point of view, the main challenge is that the choice set cannot be enumerated due to the combinatorial structure of the set of valid schedules. We propose to address this challenge by performing an explicit enumeration at the activity level for decisions related to activity location and transportation mode and an implicit enumeration for activity participation and scheduling decisions.

For each activity the agent considers, we explicitly enumerate all possible combinations of the associated locations and modes. Each of these combinations is considered as a separate activity in the model. Therefore, each activity a considered by the agent is modelled by the analyst using up to ML_a mutually exclusive activities, each associated with a unique location ℓ_a and a unique mode of transportation m_a. In addition, we impose the constraint that at most one of these duplicate activities can be selected in a given schedule. This explicit enumeration leads to K groups G_k of mutually exclusive activities. We can, therefore, simplify some notations:

- the feasible time interval of activity a can be denoted $[\gamma_a^-, \gamma_a^+]$,

- the travel time between two activities $a, b \in A, a \neq b$ can be denoted

$$\rho_{ab} = \rho(\ell_a, \ell_b, m_a), \tag{2.5}$$

and similarly,

- the travel cost between two activities can be denoted

$$\kappa_{ab} = \kappa(\ell_a, \ell_b, m_a). \tag{2.6}$$

The implicit enumeration involves solving the scheduling problem the agent considers using a standard optimisation algorithm that identifies the optimal solution without complete enumeration.

Before describing the scheduling problem, we introduce the model of the utility U_S associated with each agent's schedule. We define it as the sum of a generic utility U associated with the whole schedule and utility components capturing the activity-travel behaviour:

$$U_S = U + \sum_{a \in A} \left(U_a^{\text{participation}} + U_a^{\text{start time}} + U_a^{\text{duration}} + \sum_{b \in A} \left[U_{a,b}^{\text{t}} + U_{a,b}^{\text{travel time}} \right] \right). \tag{2.7}$$

The components and the associated assumptions are defined as follows:

1. A generic utility U that captures aspects of the schedule that are not associated with any specific activity. For instance, the agent may prefer that all shopping activities occur in the afternoon or dislike days with too many activities.

2. The utility $U_a^{\text{participation}}$ associated with the participation of the activity a, irrespective of its starting time and duration. This term may include any variable such as level of service, cost, etc. Here, we illustrate the framework with a specification involving cost. It may also include an error term, capturing the unobserved variables.

$$U_a^{\text{participation}} = \beta_{\text{cost}} * c_a + \varepsilon_{\text{participation}} \tag{2.8}$$

3. the utility $U_a^{\text{start time}}$ associated with starting time. This term captures the perceived penalty created by deviations from the preferred starting time. Here, we illustrate this using a deterministic (dis)utility:

$$U_a^{\text{start time}} = V_a^{\text{start time}} \tag{2.9}$$

with:

$$V_a^{\text{start time}} = \theta^{e}_{a_k} \max(0, x_a^- - x_a) + \theta^{\ell}_{a_k} \max(0, x_a - x_a^+), \tag{2.10}$$

where $\theta^{e}_{a_k} \leq 0$ and $\theta^{\ell}_{a_k} \leq 0$ are unknown parameters to be estimated from data. The first (resp. second) term captures the disutility of starting the activity earlier (resp. later) than the preferred starting time, as illustrated in Figure 2.2. Note that the amplitude of the penalty, captured by the parameters θ, may vary across groups of activities. The index k captures the level of flexibility with respect to the scheduling of the activity.

4. the utility U_a^{duration} associated with duration. This term captures the perceived penalty created by deviations from the preferred duration. Here, we illustrate this using a deterministic (dis)utility:

$$U_a^{\text{duration}} = V_a^{\text{duration}} \tag{2.11}$$

with:

$$V_a^{\text{duration}} = \beta^{s}_{a_{a,k}} \max(0, \tau_{a_k}^- - \tau_a) + \beta^{\ell}_{a_k} \max(0, \tau_a - \tau_a^+), \tag{2.12}$$

where $\beta^{s}_{a_k} \leq 0$ and $\beta^{\ell}_{a_k} \leq 0$ are unknown parameters to be estimated from data. Similarly to the specification of start time, the first (resp. second) term captures the disutility of performing the activity for a shorter (resp. longer) duration than the preferred one,

5. For each pair of locations (ℓ_a, ℓ_b), respectively, the locations of activities a and b with $a \neq b$, the utility $U^{\text{t}}_{a,b}$ associated with the trip from ℓ_a to ℓ_b, irrespective of the travel time. This term may include variables such as cost, level of service, etc. Here, we illustrate the framework with a specification involving travel costs. It may also include an error term, capturing the

unobserved variables.

$$U^t_{a,b} = \beta_{t,\text{cost}} * c_{t,ab} + \varepsilon_t \tag{2.13}$$

6. For each pair of locations (ℓ_a, ℓ_b), the utility $U^{\text{travel time}}_{a,b}$, which captures the penalty associated with the travel time from ℓ_a to ℓ_b. Here, it is assumed to be deterministic:
$$U^{\text{travel time}}_{a,b} = V^{\text{travel time}}_{a,b} \tag{2.14}$$
with
$$V^{\text{travel time}}_{a,b} = \theta_t \rho_{ab}, \tag{2.15}$$
where θ_t is an unknown parameter to be estimated from data, and ρ_{ab} is the travel time to the next location.

As a reminder, no utility is associated with the dummy activity "dusk". We also normalise
$$U^{\text{particitipation}}_{dawn} = U^{\text{start time}}_{dawn} = U^{\text{duration}}_{dawn} = 0. \tag{2.16}$$
Indeed, as only differences of utility matter, the two dummy activities serve as references, and their utility is zero[2].

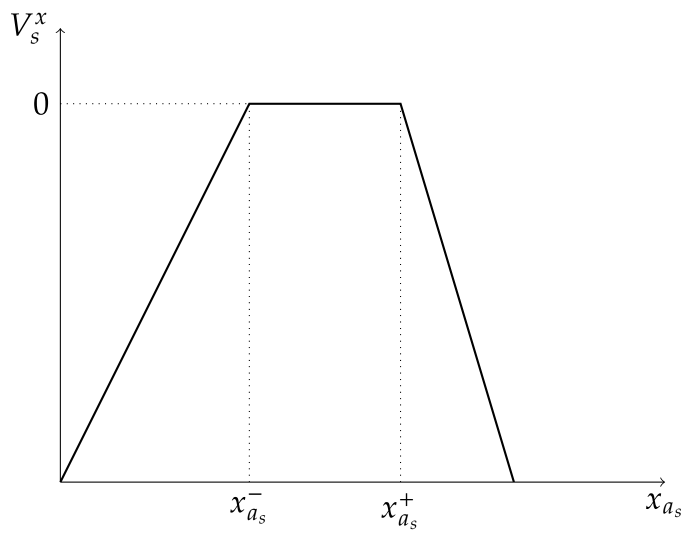


Figure 2.2: Utility associated with deviations from the preferred starting time of an activity

[2]In this specification both *dusk* and *dawn* can have a non-zero duration τ, and the associated parameters are set to 0. In the case where in-home activities are explictly considered, the duration of *dusk* and *dawn* can be set to 0, and the *home* activities associated with a non-zero duration

2.4.3 Schedule optimisation

Consistent with random utility theory, the agent is assumed to select the valid schedule with the highest utility. She, therefore, solves an optimisation problem to maximise the utility function under the validity constraints. However, from the point of view of the analyst, the utility function (2.7) is captured by a random variable, and the model associates a choice probability with each valid schedule. To deal with this uncertainty, we propose a simulation approach, where the optimisation problem is explicitly solved for several realisations of the random utility. This is done by drawing from the distributions of the random terms (e.g. $\varepsilon_{\text{participation}}$ and ε_t in the specification illustrated above) and solving the optimisation problem. Assuming a normal distribution for these quantities makes the sampling more convenient but is not required by the framework. The resulting schedule is a realisation from the choice model. The advantage of this approach is that each generated schedule is valid by design, explicitly capturing the trade-offs made by the agent.

For each activity a, we generate realisations of $U^{\text{participation}}$, that we denote by $V_a^{\text{participation}}$. For each pair (ℓ_a, ℓ_b) of locations, we also generate realisations of U^t, that we denote by V_{ab}^t. We characterise the decision of the agent using the following decision variables:

- ω_a: binary variable that is 1 if activity a is selected in the schedule, and 0 otherwise,
- z_{ab}: binary variable that is 1 if activity b is scheduled immediately after activity a, where $a \neq b$,
- x_a: starting time of activity a,
- τ_a: duration of activity a,
- α_a^m: indicator variable that is 1 if private mode m (e.g. car or bicycle) is available for activity a, and 0 otherwise.

We denote the corresponding vectors by ω, z, x, τ, α^m. We consider a realisation of the generic utility U, denoted by $U(\omega, z, x, \tau, \varepsilon)$, to emphasise that it depends on the decision variables and on the error terms.

The objective function is derived from (2.7):

$$\begin{aligned}
&\max_{\omega,z,x,\tau} U(\omega, z, x, \tau, \varepsilon) && (2.17)\\
&\qquad + \sum_{a=0}^{A} \omega_a \left[V_a^{\text{participation}}(\omega) + V_a^{\text{start time}}(x) + V_a^{\text{duration}}(\tau) \right] \\
&\qquad + \sum_{a=0}^{A} \sum_{b=0}^{A} z_{ab} \left[V_{ab}^{t}(z) + V_{ab}^{\text{travel time}}(z) \right] .
\end{aligned}$$

The constraints are

$$\sum_a (\omega_a \tau_a + \sum_b z_{ab} \rho_{ab}) = T, \tag{2.18}$$

$$\sum_a (\omega_a c_a + \sum_b z_{ab} \kappa_{ab}) \leq B, \tag{2.19}$$

$$\begin{aligned}
\omega_{\text{dawn}} = \omega_{\text{dusk}} &= 1, && && (2.20)\\
\tau_a &\geq \omega_a \tau_a^{\min}, && \forall a \in A, && (2.21)\\
\tau_a &\leq \omega_a T, && \forall a \in A, && (2.22)\\
z_{ab} + z_{ba} &\leq 1, && \forall a, b \in A, a \neq b, && (2.23)\\
z_{a,\text{dawn}} = z_{\text{dusk},a} &= 0, && \forall a \in A, && (2.24)\\
\sum_a z_{ab} &= \omega_b, && \forall b \in A, b \neq \text{dawn}, && (2.25)\\
\sum_b z_{ab} &= \omega_a, && \forall a \in A, a \neq \text{dusk}, && (2.26)\\
(z_{ab} - 1)T &\leq x_a + \tau_a + z_{ab}\rho_{ab} - x_b, && \forall a, b \in A, a \neq b, && (2.27)\\
(1 - z_{ab})T &\geq x_a + \tau_a + z_{ab}\rho_{ab} - x_b, && \forall a, b \in A, a \neq b, && (2.28)\\
\sum_{a \in G_k} \omega_a &\leq 1 && k = 1, \ldots, K, && (2.29)\\
\alpha_a^m &= 1 && \forall a \in G_{\text{home}} && (2.30)\\
\omega_a &\leq \alpha_a^m && \forall a \in A^m && (2.31)\\
\alpha_a^m &\geq \alpha_b^m + z_{ab} - 1 && \forall a \in A, b \in A \setminus G_{\text{home}} && (2.32)\\
\alpha_b^m &\geq \alpha_a^m + z_{ab} - 1 && \forall a \in A, b \in A \setminus G_{\text{home}} && (2.33)\\
x_a &\geq \gamma_a^-, && \forall a \in A, && (2.34)\\
x_a + \tau_a &\leq \gamma_a^+, && \forall a \in A. && (2.35)
\end{aligned}$$

Equation (2.18) constrains the total time assigned to the activities in the schedule (sums of durations and travel times) to be equal to the time horizon. Similarly, equation (2.19) constrains the total cost of the schedule (sums of the costs of participating and travelling to the activities in the schedule) not to exceed the maximum budget. Equation (2.20) ensures that each schedule begins and ends with the dummy activities *dawn* and *dusk*. Equations (2.21) and (2.22) enforce consistency with the activity duration by requiring the activity to have a duration greater or equal to the minimal duration (2.4) and for the activity to have zero duration if it does not take place. Equations (2.23)-(2.27) constrain the sequence of the activities: (2.23) ensures that two activities a and b can only follow each other once (thus can only be scheduled once). As it is defined for distinct activities, it also ensures that an activity cannot follow itself. Equations (2.24)-(2.26) state that each activity has only one predecessor (excluding the first activity), and each activity only one successor (excluding the last activity). Equation (2.27) enforces time consistency between two consecutive activities (with travel time ρ_{ab}). Equation (2.29) ensures that only one activity within a group of duplicates G is selected. Equations (2.30)-(2.33) define the constraints related to the choice of mode of transportation. (2.30) ensures that all private modes m are always available for activities (or trips) starting from home[3]. (2.31) only allows alternatives associated with a private mode m to take place if m is available, while (2.32) and (2.33) enforce mode consistency between two consecutive activities, excluding returns home where a different (private) mode can be chosen. Finally, (2.34) and (2.35) are time-window constraints.

Note that the model is non-linear in the objective function. Several methods exist to linearise the specification to solve it with standard mathematical programming techniques. For this research, the model was solved directly using the IBM-CPLEX solver, which applies spatial branch-and-bound to find a global optimal solution (Bliek et al., 2014).

2.4.4 Flexibility of the framework

The form of the utility function specified in the previous section is highly flexible and allows for the modeller to: (i) impose arbitrary behavioural assumptions using different constraints, (ii) introduce additional choice dimensions.

[3]This assumption can be relaxed to take into account that household dynamics influence the share of privately owned vehicles.

We have shown that some specific activity-travel behaviour can be included in the model through the constraints, such as mode consistency between consecutive alternatives or mode changes at home. The constraints do not impact the specification of the utility functions, which allows for straightforward generalisation of the model to varied behaviours and scenarios. In the next section, we introduce an application of the framework for planning a single day. Still, the time horizon can be specified as any arbitrary period (e.g. a week). For extended periods, including *linked activities* is essential to ensure consistent behaviour. Linked activities can be activities that must be included in a strict sequence (i.e. one activity performed immediately after the other), in a particular order (i.e. so that other activities may be performed in between), or that either all or none of these activities must be included in the schedule. It is also possible to associate different potential *home* locations to model long-distance commuters, for instance, who may spend some nights out of home.

Similarly, it is straightforward to include further choice dimensions without altering the specification of the utility functions. OASIS illustrates the inclusion of mode choice. However, the process can be generalised to any desirable choice addition (or restriction) by including it in the definition of a considered activity. For instance, extending the framework to include route choice is straightforward by associating each activity a to a specific route r_a and duplicating the activities as many times as possible route alternatives.

These extensions come at the cost of computational burden, and the trade-off between computational time and model realism must be carefully considered.

2.5 Empirical investigation

To illustrate the optimisation-based simulation concept introduced in Section 2.4, we rely on a real-world dataset of historic activity schedules to generate the inputs. The objective is to show that, given sets of possible activities, locations, modes and timing preferences, the model can generate realisations of chosen daily schedules.

The MTMC is a Swiss nationwide survey gathering insights on the mobility behaviours of residents (BfS and ARE, 2017). Respondents provide their socio-economic characteristics (e.g. age, gender, income) and those of the other household members. Information on their daily mobility habits and detailed records of their trips during a reference period (1 day) are also available. The 2015 edition of the MTMC contains 57,090 individuals and 43,630 trip diaries. We use only the data corresponding to the residents of Lausanne (2,227 diaries). Further details on the MTMC and the preprocessing performed to generate the required inputs are detailed in Appendix B.1.

2.5.1 Inputs

The required inputs (activities, locations, feasible and desired start times and durations, flexibility, etc.) are not always available in traditional travel surveys, including the MTMC. The challenge is thus to provide heuristics to obtain estimators for the missing attributes.

Table 2.2 summarises the data requirements for the operational model and two possible solutions to overcome the lack of information for each requirement. The *rigorous solution* column describes a methodology to obtain the associated information with minimal simplifying assumptions or proxies. These solutions might require a dedicated model or additional data. Therefore, we have provided the *heuristic* column with less rigorous but more straightforward to-implement alternatives. The methods described in the *heuristic* column have been applied in this paper, with results presented in Section 2.5.3.

2.5.2 Utility specification

Allowing for the available inputs for this case study, the schedule utility function expressed in Equation 2.7 has been simplified as follows:

1. We assume that the random terms are randomly distributed: $\varepsilon_s \sim \mathcal{N}\left(0, \sigma^2\right)$, with variance σ^2 set to 1.

2. The ranges of start time preferences $[x_a^-, x_a^+]$ are such that $x_a^- = x_a^+ = x^*$, and the associated utility $V^{\text{start time}}$ is therefore defined as:

$$V^{\text{start time}} = \theta^e_{a_k} \max(0, x^*_a - x_a) + \theta^\ell_{a_k} \max(0, x_a - x^*_a), \tag{2.36}$$

The same assumption is made for the preferred durations and their associated utility V^{duration}, similarly defined as:

$$V^{\text{duration}} = \beta^e_{a_k} \max(0, \tau^*_{a_k} - \tau_a) + \beta^\ell_{a_k} \max(0, \tau_a - \tau^*_a), \tag{2.37}$$

Table 2.2: Data requirements for operational model

Requirements	Rigorous solution	Heuristic
Considered activities A	Activity choice set generation algorithm for each individual	Description of actual schedule from dataset
Considered modes M	Mode choice set generation algorithm for each individual	Consider all five main modes (driving, passenger, public transport, walk, cycle)
Considered locations L_a	Location set generation algorithm for each individual	Description of actual schedule from dataset
Desired start time and duration ranges $[x_a^-, x_a^+]$ and $[\tau_a^-, \tau_a^+]$,	Habit analysis and identification of typical timings in multi-day diaries	Ranges replaced by recorded values in dataset
Flexibility k	Habit analysis in multi-day diaries — flexibility would be the timing variability	Assign a discrete flexibility profile to each activity based on literature classification.
Penalty values (θ, β)	Calibrated on data — n-dependent	From literature, homogeneous across all population
Feasible time windows $[\gamma_{a\ell}^-, \gamma_{a\ell}^+]$	Data collection	Out-of-sample distributions of start and end times for each activity, across the population
Minimum duration $\tau_a^{\min}$	Habit analysis in multi-day diaries	Set to 0

3. The flexibility in time k is modelled using a discrete indicator that can describe three possible behaviours (Figure 2.3):

    (a) Flexible (F): deviations from preferences for activity a are relatively unimportant and thus are less penalised.

    (b) Moderately flexible (MF): deviations from preferences are moderately undesirable and penalised more than in the flexible case.

    (c) Not flexible (NF): deviations from preferences are strongly undesirable and are consequently highly penalised.

Each activity is associated with one level of flexibility, and specific values of the penalty parameters characterise each level. The flexibility assignments for each activity are summarised in Tables 2.3 and 2.4. For the sake of simplicity, we consider that the parameters are deterministic instead of randomly distributed across the population. We have chosen values based on results from the departure time choice literature (Small, 1982). Similarly, we have used cost variables (travel cost c_t and cost of activity participation c_a) and associated parameters ($\beta_{t,\text{cost}}$ and β_{cost}) from the value of time literature, and specifically case studies in Switzerland:

1. National averages of travel cost per mode and distance (BfS, 2021) were used to approximate c_t,

2. The travel cost parameters $\beta_{t,\text{cost}}$ were derived from national averages of the value of time for each mode (Weis et al., 2021),

3. The Swiss Household Budget Survey (BfS, 2007) provides average expenditures for activities as a percentage of the household budget. These were used to define c_a. For the sake of simplicity, the cost of activities not associated with the consumption of goods (e.g. work) was set to 0.

4. The activity cost parameters β_{cost} were derived from the average value of leisure and value of time assigned to work estimated for Zurich (Schmid et al., 2021).

Table 2.3: Categories and flexibility profiles for activities in the MTMC.

Activity	Category	Flexibility profile[a] Start	Duration
Work Education Business trip	Mandatory[b]	Early: NF Late: MF	Short: NF Long: NF
Errands, use of services Escort	Maintenance	Early: MF Late: MF	Short: MF Long: F
Home[c] Shopping Leisure	Discretionary	Early: F Late: MF	Short: F Long: F

[a] F = Flexible, MF = Moderately flexible, NF = Not flexible.
[b] In this example, we use the term *mandatory* to refer to non-flexible activities with high utilities.
[c] Not including mandatory home stays *dawn* and *dusk*.

Table 2.4: Penalty values by flexibility, in units of utility

Deviation	Flexibility	Penalty θ
Early start	Flexible (F)	0
	Moderately flexible (MF)	-0.61
	Not flexible (NF)	-2.4
Late start	F	0
	MF	-2.4
	NF	-9.6
Short duration	F	-0.61
	MF	-2.4
	NF	-9.6
Long duration	F	-0.61
	MF	-2.4
	NF	-9.6

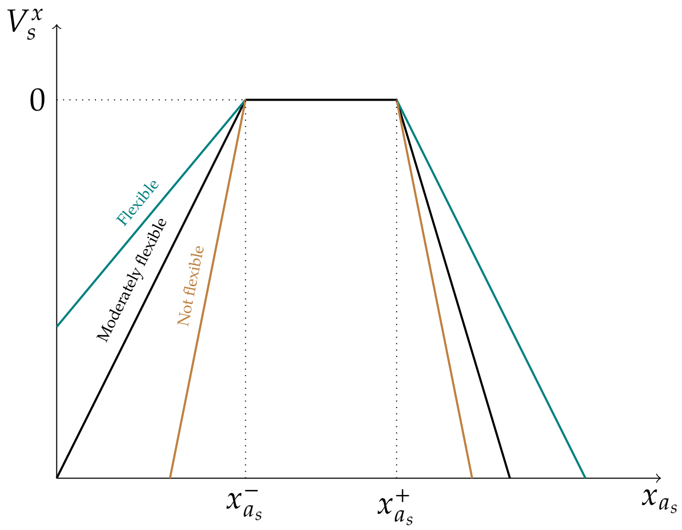


Figure 2.3: Utility associated with deviations from the preferred activity start time (early or late) and levels of flexibility

2.5.3 Results

We present four examples from the MTMC: two students, Alice and Bryan, a worker, Claire, and an unemployed person, Dylan. Each individual's set of considered activities, timing preferences, activity locations and modes are reported in Table 2.5. Specific activities were duplicated to offer different mode and location options. We take separate draws of the error terms ε for each individual and use them to draw different optimal schedules according to the utility specification. The schedules for each individual are shown in Figures 2.4 to 2.7. As for any simulation analysis, a large number of draws is necessary. In this example, we have generated 100 realisations of the schedules, out of which we have arbitrarily selected three for illustration.

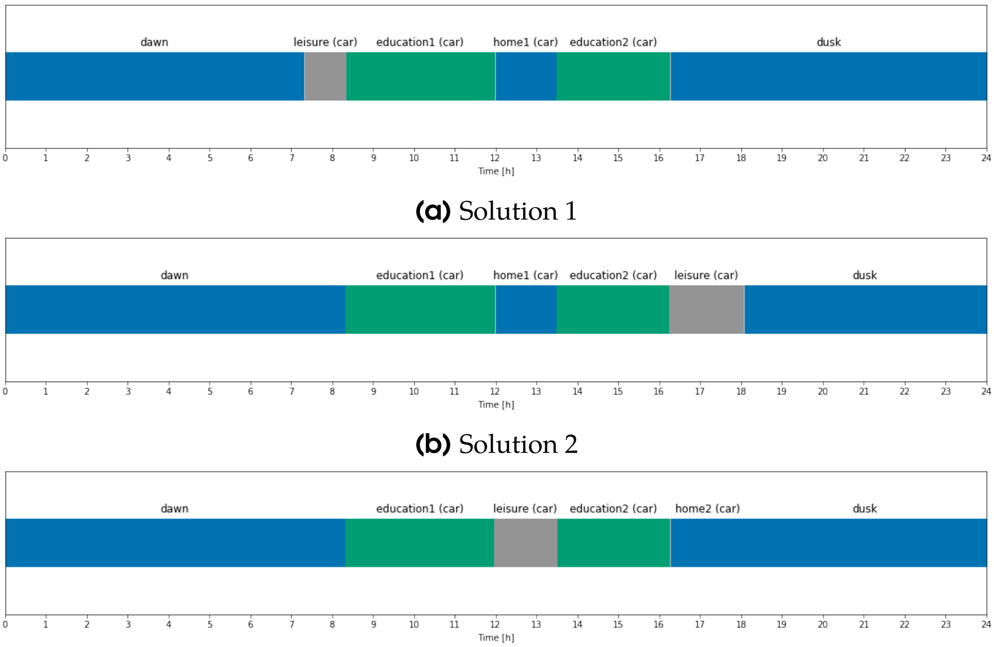
For Alice, all solutions show sequences where both of the *education* instances are scheduled. Regarding the *leisure* activity, only the second schedule (Figure 2.4b) includes it with timings consistent with her preferences. For the other two solutions (Figures 2.4a and 2.4c), this activity is scheduled at a different time of day than the desired times (in the morning and at lunchtime, respectively).

For Bryan, the first two solutions include shopping at different locations. In the third solution (Figure 2.5c), the shopping activity does not appear in the schedule, indicating that staying at home has a higher overall utility.

Table 2.5: Considered activities and preferences for each individual.

Person	Activity	x_a^* (hh:mm)	τ_a^*(hh:mm)	Location[a]	Mode
Alice	Education (AM)	8:20	3:40	Campus	Car
	Education (PM)	13:30	2:45	Campus	Car
	Education (AM)	8:20	3:40	Campus	PT
	Education (PM)	13:30	2:45	Campus	PT
	Leisure	17:10	0:50	Campus	Car
Bryan	Education	7:30	4:40	Campus	Car
	Shopping	16:30	2:00	Downtown	Car
	Shopping	16:30	2:00	Campus	Car
Claire	Work (A)	14:25	4:25	Office	Car
	Work (B)	14:25	4:25	Office	PT
	Work (C)	14:25	4:25	Library	Car
	Errands	9:45	0:15	Chemist	Car
	Escort	14:10	0:01	Downtown	Car
	Leisure	8:00	1:00	Downtown	Car
	Shopping	13:00	2:00	Shop	Car
Dylan	Escort (Afternoon)	15:10	0:50	School	Car
	Errands	16:40	1:50	Shop	Car
	Escort (Evening)	18:50	0:03	School	Car
	Leisure	19:20	1:30	Gym	Car
	Leisure	19:20	1:30	Gym	Cycling

[a] Each location is assigned unique coordinates for estimating travel times.



(a) Solution 1

(b) Solution 2

(c) Solution 3

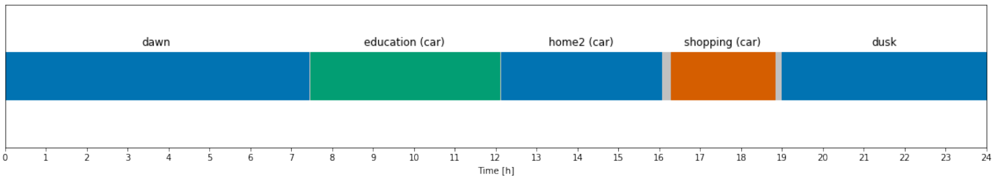
Figure 2.4: Generated schedules for Alice

The solutions for Claire (shown in Figure 2.6) are similar in that all include *work*, with timings that do not diverge substantially from the preferences. On the other hand, the discretionary activities provided as input (in this case, errands, escort, leisure and shopping) are not always scheduled. When they are, the scheduled timings can be far from the preferences (e.g. Figure 2.6c).

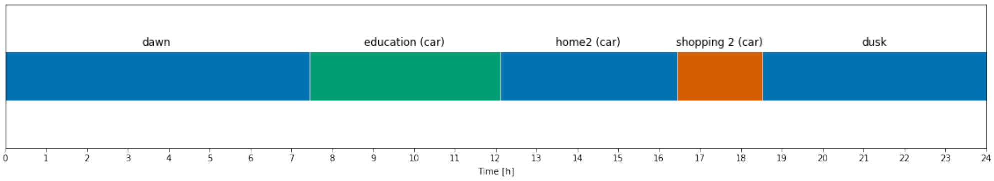
Dylan differs from the other selected individuals in that his set of considered activities does not contain any highly constrained activity such as work or education. The leisure activity is included in all three generated schedules but with varying durations. When included, the escort and errands activities stay relatively close to the preferences.

None of the solutions include public transport as a choice of transportation mode. This indicates a consistently higher attractiveness of the car mode for the given parameters.

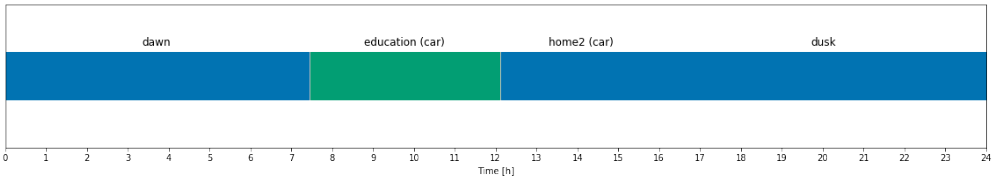
These results show that for the parameters used in this study, the variations in solutions affect mainly the discretionary activities, which have lower penalties for schedule deviations than less flexible activities. Note that we have selected only a small number of unique solutions out of all the generated solutions. The



(a) Solution 1

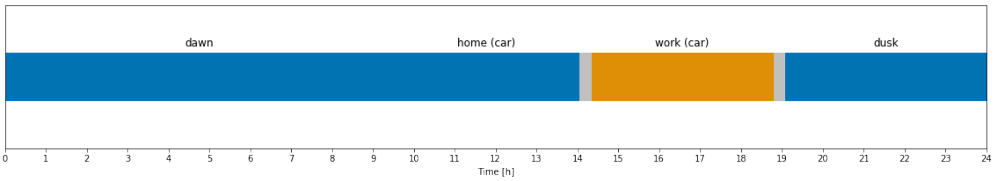


(b) Solution 2

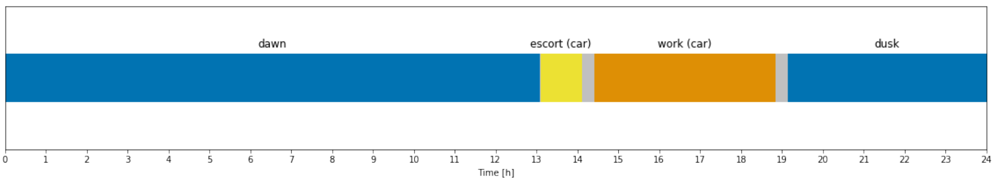


(c) Solution 3

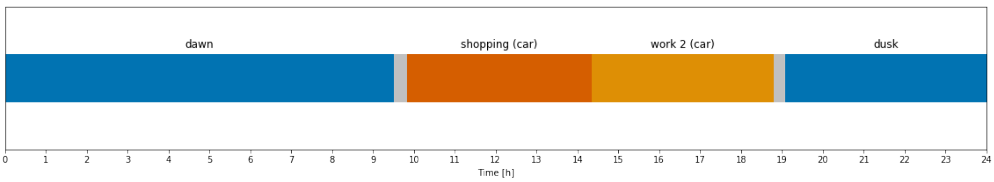
Figure 2.5: Generated schedules for Bryan



(a) Solution 1

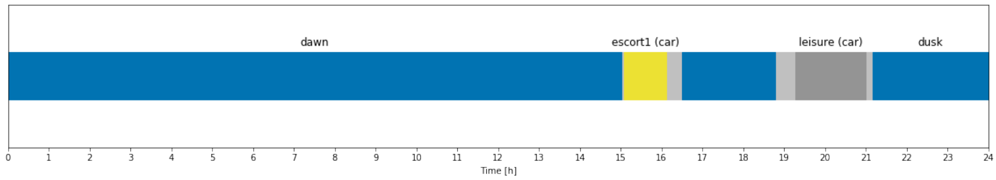


(b) Solution 2

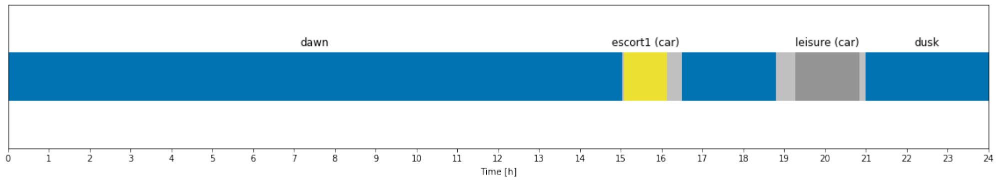


(c) Solution 3

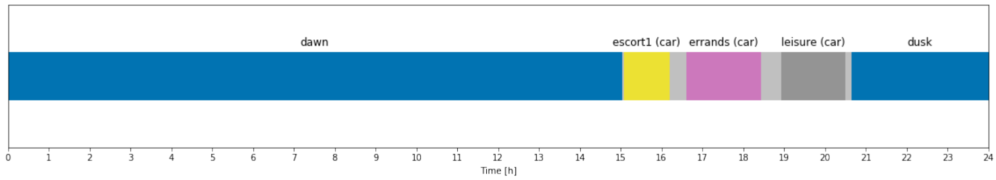
Figure 2.6: Generated schedules for Claire



(a) Solution 1



(b) Solution 2



(c) Solution 3

Figure 2.7: Generated schedules for Dylan

heterogeneity of the solution space (i.e. the distribution from which schedules are drawn) is driven by the relative values of the parameters and the error terms. More specifically, very high penalties (compared to the error variances) lead to semi-deterministic problems where the scheduler consistently outputs very similar (or the same) schedules. On the other hand, error terms with very high variance (compared to the penalties) will lead to a diverse set of solutions. Therefore, an appropriate scale for the error terms must be determined so that the model can generate varied and meaningful solutions.

2.5.4 Distributions of schedules

As mentioned in Section 2.4, the outcome of OASIS is a distribution of schedules realisations. To illustrate this concept, we return to the example of Claire, presented in the previous section.

OASIS is designed to capture the interactions of the activities in the schedule, leading to complex distributions of activity participation, start-time, and duration for each considered activity. To show the ability of the framework to draw schedules from a continuous distribution, we repeatedly draw different values of the error terms and generate the optimal associated schedule. The distribution is then compared to the empirical distribution in the data. We illustrate this example using Claire and make 1000 draws from the schedule distribution. The results are shown in Figures 2.8 to 2.11.

Regarding activity participation (Figure 2.8), in-home and out-of-home schedules can be defined. The former are schedules in which no out-of-home activity (i.e. activity requiring a journey to its destination) is scheduled. Similarly, out-of-home schedules contain at least one trip. 37.1% of the generated schedules include out-of-home activities (as opposed to a full day spent at home). In the out-of-home schedules, *work* is among the most scheduled activities. Out of the discretionary activities, only *escort* is present in about 20% of the out-of-home schedules. The other activities are rarely scheduled, likely due to their high participation cost.

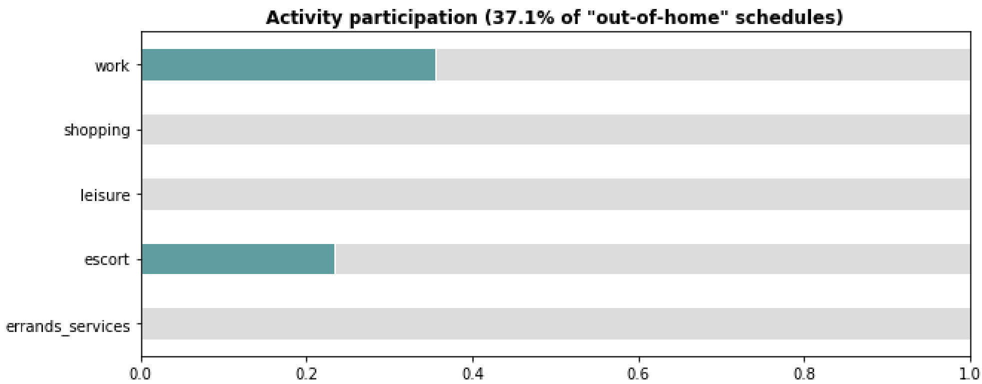


Figure 2.8: Proportion of activity participation in out-of-home schedules (1000 runs)

The simulation results are driven by the random quantities in the utility function, such as the error term ε_S.

To simulate the effect of the variance of the error term on the activity participation, we fix the variances of the error terms $\sigma^2_{\text{start time}} = \{1, 10\}$ and generate 1000 schedules for each value. The ratio of schedules containing each activity is then computed and shown in Figure 2.9. Schedules generated with a higher variance include more frequently discretionary activities. Indeed, we expect the variance to have a large enough magnitude to mitigate the exclusionary effect of the participation costs.

The distributions of start times (Figure 2.10) for each activity over 1000 runs show different profiles. Still, all seemingly biased towards the desired start time —

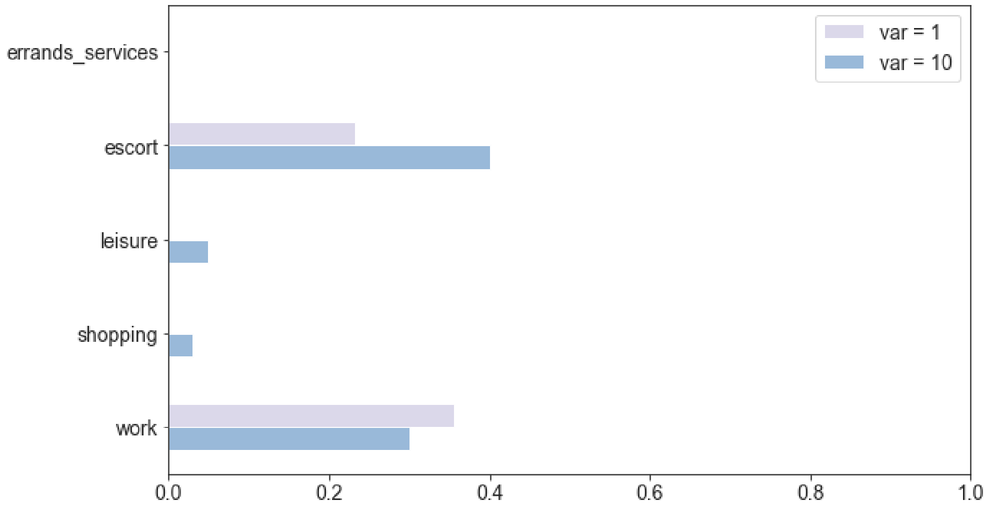


Figure 2.9: Distribution of activity participation, for different variances of the random term

except the “home" activity[4]. The distribution of *work* appears unimodal, centred around the desired start time with very low variance. This is due to the high penalties associated with schedule deviations for this activity (cf. Table 2.4). Notably, the *escort* and *shopping* activities are close to but not centred around the desired time. Given that these two activities had conflicting timings, this result shows the trade-off made during the optimisation process: in most schedules, these activities are started earlier to accommodate other activities for which the penalties for schedule deviations are higher.

Similar observations can be made for the distributions of durations (Figure 2.11): the duration assigned to *work* is almost deterministic, with very low variance, and centred around the desired duration, while the durations allocated to flexible activities are more dispersed. Again, when the desired durations involve schedule conflicts, the distributions are not centred around the desired duration and tend to have a large spread (e.g. escort).

These distributions are also affected by the random terms. For instance, Figure 2.10 shows that increasing the variance of the error terms to 10 does not significantly impact the distribution of start times for the *work* activity. On the other hand, the *escort* activity is more spread in time. As previously noted, the *leisure* and *shopping* activities are more often scheduled, leading to greater variety in the generated

[4]Regarding the *home* activity, given the constraint that the day must start and end at home, we only show the time of the last return home.

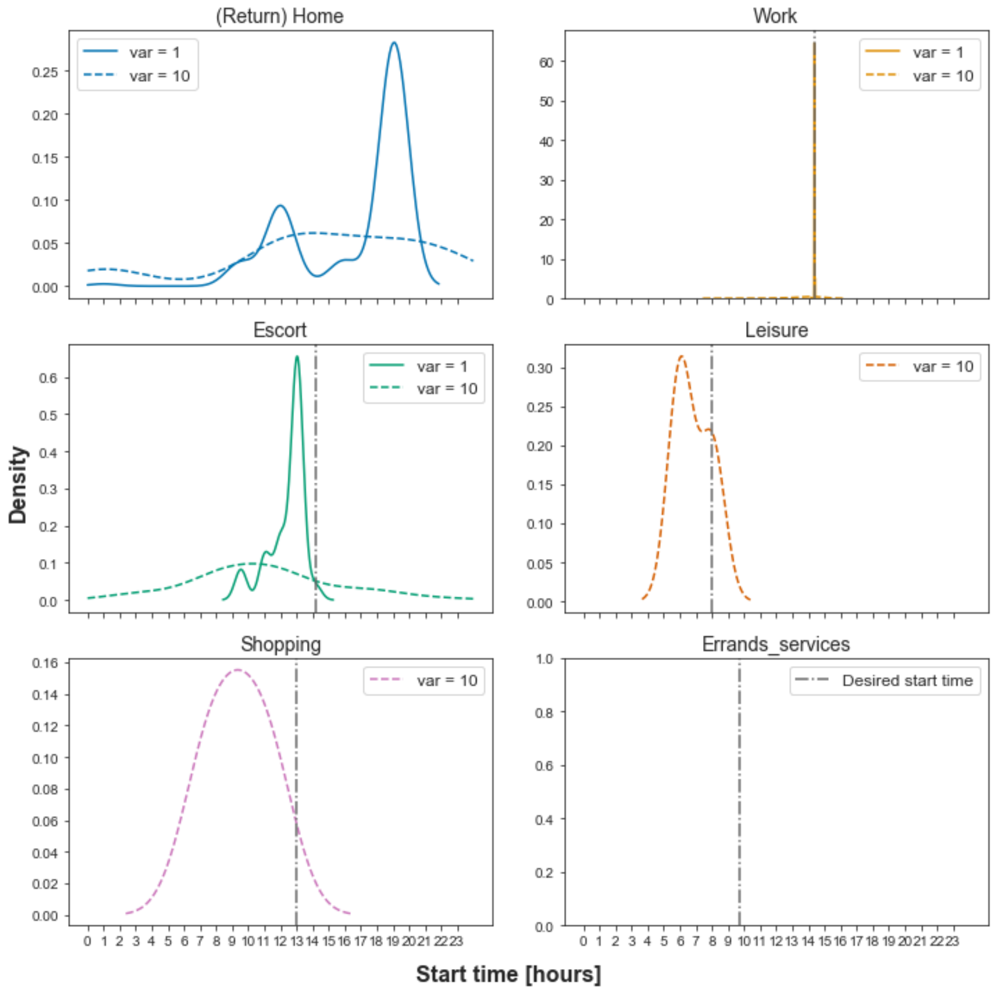


Figure 2.10: Distribution of start times per activity and variance of the random term

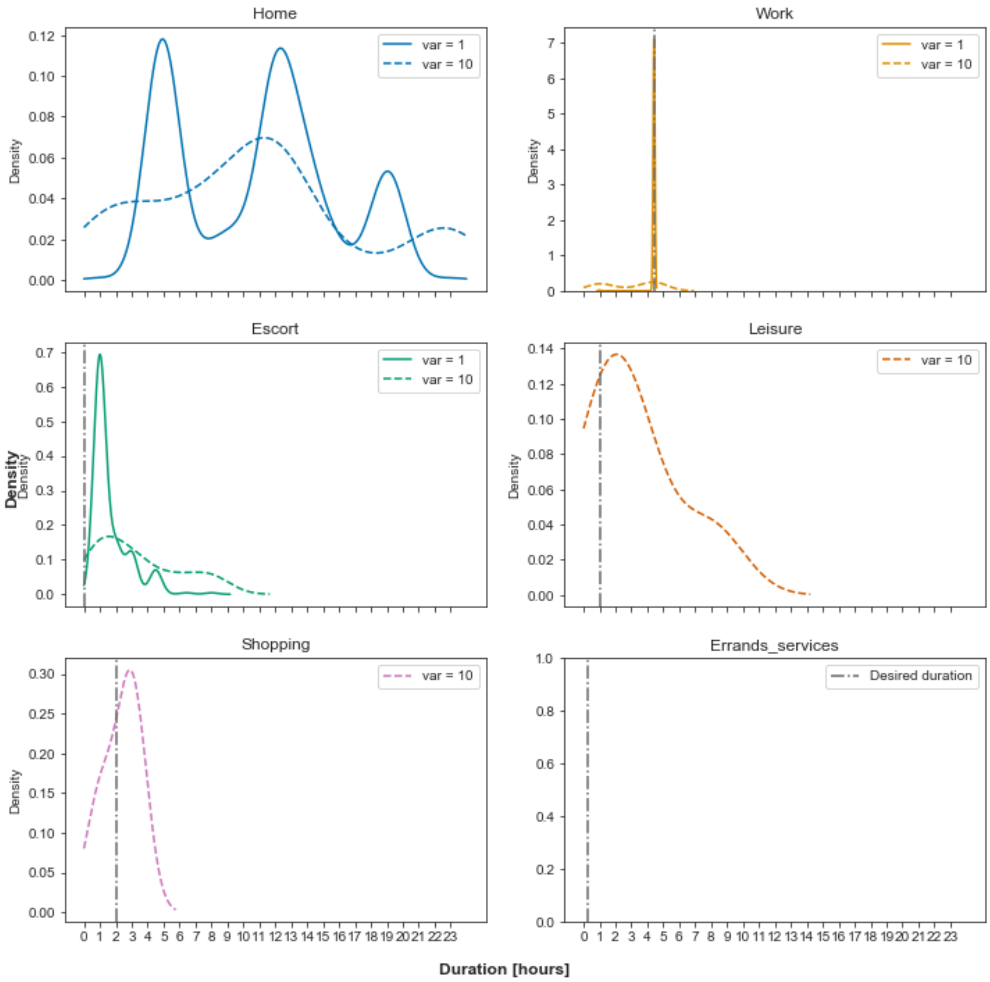


Figure 2.11: Distribution of duration per activity and variance of the random term

solutions. However, all distributions still seem to have a mode relatively close to or centred around the desired start time.

The experimental results show that the framework can generate different realisations of chosen schedules for given sets of considered activities, locations, modes, and timing preferences.

The multimodal distributions of the decision variables (start times and durations) highlight the scheduling trade-offs made during optimisation. These variations impact "flexible" activities in particular, which are characterised by lower penalties for schedule deviations.

Furthermore, the distributions emphasise the influence of the model's parameters on its outputs and, consequently, the importance of selecting ranges of values that ensure varied and stable solutions.

We now compare a distribution generated by our model and the true empirical distribution. We have selected a small subset of individuals from the MTMC (students living in Lausanne) and plotted the schedule frequency (given by the frequency of activity scheduled at a given time of day). We have collected the activities and locations from this sample. The modes of the distributions of start times and duration for each activity were computed and used as proxies for the desired start times and durations input required by the optimisation model. The *education* activity has been set to a lower flexibility level than the other activities (k = Not Flexible). The values of each parameter are summarised in Table 2.4. We have run several iterations of the model and aggregated the results to obtain a schedule distribution over a day. The empirical and simulated distributions are shown in Figure 2.12.

In the empirical distribution, education takes up most of the day, from 7:00 to 22:00, with a higher frequency between 8:00 - 12:00 and 13:00 - 16:00. The second most frequent activity is *leisure*, which is spread throughout the day between 9:00 - 4:00 (frequency between 20-30% for each hour between 12:00 and 21:00). A small proportion of students work or go shopping during the day. In the simulated distribution, there are fewer out-of-home schedules (i.e., schedules containing at least one out-of-home activity). Still, the *education* activity presents a similar profile to the empirical one. The flexible activities such as *leisure* or *shopping* have not been simulated as well: leisure is not scheduled after 16:00, and shopping is more significant in the simulated schedules than in the observed ones.

This result shows that the simulator can generate a reasonable schedule distribution for a given population. The problem's parameters (flexibility, penalties, desired timings, etc.) must be fine-tuned to adequately capture the trade-offs between activities, especially regarding flexible activities.

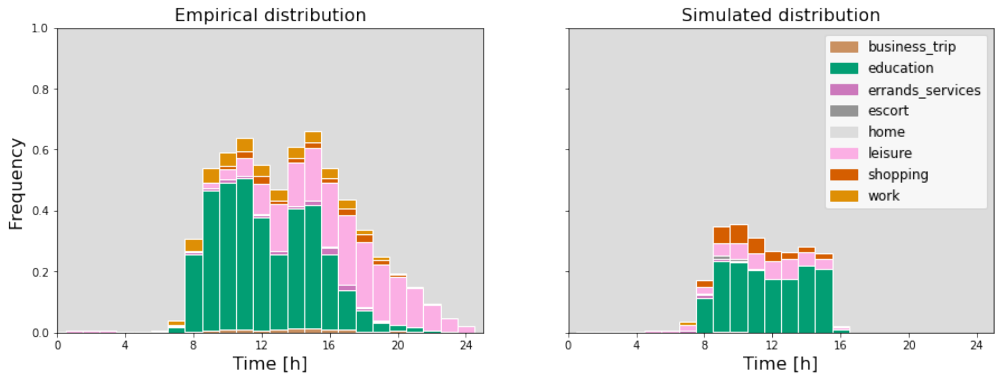


Figure 2.12: Comparison of empirical and simulated distribution of activities, for Lausanne students

2.6 Conclusion

This chapter presents OASIS, an integrated framework to model the trade-offs made by individuals when scheduling activities. The main characteristics of our methodology are as follows:

- All choices about daily mobility (activity scheduling, mode choice, activity location) can be considered simultaneously, and trade-offs between these choices are easily modelled.
- A schedule is associated with a utility, consistently with random utility theory. (Manski, 1977)
- The scheduling choice is explicitly modelled as a mixed integer optimisation problem solved by the decision maker.
- Due to the complexity of the choice model, there is no close form probability formulation. Instead, the framework allows the empirical distribution of the choice model to be estimated using simulation.

Following this first application of the framework, we have identified several strengths and weaknesses. We have used a utility specification which includes only activity- and travel-specific variables. A linear impact on the utility has been assumed for each of them. Such a simple formulation may not capture complex behaviours and interactions.

One strength of the framework is its flexibility, which allows the modeller to increase the complexity of the representation without decreasing the practicality of the formulation. As demonstrated with the inclusion of constraints on mode choice (Section 2.4), many extensions of the model can be implemented straightforwardly by adding or removing constraints or by modifying the objective function (utility). While this might increase the computational expense, it does not require any technical or methodological change to accommodate the additions, and the results can still be interpreted from first principles. This characteristic makes the framework particularly interesting for practical applications or to be integrated into a larger modelling environment with predefined inputs and constraints.

The representation of the modelling elements has also been simplified. Using single combinations of activity, mode of transport, and destination as the unit of analysis offers the advantage of simultaneously predicting different choices for each dimension. However, the generation of these combinations relies heavily on assumptions that can limit the model's ability to deal with specific cases. For this reason, the current implementation does not allow for solid dependencies between activities (e.g. bundles of activities). A careful consideration of how activities are represented in the context of our framework is necessary, with the limitation of available data to confirm our hypotheses.

The search for an optimal exact solution comes with its own set of limitations: the performance and speed of the model depend on its complexity, and the estimation times can quickly become prohibitive for an implementation in practice that often deals with vast synthetic populations and large amounts of data. Heuristics can be used to reach a solution in a shorter time - but the issue of the validity of the resulting schedule remains. In Chapter 4 and appendix C, alternative formulations of the optimisation framework relying on constraint programming are explored. This work specifically focuses on maintaining the flexibility of the current approach.

In the above case study, we assumed the model's parameters were known. It is usually not the case in practice: they must be estimated from data, using, for instance, maximum likelihood estimation. One significant challenge for applying maximum likelihood estimation to the activity-based context is the combinatorial nature of the choice set. As the alternatives, or possible schedules, cannot be enumerated, it is necessary to rely on samples of alternatives to estimate the model. We develop this methodology in Chapter 3.

Chapter 3

Estimation of parameters and utility specification

This chapter is based on the following journal publication:

> Pougala, J., Hillel, T., and Bierlaire, M. (2023c). OASIS: Optimisation-based Activity Scheduling with Integrated Simultaneous choice dimensions. *Transportation Research Part C: Emerging Technologies*, 155:104291 DOI: 10.1016/j.trc.2023.104291

And the following conference proceedings:

> Pougala, J., Hillel, T., and Bierlaire, M. (2021). Choice set generation for activity-based models. In *Proceedings of the 21st Swiss Transport Research Conference*, Ascona, Switzerland

> Pougala, J., Hillel, T., and Bierlaire, M. (2022b). Parameter estimation for activity-based models. In *Proceedings of the 22nd Swiss Transport Research Conference*, Ascona, Switzerland

The candidate has performed this work under the supervision of Prof. Michel Bierlaire and Dr. Tim Hillel.

3.1 Introduction

In chapter 2, we have introduced OASIS, an activity-based model to simultaneously estimate activity participation, scheduling, travel mode and location choices. The model involves aspects of the utility- and rule-based approaches and uses mixed-integer optimisation to simulate realisations of feasible activity schedules. The primary benefit of the simultaneous approach over traditional sequential methods (that describe the activity-travel process as a sequence of individual choices with varying degrees of interaction) is that the simultaneous approach inherently captures trade-offs between activity scheduling decisions. This opens the way for a flexible integration of behavioural extensions, including complex context-specific constraints and interactions.

A significant limitation and challenge of the simultaneous approach is the estimation of stable and significant parameters. In the previous chapter, we did not estimate the parameters of the utility function and instead used a set of accepted values from the literature to illustrate the framework's principles. Parameter estimation is generally challenging in activity-based models due to the problem's size, the structure's complexity due to the spatio-temporal constraints, and, often, the lack of appropriate data. In sequential models, the set of parameters can be estimated in stages (e.g., Bowman and Ben-Akiva, 2001; Chen et al., 2020), which considerably simplifies the problem but at the expense of model flexibility and behavioural realism. Choice sets are usually considered given or constructed with mostly arbitrary decision rules. Considering each choice dimension simultaneously makes the estimation problem significantly more complex, as the resulting combinations cannot be fully observed or enumerated, and the correlations between choice dimensions and between alternatives are difficult to properly account for within a tractable mathematical process.

In this chapter, we introduce a methodology to estimate the behavioural parameters of the simultaneous model, consisting of two elements: (i) choice set generation, where we generate a sample of competitive alternative schedules by applying the Metropolis-Hasting algorithm to historic schedules and (ii) discrete choice parameter estimation, where the scheduling process is formulated as a discrete choice problem, in which each individual chooses a full daily schedule from a finite set of possible schedules..

Sampling a finite choice set is essential for the application of classical maximum likelihood estimation, which: (i) greatly simplifies the estimation procedure, (ii) formally and explicitly links behaviour and activity schedules by providing interpretable parameter estimates, (iii) provides extensive econometric theory to support our analyses.

We test different model specifications and evaluate the quality of the parameter estimations and their impact on the simulations for a sample of individuals of the MTMC (BfS and ARE, 2017).

3.2 Relevant literature

A significant challenge in activity-based modelling is the estimation of the model parameters. This is especially crucial for utility-based models: while the activity-based problem can be solved by taking advantage of random utility maximisation theory and econometric concepts and properties, calibrating the model to data is not straightforward - often due to the lack of available data. In addition, the methodology and assumptions of classical discrete choice modelling cannot easily be transferred to an activity-based context. When the scheduling of activities and travel across time and space is formulated as a choice between discrete alternatives, the problem is multidimensional (involving continuous and discrete choice dimensions such as activity participation, scheduling, mode, destination, route..., etc.) and combinatorial. The modeller or the decision-maker cannot enumerate or fully observe the complete set of solutions. In addition, while the schedules in the choice set are overall distinct, they might present significant overlaps in their components. Finally, the constraints further increase the complexity of the problem, limiting the derivation of closed-form probabilities (Recker et al., 2008). These issues are even more challenging when the choice dimensions are considered simultaneously.

There are two main issues: generating a choice set for parameter estimation and formulating a tractable model specification to capture multidimensional correlations.

3.2.1 Choice set generation

Little work in the field of activity-based modelling specifically tackles choice set generation for the estimation of model parameters. While precise choice generation methodologies have not been extensively explored in ABM, it is an issue that has seen more focus in spatial applications such as route, destination or residential choice modelling. Two main approaches can be found in the literature: deterministic and stochastic choice set generation models (Pagliara and Timmermans, 2009). Models that use a deterministic approach typically include a choice set predefined by the modeller or samples of alternatives obtained with decision rules reflecting the domain knowledge. On the other hand, stochastic methods do not assume that the choice set is universal and known but rather model its uncertainty.

In addition to the assumption that choice sets are not universal (i.e. homogeneous across the population) and fully known to the modeller, realistic choice set generation implies considering dynamic choice sets (i.e. that evolve with time and additional endogenous or exogenous information) that may not be fully known to the decision-makers themselves. This is especially true in spatiotemporal applications, which often involve combinatorial spaces. Shocker et al. (1991) distinguishes three different sets:

1. the *awareness set*, the set of alternatives within the universal set that the consumer knows of and which are appropriate to satisfy their goals,

2. the *consideration set*, which is the set of alternatives from the awareness set that are accessible at a particular point in time,

3. the *choice set*, which is the set that the consumer considers immediately before making a choice.

As the awareness and consideration sets are not always available in traditional data sources (e.g. time use surveys and travel diaries), developing a strategy to generate them efficiently and realistically is essential.

The combinatorial nature of the problem prevents a complete enumeration of the possible alternatives. There exist strategies to estimate parameters on subsets of alternatives (e.g., Guevara and Ben-Akiva, 2013). Still, the challenge is to form the said set of alternatives to be informative enough to estimate the parameters and sufficiently varied to minimise bias.

Both deterministic and stochastic models exist to generate spatio-temporal choice sets (Pagliara and Timmermans, 2009) for parameter estimation. Stochastic models for choice set generation have been thoroughly investigated in route choice modelling (e.g., Flötteröd and Bierlaire, 2013; Frejinger et al., 2009).

In route choice modelling, Flötteröd and Bierlaire (2013) describe a methodology to sample paths from a given distribution in a network, which produces a choice set that meets these requirements. They use the MH algorithm (Hastings, 1970) to explore the solution space in an efficient way:

1. First, they propose an initial shortest path between an origin and a destination,

2. they perform random modifications on the path with a known probability and accept or reject the change based on an acceptance probability defined by the modeller. The process is carried out until the defined Markov chain reaches stationarity.

In the paper, the changes to the current state are applied using *operators*: the *splice* operator, the *shuffle* operator, and the combination of both. Splicing the path involves randomly drawing an insertion node with a given probability and then recomputing the shortest path. In the shuffle operation, the order of the existing nodes in the path is changed with a given probability, and the shortest path is recomputed.

Danalet and Bierlaire (2015) have adapted and applied the methodology proposed by Flötteröd and Bierlaire (2013) to sample alternatives in an activity-based context. The alternatives are activity schedules, represented as paths in a defined network. The nodes of the network are activities potentially performed for a unit of time, and the edges connecting them represent successful performance and succession between activities. Therefore, they consider a network with $KT + 2$ nodes and $2K + K^2T - 1$ edges, where K is the number of activity types, and T is the number of time units in the given temporal horizon. As they want to include attractive alternatives in their choice set, they define an attractivity measure for each node based on their observation frequency and the frequency of the length of activity episodes in the network. They validate the method on a synthetic network and on a real dataset describing pedestrian behaviour by calibrating the parameters of a discrete choice model with a utility associated with each activity path. They find that importance sampling with the Metropolis-Hastings algorithm provides a better model fit than randomly sampling the choice model.

However, stochastic methods are not straightforward to apply to activity-based models because their multi-dimensionality and deterministic approaches are usually preferred in the literature.

Models that use a deterministic approach typically include a choice set predefined by the modeller or samples of alternatives obtained from decision rules reflecting the domain knowledge (e.g., Bowman and Ben-Akiva (2001) enumerate the feasible combinations of primary activity, primary tour type, and number and purpose of secondary tours). In some rule-based models, the choice set generation process involves generating a limited set of activities based on rules and then enumerating the combinations (e.g., Arentze and Timmermans, 2000). On the other hand, stochastic approaches do not assume that the choice set is universal and known but rather model its uncertainty. Deterministic choice sets are used in early activity-based models.

3.2.2 Parameter estimation

Several methods are adopted for the estimation of utility parameters, including heuristics and maximum likelihood estimation using discrete models (e.g. Nijland et al., 2009; Arentze et al., 2011a; Xu et al., 2017; Chen et al., 2020). Nijland et al. (2009) estimate the parameters of Arentze and Timmermans's need-based ABM, which assumes that utilities of activities are a function of needs of individuals and households and that these needs grow over time following a logistic function. They use a logit model for the choice of performing an activity on a specific day d, given that the activity was last performed on day s.

Because the assumptions of the logit model are too restrictive to adequately capture the randomness and unobserved factors in the need-building process, Arentze et al. (2011a) also estimate the parameters of the need-based model, but with an error components mixed logit model. The setup of both models greatly simplifies the choice set considerations: as only one choice dimension is considered (day of week of participation), the choice set can easily be enumerated. In addition, as they do not explicitly model activity duration and timing decisions, they do not consider the effect of activity-travel interactions (e.g. timing trade-offs between activities).

Regue et al. (2015) and Xu et al. (2017) explicitly address the estimation of the parameters of Recker's HAPP. The utility function of the HAPP defines the objective function of a maximisation problem subject to individual spatio-temporal constraints. Regue et al. (2015) calibrate activity-specific priority parameters for different household clusters (with respect to scheduling deviations from cluster mean) using goal programming. They find an overall improvement in the model performance using edit distance as an error measure, as opposed to a case where the priorities are equal. Their methodology cannot provide insights into unchosen activity patterns as they calibrate their model parameters by confronting their simulated and observed patterns. On the other hand, Xu et al. (2017) attempt to improve the behavioural interpretation of the model simulations with estimated parameters while preserving the constraints of the optimisation problem. They solve a path-size logit model, where the choice alternatives are clusters of representative patterns from the observed data. The choice set is the combination of alternatives from unchosen clusters that leads to the minimal D-error. Their methodology is one of the first applications of discrete choice estimation for an optimisation-based activity-travel model. It shows the added behavioural value of their approach to the framework. However, it does not ensure unbiased estimators. Indeed, they do not correct their maximum likelihood estimation to account for the calibration on a sample of alternatives and not the complete choice set. In addition, the methodology to generate choice sets creates endogeneity and is biased towards alternatives with a high probability of being chosen: the unchosen alternatives are representative patterns from the observed sample, and the final choice set maximises the information gain. This leads to overfitting, which would reduce the ability of the model to be applied to different contexts and datasets.

Chen et al. (2020) estimate the parameters of their simulation-based activity-based model using gradient descent methods. The model is a nested logit model where each level contains one or more choice models π.

They illustrate their method on a sequential activity-based model with three levels (day pattern, tour, and intermediate stops). Their approach outperforms traditional gradient descent methods, but the behavioural insights gained from their strategy are limited to counting aggregate statistics. In addition, the approach can be suited to sequential ABM to analyse single days and individuals. Still, it cannot easily be extended to more complex interactions (simultaneous choices, multiday analyses, household interactions, etc.). Finally, the choice set is assumed to be known and enumerable.

Najmi et al. (2020) propose a calibration procedure for models integrating multimodal activity routing and network assignment. The model's parameters are calibrated using *splitting ratios*, system-level characteristics (e.g. repartition of trip purposes or time slots).

There are examples in the literature where authors use a method other than discrete choice modelling. For instance, Recker et al. (2008) and Allahviranloo and Axhausen (2018) use a genetic algorithm to estimate the utility function parameters of their household activity-based model. They introduce distance metrics to compute the errors between observed and predicted multidimensional sequences (Euclidian norm for continuous values such as time variables and Levenshtein distance for discrete components such as travel decisions), used to define the fitness function of the genetic algorithm.

However, the general limitations of the genetic algorithm not only apply here, but the nature of the problem exacerbates them: genetic algorithms are slow to converge due to the repeated evaluations of the fitness function. The authors perform a multi-dimensional sequence alignment at each iteration to compute the distance between predicted and observed schedules in continuous and discrete dimensions. This involves an enumeration of element-wise combinations, which can be incredibly costly with increasing complexity.

As the algorithm is searching for optimal solutions with respect to the fitness function, it is essential to purposefully ensure the diversity of the population (e.g. by modifying specific hyperparameters such as the rate of mutations or introducing random sequences in the populations) to reduce the bias in the utility parameters estimated with this method.

Chow and Recker (2012) also tackle estimating the household activity pattern problem parameters. They formulate an inverse optimisation problem to find the combination of parameters for which the schedule is optimal. A limitation of this approach is the one-to-many nature of the inverse problem, which means that, as the problem is under-identified, the found solutions and associated parameters might not be behaviourally interpretable.

Table 3.1 summarises the papers described in this section and the methodologies developed or applied by the authors for generating individual choice sets and estimating parameters.

In this chapter, we describe the methodology to estimate the parameters of the OASIS utility function based on maximum likelihood estimation on a strategically sampled choice set. To generate an appropriate choice set, we extend the works of Flötteröd and Bierlaire (2013) and Danalet and Bierlaire (2015): we implement a random walk where the candidate schedules are obtained through the application of heuristics (operators). The critical difference with Danalet and Bierlaire's work is the representation of the schedule. While they consider only time-dependent activity paths, we integrate additional choice dimensions such as location and mode choice. These dimensions are also considered simultaneously within the framework to capture trade-offs and interrelations between choices.

Expanding on generating neighbouring states with minor changes, we intro-

Table 3.1: Relevant literature

Paper	Type of ABM	Choice set generation	Parameter estimation
Recker et al. (2008)	HAPP	-	Genetic Algorithm
Nijland et al. (2009)	Needs-based model	Full enumeration	Logit model
Arentze et al. (2011a)	Needs-based model	Full enumeration	Mixed logit
Chow and Recker (2012)	HAPP	-	Inverse optimisation problem
Danalet and Bierlaire (2015)	Network-based	Metropolis-Hastings sampling	-
Regue et al. (2015)	HAPP	-	Pattern clustering and goal programming
Xu et al. (2017)	HAPP	Pattern clustering and importance sampling	Path Size logit
Chen et al. (2020)	Sequential ABM	-	Nested logit model
OASIS	Simultaneous ABM	Metropolis-Hastings sampling	Logit model

duce new operators that can modify specific schedule aspects over each choice dimension. These operators are described in section 3.3.

The estimation process consists of two elements: (i) choice set generation, and (ii) discrete choice parameter estimation. The simulation framework, presented in Chapter 2, outputs a distribution of feasible schedules for given individuals, each with socio-demographic characteristics and timing preferences (desired start time and duration for each activity or group of activities). These features impact the utility each individual gains from their daily schedule, according to the estimates of the parameters. These estimates are obtained by defining the scheduling process as a discrete choice problem and deriving the parameters that maximise the likelihood function.

3.3 Choice set generation

3.3.1 Definitions

We recall and update some fundamental definitions presented in section 2.4:

- **Time:** we assume here that time is discretised in time blocks of equal length t, with T the time horizon (e.g. $T = 24$h),

- **Space:** space is discretised in a finite set of locations $\mathcal{L}$. Each location is associated with at least one activity.

- **Activity:** an activity a is uniquely defined as an action taking place in a physical location $\ell_a \in \mathcal{L}$, having a start time x_a and a duration τ_a. The sequence of activities $\{a, a+1\}$ generates a trip from location ℓ_a to ℓ_{a+1}, that can be performed using mode $m_a \in \mathcal{M}$. $\mathcal{M}$ is the set of modes of transportation available to the individual. Note that if the next activity occurs at the same location, the duration of the trip is simply zero.

- **Schedule:** a schedule $\mathcal{S}$ is the outcome of the decisions of the person n with respect to activity participation, activity location, activity scheduling, transportation mode choice, and any other dimension added at the discretion of the modeller (e.g. route choice). More specifically, a schedule $\mathcal{S}$ is a sequence of S activities $(a_0, \dots, a_S)$, starting with a first (dummy) activity called "dawn", and finishing with a (dummy) activity called "dusk", both of which take place at home.

A schedule is *valid* if

- it spans the whole time horizon, that is, if

$$\tau_{\text{dawn}} + \tau_{\text{dusk}} + \sum_{a,b \in A} \big(\tau_a + \rho(\ell_a, \ell_{a+1}, m_a)\big) = T, \tag{3.1}$$

- it does not exceed the maximum budget, that is, if

$$\sum_{a,b \in A} (c_a + \kappa(\ell_a, \ell_b, m_a)) \leq B, \tag{3.2}$$

- each activity b starts when the trip following the previous activity a is finished, that is

$$x_b = x_a + \tau_a + \rho(\ell_a, \ell_b, m_a), \tag{3.3}$$

- the duration of each activity is valid, that is, if

$$\tau_a \geq \tau_a^{\min} > 0 \tag{3.4}$$

- only one activity from a set of considered duplicates (i.e. same activity with different associated locations or modes) is included in the schedule.

Each valid schedule $\mathcal{S}$ is associated with a time-dependent utility function, which is the sum over the utilities of each scheduled activity $a \in \mathcal{S}$. These utilities include the utility of participating in the activity, the (dis)utility of travelling, or deviating from a preferred schedule.

- **Choice set:** We adopt a definition similar to the one proposed by Shocker et al. (1991), discussed in section 3.2. An entire schedule (including activity participation, timings, locations and modes of transportation) is one alternative an individual can choose. The choice set, therefore, contains several distinct alternatives. We call *feasible set* $\mathcal{F}^n$ the ensemble of valid schedules. This is the complete choice set of the problem, which is combinatorial and, therefore, cannot be enumerated. Out of all possible schedule alternatives, the individual is only aware of a sample that defines the *considered set* C^n. While finite, this set is not readily available to the modeller, which instead has to rely on the schedule chosen and recorded to infer behaviour. The *realised schedule* is the chosen alternative.

Figure 3.1 illustrates the definition of the choice sets and how they relate.

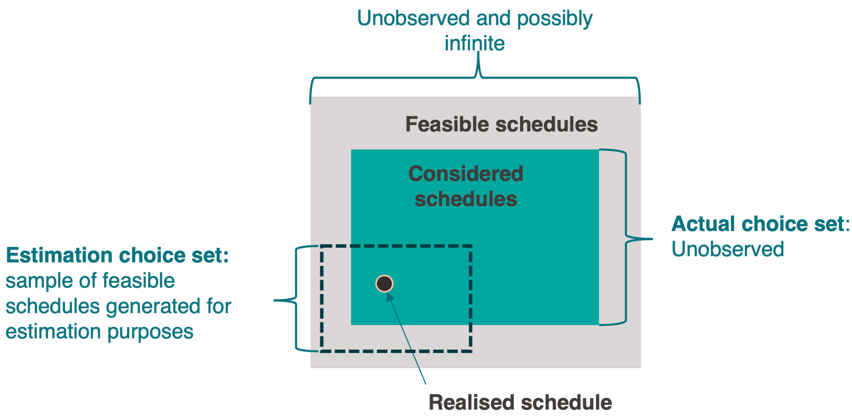


Figure 3.1: Definition of choice sets

3.3.2 Methodology

The estimation of parameters using maximum likelihood estimation requires an evaluation of the likelihood function for each alternative of the choice set $\tilde{C}_n$. If $\tilde{C}_n$ is a subset of the universal choice set of alternatives C_n, the likelihood function must be corrected with the probability of sampling the choice set $\tilde{C}_n$ given the chosen alternatives (3.12). This probability depends on the generation protocol for the sample. The procedure must, therefore, be able to produce tractable probabilities while ensuring the generation of a pertinent choice set for the estimation of parameters.

More specifically, the choice set should contain alternatives with a high probability of being chosen to represent a choice set that the individual would consider. However, estimating a model with such a choice set would lead to biased model parameters, which would, in turn, decrease the accuracy and realism of the model predictions. On the other hand, the size of the solution space requires a strategic procedure to sample alternatives to avoid only selecting non-informative or low-probability schedules. The strategy to build the choice set must generate an ensemble of high-probability schedules to estimate significant and meaningful parameters while still containing low-probability alternatives to decrease the model bias. (Bierlaire and Krueger, 2020).

The importance sampling of alternatives with the MH algorithm (Flötteröd and Bierlaire, 2013; Danalet and Bierlaire, 2015) is an excellent strategy to achieve this objective while keeping tractable probabilities to derive the sample correction for the likelihood function.

The MH (Hastings, 1970) is a Markov Chain Monte-Carlo (MCMC) method used to generate samples from a multidimensional distribution using a predefined acceptance/rejection rule. The procedure is summarised in algorithm 1 and illustrated with fig. 3.2.

Algorithm 1 Metropolis-Hastings algorithm (Gelman et al., 1995)

Choose starting point X_0 from starting distribution $p(X_0)$
for $t = 1, 2, \dots$ **do**
  Sample a candidate point $X*$ from a transition distribution $q(X * | X_{t-1})$
  Compute acceptance probability $\alpha(X_{t-1}, X^*) = \min\left(\frac{p(X^*)q(X_{t-1}|X^*)}{p(X_{t-1})q(X^*|X_{t-1})}\right)$
  With probability $\alpha(X_{t-1}, X^*)$, $X_t \leftarrow X^*$, else $X_t \leftarrow X_{t-1}$

Each iteration of the random walk is, therefore, composed of two main steps:

1. Generation of a candidate point,
2. Acceptance or rejection of the candidate point.

In the context of the activity-based framework, each point (or state) is a schedule, and the target distribution is the schedule utility function (Equation 2.7).

Generation of a candidate point

We define X_t as the state (or point) at time t. X_t is a 24 hour schedule, discretised in *blocks* of duration $\tau \in [\tau_{min}, 24 - \tau_{min}]$ (with τ_{min} the minimum block duration). The new candidate point is a *neighbouring* schedule X^*, i.e. a schedule that only differs in one dimension (time, space, or activity participation - see fig. 3.3). We define heuristics (operators) $\omega \in \Omega$ to create X^* by modifying the current state. X^* is then accepted or rejected with a given acceptance probability.

Each operator ω can be selected with a probability P_ω, decided by the modeller.

Each schedule X_t is characterised by one or more *anchor* nodes v at the start of a block, indicating the position where the change of the operator will be applied. In this context, the block length corresponds to the temporal magnitude of the

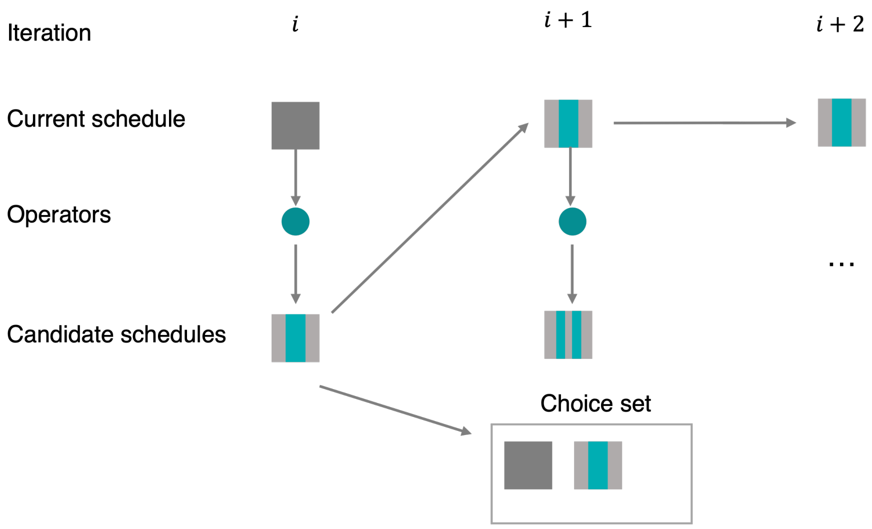


Figure 3.2: Choice set generation process

change.

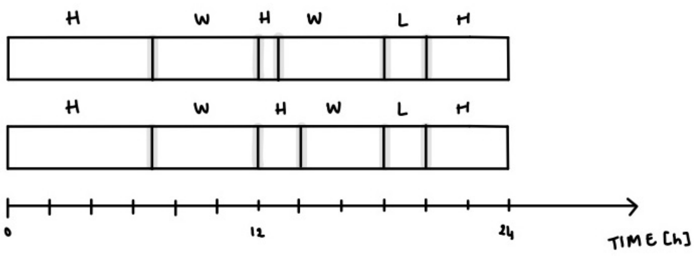


Figure 3.3: Example of neighbouring schedules. The schedules differ in the time spent at home during lunchtime.

Each operator must generate a feasible schedule, as defined in Section 3.5.2. In addition, the following conditions must be satisfied by the algorithm:

- Each iteration of the MH algorithm must be irreducible, meaning that each state of the chain can be reached in a single step:

$$Q(X_t|X_{t-1}) > 0 \qquad \forall X_t, X_{t-1} \tag{3.5}$$

  For this reason, each operator should apply single changes, or the combination of operators should lead to a state that can only be reached with this combination.

- Each iteration of the MH algorithm must be reversible, i.e. the forward probability (probability to do the change) and backward probability (probability to undo the change and go back to the previous state) must be strictly positive.

$$Q(X_t|X_{t-1}) > 0 \qquad \forall X_t, X_{t-1} \tag{3.6}$$
$$Q(X_{t-1}|X_t) > 0 \qquad \forall X_t, X_{t-1} \tag{3.7}$$

Defining single change operators enables the derivation of tractable probabilities.

The following list describes examples of operators that meet these requirements. Other operators can be created according to the modeller's needs and specifications. We illustrate their effect on an example schedule, shown in Figure 3.4. In its initial state, we assume time to be discretised in 24 blocks of length $\delta = 1h$. We consider two activities: *work* and *leisure*, each associated with a start time x_w and x_l, a duration τ_w and τ_l, and locations ℓ_w, ℓ_l. Considering that home is at location ℓ_h (and $\ell_h \neq \ell_w \neq \ell_l$), the individual travels to the other activities using modes m_w and m_l.

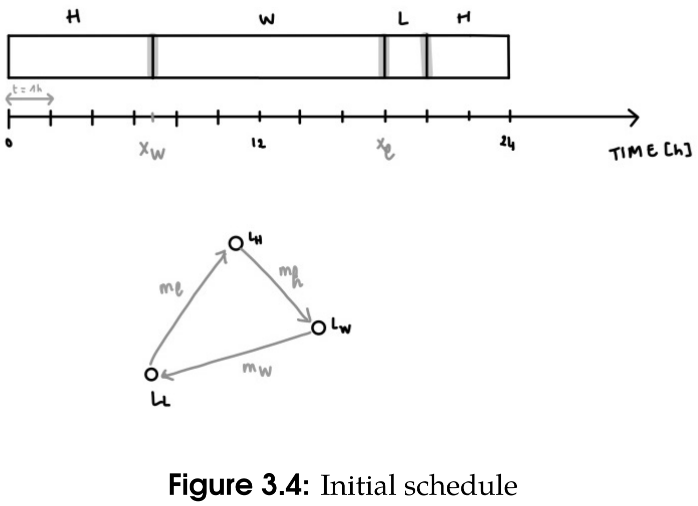


Figure 3.4: Initial schedule

Anchor The anchor operator ω_{anchor} adds an anchor node v in the schedule. This change does not affect the activity sequence but allows a change in the position of the potential modifications of the other operators.

The transition probability associated with this change is the probability of selecting one of the existing blocks as the anchor node.

Assign The assign operator ω_{assign} assigns an activity $j \in \mathcal{A}$ to a block of duration δ at position ν, previously assigned to activity i. $\mathcal{A}$ is a set of N possible activities. The assignment is done with replacement, meaning $P(i = j) > 0$. The resulting schedule must always start and end at home to respect validity requirements.

Figure 3.5 illustrates an example of modification applied by the *assign* operator on the initial schedule.

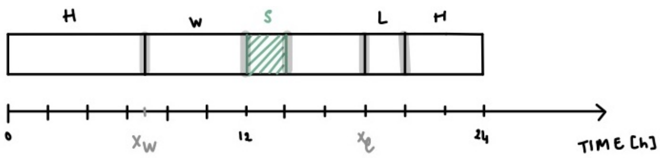


Figure 3.5: Change applied by the *assign* operator

Block The block operator ω_{block} modifies the time discretisation by changing the length δ of the schedule blocks (e.g. from $\delta = 30$ to $\delta = 15$ minutes). This change does not affect the activity sequence but allows the change in the scale of the potential modifications of the other operators.

The transition probability associated with this change is the probability of selecting one of the possible discretisations.

Figure 3.6 illustrates an example of modification applied by the *block* operator on the previously introduced initial schedule.

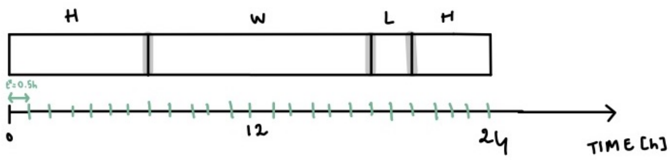


Figure 3.6: Change applied by the *block* operator

Inflate/Deflate The *inflate/deflate* operator $\omega_{\text{inf/def}}$ randomly increases the duration (i.e. adding one block of length δ) of the activity i at position ν and deflating the duration (i.e. removing one block of length δ) of an activity j of the schedule. The direction of the inflation and deflation (affecting the previous or following block of the selected one) is randomly chosen. If $i = j$, the operator only shifts the activity's start time while maintaining its duration. This operator modifies durations without generating infeasible schedules (e.g. schedules with a total duration different from the time budget). To ensure the validity constraint that the schedule must start and end at home, the schedule's first and last time block cannot be modified.

Figure 3.7 illustrates an example of modification applied by the *inflate/deflate* operator on the initial schedule.

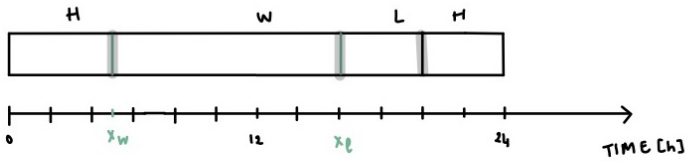


Figure 3.7: Change applied by the *inflate/deflate* operator

Mode The *mode* operator ω_{mode} changes the mode m of the outbound trip of a randomly selected activity i at position ν. The new mode is selected from a set of modes $\mathcal{M}$ that is considered known. The travel times following this change are recomputed, and any excess or shortage of time compared to the available budget is absorbed by the time at home. For this reason, and to remain compliant with validity constraints, the resulting change cannot exceed the time budget by more than the minimum time at home (i.e. 2δ). Therefore, a mode must be selected according to a distribution $P_m(\rho)$, conditional on the travel times ρ. We assume that this distribution is exogenous to the choice-set generation algorithm. The last home activity is not linked to an outbound trip, so it cannot be selected for a mode change.

Figure 3.8 illustrates an example of modification applied by the *mode* operator on the initial schedule.

Location Similarly to the *mode* operator, the *location* operator ω_{loc} changes the location ℓ_i of a randomly selected activity i at position ν, with probability P_{loc}. The new location is selected from a set of locations $\mathcal{L}$ that is considered known. The travel times following this change are recomputed, and any excess or shortage of time compared to the available budget is absorbed by the time at home. For this reason, and to remain compliant with validity

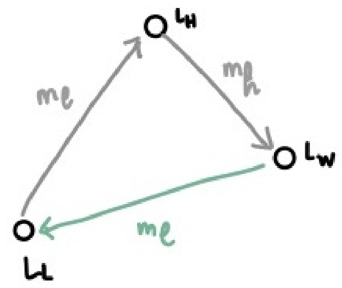


Figure 3.8: Change applied by the *mode* operator

constraints, the resulting change cannot exceed the time budget by more than the minimum time at home (i.e. 2δ). In addition, the home location ℓ_h cannot be changed. The location selection must, therefore, be done according to a distribution $P_\ell(\rho)$, which is conditional on the travel times ρ. We assume that this distribution is exogenous to the choice-set generation algorithm.

Figure 3.9 illustrates an example of modification applied by the *location* operator on the initial schedule.

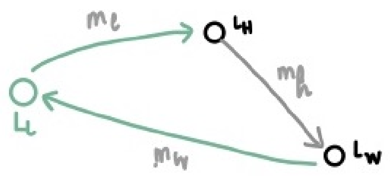


Figure 3.9: Change applied by the *location* operator

Swap The operator ω_{swap} randomly swaps two adjacent blocks. A block at position v, b_v, is randomly selected and then is swapped with the following block. The resulting schedule must always start and end at home to respect the validity requirements.

Figure 3.10 illustrates an example of modification applied by the *swap* operator on the initial schedule.

Combination This meta-operator ω_{meta} combines n distinct operators from the full set of operators Ω. n is an arbitrary number such that $n \in 2, ..., N_{op}$,

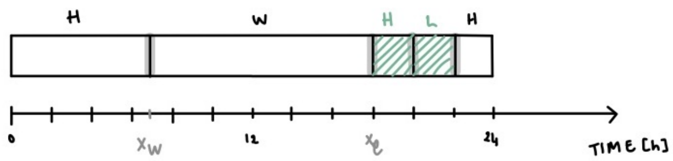


Figure 3.10: Change applied by the *swap* operator

with N_{op} the number of available operators. The transition probabilities of the change are the combined forward (resp. backward) probabilities of the selected operators. Combining operators through a meta-operator instead of randomly selecting them "on the fly" during the random walk process offers the advantage of making it easier for the modeller to track the behaviour of the process. Specifically, the impact of each operator, whether applied individually or in conjunction with others, can be evaluated.

We summarise the previous list in Table 3.2. As previously mentioned, this list is not exhaustive: other operators can be created or combined to fit the requirements of the intended applications or to improve the performance of the MH algorithm.

Table 3.2: Example of operators

Name	Choice dimension	Description	Probability
Anchor	-	Adds or deletes an anchor node	P_{anchor}
Assign	Activity participation	Assigns activity to a given block	P_{assign}
Block	-	Modifies time discretisation of the schedule	P_{block}
Inflate, Deflate	Time	Inflates or deflates the duration of a given activity	$P_{\text{inf, def}}$
Mode	Mode of transportation	Changes the mode of transportation associated with activity	P_{mode}
Location	Location	Changes the location associated with activity	P_{loc}
Swap	Activity participation, Time	Swaps the activities of two adjacent blocks	P_{swap}
Combination	All	Combines two or more operators	P_{meta}

Acceptance of candidate points

The target distribution of the MH algorithm is the schedule utility function (Equation 2.7), conditional on the distribution of the error terms, and with unknown parameters to be estimated. The acceptance probability is defined by:

$$\alpha(X_{t-1}, X^*) = \min\left(\frac{p(X^*)q(X_{t-1}, X^*)}{p(X_{t-1})q(X^*, X_{t-1})}\right) \tag{3.8}$$

Where X^* is the candidate state, $p(i)$ is an unnormalised positive weight, proportional to the target probability (Flötteröd and Bierlaire, 2013) and $q(i, j)$ is the transition probability to go from state i to state j.

Similarly to Danalet and Bierlaire (2015), for each state X_t, the target weight $p(X_t)$ is defined by:

$$p(X_t) = \tilde{U_S}(X_t) \tag{3.9}$$

Where $\tilde{U_S}$ is a schedule utility function with the same specification as the target (Equation 2.7) but with parameters calibrated on a randomly generated choice set.

The transition distribution q is directly obtained from the working operator.

Therefore, the general algorithm (algorithm 1) can be adapted to the ABM context, as summarised in Algorithm 2.

Algorithm 2 Choice set generation for the ABM with Metropolis-Hastings

```
t ← 0, initialise state with random schedule X_t ← S_0
Initialise utility function with random parameters Ũ_S
for t = 1, 2, ... do
    Choose operator ω with probability P_ω
    X*, q(X_t, X*) ← ApplyChange(ω, X_t)
    function ApplyChange(ω, state X)
        return new state X′, transition probability q(X, X′)
    Compute target weight p(X*) = U_S~(X*)
    Compute acceptance probability α(X_t, X*) = min( p(X*)q(X_t|X*) / p(X_t)q(X*|X_t) )
    With probability α(X_t, X*), X_{t+1} ← X*, else X_{t+1} ← X_t
```

Following Ben-Akiva and Lerman (1985), we define for each n the alternative specific corrective term for a choice set C_n of size $J+1$ with $\tilde{J}$ unique alternatives (Equation 3.10). Each alternative j is sampled from the target distribution of the Metropolis-Hastings algorithm with probability q_{jn}, such that $q_{jn} = 0$ if $j \notin C_n$.

$$q(C_n|i_n) = \frac{1}{q_{in}} \prod_{j \in C_n} \left(\sum_{j \in C_n} q_{jn} \right)^{J+1-\tilde{J}} \tag{3.10}$$

Implementation notes

Selection probabilities for operators The probabilities of selecting and applying an operator are arbitrary and to be defined by the modeller. An iterative approach to the choice set generation might highlight an imbalance in the rate of accepted schedules per generating operator. In this case, an equilibrium can be achieved by fine-tuning the operator choice probabilities, e.g. by selecting fewer times the operators that are more likely to produce accepted changes.

Schedule feasibility The states generated by the process must meet validity criteria such as starting and ending at home or having consistent timings between consecutive activities. One risk when defining operators is that they change a current feasible schedule into an infeasible state. For example, changing the duration of an activity may lead to a total duration that differs from the available time budget. One solution is to define operators that do not inherently induce infeasibility. This provides the advantage of making the transition probabilities easier to compute but limits the possible changes that can be applied. On the other hand, allowing for infeasibility in the operators' results can lead to more varied results. An operator that restores feasibility at the end of the process (e.g. modifying the time spent at home to absorb timing gaps or excesses in the schedule). However, as these changes would depend on the current state, computing the associated transition probabilities would prove more difficult.

Target weights The target weights for each state X_t are defined as the utility function evaluated at X_t. However, the function evaluation is conditional on the values of its parameters, which we attempt to estimate with the random walk. Lemp and Kockelman (2012) proposes an iterative process to compute the weights in importance sampling by updating the weights with the estimates of the previous iterations. For example, Danalet (2015) use parameters calibrated on a randomly generated choice set as a starting point for their Metropolis-Hastings process.

Initial schedule The methodology requires the initialisation of a starting point, which is arbitrarily chosen. A randomly generated schedule can be used for this task, but for the sake of model efficiency and realism of the resulting choice, starting with a known high-probability schedule (e.g. a daily schedule recorded in a travel survey) can be considered. This allows the selection of alternatives that the individual will likely consider more efficiently. However, as discussed previously, one must be careful also to include lower probability alternatives. The random walk parameters (e.g., acceptance ratio) must thus be adjusted to avoid such biases.

3.3.3 Empirical tests

We use the MH algorithm to generate a choice set for the *student* population of Lausanne (236 schedules) of the MTMC, the same sample used in Chapter 2.

Initialisation

The initial parameters of the model, used to evaluate the weights characterising the target distribution, are calibrated on a larger sample of Lausanne residents (students and non-students) with 1118 diaries. Table 3.3 gives the values of the significant estimated parameters. This calibration was performed by estimating the parameters using a choice set of size $N = 100$, with 99 randomly generated schedules and the chosen schedule recorded in the survey. Note that *home* is selected as the reference alternative. Consistently with random utility theory, the constants of the other activities can, therefore, be interpreted as the utility gained from performing out-of-home activities instead of staying at home, all else being equal.

We initialise the following operators for the random walk: *Block, Assign, Swap, Inflate/Deflate and Combination.* For the sake of simplicity, we omit the travel dimension and assume that each activity takes place at the same location. Therefore, we only focus on the time scheduling aspect. As mentioned earlier, we also assume an equal probability of selecting the operators.

Table 3.3: Parameters calibrated on randomly generated model.
NS: Not significant

Activity	Constant	Duration [h]	Start time[h]	Early	Late	Short	Long
Business trip	3.34	13.29	7.44	-2.65	-0.29	-0.25	-38.35
Education	5.78	5.97	6.00	-1.92	-0.22	-1.17	-0.22
Errands, services	2.61	NS	17.56	-0.0087	-1.15	NS	-0.75
Escort	3.90	NS	11.99	-0.32	-0.36	NS	-0.91
Home	-	23.98	-	-	-	-0.30	-266
Leisure	4.29	0.51	8.46	-1.55	-0.21	0	NS
Shopping	34.67	NS	8.42	-2.50	-0.24	0.12	-0.98
Work	7.33	11.22	6.49	-1.97	-0.54	-0.69	-1.25

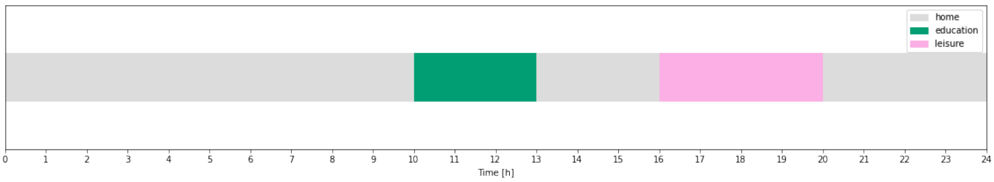
Eight activities can be scheduled: *home* (not including mandatory start and end of the schedule), *work, education, shopping, errands or use of services, business trip* (e.g. work activity outside of the typical workplace), *leisure* and *escort* (e.g. accompanying someone to an activity). These categories are a simplification of the original classification reported in the dataset. We have assumed that the probability of scheduling a type of activity (specifically for the *assign* operator) was not equal across types. Instead, we have used the frequency of each activity type $a \in \mathcal{A}$ in the student sample as a proxy for the probability of choosing to perform it at a given time. The frequency is the number of schedules in the sample in which the activity is present. The values are reported in table 3.4.

Table 3.4: Frequency values in sample, per activity

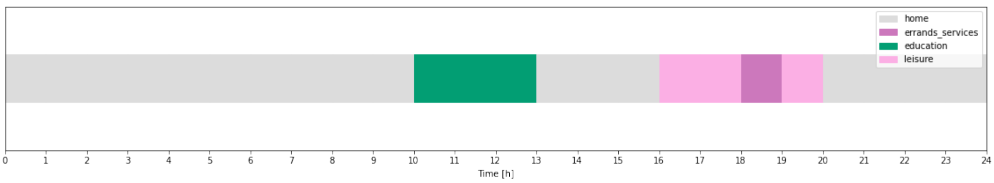
Activity	Frequency [%]
Home	38.8
Leisure	23.0
Education	20.6
Shopping	8.7
Escort	2.8
Errands, services	2.8
Work	2.5
Business trip	0.8

Examples

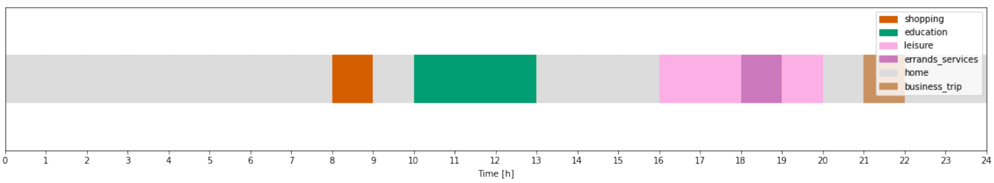
The first example is a choice set generated for one individual, randomly selected in the sample. We run 10,000 iterations of the algorithm and keep 20 accepted schedules after a warm-up period. Figure 3.11 shows the initial schedule used as input of the procedure and four generated schedules. As the selected schedules were consecutive, we can visualise the result of each accepted change. Visually, most of the accepted moves seem to be *assigning* new activities. Schedule 4 (Figure 3.11e) is interesting: it does not appear to be a reasonable schedule, with many splits of activities and short durations. This result indicates that the process can generate attractive schedules (with respect to the utility function) such as Figures 3.11b and 3.11c, and alternatives with lower choice probabilities.



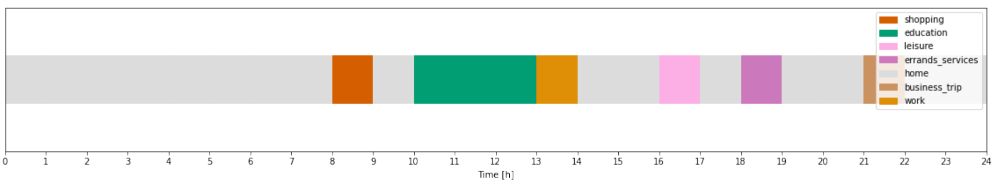
(a) Initial schedule



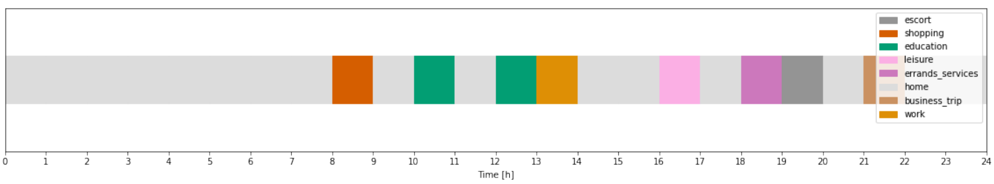
(b) Schedule 1



(c) Schedule 2



(d) Schedule3



(e) Schedule 4

Figure 3.11: Example alternatives from choice set

We repeated the procedure for all the individuals in the sample. We ran 10,000 iterations of the algorithm and sampled accepted schedules after a warm-up period. We generated 5,000 schedules across the population. Figure 3.12 shows the distribution of start times for the different activity types across all the generated alternatives. For most activities, the start times appear uniformly scheduled during the day. On the other hand, *education* and *leisure* have more defined peaks. Looking at the scheduling frequency of each activity (Figure 3.13), we notice that they are the two activities present in every generated schedule. This result is unsurprising, as they are the most frequent out-of-home activities among Lausanne students (Table 3.4), and the observed schedules were used as starting points of the random walk.

We are interested in understanding the impact of each operator on the acceptance of a generated schedule. Figure 3.14 illustrates the proportion of each operator among accepted moves. In the current set-up, and considering an equal probability of selecting one of the operators at each iteration, combining multiple changes (meta-operator) seems the most promising to achieve a schedule that will be accepted, followed by the *assign* operator. This makes sense: because the constants for participating in each activity type are positive and often more prominent in scale than the penalties for schedule deviations (Table 3.3), adding activities is more favourable in terms of utility gain than the other operations. The *block* operator applied alone produces no accepted schedule. This also makes sense, as this operator does not fundamentally change the current state and must be used with other operators.

Taking a closer look at the combinations of operators (meta-operators), we can note that longer combinations (up to 4 operators) are more likely to produce accepted schedules (Figure 3.15). Figure 3.16 shows the prevalence of each operator in the accepted meta-operator combinations. The *assign* operator is the most frequent, especially when drawn multiple times. The *swap* operator is the second most combined operator, specifically in combination with *InflateDeflate* or applied numerous times in a row. Note that the map is not symmetric; for instance, applying the *Block* operator after *InflateDeflate* is a combination that is less present among accepted schedules than the other way around.

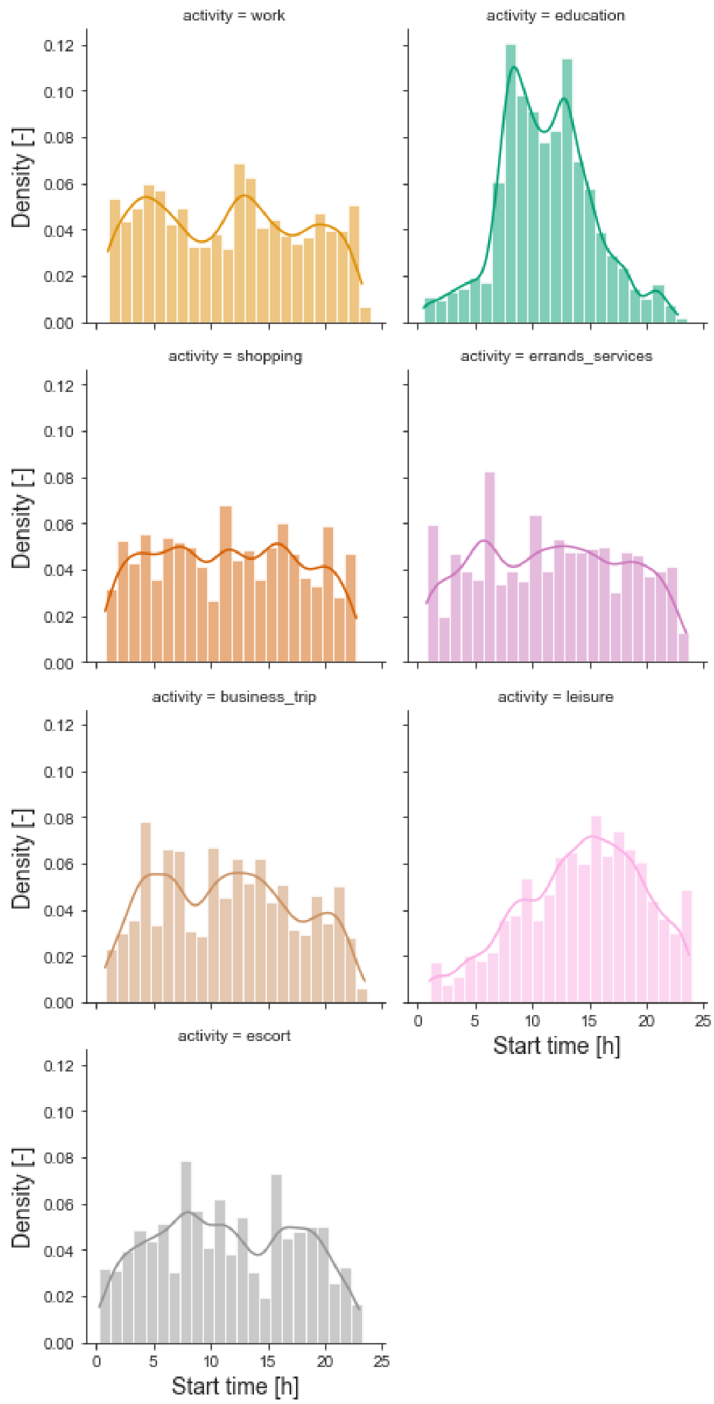


Figure 3.12: Distribution of start times in the generated choice sets

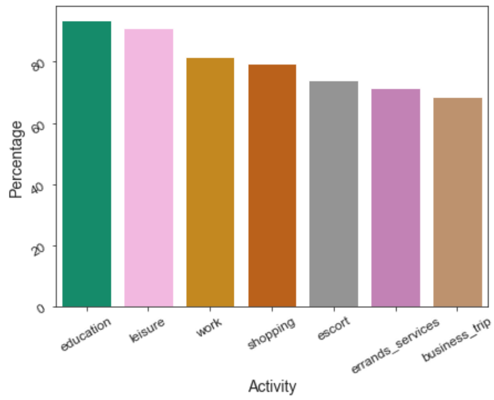


Figure 3.13: Frequency of activity types in the generated choice sets

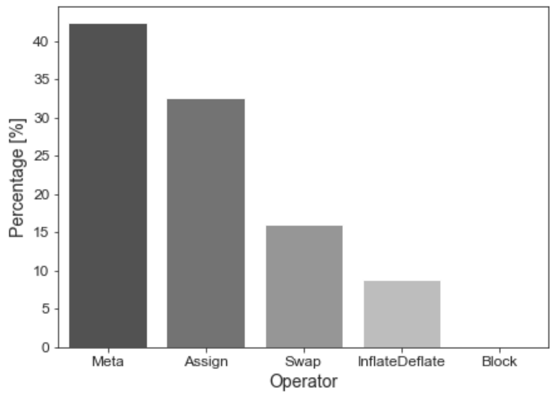


Figure 3.14: Frequency of operator types in accepted schedules

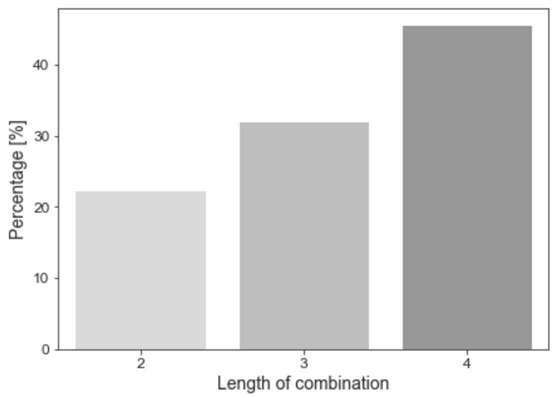


Figure 3.15: Typical lengths of combinations for accepted meta-operators

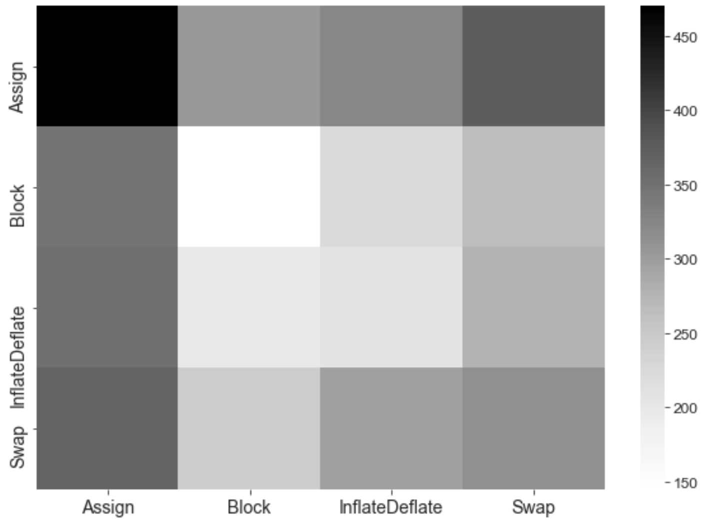


Figure 3.16: Frequency of pairs in accepted meta-operators. *y-axis: first operator, x-axis: second operator*

3.4 Parameter estimation

The scheduling process can be considered a discrete choice model where the alternatives are full daily schedules, each associated with a utility. The likelihood function (Equation 3.11) gives the probability that the model outputs the schedule i that each n has chosen (i.e. the observed schedule) (Train, 2009).

$$\max_{\beta} \mathcal{L} = \max_{\beta} \prod_{n} \prod_{i} P_{in}^{y_{in}} \tag{3.11}$$

The estimates of the parameters β are the values that maximise this function. In principle, maximum likelihood estimation requires a complete enumeration of the alternatives in the choice set. It is possible, though, to estimate the parameters using only a sample of alternatives. This is necessary in the activity-travel context, where the complete choice set C_n of alternatives is combinatorial and characterised by complex constraints. For each n in the sample, we consider a selection of alternatives $\tilde{C}_n$. The maximisation of the likelihood function yields consistent parameter estimates if a correction term $\ln P_n(\tilde{C}_n|i)$ is introduced to take into account sampling biases (Ben-Akiva and Lerman, 1985):

$$P_{in} = P_n(i|\tilde{C}_n) = \frac{e^{\mu V_{in} + \ln P_n(\tilde{C}_n|i)}}{\sum_{j \in \tilde{C}_n} e^{\mu V_{jn} + \ln P_n(\tilde{C}_n|j)}} \tag{3.12}$$

The alternative-specific correction term $\ln P_n(\tilde{C}_n|i)$ is the logarithm of the conditional probability of sampling the choice set $\tilde{C}_n$ given that i is the alternative chosen by person n. This value depends on the protocol to generate the choice set (Equation 3.10).

This formulation implies that if every alternative has an equal probability of being chosen, $\ln P_n(\tilde{C}_n|i) = 0$ and the estimation of the model on the subset is the same as the estimation on the complete choice set (Frejinger et al., 2009).

Each component of the utility function (Equations (2.8) to (2.14)) is associated with a random term. This defines a mixed logit model with error components by creating correlations between alternatives with the same values for each dimension. The model reduces to a simple logit model if we assume the error terms to be i.i.d. and Extreme Value distributed, meaning there is no correlation between alternatives. This assumption is adopted in the case study presented in Section 3.5.

3.5 Empirical investigation

We sample choice sets of daily schedules for each individual in the Lausanne student sample of the MTMC. Each choice set comprises ten alternatives, including the chosen (recorded) schedule.

The second step, once the choice sets have been generated, is to estimate the parameters of the utility function for the sample. For each individual and each alternative in their respective choice sets, we evaluate the sample correction term for the choice probability (Equation 3.12).

3.5.1 Choice sets

For each person in the training dataset, we generate a choice set of 10 alternatives (including the observed schedules) randomly, using the clustering method developed by Allahviranloo et al. (2014), and following the methodology presented in Section 3.3.

Random generation (benchmark)

We generate each alternative using the following procedure:

1. Randomly choose an activity a from a set of possible activities A, a mode $m \in M$ and a location $\ell \in L$,
2. Randomly choose a start time x_a, in minutes after midnight. For the second activity and onwards, the start time is deterministically assigned to the end time of the previous activity, including the travel time between both locations,
3. Randomly choose a duration τ_a, such that $\tau_a \leq \tau_r$, with τ_r the remaining duration until midnight.
4. Repeat until there is no time remaining.

Assuming that every alternative generated this way has an equal probability of being selected, the sampling correction term in Equation 3.12 cancels out.

Empirical choice set (benchmark)

We generate a choice set using the two-step clustering method developed by Allahviranloo et al. (2014) to extract representative activity patterns from a given dataset. Xu et al. (2017) further developed this procedure to generate a choice set suitable for discrete choice estimation of parameters. The methodology is as follows:

1. Identify representative patterns using a two-step clustering algorithm (combination of affinity propagation and k-means clustering). Similar schedules are clustered based on two dedicated metrics (agenda dissimilarity measure and the edit distance),
2. Create a choice set for each n by drawing patterns from non-chosen patterns.[1]

With this method, the choice set comprises actual activity patterns from the dataset.

OASIS generation

The initial state X_0 of the random walk is the observed schedule. We implement six operators: *Block* and *Anchor*, which influence the impact of the other operators, and *Assign*, *Swap*, *Inflate/Deflate*, which modify the schedule directly. A *Meta*-operator is implemented to combine the actions of two or more operators. Each operator can be chosen with a uniform probability $P_{\text{operators}}$.

The target distribution of the random walk is the utility function of the activity-based model (Equation 2.7), with a set of parameters β_0 that were estimated using randomly sampled choice sets. The target weights are evaluations of this utility function for the current state.

The random walk (Algorithm 2) is performed for many iterations n_{iter}. We discard $n_{\text{warm-up}}$ of these iterations to sample from a stabilised distribution. We draw nine alternatives to create the choice set by only keeping 1 out of n_{skip} schedules.

[1] Xu et al. (2017) implement an additional step where they personalise the resulting choice set by enforcing individual-specific constraints. We do not, however, have access to such constraints in our case study and, therefore, consider that each schedule is feasible and that all clusters have an equal probability of being chosen.

Table 3.5: Experimental set-up of the random walk

Feature	Definition	Value
Ω	Set of operators	Block, Assign, Anchor, Swap, Inf/Def, Meta
$N_{\text{operators}}$	Number of operators	6
$P_{\text{operators}}$	Operator selection probability	$1/N_{\text{operators}}$
n_{iter}	Number of iterations	100'000
$n_{\text{warm-up}}$	Warm-up iterations	50'000
n_{skip}	Skipped iterations	20

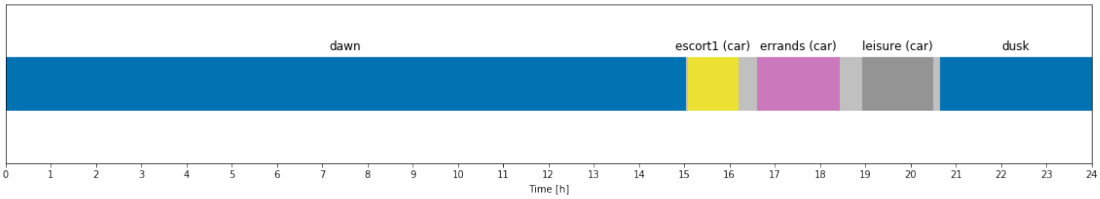


Figure 3.17: Example of a daily schedule. The light grey patches between activities indicate travel. *Dawn* and *dusk* are the first and last *home* activities of the day.

The algorithm was run on a server (2 Skylake processors at 2.3 GHz and 192GB RAM, with 18 CPUs running in parallel) for each of the 236 students in the sample for a total runtime of 2.22 minutes.

3.5.2 Scheduling framework and utility functions

We use the same schedule definition as Pougala et al. (2022a): a sequence of *activities*, starting and ending at home, over a time horizon T. An activity a is uniquely characterised by a location ℓ_a, a start time x_a, a duration τ_a, a cost of participation c_a and an outbound trip to the location of the following activity with a mode of transportation m_a. The boundary conditions (start and end of the schedule at home) are modelled as two dummy activities "dawn" and "dusk".

Figure 3.17 shows an example of a schedule for one person, which includes three out-of-home activities (escort, errands, and leisure). The trips between each location are made by car.

Each schedule S is associated with a utility function U_S, which captures the individual's preferences for the schedule. We test multiple specifications of U_S: a linear-in-parameters utility function, where time sensitivity can be included through scheduling preferences for each activity (chapter 2), and a utility specification initially proposed for the scoring of activity schedules in the MATSim microsimulator (Feil, 2010), where the utility for activity duration is assumed to have an S-shape.

Utility specification with linear penalties

As defined by Equation 2.7, the schedule utility U_S is the sum of a generic utility U associated with the whole schedule and utility components capturing the activity-travel behaviour (utility with respect to start time, duration, and travel).

The parameters involved in the utility function are summarised in Table 3.6. Indices S, a, and n denote a schedule, an activity and an individual. The *Estimated* column indicates which parameters are estimated in the current study, with results presented in Section 3.5. In this model, the error terms are assumed to be i.i.d. and Extreme Value distributed, with a scale parameter μ fixed for identification purposes.

Utility function with S-shape duration term

We test the utility specification proposed by Feil (2010), which is a modification of the default MATSim utility function (Charypar and Nagel, 2005). The utility function considers the impact of activity duration with an asymmetric S-shaped curve with an inflection point, as formalised by Joh et al. (2005) (Eq. 3.14). In their specification, they do not consider the effect of start time. The parameters of the S-shape are the inflection point α_a, the slope β_a, and the relative vertical position of the inflection point ζ_a. When $\zeta_a = 1$, α_a can be considered the duration where the utility reaches its maximum. The parameters involved in the utility function are summarised in Table 3.7. Indices S, a and n denote a schedule, an activity and an individual. The *Estimated* column indicates which parameters are estimated in the current study, with results presented in Section 3.5.

$$U_S = \sum_{a=0}^{A-1} (U_a^{\text{act}} + U^{\text{travel}}) \tag{3.13}$$

$$U_a^{\text{act}} = U_a^{\min} + \frac{U_a^{\max} - U_a^{\min}}{(1 + \zeta_a \exp \beta_a [\alpha_a - \tau_a])^{1/\zeta_a}} \tag{3.14}$$

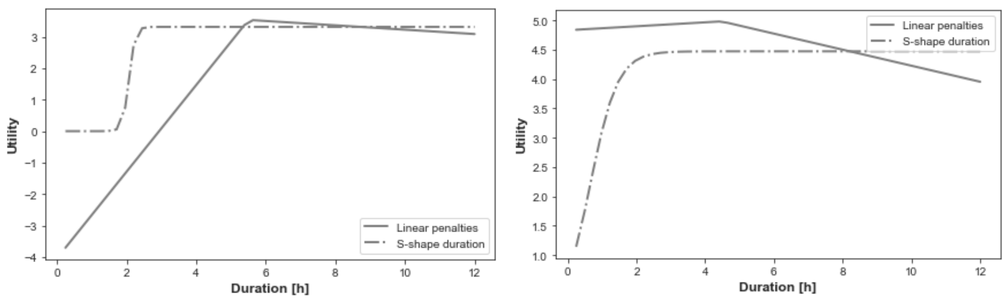
Table 3.6: Parameters of the linear penalties utility function. The *Estimated* column indicates whether the parameter is estimated in the logit specification

Parameter	Notation	Associated variable	Estimated
Alternative-specific constants	$\gamma_{S,n}$	-	
Activity-specific constant	$\gamma_{a,n}$	-	Yes
Cost of activity participation	β_{cost_a}	Cost c_a	
Penalty start time (early)	θ_a^{early}	Deviation start time δ_{e,x_a}	Yes
Penalty start time (late)	θ_a^{late}	Deviation start time δ_{ℓ,x_a}	Yes
Penalty duration (short)	θ_a^{short}	Deviation duration δ_{s,τ_a}	Yes
Penalty duration (long)	θ_a^{long}	Deviation duration δ_{ℓ,τ_a}	Yes
Travel cost	$\beta_{t,\text{cost}}$	Cost c_t	
Travel time	$\beta_{t,\text{time}}$	Time ρ_{ab}	
Error term (participation)	$\varepsilon_{\text{participation}}$	-	
Error term (start time)	$\varepsilon_{\text{start time}}$	-	
Error term (duration)	$\varepsilon_{\text{duration}}$	-	
Error term (travel time)	$\varepsilon_{\text{travel}}$	-	

Table 3.7: Parameters of the S-shape utility function. The *Estimated* column indicates whether the parameter is estimated in the logit specification

Parameter	Notation	Estimated
Maximum utility	$U_a^{\max}$	Yes
Minimum utility	$U_a^{\min}$	
Inflection point	α_a	Yes
Slope	β_a	Yes
Position of inflection	ζ_a	

Figure 3.18 illustrates the utilities of *work* and *leisure* for both specifications and different values of duration.



(a) Work **(b)** Leisure

Figure 3.18: Effect of duration on utility for the tested specifications.

3.5.3 Model specification

We consider 5 different activities: *home*, *work*, *education*, *leisure* and *shopping*.

You may recall that travel is not considered a standalone activity but is always associated with the origin activity of the trip, if applicable.

We make the following additional simplifications:

- We do not estimate travel parameters and consider them null in Equation 2.7,
- The scheduling preferences (desired start time and durations) are derived from the dataset. For each activity, we fit a distribution (either standard or log-normal) across the student population. The calibrated parameters are reported in table 3.8. We draw values of desired start times and durations for each person from these distributions.
- For the S-shaped utility function Equation 3.14, we assume, as done in

Feil (2010), $U_a^{\min} = 0$ and $\zeta_a = 1 \; \forall a$. This assumption implies a symmetric S-shape with positive support.

Table 3.8: Desired times distributions in sample

Activity	Start time	Duration
Home	-	$\mathcal{N}\,(17.4, 3.4)$
Work	Log-$\mathcal{N}\,(0.65, 4.2, 3.4)$	$\mathcal{N}\,(7.6, 3.7)$
Education	Log-$\mathcal{N}\,(0.4, 6.2, 1.7)$	$\mathcal{N}\,(6.7, 2.1)$
Leisure	$\mathcal{N}\,(14.3, 3.5)$	$\mathcal{N}\,(3.5, 2.7)$
Shopping	Log-$\mathcal{N}\,(0.3, 4.6, 9.0)$	Log-$\mathcal{N}\,(1.3, 0.15, 0.32)$

Table 3.9 summarises the model specifications implemented in this paper. The models differ in the specification of the utility function and/or the parameter estimation procedure:

1. **Benchmark 1 - Literature parameters:** A generic utility function with parameters from the literature (not estimated). The utility function is given by Equation 2.7.

2. **Benchmark 2 - Random choice set:** An activity-specific utility function where we estimate all activity-specific parameters and constants. The choice set is generated randomly. The activity-specific utility function is given by Equation 3.15:

$$
\begin{aligned}
U_S^{\text{act. sp.}} = \gamma_a + \sum_a [\theta_a^{\text{early}} \max(0, x_a^* - x_a) + \theta_a^{\text{late}} \max(0, x_a - x_a^*) \\
+ \theta_a^{\text{short}} \max(0, \tau_a^* - \tau_a) + \theta_a^{\text{long}} \max(0, \tau_a - \tau_a^*)] + \varepsilon_S
\end{aligned}
\tag{3.15}
$$

3. **Benchmark 3 - Empirical choice set:** An activity-specific utility function where we estimate all activity-specific parameters and constants. The choice set is generated by drawing from clusters of representative patterns. The activity-specific utility function is given by Equation 3.15.

4. **Model 1 - OASIS with flexibility-level parameters**: A generic utility function where we classify activities according to two levels of flexibility and estimate the corresponding parameters for both categories. The choice set is generated using algorithm 2. The utility function with flexibility-level

parameters is given by Equation 3.16:

$$U_S^{\text{flex}} = \gamma_a + \sum_f \lambda_f^a [\theta_f^{\text{early}} \max(0, x_a^* - x_a) + \theta_f^{\text{late}} \max(0, x_a - x_a^*)$$
$$+ \theta_f^{\text{short}} \max(0, \tau_a^* - \tau_a) + \theta_f^{\text{long}} \max(0, \tau_a - \tau_a^*)] + \varepsilon_S \quad (3.16)$$

with f a category of flexibility $f \in$ {Flexible, Not Flexible}. λ_f^a is an indicator variable that is 1 if activity a belongs to category f, and is an input to the model. In this case study, education and work are not flexible, while leisure, shopping and home are considered flexible.

5. **Model 2 - OASIS with activity-specific parameters**:. An activity-specific utility function, where we estimate all activity-specific parameters and constants. The choice set is generated using algorithm 2. The activity-specific utility function is given by Equation 3.15.

6. **Model 3 - OASIS with MATSim scoring function:** An activity-specific S-shaped utility for the duration, with a choice set generated using algorithm 2. The utility function is given by Equation 3.13.

We consider the default model of the OASIS framework to be the activity-specific model (Model 2). The comparison with the other specifications provides the following insights:

- Benchmark 1: This model serves as a benchmark for the improvement of estimating the parameters instead of fixed values.

- Benchmark 2 and 3: These models serve as benchmarks for the improvement of strategically sampling the choice set instead of other methods (random generation, selection of representative patterns),

- Model 1: This model is used to evaluate the improvement of estimating activity-specific parameters as opposed to generic (aggregated) ones,

- Model 3: This model is used to evaluate the improvement of a more complex (non-linear) utility specification, specifically with respect to activity duration.

The models are estimated with PandasBiogeme (Bierlaire, 2020). The estimation process is done using 70% of observations in the sample data, where one observation is the daily schedule of one individual.

Finally, we simulate daily schedules for the Lausanne sample. We compare the schedule distributions and distributions of start times and durations resulting from the specified models with observed distribution from the dataset.

Table 3.9: Simulation scenarios

Model	Bench. 1	Bench. 2	Bench. 3	1	2	3
Name	Literature	Random choice set	Empirical choice set	OASIS Flexibility parameters	OASIS Activity-specific	OASIS MATSim
Estimated parameters		✓	✓	✓	✓	✓
MH-Sampled choice set				✓	✓	✓
Activity-specific constants		✓	✓	✓	✓	✓
Activity-specific penalties		✓	✓		✓	✓

3.5.4 Parameters

Benchmark 1: Literature parameters

The parameters from the literature were used in the first implementation of the framework, as described in section 2.5.2. Values from the departure time choice literature (e.g. ratios from Small (1982)) were used to derive the parameters defined in table 3.10. The penalty parameters are specific to each flexibility category (flexible (F) or non-flexible (NF) activities). In this set of parameters, we do not consider activity-specific constants ($\gamma_a = 0 \; \forall a \in A$). The assumption is that the inherent preference to perform any activity (home included), all else being equal, is fully included in the random term of the schedule ε_S, and the error term has zero mean even without the inclusion of activity-specific constants.

Table 3.10: Parameters from the literature

	Parameter	Param. estimate
1	θ_F^{early}	0.0
1	θ_F^{late}	0.0
2	θ_F^{long}	-0.61
2	θ_F^{short}	-0.61
3	θ_{NF}^{early}	-2.4
4	θ_{NF}^{late}	-9.6
5	θ_{NF}^{short}	-9.6
6	θ_{NF}^{long}	-9.6

Benchmark 2: Random choice set

The home activity is a reference, such that $\gamma_{\text{home}} = 0$. The magnitudes and signs of the other constants are relative to the baseline behaviour of staying at home. The estimated parameters are summarised in table 3.11. Using the random choice set, many parameters result statistically insignificant ($p < 0.05$), such as the early and long penalties for education or the constants for *leisure* and *work*.

We can note that the penalty for a short leisure duration is not statistically significant, which is also expected for an activity assumed to be flexible. The same comment can be made for the *shopping* activity, although the parameter's value is very high compared to the other magnitudes. This can reflect a lack of alternatives in the choice sets where the shopping activities have longer durations than the observed schedule. Interestingly, for *work*, the duration parameters are not significant, and the start time deviations are penalised symmetrically.

Benchmark 3: Empirical choice set

The home activity is a reference, such that $\gamma_{\text{home}} = 0$. The magnitudes and signs of the other constants are relative to the baseline behaviour of staying at home. The estimated parameters are summarised in table 3.12.

Similarly to the random choice set, many parameters result in statistically insignificant ($p < 0.05$), especially for the *shopping* and *work* activities. In addition, the penalty for a short duration for *work* is significant but is positive, which is a counterintuitive result, as it implies that individuals reward scheduling

Table 3.11: Estimation results for the Random choice set model on the student population. The asterisk (*) indicates parameters that are not statistically significant based on their p-value.

	Parameter	Param. estimate	Rob. std err	Rob. t-stat	Rob. p-value
1	$\gamma_{\text{education}}$	5.28	1.4	3.76	0.000172
2	$\theta^{\text{early}}_{\text{education}}$	-1.76	1.38	-1.27	0.204*
3	$\theta^{\text{late}}_{\text{education}}$	-1.13	0.373	-3.02	0.00251
4	$\theta^{\text{long}}_{\text{education}}$	-0.266	0.288	-0.924	0.355*
5	$\theta^{\text{short}}_{\text{education}}$	-10.2	4.43	-2.3	0.0212
6	γ_{leisure}	0.507	0.592	0.856	0.392*
7	$\theta^{\text{early}}_{\text{leisure}}$	0.0779	0.103	0.757	0.449*
8	$\theta^{\text{late}}_{\text{leisure}}$	-1.2	0.157	-7.64	0.0
9	$\theta^{\text{long}}_{\text{leisure}}$	-0.228	0.075	-3.03	0.00242
10	$\theta^{\text{short}}_{\text{leisure}}$	0.0	-.	0.	1.*
11	γ_{shopping}	5.7	1.19	4.77	1.85e-06
12	$\theta^{\text{early}}_{\text{shopping}}$	-2.9	0.711	-4.08	4.5e-05
13	$\theta^{\text{late}}_{\text{shopping}}$	-0.482	0.173	-2.78	0.00541
14	$\theta^{\text{long}}_{\text{shopping}}$	-1.4	0.597	-2.34	0.0191
15	$\theta^{\text{short}}_{\text{shopping}}$	-117.0	23.8	-4.9	9.56e-07
16	γ_{work}	0.324	1.44	0.225	0.822*
17	$\theta^{\text{early}}_{\text{work}}$	-0.66	0.21	-3.14	0.00169
18	$\theta^{\text{late}}_{\text{work}}$	-0.533	0.398	-1.34	0.181
19	$\theta^{\text{long}}_{\text{work}}$	-0.0326	0.155	-0.21	0.834*
20	$\theta^{\text{short}}_{\text{work}}$	0.968	0.857	1.13	0.258*

$\bar{\rho}^2 = 0.013$
Estimation time: 1.93 [sec]

work for shorter durations than preferred. This indicates that either the preferred duration (mean of the corresponding cluster) or the choice set is inappropriate (e.g. every alternative except for the chosen one has a long work duration). To correct this, an additional step after the choice set generation is required to ensure the mathematical feasibility of the sampled schedules and their concordance with individual-specific constraints, as suggested by Xu et al. (2017).

Table 3.12: Estimation results for the empirical choice set model on the student population. The asterisk (*) indicates parameters that are not statistically significant based on their p-value.

	Parameter	Param. estimate	Rob. std err	Rob. t-stat	Rob. p-value
1	$\gamma_{\text{education}}$	3.91	0.76	5.15	2.61e-07
2	$\theta^{\text{early}}_{\text{education}}$	0.924	0.36	2.57	0.0102
3	$\theta^{\text{late}}_{\text{education}}$	-0.533	0.115	-4.63	3.63e-06
4	$\theta^{\text{long}}_{\text{education}}$	-0.379	0.093	-4.07	4.66e-05
5	$\theta^{\text{short}}_{\text{education}}$	-0.949	0.766	-1.24	0.215*
6	γ_{leisure}	5.75	0.624	9.21	0.0
7	$\theta^{\text{early}}_{\text{leisure}}$	-0.453	0.0879	-5.15	2.57e-07
8	$\theta^{\text{late}}_{\text{leisure}}$	-0.788	0.211	-3.73	1.94e-04
9	$\theta^{\text{long}}_{\text{leisure}}$	-0.572	0.144	-3.96	7.42e-05
10	$\theta^{\text{short}}_{\text{leisure}}$	-1.15	0.803	-1.43	0.153*
11	γ_{shopping}	3.05	1.05	2.90	3.75e-03
12	$\theta^{\text{early}}_{\text{shopping}}$	-0.262	0.343	-0.765	0.445*
13	$\theta^{\text{late}}_{\text{shopping}}$	-0.486	0.220	-2.20	0.0275
14	$\theta^{\text{long}}_{\text{shopping}}$	0.651	1.01	0.642	0.521*
15	$\theta^{\text{short}}_{\text{shopping}}$	5.90	3.37	1.75	0.0798*
16	γ_{work}	1.90	1.60	1.19	0.235*
17	$\theta^{\text{early}}_{\text{work}}$	-0.97	0.188	-5.16	2.51e-07
18	$\theta^{\text{late}}_{\text{work}}$	-12.5	1.29	-9.73	0.00
19	$\theta^{\text{long}}_{\text{work}}$	0.535	0.346	1.55	0.122*
20	$\theta^{\text{short}}_{\text{work}}$	3.69	0.784	4.71	2.49e-06

$\bar{\rho}^2 = 0.54$
Estimation time: 3.79 [sec]

Model 1: OASIS with flexibility-level parameters

The home activity is a reference, such that $\gamma_{\text{home}} = 0$. The magnitudes and signs of the other constants are relative to the baseline behaviour of staying at home. The estimated parameters are summarised in table 3.13. For flexible activities, the parameters indicate a similar behaviour to what is found in the literature: being late is more penalised than being early (approximately by a factor of 2). The penalties associated with duration have comparable magnitudes, although they are not statistically significant ($p > 0.05$). On the other hand, being early seems to be more negatively perceived than being late for non-flexible activities. The duration penalties are symmetrical.

Table 3.13: Estimation results for OASIS flexibility-level model on student population. The asterisk (*) indicates parameters that are not statistically significant based on their p-value.

	Parameter	Param. estimate	Rob. std err	Rob. t-stat	Rob. p-value
1	$\theta_{\text{F}}^{\text{early}}$	-0.175	0.12	-1.46	0.145*
2	$\theta_{\text{F}}^{\text{late}}$	-0.333	0.14	-2.38	0.0171
3	$\theta_{\text{F}}^{\text{long}}$	-0.105	0.0722	-1.45	0.146*
4	$\theta_{\text{F}}^{\text{short}}$	-0.114	0.194	-0.585	0.559*
5	$\theta_{\text{NF}}^{\text{early}}$	-1.14	0.367	-3.10	0.00191
6	$\theta_{\text{NF}}^{\text{late}}$	-0.829	0.229	-3.61	0.0003
7	$\theta_{\text{NF}}^{\text{long}}$	-1.20	0.393	-3.05	0.00231
8	$\theta_{\text{NF}}^{\text{long}}$	-1.19	0.468	-2.54	0.0011
9	$\gamma_{\text{education}}$	16.0	2.46	6.49	8.63e-11
10	γ_{leisure}	8.81	1.7	5.17	2.28e-07
11	γ_{shopping}	6.85	1.80	3.80	0.000146
12	γ_{work}	16.0	2.58	6.18	6.57e-10

$\bar{\rho}^2 = 0.06$
Estimation time: 0.34 [sec]

Model 2: OASIS with activity-specific parameters

We consider both activity-specific constants and schedule deviation penalties. The home activity is set as a reference for all parameters, such that $\gamma_{\text{home}} = 0$. As for model 1, the magnitudes and signs of the other coefficients are, therefore, relative to the home baseline. We estimate 20 parameters for this model (5 per activity), summarised in table 3.14.

For education, all of the parameters are statistically significant. Being early is slightly less penalised than being late, although the penalties are almost symmetrical. The same observation can be made for the penalties associated with duration. For work, the penalty for being late is not statistically significant (p-value > 0.05), while being early is significantly penalised. The penalties associated with duration negatively impact the utility function; particularly, the activity running for longer than desired is highly penalised.

Interestingly, most of the parameters associated with leisure are not statistically significant. This could indicate that leisure is not a particularly time-constrained activity for students. It is less likely to trigger trade-offs in the scheduling process than the other activities.

On the other hand, shopping displays high penalties for scheduling deviations, especially with respect to start time. This behaviour does not support the assumption used in the previous model that shopping is a flexible activity.

Figure 3.19 illustrates some schedules generated with activity-specific parameters.

Model 3: OASIS with MATSim specification

We estimate the parameters $U_{\mathrm{a}}^{\max}, \alpha_a, \beta_a$ for all activities. For identification purposes, we fix $U_{\mathrm{a}}^{\min} = 0$ and $\zeta_a = 1$. Similarly to the other models, *home* is associated with a null utility. This assumption also means that the duration at home is the remaining budget time after performing out-of-home activities.

All parameters are significant based on their $p-$value.

For *education* and *work*, the α parameter (inflection point) is around 2 hours, which means that beyond this duration, the utility increases at a decreasing rate (satiation effect). The fact that longer durations are usually scheduled for these activities (as seen in the observed data, fig. 3.20a) suggests that the time allocation for education and work is more constraint-driven than utility-driven. For *shopping*, we observe the opposite. The inflection point is at a very high duration as compared to the typical values in the dataset. However, the negative slope suggests a decreasing utility. This seems to indicate a behaviour that the sole participation in the activity (characterised by a duration $\tau_{\text{shopping}} > 0$) has a positive impact on the utility function but that this utility decreases with duration.

Table 3.14: Estimation results for OASIS activity-specific model on student population. The asterisk (*) indicates parameters that are not statistically significant based on their p-value.

	Parameter	Param. estimate	Rob. std err	Rob. t-stat	Rob. p-value
1	$\gamma_{\text{education}}$	18.7	3.17	5.89	3.79e-09
2	$\theta^{\text{early}}_{\text{education}}$	-1.35	0.449	-3.01	0.00264
3	$\theta^{\text{late}}_{\text{education}}$	-1.63	0.416	-3.91	9.05e-05
4	$\theta^{\text{long}}_{\text{education}}$	-1.14	0.398	-2.86	0.00428
5	$\theta^{\text{short}}_{\text{education}}$	-1.75	0.457	-3.84	0.000123
6	γ_{leisure}	8.74	1.94	4.50	6.79e-06
7	$\theta^{\text{early}}_{\text{leisure}}$	-0.0996	0.119	-0.836	0.403*
8	$\theta^{\text{late}}_{\text{leisure}}$	-0.239	0.115	-2.07	0.0385
9	$\theta^{\text{long}}_{\text{leisure}}$	-0.08	0.0617	-1.30	0.195*
10	$\theta^{\text{short}}_{\text{leisure}}$	-0.101	0.149	-0.682	0.495*
11	γ_{shopping}	10.5	2.20	4.78	1.74e-06
12	$\theta^{\text{early}}_{\text{shopping}}$	-1.01	0.287	-3.51	0.000443
13	$\theta^{\text{late}}_{\text{shopping}}$	-0.858	0.237	-3.63	0.000284
14	$\theta^{\text{long}}_{\text{shopping}}$	-0.683	0.387	-1.76	0.0779*
15	$\theta^{\text{short}}_{\text{shopping}}$	-1.81	1.73	-1.04	0.297*
16	γ_{work}	13.1	2.64	4.96	7.16e-07
17	$\theta^{\text{early}}_{\text{work}}$	-0.619	0.217	-2.85	0.00438
18	$\theta^{\text{late}}_{\text{work}}$	-0.338	0.168	-2.02	0.0438
19	$\theta^{\text{long}}_{\text{work}}$	-1.22	0.348	-3.51	0.000441
20	$\theta^{\text{short}}_{\text{work}}$	-0.932	0.213	-4.37	1.23e-05

$\bar{\rho}^2 = 0.62$
Estimation time: 1.41 [sec]

Interestingly, for *leisure* $U^{\max}_{\text{leisure}}$ is almost the same as for education, although it is reached much sooner according to the α parameter. This suggests a more substantial satiation effect for this activity as compared to *education*, which is expected.

Table 3.15: Estimation results for OASIS with MATSim specification model on student population.

	Parameter	Param. estimate	Rob. std err	Rob. t-stat	Rob. p-value
1	$U^{\max}_{\text{education}}$	4.79	0.443	10.8	0.00
2	$\alpha_{\text{education}}$	1.57	0.202	7.75	9.1e-15
3	$\beta_{\text{education}}$	7.56	4.84	1.56	0.119
4	$U^{\max}_{\text{leisure}}$	4.47	0.379	4.50	9.1e-15
5	α_{leisure}	0.668	0.213	3.13	0.00172
6	β_{leisure}	2.53	0.686	3.69	0.000225
7	$U^{\max}_{\text{shopping}}$	2.12	0.333	6.36	2.04e-10
8	α_{shopping}	3.66	0.975	3.75	0.000175
9	β_{shopping}	-4.85	2.3	-2.1	0.0353
10	$U^{\max}_{\text{work}}$	3.31	0.637	5.19	2.08e-07
11	α_{work}	2.07	0.0459	45.	0.00
12	β_{work}	11.5	0.792	14.5	0.00
$\bar{\rho}^2 = 0.56$					
Estimation time: 12.22 [sec]					

3.5.5 Simulation results

Using the parameters described in the previous section, we simulate schedules for the test dataset. The simulation procedure was introduced in section 2.5.4: at each iteration $i \leq n_{\max}$, we draw a random term ε_i from a known distribution. We solve the utility maximisation problem for this error instance to obtain a draw from the underlying schedule distribution. We draw $n_{\max} = 20$ schedules for each individual in the sample.

To compare the results of each model with the original data, we analyse the simulated frequencies of activity participation per hour of the day, simulated durations and start times for each activity. We compute the Kolmogorov-Smirnov (KS) statistic between the original and simulated distributions for a quantitative evaluation of the goodness-of-fit of these distributions.

Figure 3.19: Examples of simulated schedules (Model 2)

Simulated statistics

We compare descriptive statistics of the simulated sample with those observed in the dataset. These statistics are daily averages of the time spent out-of-home (total and for each activity) and the proportion of scheduled activity types. These statistics are derived exclusively for schedules containing at least one out-of-home activity. It is worth noting that all models generate significantly more fully-at-home days (about five times more than what is observed in the MTMC data).

The results are summarised in Table 3.16 and Table 3.17, respectively. The estimated models (Models 1, 2 and 3) generate average durations that are closer to the observed ones than the model with parameters from the literature. They are especially accurate for the average total time, but the proportions across activities are not as well captured. For example, the average duration spent in education is underestimated by about 1 hour. In contrast, the time spent in leisure is overestimated (by 2 hours in the case of the activity-specific model).

Table 3.16: Average out-of-home duration, in hh:min

Activity	Data	Literature	Random	Empirical	OASIS Flexibility	OASIS Act.-spec.	OASIS MATSim
Total	04:53	02:54	06:38	04:23	04:10	05:19	8:20
Education	03:32	01:11	04:43	02:08	02:25	02:29	02:43
Leisure	00:39	00:58	01:34	00:49	01:17	02:32	04:43
Shopping	00:08	00:22	00:08	01:07	00:21	00:10	00:10
Work	00:26	00:05	00:13	00:18	00:07	00:08	00:20

Regarding the proportion of scheduled activity(table 3.17), Model 2 (OASIS with activity-specific parameters) significantly underestimates the frequency of each activity. This is likely due to the approximation of the desired start times, which are computed for only one activity instance and do not adequately account for bimodality or asymmetry in timing preferences (e.g. different preferred start times for doing work in the morning or the afternoon). This point is discussed further in Section 3.5.5. On the other hand, the MATSim specification seems to provide more realistic results.

Table 3.17: Proportion of scheduled activities [%]

Activity	Data	Literature	Random	Empirical	OASIS Flexibility	OASIS Act.-spec.	OASIS MATSim
Home	71.3	85.3	85.9	85.1	89.3	89.5	66.5
Education	11.2	6.1	5.2	6.4	4.6	3.1	13.0
Leisure	12.8	5.7	7.3	4.0	4.3	6.3	14.5
Shopping	3.7	2.3	0.7	1.6	1.5	0.93	4.2
Work	1.13	0.61	1.0	3.0	0.35	0.20	1.4

Time of day participation

Figure 3.20a shows the typical distribution of daily activities for schedules, including at least one activity out of the home. The height of each bar represents the proportion of the sample participating in each activity at a given moment. Before 7:00, almost all of the individuals in the sample are home. The proportion of people undertaking their main *education* activity steadily increases during the morning, to reach a peak at 11:00 (50%). The ratio decreases at lunchtime (40% to 25% between 12:00 and 13:00) and goes up again in the afternoon. The *leisure* activity is the second most frequent activity from 10:00 to 15:00. From 16:00 onward, it surpasses *education*. *Work* is the third most frequent activity, although in much smaller proportions than the previous two. Its profile is similar to *education*.

Figures 3.20b to 3.20g show the distributions for out-of-home schedules[2] resulting from the simulator framework with the six mentioned configurations: with parameters from the literature (fig. 3.20b), activity-specific parameters with random (fig. 3.20c) and empirical choice set (fig. 3.20d), OASIS generic (fig. 3.20e), and activity-specific (fig. 3.20f) model, and MATSim function (fig. 3.20g). All configurations, except the MATSim specification, can capture the importance of *education* relative to the other activities in the schedule. However, as mentioned in the previous section, for all models, most generated schedules are full days at home (i.e. no out-of-home activity scheduled).

The original profile of the education activity, with a distinct peak period, is best captured with the OASIS estimated parameters, both flexibility- and activity-specific. In both cases, the peak is reached before 9:00, as opposed to the observed

[2]Out of the 20 simulated schedules for each individual in the sample.

11:00 peak. This discrepancy is likely due to the assumption of an unimodal desired start time; a multimodal distribution (closer to the observed one) would improve the fit of the simulated distribution.

Interestingly, the *leisure* activity — and by extension, all activities previously defined as flexible — has very different simulated profiles from the observed one. With the literature parameters and the MATSim specification, the share of leisure is constant for most of the day and comparable to the percentage of education. On the other hand, with the OASIS activity-specific parameters, the activity is overrepresented during the night (midnight to 7:00), compared to the other simulated activities and the leisure observations in the data for this period. The profile is similar to the real one for the rest of the day.

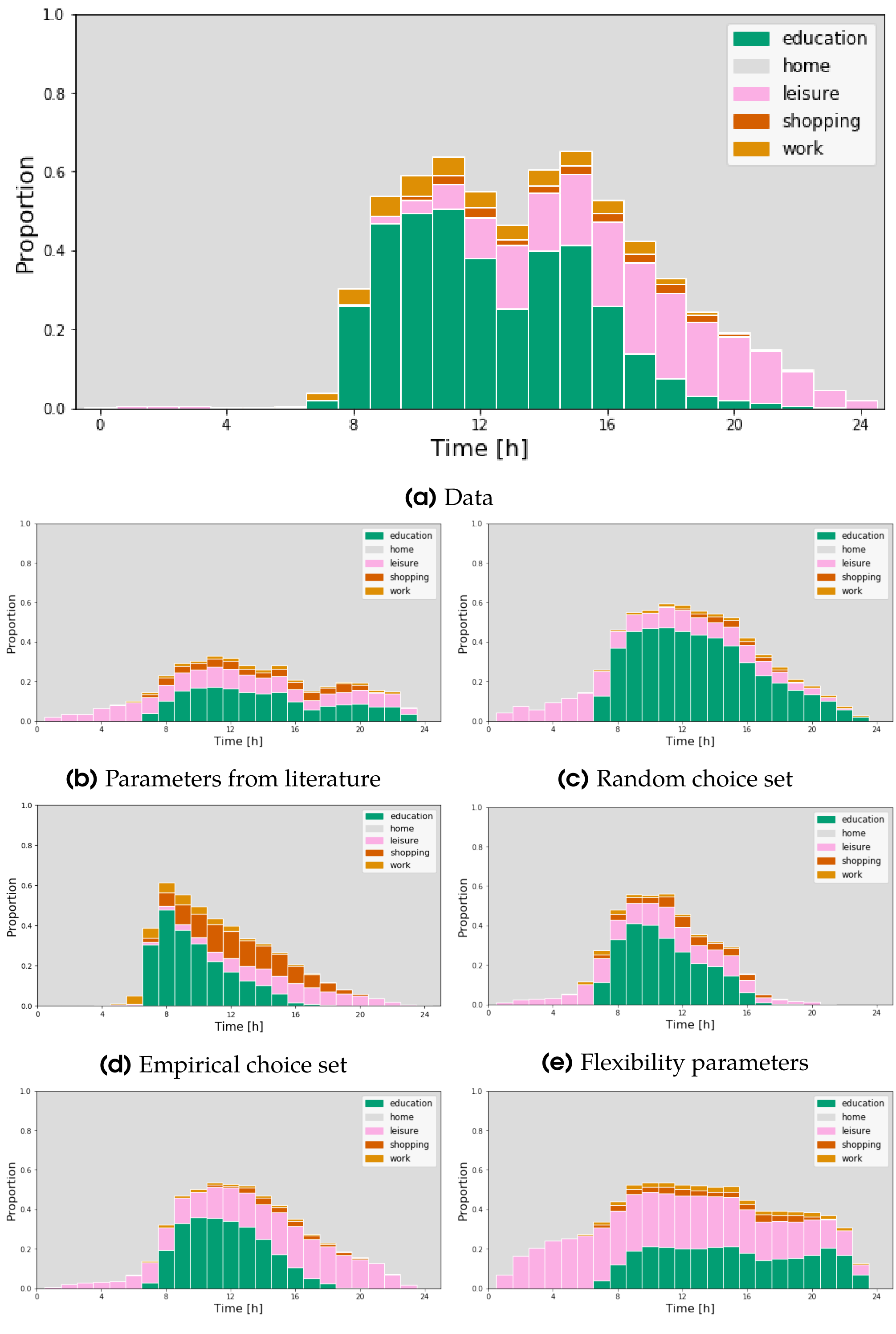
The *shopping* activity is overrepresented in the schedules simulated with the empirical choice set. This is due to the estimated penalties for shopping, which are either insignificant or positive (table 3.12).

For the MATSim specification, we notice that the time of day activity frequency is not correctly captured for most activities, but especially for *leisure* and *education*, which are respectively over- and underrepresented at most times during the day (around 20% of participation). This is because the start time is not included in the specification. This result supports the assumption that the satiation effect for activity duration differs depending on the time of day.

Start time

We compare the simulated start times per activity and model by visualising the kernel density estimations of the models with parameters from the literature, generic and activity-specific parameters (fig. 3.21), and respective KS statistic compared to the observed dataset (a lower KS indicates a better fit). We compare the estimated models (flexibility-level parameters, activity-specific parameters, and MATSim specification) to the benchmark (parameters from the literature).

Except for *education*, the activity-specific model is the model that better reproduces the distributions of start time (lowest KS). The observed distribution of *education* is truly bimodal, which is not adequately captured by either of the estimated models. This is likely due to the approximation of desired times to an unimodal distribution. The model with parameters from the literature produces a relatively good fit, but this distribution varies very little from one activity to another.



(a) Data

(b) Parameters from literature

(c) Random choice set

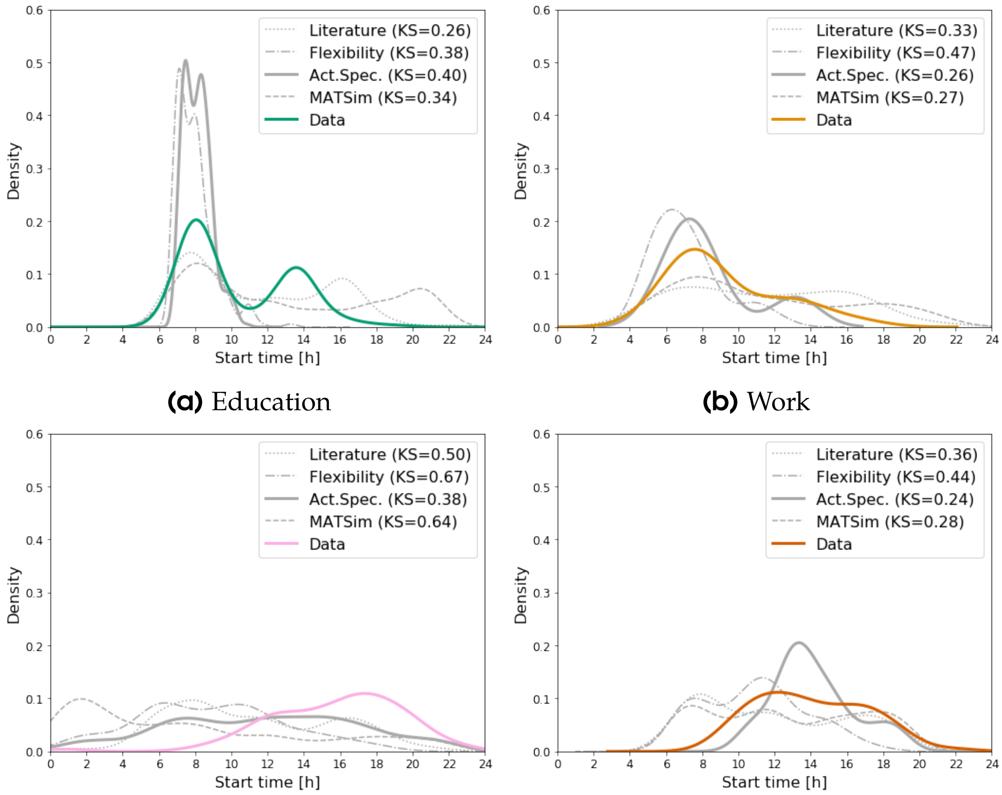
(d) Empirical choice set

(e) Flexibility parameters

(f) Activity-specific parameters

(g) MATSim specification

Figure 3.20: Time of day activity frequency. The height of the bars is the proportion of people participating in each activity at a given moment.



(a) Education

(b) Work

(c) Leisure

(d) Shopping

Figure 3.21: Simulated start times, per model and activity

Duration

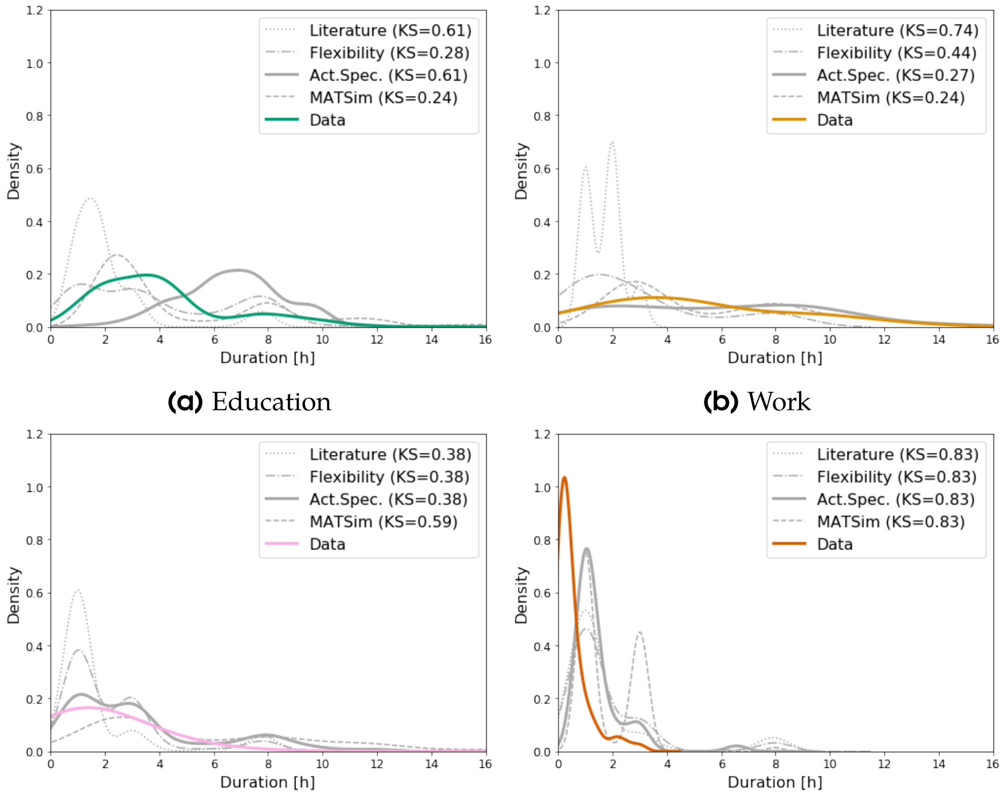
Similarly, we compare the simulated durations per activity and model by visualising the kernel density estimations of each model (fig. 3.22) and computing their respective KS statistic.

For all activities, the model with parameters from the literature tends to generate short activities ($\tau_a \leq 2$ hours) more frequently and in more minor proportions activities with a duration of about 8 hours (for education, leisure and shopping). The three OASIS models generate more diverse patterns with respect to duration: the flexibility-level model seems to capture well the bimodality of *education*. On the other hand, the activity-specific model generates better distributions for *work* and *leisure*. The MATSim specification yields the best results in terms of KS statistic for *education* and *work*. All models tend to generate short instances of the *shopping* activity. However, there is a non-negligible number of schedules with very long shopping activities (8 hours), which is not close to what was observed nor remarkably realistic. This limitation is also reflected by the high value of the KS statistic.

Discussion

This empirical investigation using the MTMC has demonstrated the added value of estimating the parameters for the accuracy and realism of the simulated schedules, as opposed to using constant parameters from the literature. Removing a layer of abstraction by estimating activity-specific parameters instead of generic parameters aggregated over the set of activities has provided results fitting the observed distribution better.

As shown by comparing benchmark 2 (model with random choice set) with models 1-3, the parameters obtained with the MH algorithm yield simulation results more consistent with the observations than those generated with a random choice set. This indicates the importance of sampling strategically from the solution space to ensure that the choice set contains meaningful (or high probability) alternatives. In addition, comparing the values and statistical significance of the estimated parameters highlights the impact of sampling informative schedules as opposed to random ones, especially with such a low number of alternatives. For the random choice set, many alternatives are required to achieve consistent and comparable results with the observed data, as illustrated by fig. 3.23. A low number of alternatives for the MH choice set already yields



(a) Education **(b)** Work

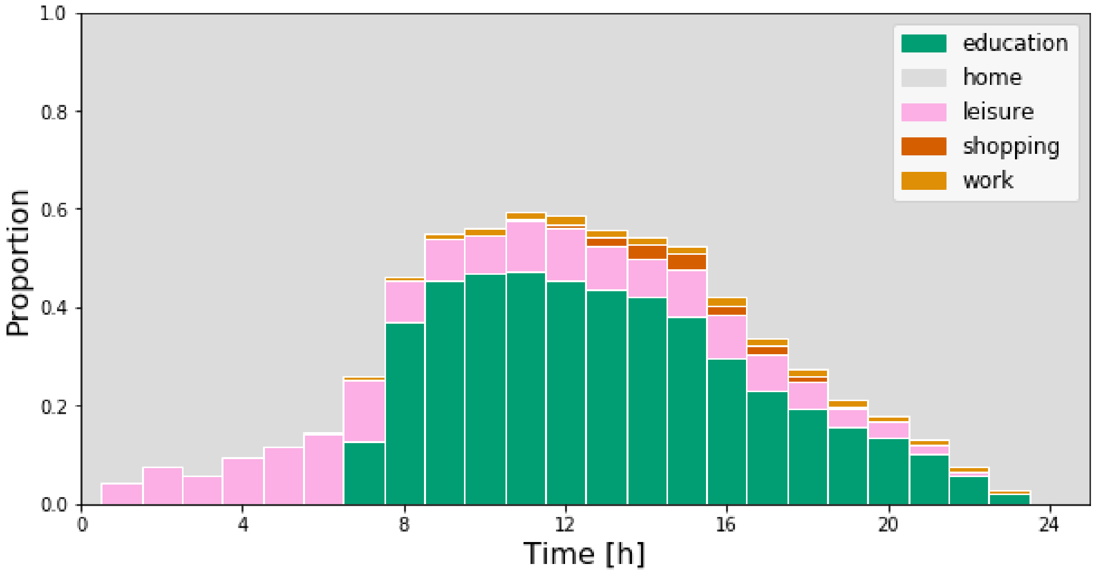
(c) Leisure **(d)** Shopping

Figure 3.22: Simulated durations, per model and activity

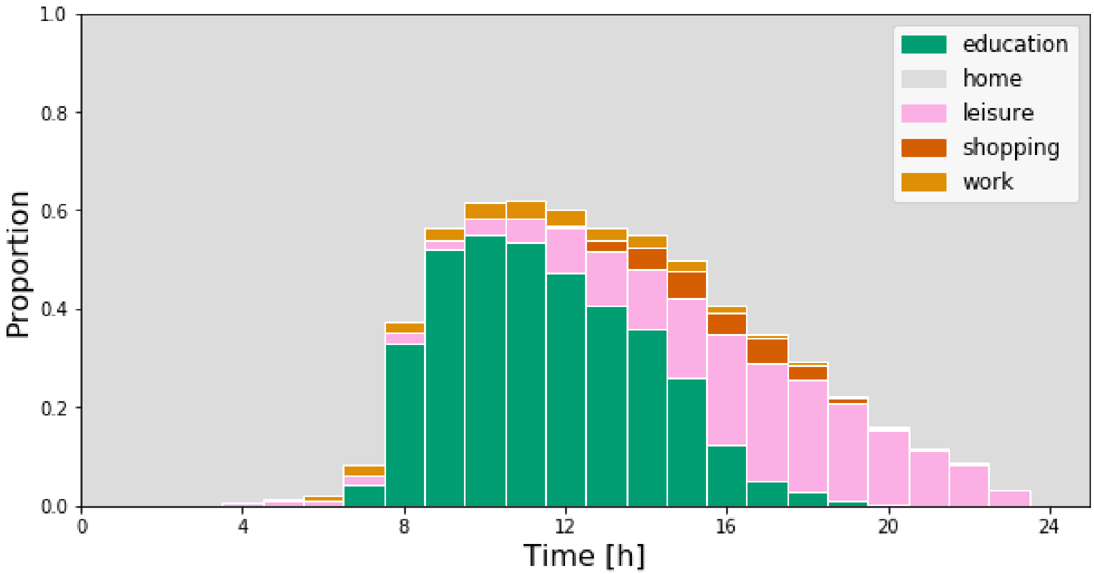
satisfactory results. This concern is also valid for the choice set obtained by sampling from the clusters of representative patterns (benchmark 3). This method is faster than the Metropolis-Hastings algorithm. Still, the number of alternatives that can be sampled is limited by the number of representative clusters (sampling with replacement is an option, but the consequent bias must be addressed). This method would, therefore, require more data than the OASIS generation procedure. In addition, Xu et al. (2017) do not correct for importance sampling, which introduces an additional bias. The resulting parameters may, therefore, not be consistent.

The application of the methodology has also highlighted some limitations: the simplifying assumptions formulated to estimate the problem significantly impact the quality of the solutions. For instance, the distributional assumptions of the desired times are too restrictive in this case. More specifically, multimodal distributions for the activity start times seem more appropriate and reflective of the observations. This change requires reconsidering the definition of activities, as it implies that the behaviour towards an activity of the same type (e.g. work) would differ depending on when it is scheduled.

Another finding is that, while the simulated profiles are close to the observed ones, all tested models simulate significantly more schedules with no out-of-home activities than what is observed. The fact that this phenomenon is also observed with parameters from the literature suggests that the specification itself does not appropriately model the reality. Indeed, because of its restrictive assumptions on the independence of alternatives, the logit model does not account for the correlations, interactions and unobserved behaviour that clearly impact the scheduling decisions (specifically, the decision to travel out of home). More complex specifications must be investigated, starting with mixed logit models, which relax the Independance from Irrelevant Alternatives (IIA) assumption.



(a) N = 10



(b) N = 100

Figure 3.23: Impact of choice set size on time of day distribution for random choice set model

3.6 Towards individual-specific parameters

In this chapter, we have assumed uniform parameters across the population to simplify the process. A more realistic behavioural assumption would be to consider these parameters distributed across the population, thus specifying a more complex choice model (e.g. mixed logit). Specifically, the parameters penalising the schedule deviations (both start time and duration) must be considered carefully, as they not only translate sensitivity towards time but may also be influenced by some latent components (preferences, habits) that are not explicitly accounted for in the current specification.

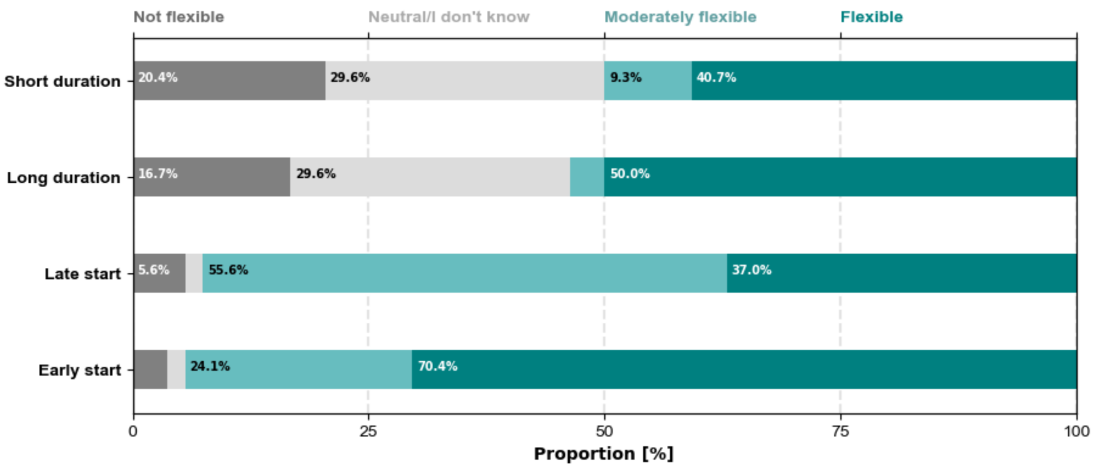
The lack of data is the main obstacle to moving towards more complex specifications, including individual-specific parameters or latent class models. Indeed, classical travel surveys do not provide sufficient information to estimate such models. While longitudinal surveys can give evidence for momentum and periodicity in activity-travel behaviour (which can be in turn used as a proxy to define *habits*, as done in chapter 4), they are also limited to revealed preference data, and therefore cannot inform on considered choices of activities, modes and locations.

Unfortunately, very few activity and time-use surveys with these characteristics exist. We can cite the CHASE survey (Doherty and Miller, 2000) and its extension REACT (Lee et al., 2001), which are household activity surveys focusing on identifying the underlying scheduling process. There is, therefore, a significant gap in the literature to fill.

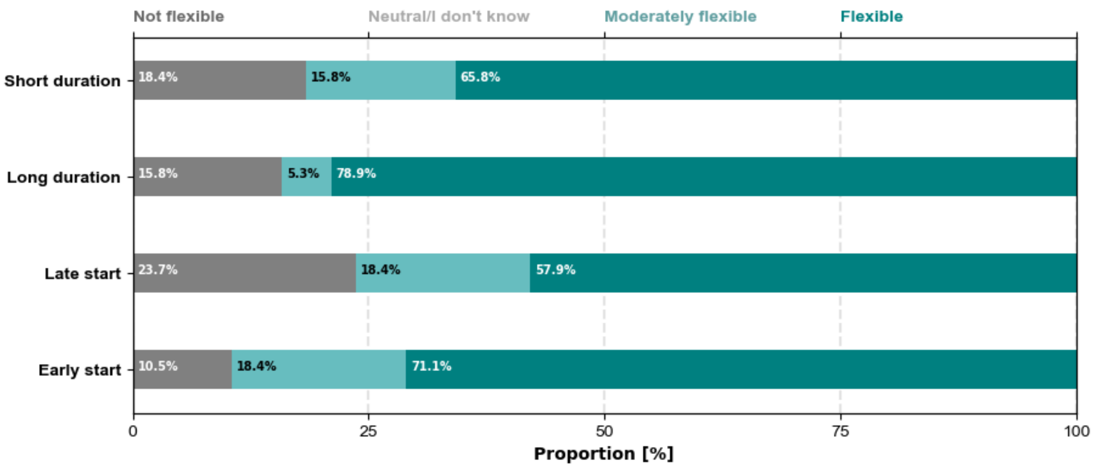
As an exercise, we have designed a survey to collect activity planning information at the weekly and daily levels. The respondents are asked at the beginning of the week which activities they consider or plan on doing during the weeks, as well as basic questions designed to map the structure of a weekly schedule (frequency of activities, considered days, modes, etc.). Then, the respondents are asked every day to communicate their planned schedule for the next day, including start and end times and considered locations (if applicable, for example, multiple grocery shops). The respondents were also asked to indicate their flexibility on a scale from -1 (not flexible) to 1 (very flexible) towards deviations from their planned activity timings. The full description of the survey and the questions are provided in Appendix B.2.

Figures 3.24 and 3.25 show examples of insights from the survey, applied to a sample of 7 testers. Figure 3.24 gives the Likert scales of scheduling flexibility for each activity, and Figure 3.25 highlights differences in desired times between two individuals. These outputs can help enrich the estimation of an existing activity-based model or help develop a latent class model.

Ideally, this quantitative survey should be used with a revealed preference travel diary to properly and fully calibrate an activity-based model. Identifying the discrepancies between planned and realised activity schedules is necessary to understand what elements trigger scheduling adjustments and trade-offs and better inform our models and assumptions.

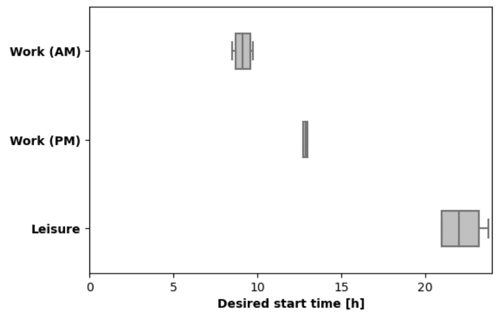


(a) Work (54 answers)

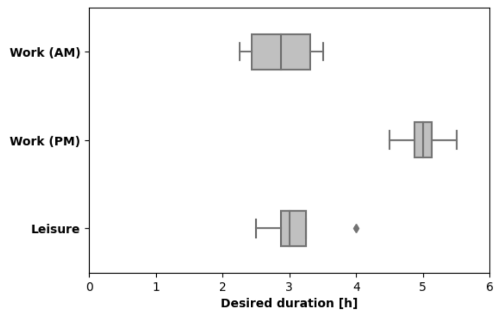


(b) Leisure (34 answers)

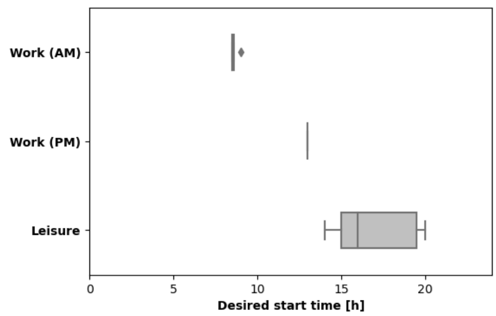
Figure 3.24: Survey responses for scheduling flexibility



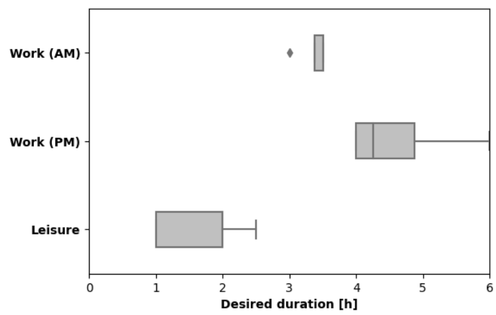
(a) Start time (Individual A)



(b) Duration (Individual A)



(c) Start time (Individual B)



(d) Duration (Individual B)

Figure 3.25: Reported desired times and durations for two individuals

3.7 Conclusion

We have presented a procedure to estimate the parameters of the OASIS framework, which includes the optimisation-based simulator introduced in chapter 2. The estimation process includes: (i) the generation of choice set for parameter estimation, with a sufficiently wide variety of alternatives to ensure unbiased and stable parameter estimates, with tractable sample probabilities, and (ii) the discrete choice estimation of the parameters for different model specifications. We have applied our methodology to a simple case: a time-dependent and linear-in-parameters utility function and a small dataset. The resulting parameters are mostly statistically significant and behaviourally interpretable, even with relatively few alternatives in the choice set. Using the parameters as input for the activity-based simulator, we can demonstrate that the simulated distribution is closer to the observed one with the estimated parameters as opposed to a benchmark from the literature with respect to the simulated activity participation and duration. We have also estimated parameters of other state-of-the-art utility specifications, including models used within the MATSim microsimulator. These utility functions have more behavioural realistic assumptions for the impact of duration on the scheduling utility than the linear specification used so far in OASIS. In the case of the S-shape, this formulation does not require the explicit definition of the desired duration, which is a non-negligible advantage. However, the impact of start time is significant based on our analyses and should, therefore, be included in the specification.

In this chapter, we have focused on demonstrating the feasibility and added value of the methodology. This is a necessary foundation for the framework to solve problems of higher complexity, including social interactions or multi-day behaviour. Methodological improvements such as choosing appropriate model structures to manage the high correlations (e.g. mixtures of logit, latent class models) are expected to significantly improve the quality of the estimation and the associated simulation results. In addition, future work will also include estimating travel-related parameters (e.g., travel time and cost, network accessibility), which will require network data to compute attributes for chosen and unchosen alternatives. The estimation of travel parameters, alongside activity parameters, will provide valuable insights into how both dimensions interact and affect the schedule utilities.

Other simplifying assumptions, such as the distribution of desired times, which is assumed unimodal in this paper, can significantly impact the quality of the estimations and must, therefore, be carefully investigated. For preferred times specifically, they could be included as parameters to be estimated. Depending on the chosen model specification, this could require an iterative process to be solved.

We have performed the estimations on small samples in terms of observations and alternatives in the choice set. Our results show that we could estimate significant parameters with the MH algorithm. In contrast, the random choice set requires a more substantial number of alternatives to inform the estimation process properly. The next step is to find the optimal number of alternatives N^* to sample with the OASIS methodology to obtain the best trade-off between estimation quality and computational efficiency.

Regarding validation, we will investigate a multidimensional distance metric in future work to compare observed and simulated schedules, similar to the multidimensional sequence alignment technique used by Recker et al. (2008) or Joh et al. (2002). In addition, the calibration of parameters on a synthetic population would allow the evaluation of the estimation quality against known control variables.

Regardless, these results open the way for significant contributions in activity-based modelling: the methodology to estimate the parameters allows researchers to explicitly consider behaviour in the activity-based analysis, which is usually a limiting factor in econometric models. An essential contribution of the OASIS framework is that the methodology remains the same for any change of context-specific constraints and features or utility specification changes. For example, this methodology was presented for the specific context of single-day and single-individual scheduling. Extensions such as multiday or household scheduling would require careful consideration: for the choice set generation, dedicated operators should be implemented (e.g., the operator changing the day of the week of an activity or whether an activity is performed jointly with a member of the household or solo), and the utility function and constraints must be formulated such as to accommodate these interactions. These extensions do not modify the core methodology of both the estimation and the simulation. Modellers can develop flexible and tailored models for various applications to integrate into the framework straightforwardly. The parameters can then be estimated, even with limited data, positively impacting the realism of the resulting simulations.

Chapter 4

From one-day to multiday activity scheduling

This chapter is based on the following conference proceedings:

> Pougala, J., Hillel, T., and Bierlaire, M. (2023a). From one-day to multiday activity scheduling: extending the OASIS framework. In *Proceedings of the 23rd Swiss Transport Research Conference (STRC)*, Ascona, Switzerland *Available at: https://www.strc.ch/2023/Pougala_EtAl.pdf*

The candidate has performed this work under the supervision of Prof. Michel Bierlaire and Dr. Tim Hillel.

In addition, this work is part of the research project MAPS *(PIs: J. Pougala, M-E. Schultheiss)*, supported by an ENAC Interdisciplinary Cluster Grant (EPFL).

4.1 Introduction

In practice, most operational ABM have focused on single-day analyses. This common simplifying assumption significantly limits the models' behavioural realism, as they cannot adequately capture the dynamics and processes involved in the scheduling of activities over multiple days. Decisions taken daily are affected by both *habits* built over time and *forward-looking behaviour* (Bierlaire et al., 2021), where individuals decide based on the expected outcomes of future decisions. In addition, some constraints are not necessarily applicable to a 24-hour period but to longer timeframes (e.g., shopping frequency, which becomes more constraining the longer the individual goes without necessities). To realistically model the activity-travel behaviour, explicitly integrating these elements into the framework is crucial.

This chapter presents and discusses assumptions and methodological requirements to extend a single-day scheduling framework to a multiday scope, emphasising the OASIS framework, shown in chapter 2. As a proof of concept, we have implemented and tested a preliminary operational scheduler that illustrates the advantages of our approach. We discuss methodological extensions, modelling assumptions, and data requirements.

In section 4.2, we present relevant research on the development of multiday ABM. In section 4.3, we introduce the assumptions and methodology to accommodate multiday considerations into the model. Finally, we illustrate the preliminary modelling additions with selected examples from the MOBIS dataset (Molloy et al., 2022).

4.2 Literature review

Many authors have identified a significant limitation of current ABM: the majority of models focuses on the simulation of a single day, thus ignoring significant dynamics and correlations that arise from the scheduling over multiple days or longer periods (e.g. Roorda and Ruiz, 2008; Calastri et al., 2020). There exist specific intrapersonal factors that influence the scheduling process. Roorda and Ruiz (2008) formulate the hypotheses that a person's activity/travel planning behaviour depends on their behaviour on other days of the week and that there are two main components to this dynamic behaviour:

1. same-day and next-day substitution effects for activities and trips, and

2. latent propensity to engage in some activities or choose a specific transportation mode.

One reason for the lack of research on multiday dynamics is the lack of available longitudinal data, which contains sufficient information to calibrate a multiday ABM. This leads several authors to propose methodologies to derive intrapersonal indicators from single-day trip data (e.g. Arentze et al., 2011b; Hilgert et al., 2017). It is an effective solution to circumvent the data issue. Still, it can introduce significant biases in the outputs as many behavioural assumptions must be made with limited possibilities of validating them.

In ABM research, most studies on intrapersonal variability focus on specific aspects of the scheduling process but not on the activity-travel behaviour as a whole (Zhang et al., 2021). For example, some authors investigate the impact of multiday dynamics on activity generation only (e.g. Nurul Habib and Miller, 2008; Arentze et al., 2011b).

Nurul Habib and Miller (2008) address the issue of activity generation (i.e. generating sets of feasible activities to be scheduled) for a week. They solve a utility-based model for each day of the week and include a term for the previous day's frequency of participation in the utility function of each activity. They assume that the activities considered for each day are influenced by previous activities. They find that estimating individual daily models with previous-day effects yields better model fit than estimating an aggregated model over the week. One limitation is that the Markovian nature of their assumption for day-to-day dynamics can be restrictive, as only the interdependence of consecutive days is taken into account.

Arentze et al. (2011b) also investigate multiday dynamic activity generation. More specifically, they propose a methodology to generate multiple-day activities using one-day observations from trip diary data. They assume that each observation is drawn from a long-term distribution of activity patterns. They perform random utility maximisation and consider that the activity patterns' utilities depend on the time elapsed since the last performed activity. In addition, they postulate the existence of individual preferences for performing activities on certain days of the week. In this case, the multiday dynamics are solely dependent on the past. Decisions or considerations for future days are not taken into account. Inspired by the needs-based hypothesis of Arentze and Timmermans (2009); Arentze et al. (2011b), Märki et al. (2014) present a heuristic approach to generate multiple weeks of schedules: pairs of activity and location are chosen such as to reduce deviations from targets (e.g., frequency, percentage of time spent in activity) defined by recorded travel surveys. While they look beyond activity generation, they focus primarily on the activity duration and sequence aspects of scheduling.

Other authors, such as Cirillo and Axhausen (2010); Zhang et al. (2021) include the scheduling process in their multiday analyses, in addition to the choice of activity type.

Cirillo and Axhausen (2010) model the choice of activity type and their scheduling in timeframes defined by a tour decomposition of the day (e.g. morning and evening tours) using mixed logit models. They consider multiple time horizons (single activity episode, day, week and multiple weeks), and, as they assume that past performance of activities affects the current scheduling decisions, they include variables specific to each scope (e.g. activity duration at the day level, or number of days since last performance of activity at the multiweek level) in the utility function. They found that the dynamic model was able to reproduce choice patterns and day-to-day variability of activity behaviour.

Zhang et al. (2021) model intrapersonal (day-to-day) variability of full activity-travel patterns, represented as spatio-temporal networks, with a bi-level multinomial logit model (MNL). The first level models the utility of choosing a representative pattern with respect to the day of the week. In contrast, the second level explains the alternative-specific constants of the first level with socio-demographic characteristics. They apply their model to a panel travel survey of Beijing and find significant day-to-day variability for most activity-travel patterns, with more substantial differences when comparing weekdays to weekends. They also find evidence that some specific activities are more likely to occur on certain days.

One common limitation of these models is that the multiday dynamics depend solely on the past, and decisions for future days are ignored. In addition, when multiple days are considered, the focus remains on the correlations between days, and scheduling dynamics within a day take less priority.

Calastri et al. (2020) argue that both within and between days correlations must be considered to develop realistic multiday ABM. They propose different specifications of the MDCEV to integrate and test the effects of these correlations. Their first specification considers day-specific non-additive utility functions and time constraints. In the second case, they consider correlated and additive utility functions.

Hilgert et al. (2017) introduce their activity-based model actiTopp, which generates one-week activity schedules based on socio-demographic characteristics of given individuals. Their model involves a sequence of discrete choice models for the scheduling decisions (e.g., participation frequency for each activity type, mean duration, etc.). Multiday considerations are considered at the personal level, where decisions that affect the week are made (e.g., number of days for each activity type, weekly time budgets, and usual start times). The outputs of each modelling level are fed to the subsequent models. This approach presents the typical limitation of sequential models: the potential for feedback between different models is very low, and specification errors or unexpected correlations can become difficult to track.

In this research, we propose some considerations to develop a methodology for simulating multiday activity-travel scheduling within the scope of the OASIS framework. This framework integrates all choice dimensions simultaneously to capture scheduling trade-offs, which implies a significant level of complexity when the model is scaled up to simulate multiple correlated days.

4.3 Methodology

4.3.1 Hypotheses

The first behavioural principles at the core of the single-day framework still hold in the multiday case. The extension to multiday is done by relaxing the assumption that days are scheduled independently, but rather, that each day is planned by considering constraints, preferences and decisions taken within a larger time horizon. There are three main mechanisms which influence decisions over time (Bierlaire et al., 2021):

1. changes in external conditions over time,
2. habitual behaviour,
3. forward-looking planning.

The second and third points are behavioural processes that are specific to each individual. *Habits* translate the ability of the decision-maker to learn from past experiences and influence the preferences and perception of current options. On the other hand, *forward-looking planning* affects current decisions by anticipating future outcomes and their associated utility. Forward-looking behaviour is implicitly accounted for by simultaneously simulating all choice dimensions (including the day of participation). Therefore, this chapter focuses on integrating habits to introduce a correlation between days. Habitual behaviour and learning can be considered by including dedicated terms in the utility function and by calibrating the parameters such that the generated schedules match regular patterns of activities or activity motifs (Schultheiss, 2021).

4.3.2 New definitions

The multiday extension can be considered on multiple levels:

1. Input:

    - **Preferences**: The assumption that individuals have desired start times x^*_a and τ^*_a for each activity still holds in the multiday case. However, this preference might depend on the day d. For example, an individual may prefer to start working at 10:00 on Mondays but at 09:00 on Fridays so they can leave earlier. In addition, we consider the preference for activity frequency f^*_a, which is the number of times an individual prefers to perform the activity in the time horizon T. We can differentiate*regular* from *occasional* activities (e.g. work vs. leisure). We also consider a preferred day d^*_a for participation in activity a. f^*_a and d^*_a are included in the daily utility functions U^d_S.

    - **Changes in external conditions**: In the multiday case, we need to consider potential changes in external conditions from one day to the other, which could significantly impact the scheduling process and the constraints. For example, feasible time windows for activities can vary depending on the day (e.g. opening days of shops or services), which can significantly restrict the available activities for scheduling on a given day. Resource availability, such as household vehicles, might also be day-specific.

2. Model:

    - **Time budget**: Considering a time horizon T of $D = 1, 2..., d$ days, the time budget can be increased from 24h to 24D hours. This implies that a specific activity a can potentially be scheduled on any day d, depending on the preferences and flexibility of the individual. This reflects activity planning behaviour more closely by allowing some activities to be scheduled later if it increases the overall utility.

    - **Objective function:** Each day d of the time horizon is associated with a time-dependent utility function U^d_S. Similarly to the utility function of the single day case (Equation 2.7), this function includes penalties for deviations from the preferred start time (early and late) and duration (short and long) and an additional term for deviation from the preferred day of participation. The objective function is the sum of the utility functions of everyday d in the time horizon and a term that penalises the difference between actual and preferred activity frequency.

- **Decision variables**: We consider the decision variables defined for the single-day problem. In the multiday case, the decision variables $\boldsymbol{\omega}, \mathbf{z}, \mathbf{x}, \boldsymbol{\tau}$ are vectors of size T, with T the time horizon. Each element of the vector is the decision for a day d. For example, $w_{a,d} = 1$ indicates that activity a is performed on day d. In addition, we introduce the decision variable f_a, which is the frequency or number of activity occurrences a over the time horizon T. We constrain $f_a = \sum_d \boldsymbol{\omega}_{a,d}$.

- **Constraints**: In the multiday scenario, the scheduling framework optimises single-day schedules, adding multiday utility terms. Therefore, the single-day constraints still hold and are sufficient to ensure feasibility in the multiday case. Consistency conditions over multiple days should be verified (e.g. allowing for overnight activities), as well as changes in external conditions (e.g. vehicle availability, opening days of shops or services, etc.)

Table 4.1 summarises the main methodological differences between the single-day and the multiday simulator.

Table 4.1: Methodological differences between single-day and multiday framework

Feature	Single day	Multiday
Time horizon T	1 day	D days
Objective function	Schedule utility U_S	Multiday utility $\sum_{d\in T} U_S^d + U_f$
Decision variables	Participation, start time, duration, sequence	Single day variables + activity frequency
Constraints	Budget, feasibility, consistency	Single day constraints and external conditions
Preferences	Start time, duration	Daily start time and duration, frequency over T

4.3.3 Utility function

Considering each day d in the time horizon, Equation (4.1) presents the multiday utility function.

$$U_S = \sum_d \left[U_d + \sum_a \left(U_{a,d}^{\text{participation}} + U_{a,d}^{\text{start time}} + U_{a,d}^{\text{duration}} + \sum_b U_{a,b,d}^{\text{travel}} \right) \right] + \sum_a U_a^{\text{frequency}} \tag{4.1}$$

The utility terms for start time and duration are day-specific. This makes it possible to consider different sensitivities towards schedule deviations based on the day of the week.

Correlations between days are implicitly introduced with the frequency utility term (Equation 4.2). We assume that each person has a preferred frequency for each activity a (e.g. going to work five days a week). The preferred frequency f_a^* may be a number or a range of values (e.g. leisure performed 2-4 times a week). Deviations of the actual scheduled frequency ($f_a = \sum_d \omega_{a,d}$) from this quantity are penalised by negative parameters $\theta_a^{\text{frequency-}}$ (less frequent than desired) and $\theta_a^{\text{frequency+}}$ (more frequent than desired), to be estimated.

$$U_a^{\text{frequency}} = \theta_a^{\text{frequency-}} \max\left(f_a^* - \sum_d \omega_{a,d}, 0 \right) + \theta_a^{\text{frequency+}} \max\left(\sum_d \omega_{a,d} - f_a^*, 0 \right) \tag{4.2}$$

For the sake of simplicity, we consider for the rest of this chapter that deviations in either direction (frequency too high or too low compared to preference) are penalised equally, i.e. $\theta_a^{\text{frequency-}} = \theta_a^{\text{frequency+}} = \theta_a^{\text{frequency}}$ (Equation 4.3).

$$U_a^{\text{frequency}} = \theta_a^{\text{frequency}} \left| \sum_d \omega_{a,d} - f_a^* \right| \tag{4.3}$$

Finally, we assume a preference exists for conducting activities on specific days (e.g., working on weekdays instead of weekends) (Equation 4.4), captured by the day-specific parameter $\theta_{a,d}^{\text{participation}}$. It decreases the utility of the activity if it is scheduled on a day different from what is preferred.[1]

$$U_{a,d}^{\text{participation}} = \theta_{a,d}^{\text{participation}} * \omega_{a,d} \tag{4.4}$$

4.3.4 Constraints

The constraints in the multiday case are largely similar to the single-day constraints. However, given that the variables are expressed over a longer timeframe, the following constraints may be adapted:

- **Budget constraints:** It is reasonable to assume that the multiday time and cost budgets are equivalent to the sums of the budgets for every day of the time horizon. Therefore, enforcing budget constraints daily is sufficient to ensure they hold at the multiday level.

- **Consistency constraints:** In the single-day case, we have defined constraints to ensure that the resulting schedules are consistent with the scheduling decisions and their impact. For example, they ensure that activities that follow each other have consistent timings when travel is included or that mode choice is compatible with the available or previously chosen mode. These consistency measures must be carried over across days in the multiday case. For instance, if we relax the assumption that schedules must start and end at home (i.e. we allow overnight activities), we need to ensure that the first activity of the day is either the same as the last activity of the previous day (which can be *home/dusk* or other) or *travel*.

Following these observations, the constraints of the multiday optimisation problem are formulated below. Here, we define $\text{dawn}_d = S_d(0)$ as the first activity of the schedule of day d, and $\text{dusk}_d = S_d(T_d)$ the last activity of S_d. These activities can be *home* or another activity type.

$$\sum_d \sum_a (\omega_{a,d}\tau_{a,d} + \sum_b z_{ab,d}\rho_{ab,d}) = T, \tag{4.5}$$

[1]This behaviour could be replicated with constraints. For example, we can enforce that some activities never occur on specific days (e.g., work cannot occur on weekends). However, using a utility term allows for more flexibility and does not require specific knowledge of the context to formulate such constraints.

$$\sum_d \sum_a (\omega_{a,d} c_{a,d} + \sum_b z_{ab,d} \kappa_{ab,d}) \leq B, \tag{4.6}$$

$$\tau_{a,d} \geq \omega_{a,d} \tau_{a,d}^{\min}, \quad \forall a \in A, d \in T, \tag{4.7}$$

$$\tau_{a,d} \leq \omega_{a,d} T_d, \quad \forall a \in A, d \in T, \tag{4.8}$$

$$z_{ab,d} + z_{ba,d} \leq 1, \quad \forall a, b \in A, a \neq b, \forall d \in T, \tag{4.9}$$

$$z_{a,\text{dawn}_d} = z_{\text{dusk},a_d} = 0, \quad \forall a \in A, d \in T \tag{4.10}$$

$$\sum_a z_{ab,d} = \omega_{b,d}, \quad \forall b \in A, b \neq \text{dawn}, \forall d \in T, \tag{4.11}$$

$$\sum_b z_{ab,d} = \omega_{a,d}, \quad \forall a \in A, a \neq \text{dusk}, \forall d \in T, \tag{4.12}$$

$$\omega_{a=\text{dawn},d+1} = \omega_{a=\text{dusk},d}, \quad \forall d \in [0, |T|[, \tag{4.13}$$

$$(z_{ab,d} - 1) T_d \leq x_{a,d} + \tau_{a,d} + z_{ab,d} \rho_{ab,d} - x_{b,d}, \quad \forall a, b \in A, a \neq b, \forall d \in T \tag{4.14}$$

$$(1 - z_{ab,d}) T_d \geq x_{a,d} + \tau_{a,d} + z_{ab,d} \rho_{ab,d} - x_{b,d}, \quad \forall a, b \in A, a \neq b, \forall d \in T \tag{4.15}$$

$$\sum_{a \in G_k} \omega_{a,d} \leq 1 \quad k = 1, \ldots, K, \forall d \in T, \tag{4.16}$$

$$\alpha_{a,d}^m = 1 \quad \forall a \in G_{\text{home}}, \forall d \in T_m, \tag{4.17}$$

$$\omega_{a,d} \leq \alpha_{a,d}^m \quad \forall a \in A^m, \forall d \in T_m, \tag{4.18}$$

$$\alpha_{a,d}^m \geq \alpha_{b,d}^m + z_{ab,d} - 1 \quad \forall a \in A, b \in A \setminus G_{\text{home}}, \forall d \in T_m, \tag{4.19}$$

$$\alpha_{b,d}^m \geq \alpha_{a,d}^m + z_{ab,d} - 1 \quad \forall a \in A \setminus G_{\text{home}}, b \in A, \forall d \in T_m, \tag{4.20}$$

$$x_{a,d} \geq \gamma^{-}_{a,d}, \qquad \forall a \in A, d \in T, \tag{4.21}$$

$$x_{a,d} + \tau_{a,d} \leq \gamma^{+}_{a,d}, \qquad \forall a \in A, d \in T. \tag{4.22}$$

Equations (4.5) and (4.6) are constraints that apply over the time horizon. They can be verified at an aggregated level (sum over all days) or disaggregated level (each day). Equations (4.7) to (4.22) must be verified every day.

Equation 4.5 constrains the total time assigned to the activities in the schedule (sums of durations and travel times) for each day to equal the time horizon. Equation 4.6 constrains the total cost of the schedule (sums of the costs of participating and travelling to the activities in the schedule) for each day to not exceed the maximum budget over the time horizon. Equations (4.7) and (4.8) enforce consistency with the activity duration and activity participation.Equations (4.9) to (4.15) ensure consistency for sequences of activities. Specifically, Equation 4.13 constrains the last activity of the schedule on the day d to have the same type as the first activity on the following day $d + 1$. Equation 4.16 ensures that only one activity within a group of duplicates G is selected. Equations (4.17) to (4.20) define the constraints related to the choice of mode of transportation (availability, consistency). They are applicable on days when (private) mode m is available to the individual (set $T_m \in T$). Finally, eqs. (4.21) and (4.22) are time-window constraints.

4.4 Empirical investigation

We test the modified OASIS framework to simulate multiday schedules for a sample of individuals from the MOBIS dataset (Molloy et al., 2022). The MOBIS dataset is a longitudinal dataset conducted in Switzerland, which contains eight weeks of GPS traces for 3680 respondents. For the analyses presented in this paper and for efficiency, we randomly selected a subsample of 460 respondents.

First, we implement the modelling hypotheses presented insection 4.3. Then, we illustrate the output of the framework for a small instance. We discuss limitations and identify the axes that should be the focus of future research.

4.4.1 Preferences

One crucial hypothesis of the multiday analysis is that the preferences of individuals for activity timings are day-specific. This implies that deviations from the preferred schedules will be penalised differently depending on the day or type of day (e.g. weekdays – Monday to Friday – versus weekends – Saturday to Sunday).

By analysing the dataset, we observe a profile that concurs with this assumption (Figure 4.1). For the *work* activity (Figure 4.1a), the distribution of start times shows that this activity is significantly more present in weekday schedules as opposed to weekends. In addition, the weekday distribution presents two peaks at 6:00 and 11:00, whereas the weekend distribution is more uniform. The same observations can be made for *education*.

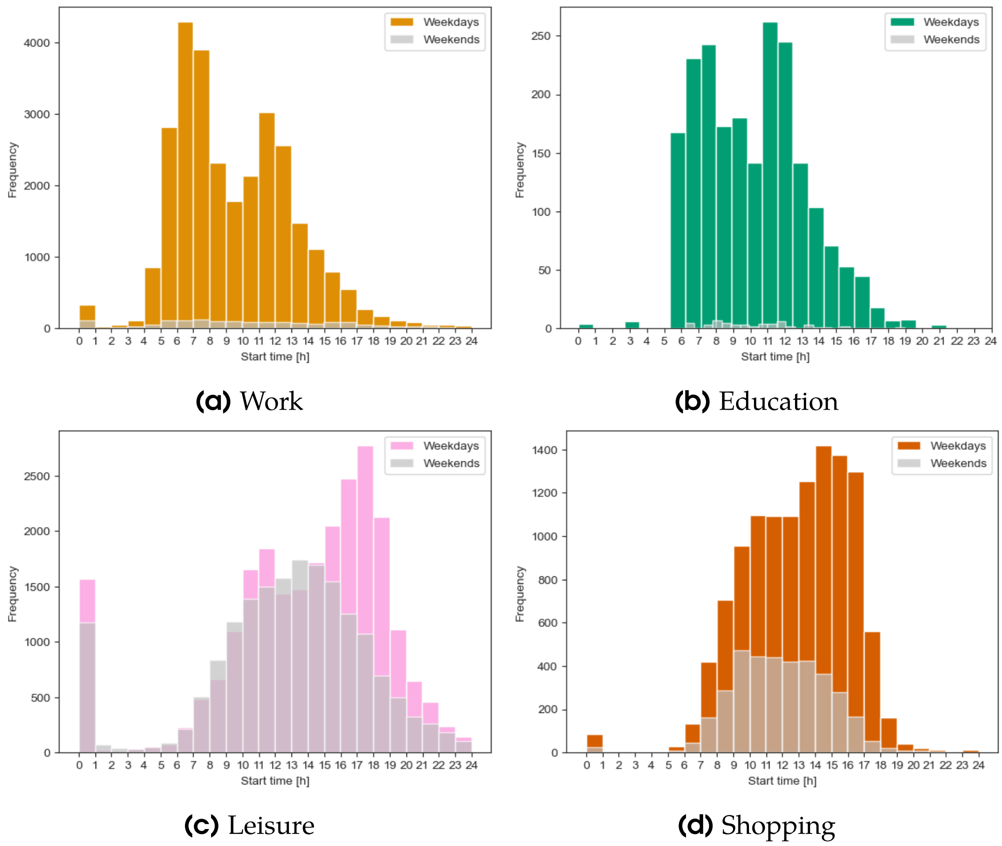
For *leisure* (Figure 4.1c), we see that the distributions for weekdays and weekends are comparable in terms of frequency counts, with a higher peak at 17:00 and earlier in the day at 13:00 for weekends. Both sets present a significant peak at midnight, indicating that leisure is often scheduled overnight.

The conclusions for *shopping* (Figure 4.1d) are similar to leisure: on weekdays, the distribution shows a peak in the second half of the day (between 14:00 and 17:00), while on weekends, the start times are more evenly distributed during the day.

We integrate these activity and day-specific preferences for start time and duration to the model by fitting log-normal distributions[2] to the observed activity distributions (start time, duration, and frequency) of the sample over eight weeks. The parameters of these distributions are reported in Table 4.2. We draw values from each simulation and individual from these distributions for their preferred start time $x^*_{a,d}$, duration $\tau^*_{a,d}$.

Regarding activity participation, we observe notable trends for the weekly frequency (Figure 4.2), which is defined as the number of days in a week when a given activity is scheduled at least once: *work* (fig. 4.2a) is a regular activity: the majority of individuals work for four days or more per week. *Education* (fig. 4.2b) is also regular but at a lower frequency (once per week). This indicates a low variability across individuals and weeks for these two activities. On the other

[2]The choice of distribution is arbitrary.



(a) Work **(b)** Education

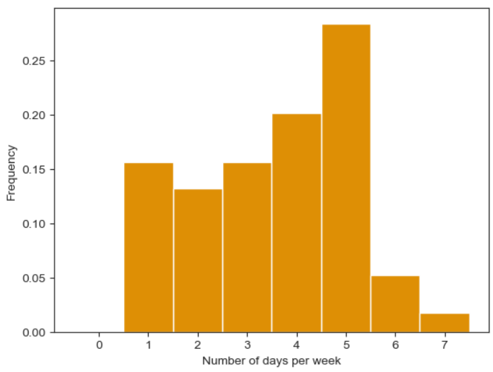
(c) Leisure **(d)** Shopping

Figure 4.1: Distribution of start times (Mon-Fri vs. Sat-Sun) for different activities.

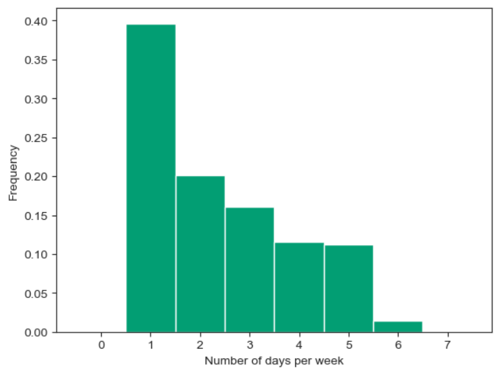
Table 4.2: Desired times distributions in sample

Day	Activity	Start time	Duration
Weekends	Work	Log-$\mathcal{N}$ $(0.15, -14.7, 24.0)$	Log-$\mathcal{N}$ $(1.4, 0, 1.6)$
	Education	Log-$\mathcal{N}$ $(0.14, -11.8, 21.8)$	Log-$\mathcal{N}$ $(0.74, -0.51, 2.3)$
	Leisure	Log-$\mathcal{N}$ $(9.1, -4.8, 4.0)$	Log-$\mathcal{N}$ $(1.3, 0, 0.88)$
	Shopping	Log-$\mathcal{N}$ $(0.015, -204.1, 216.9)$	Log-$\mathcal{N}$ $(0.85, 0, 0.27)$
Weekends	Work	Log-$\mathcal{N}$ $(0.06, -81.1, 91.3)$	Log-$\mathcal{N}$ $(1.7, 0.06, 1.4)$
	Education	Log-$\mathcal{N}$ $(0.35, 2.9, 6.9)$	Log-$\mathcal{N}$ $(1.6, 0.06, 1.4)$
	Leisure	Log-$\mathcal{N}$ $(8.8, -6.8, 4.1)$	Log-$\mathcal{N}$ $(1.3, 0, 0.68)$
	Shopping	Log-$\mathcal{N}$ $(0.012, -244.3, 256.2)$	Log-$\mathcal{N}$ $(0.90, 0, 0.30)$

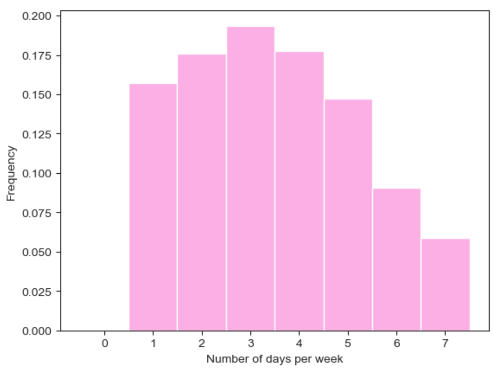
hand, *shopping* but mainly *leisure* have less defined peaks, and the participation rates remain constant across a broader range (from once to 5 times per week for leisure and from once to three times per week for shopping). Contrasted with work and education, these activities seem more occasional or irregular in terms of weekly patterns.



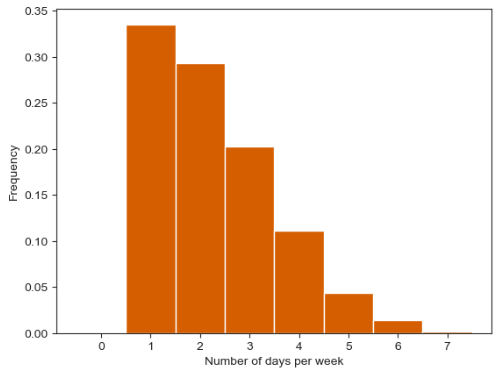
(a) Work



(b) Education



(c) Leisure



(d) Shopping

Figure 4.2: Distribution of weekly participation frequency for different activities.

The results of Figure 4.2 can be used to define the frequency preferences $f^*_{a,d}$ for each individual. In this case, we approximate this variable with the mean of the empirical distributions for each activity, as reported in Table 4.3.

Table 4.3: Desired weekly and daily activity frequencies

Activity	Weekly frequency
Work	3.5
Education	2.4
Leisure	3.5
Shopping	2.3

4.4.2 Utility function and parameters

We implement the utility function defined in Equation 4.1, with several simplifications:

- We only consider activity-related utility parameters and, therefore, do not include travel time,
- We assume that the utility of *work* and education activities are penalised by the parameter $\theta_a^{\text{weekend}}$ if they are conducted on Saturday or Sunday. The indicator $\delta^d_{\text{weekend}}$ is 1 if $d \in \{\text{Saturday, Sunday}\}$ and 0 otherwise. For *leisure* and *shopping*, $\theta_a^{\text{weekend}} = 0$.

$$U_S = \sum_a \left(\theta_a^{\text{frequency}} \left| \sum_d \omega_{a,d} - f_a^* \right| + \sum_d \theta_a^{\text{weekend}} \delta^d_{\text{weekend}} \omega_{a,d} + U_{a,d}^{\text{start time}} + U_{a,d}^{\text{duration}} \right) \tag{4.23}$$

For the parameters of the daily utility functions, we use the default OASIS activity-specific parameters, estimated in chapter 3. We assume arbitrarily that $\theta_a^{\text{frequency}} = \theta_{\text{work}}^{\text{weekend}} = \theta_{\text{education}}^{\text{weekend}} = -10$.

The values of the parameters are summarised in Table 4.4.

4.4.3 Example

To illustrate the multiday specification and methodology described in Section 4.3, e solve a week of activities for an individual of the MOBIS dataset. The observed schedules are illustrated in Figure 4.3. This person goes to work every weekday, with at least one leisure activity in the evening. They go shopping on Friday and have two overnight activities between Tuesday and Wednesday and Friday and Saturday.

For this individual, we provide as input the set of activities *{home, work, leisure, shopping}*, to be performed any day during the week, with the penalties and preferences introduced in Sections 4.4.1 and 4.4.2.

We compare the results of the multiday model with the outputs of the single-day model that we run n_{days} times to investigate the added value of our methodologi-

Table 4.4: OASIS activity-specific parameters for the multiday model. Parameters 17-19 were arbitrarily defined.

	Parameter	Param. estimate	Rob. std err	Rob. t-stat	Rob. p-value
1	$\gamma_{\text{education}}$	18.7	3.17	5.89	3.79e-09
2	$\theta^{\text{early}}_{\text{education}}$	-1.35	0.449	-3.01	0.00264
3	$\theta^{\text{late}}_{\text{education}}$	-1.63	0.416	-3.91	9.05e-05
4	$\theta^{\text{long}}_{\text{education}}$	-1.14	0.398	-2.86	0.00428
5	$\theta^{\text{short}}_{\text{education}}$	-1.75	0.457	-3.84	0.000123
6	γ_{leisure}	8.74	1.94	4.50	6.79e-06
7	$\theta^{\text{early}}_{\text{leisure}}$	-0.0996	0.119	-0.836	0.403*
8	$\theta^{\text{late}}_{\text{leisure}}$	-0.239	0.115	-2.07	0.0385
9	γ_{shopping}	10.5	2.20	4.78	1.74e-06
10	$\theta^{\text{early}}_{\text{shopping}}$	-1.01	0.287	-3.51	0.000443
11	$\theta^{\text{late}}_{\text{shopping}}$	-0.858	0.237	-3.63	0.000284
12	γ_{work}	13.1	2.64	4.96	7.16e-07
13	$\theta^{\text{early}}_{\text{work}}$	-0.619	0.217	-2.85	0.00438
14	$\theta^{\text{late}}_{\text{work}}$	-0.338	0.168	-2.02	0.0438
15	$\theta^{\text{long}}_{\text{work}}$	-1.22	0.348	-3.51	0.000441
16	$\theta^{\text{short}}_{\text{work}}$	-0.932	0.213	-4.37	1.23e-05
17	$\theta^{\text{frequency}}$	-10.0	.	.	
18	$\theta^{\text{weekend}}_{\text{work}}$	-10.0	.	.	
19	$\theta^{\text{weekend}}_{\text{education}}$	-10.0	.	.	

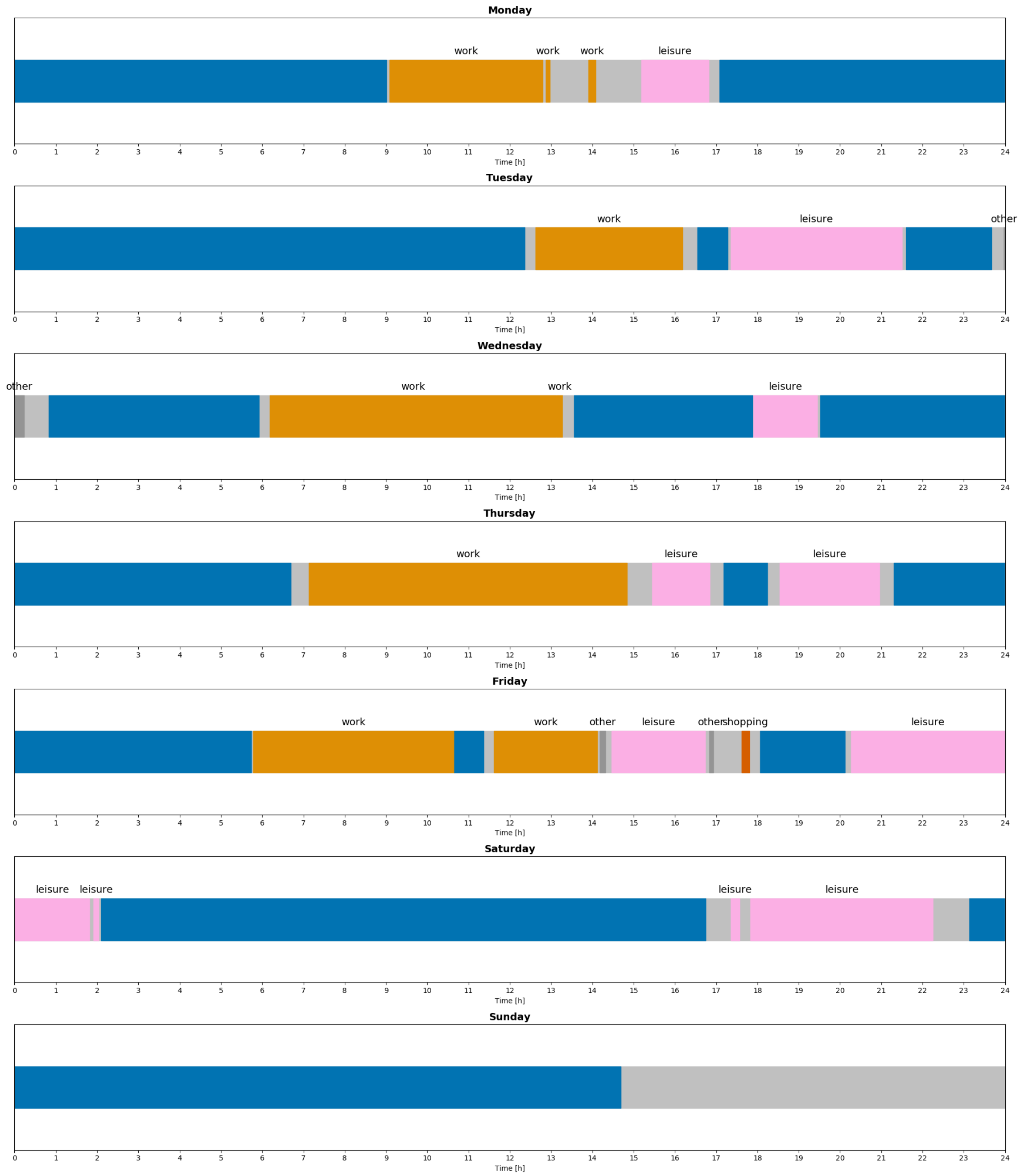


Figure 4.3: Example week from MOBIS dataset

cal extension. This procedure should be regarded as proof of concept, not formal validation.

Results

Using the original single-day and multiday models, we simulate a week of daily schedules (Monday to Sunday) for the example individual presented in the previous section. We ran the simulation ten times. In the multiday case, each resulting week corresponds to a different draw of the error terms.[3] In the single-day case, each day corresponds to a different draw of the error terms, and one week is defined as seven consecutive (and independent) draws.

Figures 4.4 and 4.5 show the results of one simulation for the single day model (fig. 4.4) and the multiday model (fig. 4.5). These specific draws of the simulators were obtained with input desired times reported in table 4.5.

In the single model, the days are effectively independent from each other, except for the desired start times and durations provided as input. Therefore, the simulator reflects the distribution of the error terms more than any underlying interaction.

Using the multiday model, weekly habits are more apparent. *Work* is scheduled every weekday (Monday to Friday) and never on the weekend, in line with the preferred frequency and daily participation. *Leisure* is scheduled daily except for Friday, with varying durations. *Shopping* is only done twice at the beginning of the week. Note that the durations and start times differ significantly from the observed week. This is due to the desired times for these values, which we have drawn from a log-normal distribution (table 4.2).

Table 4.5: Desired activity timings for simulated week W1 [hh:min]

	Weekday		Weekend	
Activity	Start time	Duration	Start time	Duration
Work	06:15	08:10	13:30	00:15
Leisure	00:35	00:05	00:00	02:40
Shopping	13:35	00:50	11:15	01:39

Figure 4.6 compares the outputs of 100 iterations of the single-day and multiday models. The left column shows the distribution of time of day participation

[3]We assume that the distribution of error terms is the same as in the single-day case.

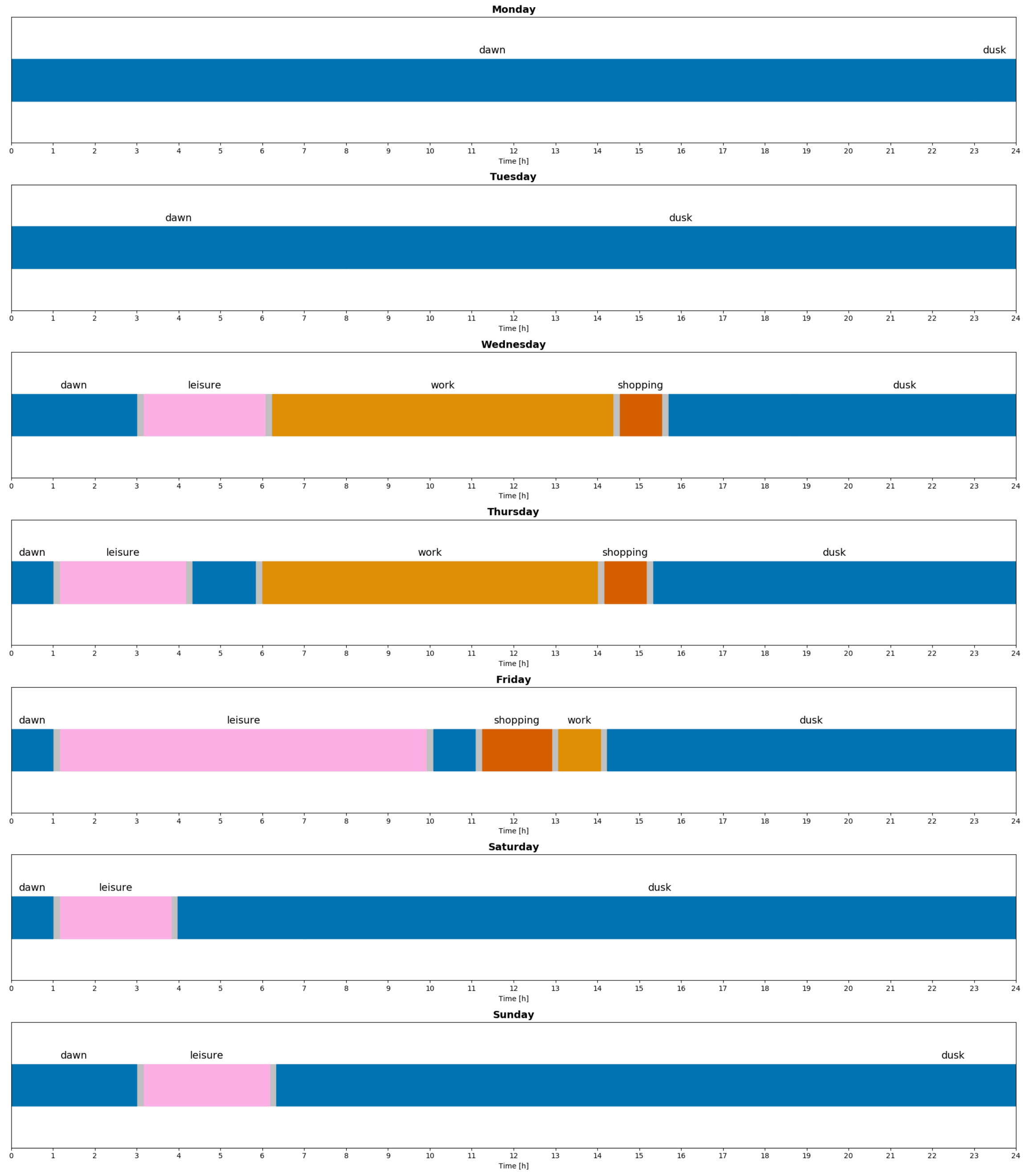


Figure 4.4: Simulated week with OASIS single model

for a typical weekday (Monday) as simulated by the single-day model (top row) and multiday model (bottom row). The right column displays the same distribution for a typical weekend day (Saturday). In the case of the single-day model, we observe no significant difference between weekdays and weekends in terms of profile, except for *shopping*, which is more prominent on Saturdays.

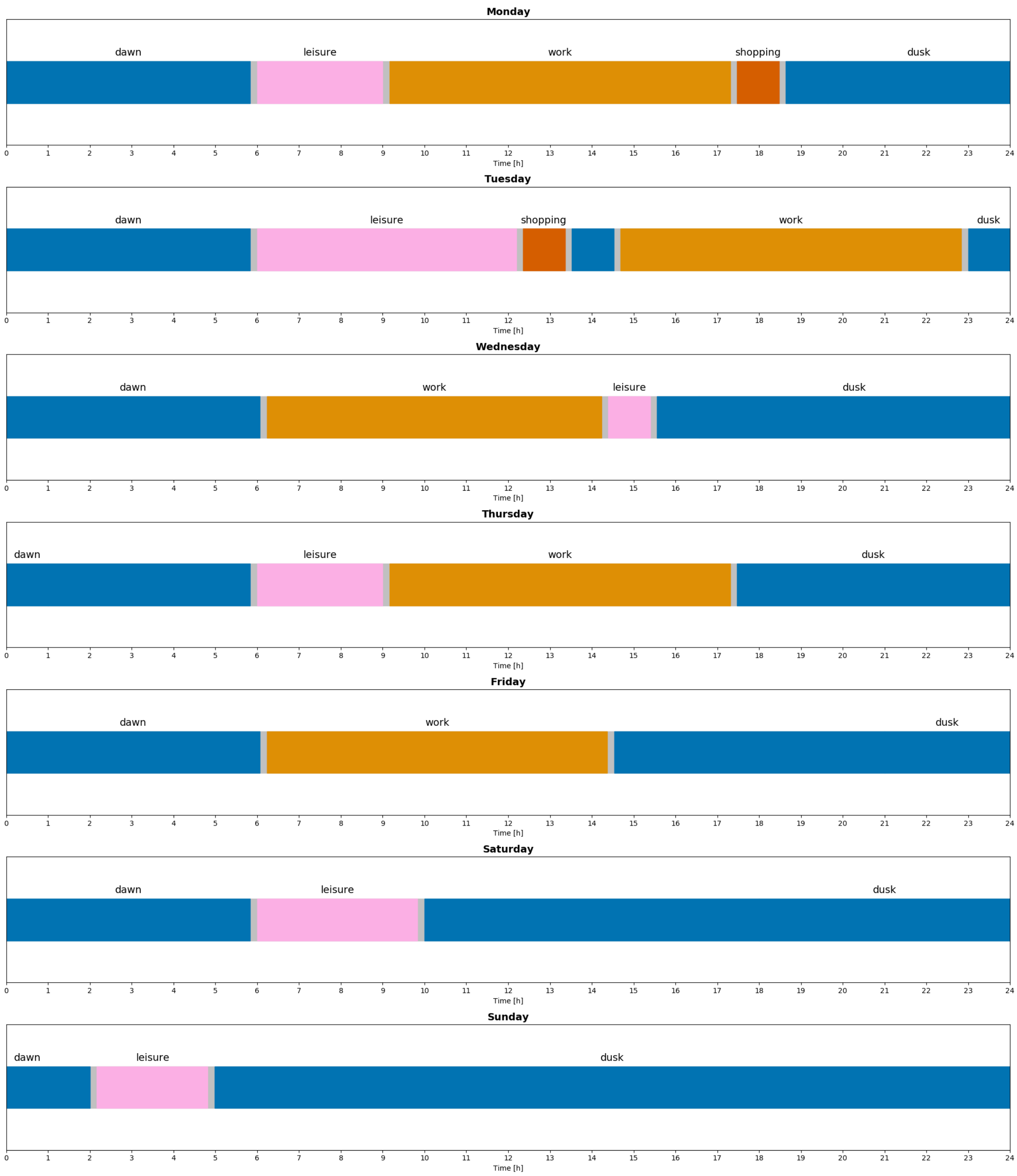


Figure 4.5: Simulated week with OASIS multiday model

This difference is due to the change in desired start time and duration between weekdays and weekends, as presented in table 4.5. The difference is more evident in the multiday case, where we explicitly account for preferences in daily participation and activity frequency. The majority of the schedules generated for Mondays include a *work* activity in the morning and most of the afternoon (7:00

to 16:00). From 16:00 onwards, *work* and *leisure* are scheduled. Still, the time is mainly spent at home (from 60-100 % of schedules). Half of the schedules contain a *leisure* activity before work (4:00-6:00). The activity profile is very different on a typical Saturday. The majority of schedules are entirely at home. For out-of-home schedules, the day is primarily spent in *leisure*, with some *shopping* at 12:00. Interestingly, both the single-day and multiday configurations tend to schedule *leisure* during the night (00:00 to 6:00), which is surprising as this is observed only once in the recorded week (fig. 4.3). This is likely because we did not estimate parameters specifically for the MOBIS dataset and are therefore not fully replicating the observed behaviour. Nevertheless, the comparison between the single-day and multiday frameworks highlights the added value and necessity of introducing day-specific variables and correlations to capture day-to-day variability, and better reflect the decision-making scheduling process.

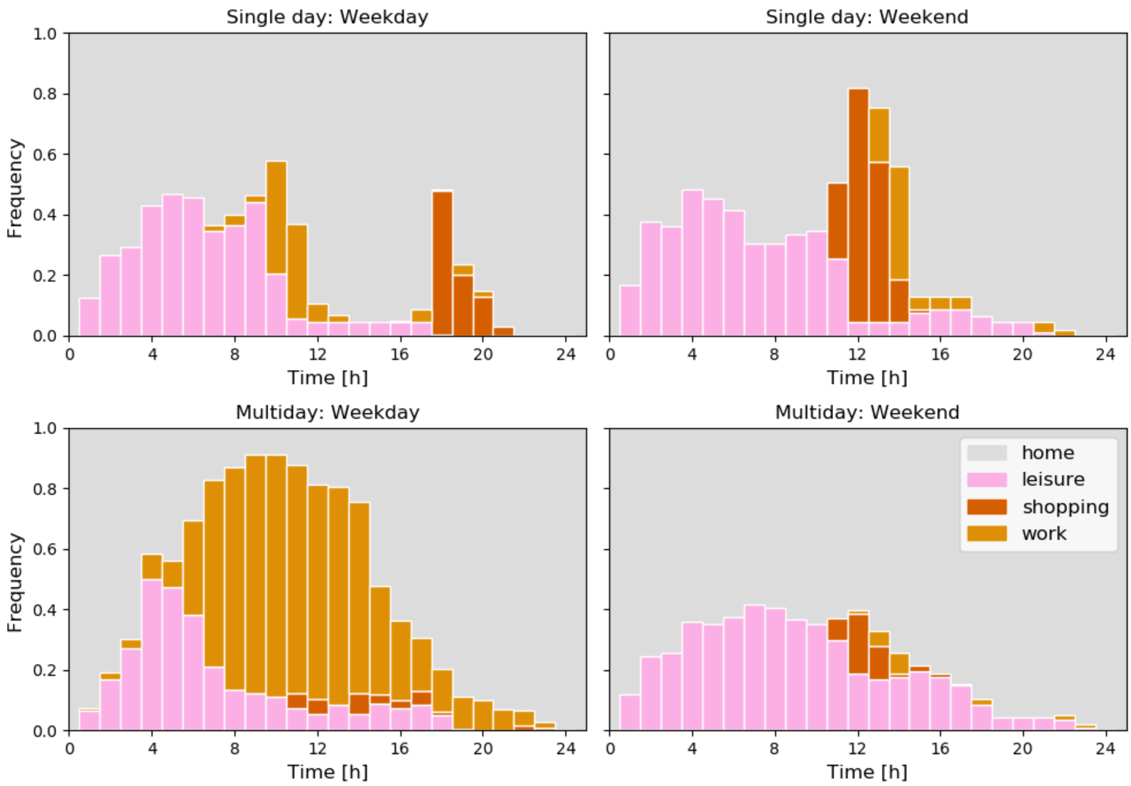


Figure 4.6: Comparison of time of day distribution of activity participation over 100 iterations, between single-day generation (top row) and multiday generation (bottom row).

4.4.4 Simulated statistics

We compare descriptive statistics of the simulated sample for both models. These statistics are the proportion of out-of-home schedules (i.e., schedules containing at least one out-of-home activity) and daily averages of the time spent out-of-home (total and for each activity, computed for out-of-home schedules).

The results are summarised in Table 4.6 and Table 4.7, respectively.

Regarding the proportion of out-of-home schedules, we note that the single-day model generates many schedules entirely at home. This does not reflect the observed behaviour over the week, where weekdays especially contain at least two unique out-of-home activities, while one or less on weekends. This trend is captured by the multiday model, which only generates out-of-home schedules on weekdays.

Table 4.6: Percentage of out-of-home schedules

Model	Weekday	Weekend
Single	23.0	23.0
Multi	100.0	97.8

On weekdays, the multiday model is generally closer to the observed schedules regarding the average duration spent in each activity. The single-day model significantly underestimates the time spent at work (by about 5 hours). Coupled with the fact that, in general, this model tends to generate days fully at home, the accuracy of this model is very unsatisfactory. For weekends, both models provide similar solutions. The *shopping* activity is overestimated for both models and categories of days. This can be explained by the chosen desired duration (50 minutes), which is far from the actual duration spent by this individual (11 minutes).

4.4.5 Runtimes

Figure 4.7 compares runtimes for different configurations of the multiday problem. The solved scenarios differ in the number of out-of-home activities n_a to be scheduled and the number of days in the time horizon n_d. There are as many locations as there are activities, and we only consider one possible mode of transportation (driving), resulting in a mode-travel time matrix of shape $1 \times n_a \times n_a$.

Table 4.7: Average out-of-home duration, in hh:min

	Weekday			Weekend		
Activity	Data	Single	Multi	Data	Single	Multi
Total	09:33	05:11	10:34	06:33	06:26	05:15
Leisure	03:25	03:55	02:56	06:33	04:37	04:27
Shopping	00:11	01:30	01:08	00:00	02:01	01:45
Work	5:56	01:07	07:58	00:00	01:09	01:00

Ten simulations were performed for each scenario. The simulations were conducted with parallel processing on a 2.8 GHz quad-core Intel Core i7 with 16 GB RAM.

The *time limit* parameter of CPLEX was set to 1,800 seconds per solver call.[4]

Unsurprisingly, the runtime increases significantly with the increasing complexity of the problem, both in terms of the number of days to be scheduled and the number of alternatives. Expanding the time horizon has the most significant impact on runtime, given that every new day is a new optimisation problem with its own decision variables and constraints. For a time horizon of $n_d = 5$, the simulations including $n_a = 4$ out-of-home activities to be scheduled reach, on average, the runtime limit and exceed it most of the time when the n_d increases to 7.

Even when the threshold is not reached, the average runtimes are too high to reasonably apply the multiday framework to a large-scale application. For example, simulating weeks of schedules with four out-of-home activities for a sample of 1,000 individuals would take around two weeks with these specifications. Increasing the computing resources would improve the performance, but some measures must be taken to speed up the process significantly.

[4]This limit includes all solving operations, such as preprocessing and internal calls to other optimisers.

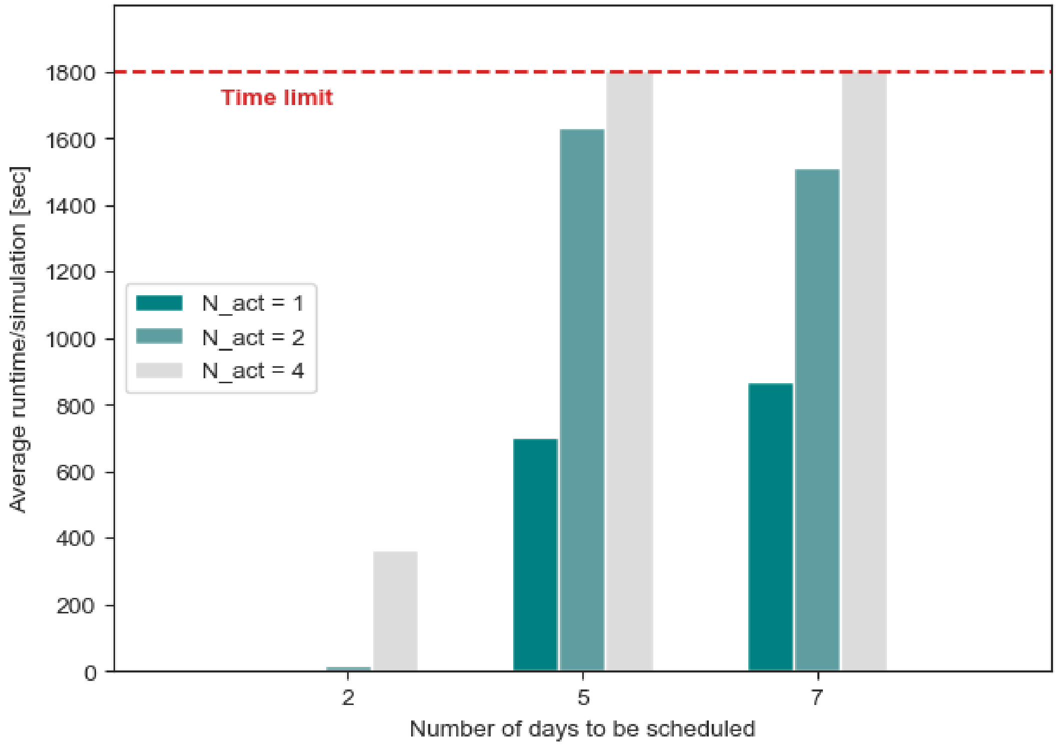


Figure 4.7: Comparisons of runtimes for different multiday configurations

4.5 Conclusion and further work

This chapter presents a preliminary investigation on the extension of the single-day OASIS framework with intrapersonal interactions in the form of behaviour over multiple days. We have started by adapting the specification of the optimisation problem by including multiday-specific variables, utility parameters and multiday constraints. Notably, we have found that relaxing some constraints is necessary to allow for specific observations, such as overnight activities.

In future work, we will improve the methodology by focusing on the following points: parameter estimation and computation performance.

4.5.1 Parameter estimation

In this first exploration of the multiday extension of OASIS, we did not calibrate the parameters to the MOBIS dataset. Instead, we used the activity-specific parameters estimated in chapter 3 and assigned arbitrary values to the new penalties for activity frequency and daily participation. This was done to simplify the simulation process and investigate the impact of multiday variables.

The next step of the analysis would be to estimate multiday parameters by adapting the estimation method (section 3.4) to reflect day-to-day interactions and correlations.

The obvious challenge is to generate a choice set adapted to the multiday scenario, which poses several issues. First, we must define the choice alternative and its temporal scale (e.g., one day, a week, a few weeks, etc.). Ideally, we should not have to estimate parameters every time we change the scheduling scope. Therefore, the choice model set up for the estimation of parameters must be carefully constructed to yield robust and transferable parameters. Secondly, the choice of operators to be included in the Metropolis-Hastings algorithm must be considered to introduce enough variability in the alternatives. If we consider a week of schedules as a choice alternative, we could imagine an operator that changes the day when a given activity is performed. However, there is a non-negligible concern for the tractability of such operators, specifically regarding the computation of forward and backward probabilities of the induced changes.

4.5.2 Computational performance

The multiday specification of the problems highlights the limitations of the mixed-integer formulation to solve this level of complexity in reasonable times.

Two avenues can be investigated:

- **Formulation improvement:** The multiday problem presented in this chapter is a direct extension of the single-day formulation, where all variables and constraints are multiplied over the time horizon. This allowed for the identification of the strengths and limitations of the framework when applied to more complex problems. Introducing some simplifying assumptions might be beneficial for the computational efficiency of the framework. For instance, the review of the literature and the analysis of the MOBIS dataset have highlighted that, while day-to-day variability exists, there is evidence for habitual behaviour resulting in reasonably similar activity schedules over a given period. This implies that it might not be necessary to simulate each day of, e.g. one given week or each week of a year. Identifying the periodicity of activity-travel behaviour could significantly simplify the problem.

For example, *activity motifs* (Schultheiss, 2021) can be used for this purpose if we extend the concept of scheduling preferences to entire schedules (e.g. we assume that decision-makers have preferences for specific day typologies, such as a full day at home, a day with a prolonged work activity, etc.). Pre-constructed motifs become inputs, alongside their frequency in the observed schedules (of the individual or the population), and the utility function can be modified to account for *similarity* between the generated schedule and the pattern and to penalise discrepancies between observed and penalised pattern frequencies.

The non-linear specification also contributes to the high solving times, and a linearisation of the optimisation problem may prove helpful when scaling up to multiple days.

- **Alternative solving methods:** The computational expense may be reduced using another problem than the Mixed Integer Programming (MIP) to optimise the multiday activity schedules. For instance, Constraint Programming is a promising solution, as it is well suited to deal with problems with vast sets of constraints. A Constraint Programming (CP) model finds feasible solutions using constraint elimination – i.e. using logical inference to eliminate infeasible solutions after given constraints have been activated. CP problems focus on achieving feasibility rather than optimality, which means that a trade-off has to be made to reduce computational time. How critical this trade-off is depends on the intended application of the simulator.

  In this case, we have implemented the multiday problem using a CP formulation with indexed variables.[5]

  Details on this implementation can be found in Appendix C. Figure 4.8 shows the decrease in runtime provided by a CP formulation of the setup presented above. For the most critical case ($n_a = 4$ and $n_d = 7$), finds a solution four times faster on average than the MIP model. This comes, however, at the expense of output quality insofar as the found solutions are feasible rather than optimal. This is shown in Figure 4.9.

[5]This implementation is based upon a baseline formulation of OASIS using CP, developed and tested by L. Bataillard, co-supervised by the candidate for a Master's semester project at EPFL (Bataillard et al., 2022).

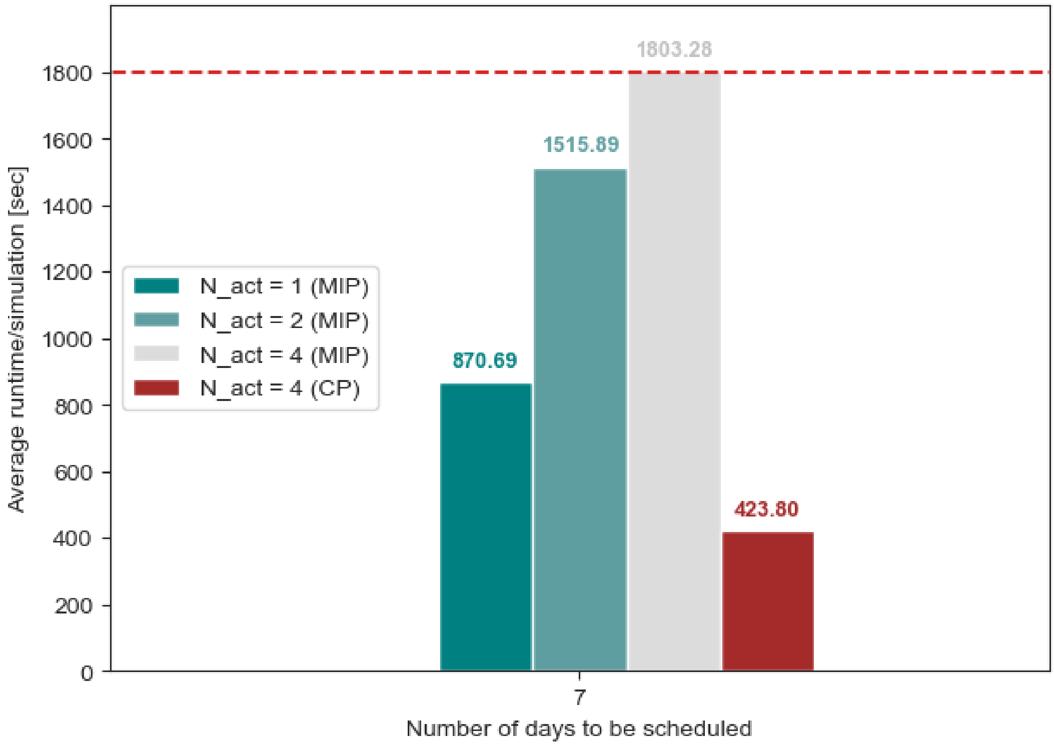


Figure 4.8: Comparisons of runtimes of MIP and CP formulations

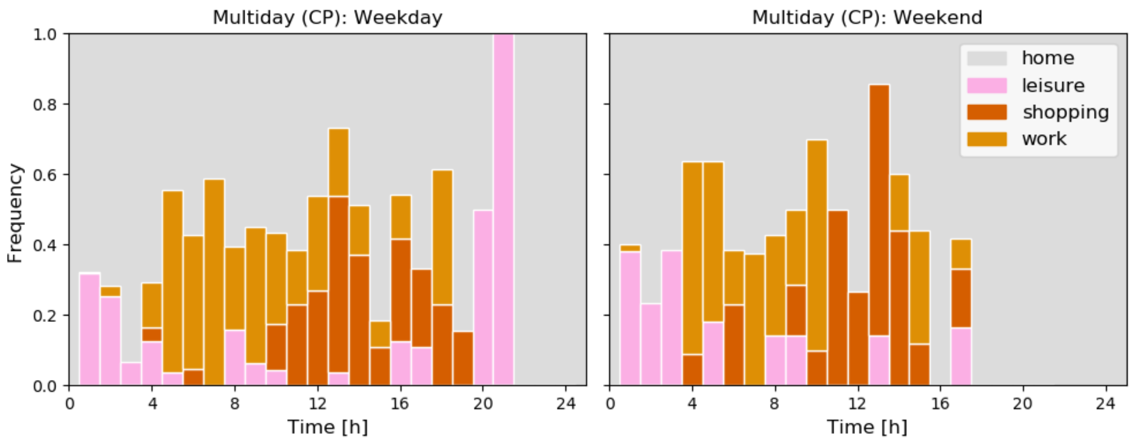


Figure 4.9: Time of day distribution of activity participation (CP)

Chapter 5

Practical applications

5.1 Introduction

This chapter summarises two research projects conducted in collaboration with academic and industrial partners. These projects have different characteristics (objectives, methods, problem complexity) but showcase the flexibility and functional modularity of OASIS. The framework's components can be used jointly or separately depending on the desired outcomes (full simulation or specific parameter estimates). They can be modified to include context-dependent constraints and ensure compatibility with other models and tools – without loss of generality.

- **Optimisation of individual mobility plans to simulate future travel in Switzerland (OPTIMS):** This project, funded by the Swiss Innovation Agency (Innosuisse), was conducted in collaboration with the Swiss Federal Railways (SBB) between September 2020 and March 2022. The outcomes of this project were described in the following publication:

  Manser, P., Haering, T., Hillel, T., Pougala, J., Krueger, R., and Bierlaire, M. (2022). Estimating flexibility preferences to resolve temporal scheduling conflicts in activity-based modelling. *Transportation*

- **e-Bike City:** This is a lighthouse project of the Department of Civil and Environmental Engineering of ETH Zürich, with support from the Swiss Federal Office of Energy (BFE). It involves multiple academic, industrial and political partners. More specifically, we have contributed to developing the *Subproject J: Estimating choice models for daily schedules.* Initial results for this project were described in the following conference proceedings:

Pougala, J., Hillel, T., and Bierlaire, M. (2023b). Modelling the impact of activity duration on utility-based scheduling decisions: a comparative analysis. In *Proceedings of the 11th Symposium of the European Association for Research in Transportation (HEART), 6-8 September 2023*, Zurich, Switzerland

The following sections briefly present these projects, the research questions we tried solving with OASIS and some illustrative results.

5.2 OPTIMS

5.2.1 Context

SBB has developed a microscopic travel demand model called SIMBA to simulate 24-hour travel days for the entire population of Switzerland.MOBi (Scherr et al., 2019, 2020). The framework contains three major components: a synthetic population, an activity-based demand model (MOBi.plans) and an agent-based traffic flow simulation model. This project focuses on the activity-based component. MOBi.plans generates a 24-hour activity-travel schedule for a given individual, including information on the tour-based choice of activity participation, mode, location and timings (duration and time of day). The schedule is generated with a sequence of discrete choice models, modelling, in order: permanent choices (such as the ownership of mobility tools and residential location), followed by daily choices (such as number and type of tours, destinations). Rules are then used to derive consistent activity plans from the outcomes of the discrete choice models. However, using a sequential approach and deterministic rules significantly limits the model's flexibility and ability to account for complex interactions.

This project aims to apply the simultaneous optimisation approach of OASIS to generate activity plans to be used as input for the SIMBA.MOBi traffic simulator. One particular challenge is maintaining key modelling characteristics (e.g. tour-based representation of activity decisions) to ensure compatibility with the rest of the framework. OPTIMS therefore refers to the combination of the OASIS simulation module and the SIMBA.MOBi framework.

Table 5.1 summarises the key methodological contributions of OPTIMS, compared to the classical SIMBA.MOBi.

Table 5.1: Methodological differences between SIMBA.MOBi and OPTIMS

Feature	SIMBA MOBi	OPTIMS
Disaggregate analysis	Yes	Yes
Daily mobility simulation	Sequential	Simultaneous
Scheduling (time of day, duration)	Rule-based	Based on real behaviour
Multimodality	Rule-based	Full multimodality
Destination choice	Limited to homogeneous zonal attraction	Disaggregate and consistent with plan
Social interaction	Rule-based, car usage only	Full behavioural response
Inclusion of unseen alternatives	Limited behavioural response	Full behavioural response
Behavioural realism	Medium	High

5.2.2 Case study

The performance of OPTIMS was assessed on a specific application and case study: generating schedules (with an emphasis on the resolution of time conflicts) at a relatively large scale (synthetic population of full-time workers living in Lausanne). Details on the methodology and results were published in (Manser et al., 2022).

The simulation procedure is two-fold:

1. **Parameter estimation**: the utility parameters that are considered are penalties for deviations from preferred time of day participation and duration, specific to the activity type and the individual flexibility (see Section 2.4.2). A discrete choice model is defined, where the alternatives are complete 24-hour activity plans. The choice set of unknown alternatives is generated by combining random alternatives and alternatives from the sequential MOBi.Plans. This ensures a mix of high and low-probability alternatives but is limited as the sampling correction term for the likelihood function cannot be calculated.

2. **Schedule optimisation**: schedules are generated for each individual in the synthetic population by maximising their utility (see Section 2.4.3).

Utility specification

The utility applied within OPTIMS (Equation 5.1) combines the OASIS utility function (Equation 2.7 and the original MOBi.Plans specification.

$$U_S = \sum_{a \in \mathcal{A}} U_{\text{start time}}(x_a) + \sum_{a \in \mathcal{S}} U_{\text{duration}}(\tau_a) + \sum_{O \in \{\mathcal{P},\mathcal{H}\}} U_{\text{duration}}(\textstyle\sum_{a \in O} \tau_a) + \sum_{a \in \mathcal{A} \setminus \{\text{dusk}\}} U_{\text{tt},a}(tt_a) \tag{5.1}$$

Where:

- $U_{\text{start time}}(x_a)$ is the utility component for deviation from the start time for each activity $a \in \mathcal{A}$. The desired start time is defined as x_a^* and x_a is the start time of activity a. Considering the parameters θ_a^{early} and θ_a^{late}, and the difference $|x_a^* - x_a|$:

  $$U_{\text{start time}}(x_a) = \theta_a^{\text{early}} \max(0;\ x_a^* - x_a) + \theta_a^{\text{late}} \max(0;\ x_a - x_a^*) \tag{5.2}$$

- $U_{\text{duration}}(\tau_a)$ is the utility component penalising deviations from preferred activity duration. This term differs from the default OASIS function as desired durations (or activity time budget) are specific to categories of activities (home, primary and secondary activities). For primary activities $a \in \mathcal{P}$ (e.g. work, education), we compare the sum of all scheduled primary activities (i.e. $\tau_a = \sum_{p \in \mathcal{P}} \tau_p$) to the desired daily duration, or primary time budget ($\tau_a^* = \tau_{\mathcal{P}}^*$). The same assumption applies to home activities. We use activity-specific desired durations for secondary activities $a \in \mathcal{S}$.

  For all categories, we consider the parameters θ_x^{short} and θ_x^{long} respectively penalising shorter and longer durations than desired, where x is either an activity or a type of activity:

  $$U_{\text{duration}}(\tau_a) = \theta_a^{\text{short}} \max(0;\ \tau_a^* - \tau_a) + \theta_a^{\text{long}} \max(0;\ \tau_a - \tau_a^*) \tag{5.3}$$

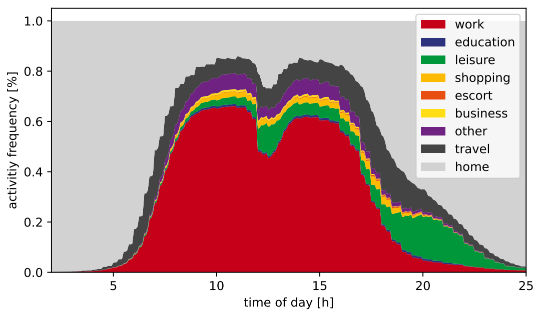
- $U_{\text{tt},a}(tt_a)$ is the (dis)utility of the time spent travelling. Similarly to the assumptions presented in chapter 2, the travel time parameter θ_{travel} is set to -1. The travel time matrix for each alternative is generated with the destination and mode choice model of SIMBA MOBi:

$$U_{\mathrm{tt},a}(tt_a) = \theta_{\mathrm{travel}}\, tt_a \tag{5.4}$$

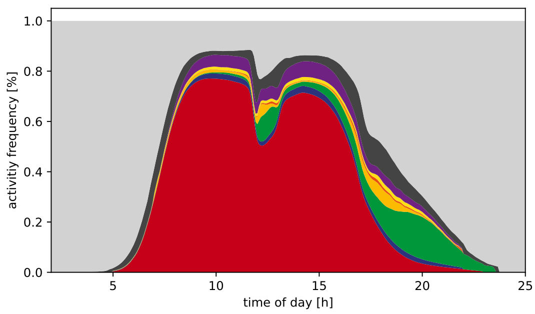
Further adaptations and input data

The optimisation model was further adapted to accommodate the tour-based requirements of the SIMBA MOBi framework.

Finally, OPTIMS was tested by drawing schedules for the agents of the synthetic sample. Figure 5.1 compares the simulated time-of-day distribution of each activity to the observed profiles in the MTMC. The results are extremely promising: the simulated outputs reproduce the real distribution very closely – except for the overnight *leisure* activities in the MTMC which the model cannot generate because of the 24-hour constraint on the time budget. In addition, *travel* between activities seems to be underestimated. This is likely due to the conservative assumption of a constant travel time parameter.



(a) Observed (microcensus)



(b) Simulated

Figure 5.1: Simulated activity profiles of the simulation compared to the MTMC (Manser et al., 2022).

This research project has been the first confrontation of OASIS with real-life requirements, including:

- large scopes of application, with thousands of agents and their respective data,
- context specificities, which require flexibility in the definition of the modelling components to be accommodated,
- modelling and performance requirements to use the framework with other

(existing) tools and modelling ecosystems.

The collaboration has been successful: the results show a real added value of using simultaneous estimation instead of sequential in this context. In addition, the workflow of SIMBA.MOBi is greatly simplified as there is no longer a need to calibrate and validate multiple sequential models. Instead, we can only estimate parameters for a single model encompassing every dimension.

5.3 e-bike City

5.3.1 Context

The *e-bike city* project was born out of the urban vision of a city where the transport system and infrastructure are focused on active modes and public transportation (Ballo et al., 2023). This is done by assigning half of the available road space to micromobility (Figure 5.2), thus decreasing the share of infrastructure allocated to private vehicles. This is expected to positively impact issues such as carbon emissions (by encouraging a shift from the use of cars to more sustainable transportation modes) or spatial equity (by improving accessibility and introducing a more balanced land use).

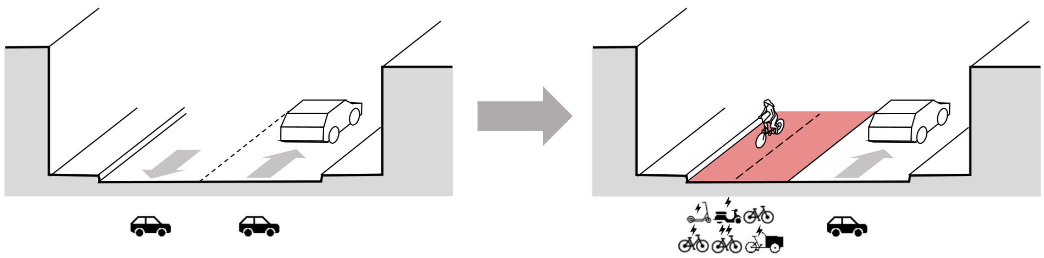


Figure 5.2: e-bike city concept (Ballo et al., 2023)

Such a drastic change in urban configuration is bound to affect activity and travel behaviour, both in observable (differences in choice of mode and location, distance travelled...) and unobservable (changes in habits and preferences) ways. Quantifying the individual modifications induced by the e-bike city is necessary to develop reliable indicators to assess the project's feasibility. In addition, understanding existing behaviour and how individuals occupy and interact with their environment in time and space is necessary to develop the e-bike city appropriately.

The primary tool used to simulate different scenarios is MATSim. Each agent in the microsimulation is characterised by a schedule of daily activities, scored by a utility function that is, among others, dependent on activity duration and network conditions (Charypar and Nagel, 2005). The scoring function parameters are not estimated; typical values from Vickrey's model for departure time choice are used. There have been attempts to estimate MATSim's parameters (e.g. Feil, 2010) but with limited success.

The objective of this collaboration is to apply the OASIS framework to: (i) estimate the parameters of the scoring function and (ii) develop a unified framework to use OASIS in conjunction with MATSim to produce behaviourally realistic simulations of the e-bike city scenarios.

At the time of writing, the research project is still ongoing.

5.3.2 Estimation of parameters

For an individual n, each activity a provides a utility U_{a_n}, composed of the following elements:

1. A *participation* term, which is constant with respect to time.
2. A utility with respect to *activity start time*.
3. A utility with respect to *activity duration*.
4. Utility terms with respect to *travel*, considering the influence of travel time and cost to the activity.

Charypar and Nagel (2005) formalised the utility function used in MATSim. The utility of activity duration has a logarithm form (Equation 5.6), which implies a decreasing marginal utility. In addition, a duration that is too short is penalised. For start time (Equation 5.7), schedule deviations such as late or early are penalised.

The parameters are: a parameter common to all activities β_{act}, a typical duration τ_a^* (considered known), a scaling factor A and a priority term ρ. $\beta^{\text{short}}, \beta^{\text{early}}, \beta^{\text{late}}$ penalise schedule deviations (δ).

$$U_S = U \sum_{a=0}^{A-1} (U_a^{\text{duration}} + U_a^{\text{start time}} + U_a^{\text{travel}}) \tag{5.5}$$

$$U_a^{\text{duration}} = \max \left[0, \beta_{\text{act}} \tau_a^* \ln \left(\frac{\tau_a}{\tau_a^* \exp(-A/(\rho \tau_a^*))} \right) \right] + \beta_a^{\text{short}} \delta_a^{\text{short}} \tag{5.6}$$

$$U_a^{\text{start time}} = \beta_a^{\text{early}} \delta_a^{\text{early}} + \beta_a^{\text{late}} \delta_a^{\text{late}} \tag{5.7}$$

As presented in Chapter 3, we have also tested the utility specification proposed by Feil (2010) for their PlanomatX model. Feil's specification modifies the default scoring function by considering the impact of activity duration with an asymmetric S-shaped curve with an inflexion point, as formalised by Joh et al. (2005) (Equation 5.9). The parameters of the S-shape are the inflection point α_a, the slope β_a, and the relative vertical position of the inflection point γ_a. When $\gamma_a = 1$, α_a can be considered the duration where the utility reaches its maximum. They do not consider start time in their utility function.

$$U_S = \sum_{a=0}^{A-1} (U_a^{\text{act}} + U^{\text{travel}}) \tag{5.8}$$

$$U_a^{\text{act}} = U_a^{\text{min}} + \frac{U_a^{\text{max}} - U_a^{\text{min}}}{(1 + \gamma_a \exp \beta_a [\alpha_a - \tau_a])^{1/\gamma_a}} \tag{5.9}$$

5.3.3 Estimation results

Following the methodology described in Chapter 3, we start by generating the choice sets of daily schedules for each individual in the sample of Lausanne students of the MTMC (see Appendix B.1). Each choice set comprises ten alternatives, including the chosen (recorded) schedule.

The models are estimated with PandasBiogeme (Bierlaire, 2020). The estimation process is done using 70% of observations in the sample data, where one observation is the daily schedule of one individual. The hold-out sample with the remaining 30% observations is used to simulate schedules.

Table 5.2 presents the parameter estimates for the MATSim scoring function.

We have chosen to display only significant parameters at a 5% level. For the estimation of the MATSim function, we have considered the same assumptions as described by Charypar and Nagel (2005) for the values of the scaling parameter ($A = -200$) and the priorities for each activity ($\rho_a = 1$ for $a \in$ {home, education, work} and $\rho_a = 3$ otherwise).

Finally, given that in the OASIS context, *home* is the reference alternative and, therefore, associated with a null utility, we have not estimated any parameter for this activity. Thus, the magnitudes and signs of the other coefficients should be considered relative to the home baseline.

The parameters of the PlanomatX function can be found in Table 3.15 (page 91).

Activity-specific parameters

For *education*, both start time deviations are penalised (being early slightly more than late) in comparable magnitudes. Being early at a leisure activity is not associated with a statistically significant penalty, as opposed to being late. For *work*, we have an insignificant parameter for being late.

Table 5.2: Estimation results for MATSim utility function. Only statistically significant parameters were included.

Parameter	Param. estimate	Rob. std err	Rob. t-stat	Rob. p-value
β_{act}	0.0514	0.00974	5.27	1.34e-07
$\theta^{\text{education}}_{\text{early}}$	-1.6	0.449	-3.57	0.00036
$\theta^{\text{education}}_{\text{late}}$	-1.01	0.291	-3.48	0.00051
$\theta^{\text{leisure}}_{\text{late}}$	-0.467	0.122	-3.84	0.00012
$\theta^{\text{shopping}}_{\text{early}}$	-0.476	0.119	-4.01	6.04e-05
$\theta^{\text{shopping}}_{\text{late}}$	-0.293	0.0842	-3.48	0.00049
$\theta^{\text{work}}_{\text{early}}$	-2.75	0.712	-3.87	0.000111
$\theta^{\text{work}}_{\text{short}}$	-1.59	0.493	-3.22	0.00126
$\bar{\rho}^2 = 0.56$				
Estimation time: 1.93 [sec]				

5.4 Conclusion

These projects have contributed significantly to developing an operational version of OASIS and offered opportunities to test the framework with different scenarios, constraints and requirements. As the philosophy behind OASIS is to produce a modular and highly flexible tool for urban planners, travel practitioners and decision-makers, these collaborations have proved invaluable. Learning from the challenges faced while applying the framework to solve these specific case studies, we have compiled a few recommendations for future applications:

- **Context:** Knowing and defining the context is paramount: identifying the possible sets of activities, locations, modes and their respective availability conditions. For this, knowledge of the population is essential, and one can benefit from supplementary surveys that include attitudinal questions. The modelling context, including scope and boundaries, must also be clearly defined beforehand. For example, what constitutes a *realistic* schedule depends on the project. Validity and feasibility criteria must be considered carefully.

- **Constraints**: Another point is to reflect on the definition of constraints, precisely, what can be considered a constraint (i.e., cannot be violated in the simulation process), and preferences or soft constraints (which are penalised in the utility function). This distinction is not universal and not always straightforward (e.g. working hours) and can significantly impact the solutions.

- **Outputs:** The framework can be applied for different end goals: here, we have shown examples of integration within an existing model and model estimation. Specific modelling requirements (e.g., performance indicators, trade-offs between runtime and quality) should be identified depending on the intended application.

Chapter 6

Conclusion

6.1 Summary of contributions

This thesis presents the development of OASIS, an activity-based simulation framework, which outputs distributions of schedules given an individual and potential activities. OASIS is our answer to two main research gaps in the activity-based literature: (i) accurately modelling the behaviour-activity-travel interactions, which explain the scheduling process while maintaining a high level of theoretical soundness and practical flexibility, (ii) dealing with and overcoming the uncertainty due to the lack of data and knowledge on these interactions to estimate and calibrate scheduling models.

Chapter 2 is the skeleton of the framework: we have presented the mixed-integer optimisation algorithm at the core of the schedule simulation process under the postulate that agents attempt to maximise the utility of their daily schedule. The following model characteristics can be noted:

- All choices about daily mobility (activity scheduling, mode choice, activity location) can be considered simultaneously, and trade-offs between these choices are easily modelled.
- A schedule is associated with a utility, consistently with random utility theory.
- The scheduling choice is explicitly modelled as a mixed integer optimisation problem solved by the decision maker.
- Due to the complexity of the choice model, there is no close form probability

formulation. Instead, the framework allows the empirical distribution of the choice model to be estimated using simulation.

The main contribution of the OASIS simulation approach is the simultaneous integration of activity-travel choice dimensions. With these characteristics, trade-offs between choice dimensions- inherent to the act of scheduling- are explicitly considered within the optimisation process. Behaviourally, this implies that we can model a balance between preferences and constraints without requiring additional ground knowledge or assumptions. This feature greatly contributes to the flexibility of the framework, which is two-fold: (i) flexible inputs, as the user-defined utility function informs the required elements. Similarly, defining the context by adding or removing constraints or changing the definition of some variables is straightforward, as demonstrated in Chapter 4 and Chapter 5. (ii) flexible outputs, as the modeller can easily control the simulation parameters. The default result of OASIS is a simulated distribution of schedules for given individuals, and the simultaneous approach alongside a robust microeconomic framework allows modellers to investigate the effects of isolated changes (e.g. new modes of transportation, transport policies, travel restrictions...) on the overall activity-travel behaviour, with minimal implementation effort.

The ability to derive maximum likelihood estimators of the utility function parameters, as presented in **Chapter 3**, greatly contributes to this flexibility. The methodology is based on a sampling procedure for unchosen alternatives based on the MH algorithm initially developed in the route choice context by Flötteröd and Bierlaire (2013). Sampling alternatives allows the derivation of the maximum likelihood estimators of the parameters, where the likelihood function is corrected to account for the estimation on a sample of alternatives instead of the entire (combinatorial) set (Ben-Akiva and Lerman, 1985). Using the parameters as input for the activity-based simulator, we can demonstrate that the simulated distribution is closer to the observed one, as measured by metrics like simulated activity participation and duration. This is a significant contribution, as parameter estimation is minimal for activity-based models. Many models either do not estimate parameters (and use common values in the literature, as we have done in Chapter 2), rely on simplifying the choice set (e.g. Arentze et al., 2011a) or use heuristic methods that are not easily transferable to other models (e.g. Recker et al., 2008). In addition, for the models that do estimate parameters, there has not been, to the best of our knowledge, an in-depth investigation of utility specifications and how different model specifications affect the simulation outputs. Here, we have presented a methodology that yields significant estimates for activity parameters related to start time and duration. We have illustrated the simulation effects of different specifications (alternative-specific vs. generic parameters, non-linear relationships, etc.). In addition, the choice set generation and parameter estimation methodology are independent of the simulation model itself. They can, therefore, be adapted and used with other frameworks and specifications.

One major limitation of current ABM is the focus on a single day as the unit of analysis, which ignores fundamental behavioural dynamics (e.g. habits, forward-looking planning) that explain in part the daily scheduling process but become crucial when extending to longer time horizons (Roorda and Ruiz, 2008). Multiday analyses are gaining traction in ABM research – but current applications tend to study specific aspects of the problem but not the activity-based process as a whole (e.g., activity generation, activity patterns variability). In **Chapter 4**, we have proposed an extension of the single-day framework for OASIS to simulate schedules over multiple days, considering adaptations at all levels (input, objective function, decision variables and constraints, and outputs). With an application on the MOBIS dataset, we have demonstrated that our extension can capture day-to-day dynamics that are not adequately accounted for in the single-day model. This result highlights the scalability of OASIS. It provides ideas to extend an existing single-day framework to a multiday scope instead of conceptualising a dedicated multiday framework from scratch. This would lead to a non-negligible gain of time, computational resources and data requirements.

Highlighting the flexibility and scalability of OASIS is a first step towards bridging the gap between theoretical concepts and operational tools. In **Chapter 5**, we have presented two practical applications of OASIS, emphasising the different project requirements (in terms of data, modelling elements, output quality) and how to integrate them in the original framework. These collaborations with the industry and academia have succeeded within the scope of the respective projects and in the overall improvement of the framework and contribution to research.

6.2 Future research directions

Not unlike a Swiss army knife, OASIS is a versatile tool that was designed to fit multiple purposes. The contributions of this work to ABM research open the door to applications and methodological extensions, which have, so far, seen little or slow progress due to the limitations of the activity-based approach. In this section, we discuss a few ideas for future research.

A potential research direction is the development of "digital twins" of urban systems, involving interactions between populations and built environment, often through the help of Information and communication technology (ICT). With increasing amounts of data and pressing environmental issues requiring fast but efficient responses, digital twins have become fundamental tools for planners and decision-makers to simulate and test policy scenarios in recent years. Simulating entire networks requires strategically integrating several systems and profoundly understanding their interactions in time and space. Using OASIS in this context would be a great benefit, as it inherently accounts for multiple dimensions simultaneously and offers enough flexibility and modularity to be integrated into and enhance the existing framework. The research opportunities that would arise from this application can be discussed at different scales:

- **Individuals:** Individuals have been the core of the research presented in this thesis, but we have barely scratched the surface in terms of behavioural modelling. There is a great synergy potential with fields such as cognitive psychology and social sciences - specifically to (i) support and enrich the behavioural layer of the model, as well as strong theory to interpret the results, and (ii) strengthen our understanding of how individuals perceive, relate to, and interact with the physical environment, and how, in turn, these interactions affect their travel behaviour (e.g. Cenani et al., 2017). This would improve the quality of the simulations and provide valuable insights into other domains, such as architecture and urban planning. Indeed, providing behaviourally informed responses to spatial features would be a valuable aid in designing urban spaces efficiently.

- **Groups:** Interpersonal interactions are essential to activity-travel behaviour. Interpersonal interactions can either be direct (e.g. joint participation in activities or sharing of a vehicle for a specific trip) or indirect (e.g. performing an activity for the benefit of the group, even though it might not be positively rewarded in individual utility), and affect the alternatives, the utility components and parameters, and the constraints. Rezvany et al. (2023) have successfully adapted OASIS to simulate household dynamics in daily activity scheduling. Building on their work, the framework can be scaled up to deal with larger social networks, including groups with looser social ties (e.g. groups of employees at the same workplace, users of the same facility, etc.). These group dynamics might not directly impact the final schedule, but they influence how the environment is perceived and consequently influence decisions. For example, expected network conditions influence departure time choice (Small, 1982), or the choice of activity destination can account for expected social similarity with other visitors (Gramsch Calvo and Axhausen, 2022). The ability to accurately capture and model interpersonal interactions opens the door for significant contributions in theoretical, strategical and operational applications: synthetic population generation, management of large-scale events, and development of emergency response frameworks, ...

- **Systems:** There is an urgent need to build or transform sustainable spaces such as to mitigate their environmental pressure and ensure the equitable welfare of their inhabitants. Modelling urban ecosystems with this purpose brings challenges that are difficult to overcome with traditional approaches. One of these challenges is the transferability to different geographical contexts. The flexibility of OASIS makes this operation possible: for example, the framework can be calibrated for different cities or geographical spaces and can be used to identify differences in activity-travel behaviour that could be accounted for, among others, social and cultural differences. However, careful consideration of each area's characteristics and particular needs must be given to avoid the common pitfalls of "one size fits all" models.

Beyond the transportation field, other domains can benefit from using an integrated activity-based framework. For example, studies on urban metabolism - and more specifically, the modelling, forecasting and regulation of resource consumption (energy, water...), have started being explored through an activity-based lens (e.g. Keirstead and Sivakumar, 2012; Pawlak et al., 2020), and could be integrated within the OASIS framework.

Appendices

Appendix A

OASIS documentation

A.1 Source code

The source code for OASIS can be downloaded from:
https://github.com/transp-or/oasis

The full documentation is available:
https://oasis-abm.readthedocs.io/en/latest/

OASIS requires the following packages:

- Python: 3.10+
- Docplex[1]: 2.25.236
- Scipy: 1.10.1+
- Numpy: 1.24.2+
- Pandas: 1.5.3+

We recommend creating a new environment using the provided `requirements.txt` file to download all dependencies.

A.2 Simulation

The `Simulation` module is comprised of the following files:

[1]This package requires a valid CPLEX license to function. Please visit IBM's official documentation for more information.

- `simulation.py`: This script stores information on the `Simulation` class and subclasses (e.g. `MIP`). These classes are used to set up and solve the optimisation problem.
- `results.py`: The `Results` class stores the outputs of the simulation (optimised schedules, runtimes, and objective functions), and handles the visualisation and simulation statistics.
- `input_data.py`: This script handles the input data, and creates `ActivityData` objects. These objects contain information on each activity to be scheduled, including preferred start time, duration, and utility parameters.
- `error_terms.py`: The `ErrorTerms` class is used to handle the utility function errors – to be drawn at each new iterations.
- `runner.py`: The main file to run the simulation.

In this section, we will go through an example to illustrate each simulation step.

A.2.1 Preparing the input

File(s): runner.py

```
import joblib
import json

DATA = joblib.load('data/example_data.joblib')
TT = joblib.load('data/example_tt.joblib')
PARAMS = json.load(open('data/example_parameters.json', 'r'))
```

Three main inputs must be provided for the simulation:

1. The set of activities (`DATA`)
2. A mode travel time matrix (`TT`)
3. The set of activity parameters (`PARAMS`)

We start with an example schedule from the MTMC dataset. This schedule contains two *work* activities and a *leisure* activities. The set of activities is provided as a `pandas DataFrame` (Figure A.1), and contains the label of the activities (a unique identifier and the activity type), the recorded start time, duration and end time (which are not mandatory for the simulation), a feasible start and end time (not mandatory, and will default to the whole day if not provided), the location of the activity (which should correspond to one entry of the travel time matrix), the mode of transportation and desired start and end times.

	act_id	act_label	label	feasible_start	feasible_end	location	mode_travel	group	desired_start	desired_duration
0	1.0	home	dawn	0	24	A	driving	dawn	0.000000	12.940332
1	2.0	work	work1	5	23	B	driving	work	6.602686	10.470977
2	1.0	home	home	0	24	A	driving	home	0.000000	12.940332
3	2.0	work	work2	5	23	B	driving	work	6.602686	10.470977
4	8.0	leisure	leisure	0	24	B	driving	leisure	16.005231	3.380537
5	1.0	home	dusk	0	24	A	driving	dusk	0.000000	12.940332

Figure A.1: Example of input schedule

The travel time matrix is a dictionary formatted as :

```
{mode: {
origin_location: {
destination_location1 : travel_time_1,
destination_location2 : travel_time_2
}}}
```

The travel time is in hours.

In the example, we consider the travel times for the `driving` mode and two different locations.

```
{'driving':
    {'A': {'A': 0, 'B': 0.0002777777777777778},
    'B': {'A': 0.0002777777777777778, 'B': 0}}}
```

Finally, the parameters should be a dictionary containing the activity-specific parameters that will be used in the utility function. The dictionary should have the format:

```
{activity_1: {parameter_1: value, parameter_2: value},
 activity_2: {parameter_1: value, parameter_2:value}}
```

In the example, we use the utility function as defined in Chapter 3, including penalties for early and late start time, short and long duration, and travel time. The parameters for the *work* activity are:

```
{'constant': 13.0838530926,
 'early': -0.618657816,
 'late': -0.3384943975,
 'short': -0.9319615942,
 'long': -1.223996357,
 'travel_time': -1}
```

The next step is to define the error terms that will be used in the utility function. In the specification of Chapter 3, we consider normally distributed error terms for each decision variable and an Extreme Value distributed error term. These random components are instances of the `ErrorTerms` class and are defined in a dedicated dictionary. During the simulation, the `draw()` method of these error objects will be called to draw a new value for each iteration.

```
from error_terms import GaussianError, EVError

UTILITY_PARAMS = {
    'error_w': GaussianError(),
    'error_x': GaussianError(),
    'error_d': GaussianError(),
    'error_z': GaussianError(),
    'error_ev': EVError()
    }
```

Finally, we call the `data_reader()` function, which transforms the schedule dataframe and parameters into `ActivityData` objects that will be used during the simulation.

```
from input_data import data_reader

dataset = data_reader(DATA,PARAMS)
```

A.2.2 Setting up and running the model

Files: runner.py, simulation.py

Once the data is imported, we can set up the simulation model. This is done by creating a `Simulation` object and passing the dataset, the utility function parameters and the simulation parameters (number of iterations and progress output) as arguments. The `verbose` argument specifies how frequently the model prints its progress.

Here, we create a simulation with 100 iterations and a MIP solver. We print the model progress every 25 iterations.

```
from simulation import MIP
N_ITER = 100

new_simulation = MIP(dataset, UTILITY_PARAMS,TT)
results = new_simulation.run(n_iter = N_ITER, verbose = 25)
```

Each new `Simulation` object instantiates a `Model` from the `docplex` library. The method `initialize()` adds decision variables and constraints to the model and can be modified directly in the corresponding script or using the `add_constraints()` function in the runner file. The CPLEX optimisation settings (e.g. time limit) can be specified when creating the `Simulation`. The default settings are a time limit of 120 seconds per solve call, and the optimality target set to `global`[2].

The utility and objective functions of the problem can be directly modified in the `utility_function()` and `objective_function()` methods of the `Simulation` object.

The `run()` method solves the optimisation problem and returns a `Results` object containing the optimised schedule(s), the runtime(s) and the value(s) of the objective function.

As we have activated the `verbose` option, the model prints its progress every 25 iterations.

```
Starting simulation: 100 iterations.
-----------------------------------------
Starting iteration 25/100.
Iteration 25 complete. Iteration runtime: 00:00:00. Time elapsed:
  00:00:25.
Starting iteration 50/100.
Iteration 50 complete. Iteration runtime: 00:00:00. Time elapsed:
  00:00:52.
Starting iteration 75/100.
Iteration 75 complete. Iteration runtime: 00:00:01. Time elapsed:
  00:01:18.
Starting iteration 100/100.
Iteration 100 complete. Iteration runtime: 00:00:00. Time elapsed:
  00:01:42.
-----------------------------------------
```

[2]See IBM's documentation for an exhaustive list of parameters.

```
Simulation complete. Total runtime: 00:01:42
```

A.2.3 Processing the outputs

Files: runner.py, results.py

The simulation outputs a `Results` object that stores the optimal schedules, runtimes and objective values for all iterations. Several methods can be helpful to visualise the results:

- `plot()`: plots the optimal schedules. The argument `plot_every` controls how many schedules to plot if more than one is provided. By default, the figure is saved as a `png` file, but this can be modified with the `save_fig` argument (either saving with a different extension or not saving the figure). The plotting function can be further customised by specifying, for example, the size, title, legend or activity colours.

  ```
  results.plot(plot_every=25)
  ```

  Figure A.2 shows the output of this command.

- `plot_distribution()`: plots the time of day distribution across all iterations. By default, the figure is saved as a `png` file, but this can be modified with the `save_fig` argument (either saving with a different extension or not saving the figure). The plotting function can be further customised by specifying, for example, the size, title, legend or activity colours.

  ```
  results.plot_distribution(figure_size= [7,4])
  ```

  Figure A.3 shows the output of this command.

- `compute_statistics()`: computes simulation statistics (e.g. proportion of out-of-home schedules, average time spent in a given activity) for a given list of activities. These statistics can be directly printed or saved to a file. This function provides bootstrap confidence intervals for each indicator. The settings for the bootstrapping can be specified in the arguments (e.g. number of samples, level of confidence).

  ```
  results.compute_statistics(['home', 'work', 'leisure'], save =
    False)
  ```

  The output of this command is:

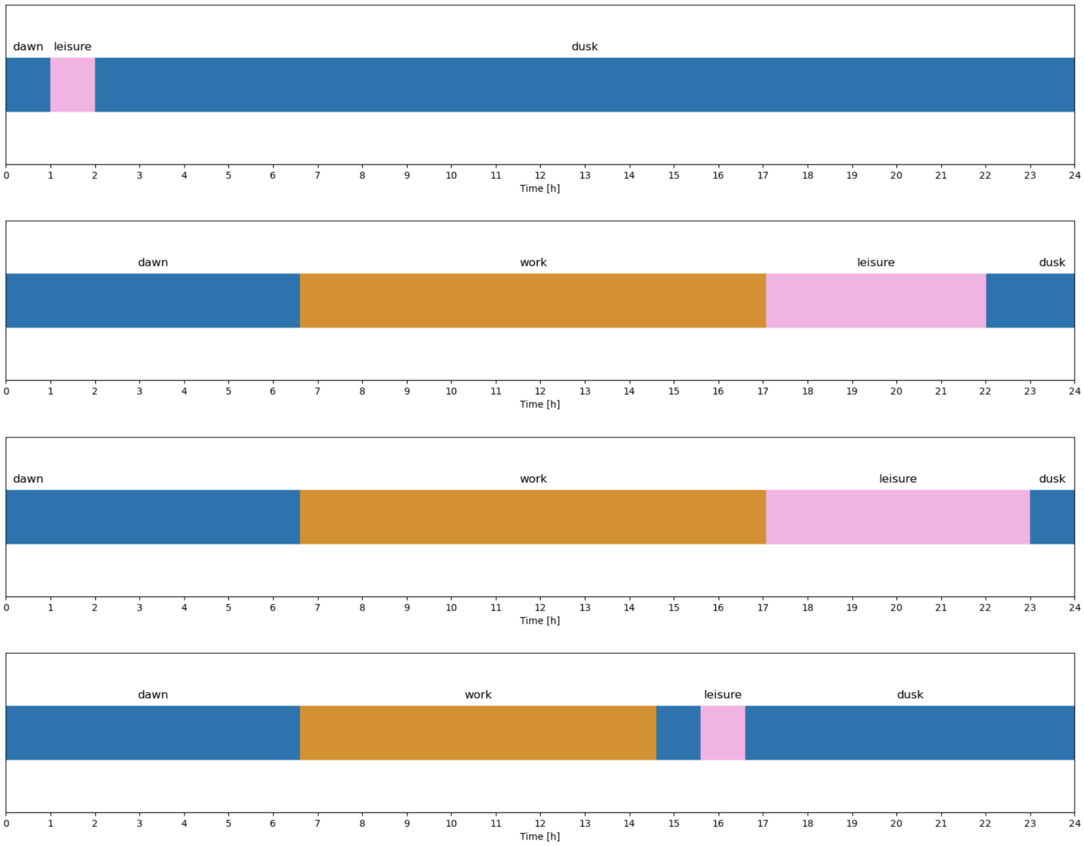


Figure A.2: Example of output schedules

```
Summary of collected statistics:
--------------------------------------------------
Total number of schedules: 100
Proportion of out-of-home schedules: 93.00 %
Average time spent out-of-home: 13.10, CI: [12.956,13.279] hours
Average number of out-of-home activities: 1.98, CI: [1.968,
  1.989]
--------------------------------------------------
Average duration of each activity:
Home: 10.88, CI: [10.702, 11.017] hours
Work: 10.06, CI: [9.970, 10.188] hours
Leisure: 3.18, CI: [3.077, 3.312] hours
--------------------------------------------------
```

A.2.4 Full script

```python
import joblib
import json

```

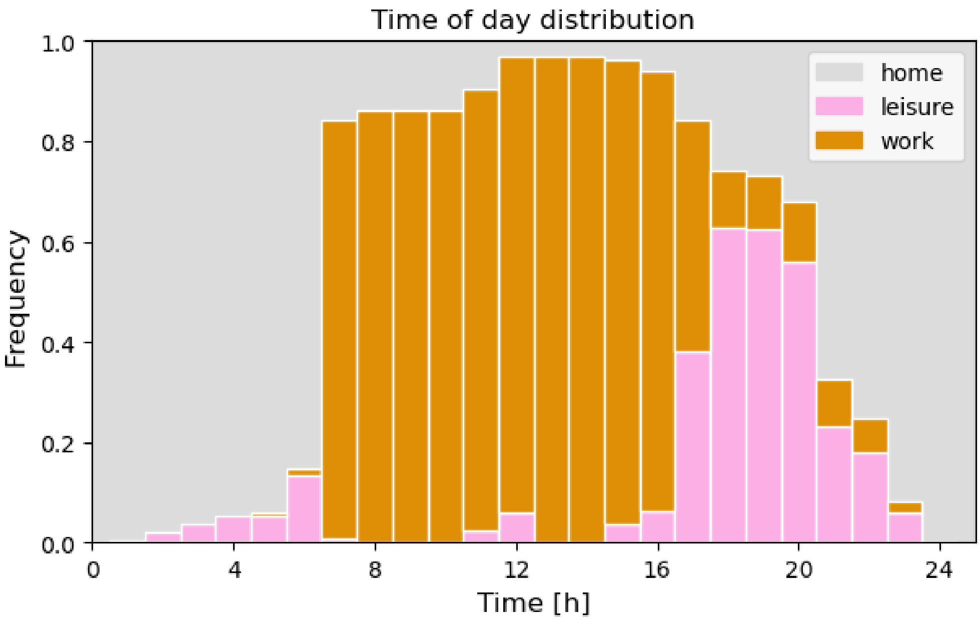


Figure A.3: Example of output distribution

```
from input_data import data_reader
from error_terms import GaussianError, EVError
from simulation import MIP


DATA = joblib.load('data/example_data.joblib')
TT = joblib.load('data/example_tt.joblib')
PARAMS = json.load('data/example_parameters.json')

UTILITY_PARAMS = {
    'error_w': GaussianError(),
    'error_x': GaussianError(),
    'error_d': GaussianError(),
    'error_z': GaussianError(),
    'error_ev': EVError()
    }

N_ITER = 100

def main():
    dataset = data_reader(DATA,PARAMS)
    new_simulation = MIP(dataset, UTILITY_PARAMS,TT)

    results = new_simulation.run(n_iter = N_ITER, verbose = 25)

```

```
    results.plot(plot_every = 25, save_fig='png')
    results.plot_distribution(save_fig='png')
    results.compute_statistics(['home', 'work', 'leisure'])

if __name__ == '__main__':
    main()
```

A.2.5 Multiday

The MultidayMIP simulation class can be called instead of the standard MIP to simulate multiday schedules. The arguments are the same as MIP, with the addition of two specific arguments:

- n_days: The number of days in the time horizon,
- day_index: An integer that identifies the day of the week. By default, we consider 1 to be Monday and 7 to Sunday. This variable is helpful to differentiate utility functions based on the type of day (e.g. to include different preferences for participation, start time and duration on weekdays or weekends).

If the preferences for each activity vary according to the type of day, they must be explicitly defined for each ActivityData. This can be done by providing the desired start time and duration for weekdays and weekends as input[3]. Another variable included in ActivityData is desired_frequency, which is defined as the preferred weekly number of occurrences of a given activity.

If successful, the multiday simulation produces a Results object that contains n_days schedules and the runtimes and optimal values of the objective function. The plot() function is modified to plot and display the name of each day. The statistics can be computed for every solution or schedule category (weekdays vs. weekends.)

An example of the multiday setup can be found below:

```
import joblib
import json

from input_data import data_reader
from error_terms import GaussianError, EVError
```

[3]This categorisation can be modified, e.g. having different desired times for each day. However, it must match the specification of the utility function.

```
from simulation import MultidayMIP


DATA = joblib.load('../data/example_data_multiday.joblib')
TT = joblib.load('../data/example_tt_multiday.joblib')
PARAMS = json.load(open('../data/example_parameters_multiday.json', '
  r'))

UTILITY_PARAMS = {
    'error_w': GaussianError(),
    'error_x': GaussianError(),
    'error_d': GaussianError(),
    'error_z': GaussianError(),
    'error_ev': EVError()
    }

N_ITER = 5
N_DAYS = 7
DAY_INDEX = [*range(1,8)]
SETTINGS =  {'optimality_target': 3, 'time_limit': 150}


def main():
    """Run multiday simulation"""

    dataset = data_reader(DATA,PARAMS)
    new_simulation = MultidayMIP(dataset, UTILITY_PARAMS,TT, n_days=
      N_DAYS, day_index=DAY_INDEX, **SETTINGS)

    results = new_simulation.run(N_ITER,verbose = 2)

    #visualise results
    results.plot(plot_iter = 2, save_fig='png') #plot iteration 2
    results.plot_distribution(days = [*range(1,6)], figure_size=
      [7,4], save_fig= 'png') #time of day distribution for weekdays
    results.plot_distribution(days = [6,7], figure_size= [7,4],
      save_fig= 'png') #time of day distribution for weekends
    results.compute_statistics(['home', 'work', 'leisure'], days = [*
      range(1,6)]) #stats for weekdays
    results.compute_statistics(['home', 'work', 'leisure'], days =
      [6,7]) #stats for weekends


if __name__ == '__main__':
    main()
```

A.3 Estimation

The following files are used for the estimation.

- `estimation.py`: This script stores information on the `ChoiceSetGenerator` class, used to run the Metropolis-Hastings algorithm, and transform the generated choice set into the appropriate format.
- `metropolis_hastings.py`: Stores the `random_walk` function, as well as other functions to handle the results (convergence assessment, statistics)
- `activity.py`: This script handles the input data, and creates `Activity` and `Schedule` objects. These objects contain information on each activity and on the structure of the schedule. They will be modified during the generation process.
- `operator.py`: The `Operator` class and subclasses (e.g. `Assign`) are used to handle the random walk operators, including functions to compute the change probabilities.
- `runner.py`: The main file to run the simulation.

In this section, we will go through an example to illustrate each step of the estimation.

A.3.1 Preparing the input

File(s): runner.py

```
import joblib
import json

DATA = joblib.load('../data/example_data_estimation.joblib')
TT = joblib.load('../data/example_tt.joblib')
PARAMS = '../data/target_params.joblib'
```

Three main inputs must be provided for the simulation:

1. The list of schedules, one schedule per individual in the population (`DATA`)
2. A mode travel time matrix (`TT`)

3. The set of activity parameters for the target distribution (`PARAMS`)

We use the same example as Appendix A.2.1 but now use the **observed** records. This means that the columns `start_time` and `duration` must exist and indicate the actual start time and duration of each activity (Figure A.4). The travel time matrix is the same, and the parameters should be the parameters of the target distribution of the Metropolis-Hastings algorithm. This distribution can be specified in the `target_distribution` function, in the `metropolis_hastings` module.

	act_id	act_label	label	feasible_start	feasible_end	location	mode_travel	group	desired_start	desired_duration	start_time	end_time	duration
0	1.0	home	dawn	0	24	A	driving	dawn	0.000000	12.940332	0.000000	9.500000	9.500000
1	2.0	work	work1	5	23	B	driving	work	6.602686	10.470977	9.533333	13.500000	3.966667
2	1.0	home	home	0	24	A	driving	home	0.000000	12.940332	13.533333	15.166667	1.633333
3	2.0	work	work2	5	23	B	driving	work	6.602686	10.470977	15.200000	20.000000	4.800000
4	8.0	leisure	leisure	0	24	B	driving	leisure	16.005231	3.380537	20.466667	20.466667	0.000000
5	1.0	home	dusk	0	24	A	driving	dusk	0.000000	12.940332	20.500000	24.000000	3.500000

Figure A.4: Example of input schedule for the estimation

To proceed with the estimation, we transform the `DataFrame` schedule into a `Schedule` object. We can do this using the `parse_df_schedule` function. The Schedule class stores information on the activities in the schedule, which are themselves `Activity` objects (storing timings, locations, modes), as well as specific functions that will be helpful during the random walk. For example, the `streamline` function restores validity conditions (e.g. 24-hour time budget, start and end at home) after an operator has applied a change.

```
from helper_func import parse_df_schedule

DATA = [parse_df_schedule(DATA, TT)]
```

A.3.2 Setting up and running the estimation

File(s): runner.py, estimation.py

We create a new `ChoiceSetGenerator`, to generate a choice set of `n_alt = 5` alternatives. We specify additional parameters for the Metropolis-Hastings algorithm, such as the number of iterations, the number of iterations for warm-up, and thinning.

```
from estimation import ChoiceSetGenerator

mh_params = {"n_iter":1000,
```

```
"n_burn": 50,
 "n_skip": 1,
 "uniform": False,
}

estimator = ChoiceSetGenerator(DATA, PARAMS, n_alt = 5, mh_params=
  mh_params)
```

Note that these parameters can also be provided directly in the `settings.py` file. This file includes, for example, default parameters for operators and activities (probabilities), as can be seen below:

```
DEFAULT_ACTIVITIES = ["home", "work","education","shopping","
  errands_services","business_trip","leisure","escort"]
DEFAULT_OPERATORS = ['Block', 'Assign', 'AddAnchor', 'Swap', '
  InflateDeflate', 'MetaOperator']
DEFAULT_P_OPERATORS = len(DEFAULT_OPERATORS)*[1/len(DEFAULT_OPERATORS
  )]
DEFAULT_MODES = ["driving", "pt", "cycling"]

DEFAULT_MH_PARAMS = {"n_iter":200000,
"n_burn": 50000,
 "n_skip": 10,
 "uniform": False,
}

DEFAULT_VARIABLES = ['start_time', 'duration', 'participation']
```

The `run()` function is called to run the Metropolis-Hastings algorithm. For large samples and number of iterations, we recommend parallelising the code using the `run_parallel()` function instead.

```
estimator.run()
```

A.3.3 Processing the outputs

Files: runner.py, metropolis_hastings.py, estimation.py

We plot a few draws using the `output` function. This function plots the schedule and returns the choice set in the desired format.

The function `collect_distributions` (from the `metropolis_hastings` file- collects and plots the distributions of the resulting choice set for different metrics (start time, duration, activity participation).

Figure A.5 shows a few draws from the choice set generated for the example individual. Note that for each choice set, the first schedule is the recorded (chosen) one.

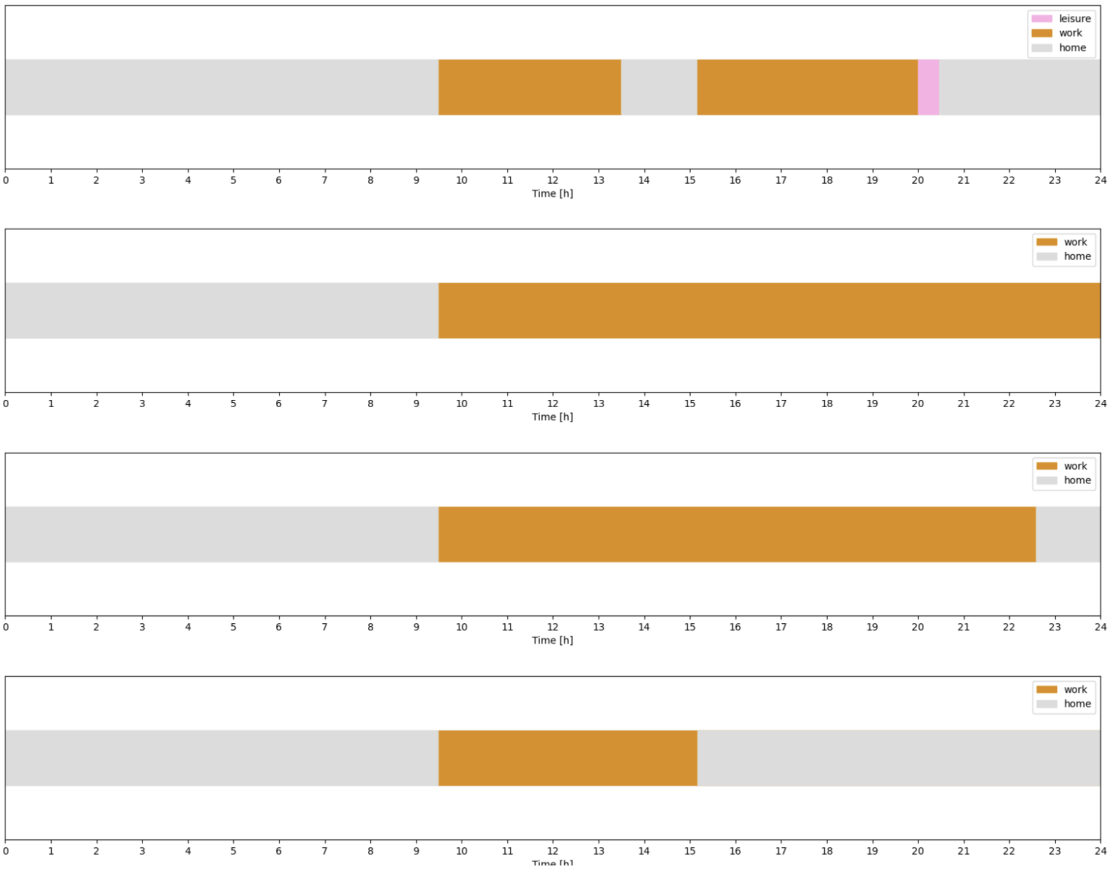


Figure A.5: Example of output for the estimation

We can use the function `train_test_sets()` to create train and test datasets for the estimation. By default, there is a 70/30 split between train and test observations. This function also computes the sample probability `prob_corr` to correct the choice probabilities and likelihood function (see Ben-Akiva and Lerman, 1985). Each individual is associated with a unique `obs_id`, and each alternative of the choice set with a unique `alt_id`, as seen in Figure A.6.

The train and test datasets can be created in `wide` or `long` format. They can then be used to estimate parameters with a discrete choice solver (e.g. Biogeme, Bierlaire, 2020)

A.3.4 Full script

	obs_id	alt_id	choice	prob_corr	home:start_time	home:duration	home:participation	work:start_time	work:duration
0	0	0	1.0	868.954605	0.0	14.699444	1	9.500278	8.832778
1	0	0	1.0	868.954605	0.0	14.699444	1	9.500278	8.832778
2	0	1	1.0	870.149372	0.0	8.936165	1	8.659382	15.063280
3	0	2	1.0	870.753124	0.0	8.659104	1	8.659382	3.299849
4	0	3	1.0	869.954605	0.0	9.500000	1	9.500278	14.499722
5	0	4	1.0	870.272664	0.0	8.659104	1	8.659382	15.340618

Figure A.6: Example of train dataset

```python
import joblib
from estimation import ChoiceSetGenerator
from helper_func import parse_df_schedule

DATA = joblib.load('../data/example_data_estimation.joblib')
TT = joblib.load('../data/example_tt.joblib')
PARAMS = '../data/target_params.joblib'

MH_PARAMS = {"n_iter":1000,
"n_burn": 50,
 "n_skip": 1,
 "uniform": False,
}

N_ALT = 5

def main():
    data = parse_df_schedule(DATA)
    estimator = ChoiceSetGenerator(DATA, PARAMS, n_alt = N_ALT,
      mh_params=MH_PARAMS)
    estimator.run()

    train_wide, train_long, test = estimator.train_test_sets()

if __name__ == '__main__':
    main()
```

Appendix B

Data

B.1 Mobility and Transport Microcensus

The Mobility and Transport Microcensus (*Mobilität und Verkehr Mikrozensus*), (BfS and ARE, 2017) is a Swiss nationwide travel survey conducted every five years by the Federal Office of Statistics (BFS) and the Federal Office for Spatial Development (ARE). This survey aims to gather insights into the mobility behaviours of residents.

The 2015 dataset contains 57'090 individuals (each representing one household) and 43'630 trip diaries. The residents of Lausanne account for a total of 2'227 diaries.

The dataset was preprocessed to:

- Clean the data from problematic observations (missing values, reporting errors, etc.). In addition, we have only kept observations where the schedule started and ended at home.
- Transform the trip-based data into an appropriate activity-based input for OASIS (Table B.1)

The trip-related features were obtained from the `Etappen` table, while all socio-economic features can be found in the `Zielpersonen` table.

OASIS requires two additional input data: the travel time and the distance matrix. The travel time matrix was computed using the code developed by Hillel et al. (2018), which uses Google Maps Direction API. For each pair of activity locations

OASIS input	MTMC variable	Processing
Activity label	`f52900`: Trip purpose	Removed travel-related purposes *Mode transfer* and *Border crossing*. Re-labeled other purposes.
Activity start time	`f51400time`: Trip arrival time	Converted to hours
Activity end time	`f51100time`: Trip departure	Converted to hours
Activity duration	-	Activity end time - start time
Activity location	`S_Y, S_X, Z_Y, Z_X`: Trip OD coordinates (WGS84)	-
Employment status	`ERWERB` 4 level employment status	Categorised into Workers, Students, and Unemployed
Geographical region	`WAGGLO2000`, `WKANTON` or `WREGION`	Used `WAGGLO2000` to sample Lausanne residents.

Table B.1: Processing of MTMC

(l_a, l_b), a typical travel time was computed for driving, cycling, public transport, and walking modes. Similarly, the distance matrix was computed using the distance matrix API.

B.2 Survey on daily and weekly activity planning

Daily activity schedules

Week : from Monday …./…. to Sunday …./….

Name :

This survey aims to capture the scheduling process of individuals when they plan their days in a given timeframe (1 week). We are specifically interested in days that start and end at home (24h).

In the section **Weekly planning** we will ask you to provide the activities that you consider doing anytime during the week (from Monday morning to Sunday evening), as well as your usual preferences in terms of times and durations. It should be filled out on the Sunday before the beginning of the recorded week.

In the section **Daily planning**, we will ask you to provide your intended schedule for a given day, and your preferences in terms of times, durations and locations for this specific day. It should be filled at the time when you are most likely to plan your day (e.g. the evening before or the morning of).

Weekly planning

1. Which out-of-home activities do you plan to do this week?

Activities (ID)	**X**	**How many times this week?**	**Which days (if specific)?**
Work (1)			
Work (not at usual workplace) (2)			
Education (3)			
Shopping (4)			
Errands/Services (5)			
Escort (6)			
Eating (7)			
Fitness (8)			
Leisure / Social activities (9)			
Other (please specify) (10)			

The activities are defined as follows:

- **Work:** usual profession performed at a specific location
- **Work (not at workplace**) : business activities performed outside of the usual work location (includes business trips and work at home)
- **Education:** only for students up to Master's level (for PhD students, you can include courses as work)
- **Shopping:** shopping for non-necessities (i.e. not food)
- **Errands/services:** shopping and use of facilities for necessities (e.g. food shopping, medical appointments)
- **Escort:** accompanying someone to an activity without participating
- **Eating:** includes all meals eaten in a catering establishment (e.g. cafeterias, restaurants etc.)
- **Fitness:** includes all sportive activities

- **Leisure/ social activities:** includes all recreational activities

2. What is your typical/preferred:

    - Minimum daily duration at home (Mon-Fri)[1]: ………….. h
    - Minimum daily duration at home (Sat-Sun): ………….. h
    - Daily duration at work/education (Mon-Fri): ………….. h
    - Earliest departure time from home (Mon-Fri): ………….. (HH:MM)
    - Earliest departure time from home (Sat-Sun): …………..
    - Latest arrival time at home (Mon-Fri): ………….. (HH:MM)
    - Latest arrival time at home (Sat-Sun): …………..

3. Are there other activities that you do regularly but will not perform this week? If so, which ones and when?

4. Which modes do you plan to use this week? (main modes only, i.e. not mode transfers)

Modes	**X**
Car (driver)	
Car (passenger)	
Public Transport	
Bike	
Walking	

Daily Planning

Please fill the following tables with the schedule you **intend to do** for each day (it does not matter If your actual day diverges from your plan).

Consider the following definitions:

- **Activities:** a one word description of your activity
- **Start/End time:** the start (resp. end) time is defined as the arrival (resp. departure) time (HH:MM) to the location where you perform the activity. If you do not have a specific preference, you can fill it with qualitative information (e.g., in the morning, after work, …)
- **Duration:** your desired duration for each activity
- **Location:** your preferred location for performing the activity. It does not have to be an address, simpler methods of identification are possible (e.g. closest public transport stop,

[1] Considering all tasks you need to do at home (e.g. sleeping, cooking, ….). It is not a constraint, i.e. it could be possible for you to spend less time at home than this duration, but you would be unhappy to do so.

name of shop/restaurant…). If you do not want to disclose your home location, please provide an estimate travel time from your home to the location of the other activities.

- **Considered locations** (if applicable): other locations where you would be willing to perform the activity.

- **Feasible time windows** (if applicable): e.g. shops opening hours. If you are considering multiple locations, specify the feasible time windows for each of them if they exist and are different.

- **Flexibility of start time (early):** scale from -1 to 1
  - -1 = I cannot be early to this activity
  - 0 = I do not mind being a little early to this activity (please specify by how many minutes)
  - 1 = I do not mind being early to this activity
- **Flexibility of start time (late):**scale from -1 to 1
  - -1 = I cannot be late to this activity
  - 0 = I do not mind being a little late to this activity (please specify by how many minutes)
  - 1 = I do not mind being late to this activity

- **Flexibility of duration (short):** scale from -1 to 1
  - -1 = This activity cannot be shorter than what I have planned
  - 0 = I can tolerate a slightly shorter duration than what I have planned (please specify by how many minutes)
  - 1 = I do not mind if the duration is shorter than what I have planned
- **Flexibility of duration (long):** scale from -1 to 1
  - -1 = This activity cannot be longer than what I have planned
  - 0 = I can tolerate a slightly longer duration than what I have planned (please specify by how many minutes)
  - 1 = I do not mind if the duration is longer than what I have planned

- **Constraints:** any requirements to perform this activity (e.g. return home after grocery shopping)

EXAMPLE SCHEDULE

Activity	Start (HH:MM)	End (HH:MM)	Duration (h)	Location	Considered Locations	Time windows	Flex. start		Flex. duration		Constraints
							Early	Late	Short	Long	
Home	00:00	08:30		Riponne-M.Béjart		00:00 – 23:59	/	/	1	1	
Work	09:00	12:00		EPFL			1	0 (20 min)			
Lunch	12:00	13:00	1	EPFL		11:30 – 14:30	0 (10min)	0 (10 min)	0 (10 min)	0 (10 min)	
Work	13:00	18:00		EPFL			1	0 (20 min)			
Grocery shopping	After work		1	Migros EPFL	Aldi Bessières	7:30 – 20:00 8:00 – 19:00			0 (20 min)	0 (10 min)	Return home to drop-off groceries
Home		20:10	1.5	Riponne-M.Béjart			1	1	0 (10 min)	0 (15 min)	
Cinema	20:30	22:30		Pathé Flon	Pathé Galeries Cinétoile Malley	20:30 – 22:30 20:10 – 22:10 21:00 – 23:00	0 (15min)	-1	-1	0 (20 min)	
Home		23:59		Riponne-M.Béjart			1	1	1	1	

Appendix C

Constraint Programming formulation

This work is based upon the following semester project, performed under the supervision of the candidate.

> Bataillard, L., Pougala, J., Haering, T., and Bierlaire, M. (2022). A comparative analysis of optimization algorithms for activity-based applications. Master semester project

The objective of this semester project was to implement an alternative formulation for the OASIS optimisation module using constraint programming (CP). It is a modelling approach to solve combinatorial optimisation problems. CP is especially well suited to deal with large numbers of constraints thanks to the following principles (Philippe et al., 2001):

1. *Constraint propagation*: Existing constraints are not only used to check the validity of the solutions but are actively used to deduce new constraints, remove values from the variables' domains, and detect inconsistencies, based on logical inference.

2. *Search algorithm*: As constraint propagation alone is insufficient to detect all possible inconsistencies, it is paired with a search algorithm (usually tree search) to explore the solution space.

3. *Locality*: The constraints must be propagated as locally as possible.

CP has been used in the literature to solve scheduling problems (of the time/resource allocation variety). Still, to our knowledge, it was never implemented to solve a full optimisation-based activity-based model.

In his report, Bataillard et al. has implemented three different CP formulations for OASIS (direct translation of the MIP, indexed model and interval model). For all of his experiments, he has found that the CP models outperformed the MIP, especially with complex inputs (i.e. increasing number of activities, modes and locations). The main limitation of the approach is that CP models generally output feasible solutions, which significantly contributes to the gain in runtime at the expense of guaranteed optimality.

In Chapter 4, we have observed that the high runtimes of the MIP become a significant limitation when we extend the framework to solve multiday instances. Therefore, we have adapted Bataillard et al.'s CP indexed model for single-day scheduling to accommodate multiday activities and constraints. Note that in the indexed model, travel time between the locations of activities a and b by mode d $\rho(m, ell_a, \ell_b)$ is described by a flattened array P of size $|M||L|^2 + 1$, where M and L are respectively the sets of possible modes of transportation and activity locations. P is indexed by the combination (m, ℓ_a, ℓ_b), such that $\rho(m, \ell_a, \ell_b) = P\left[|L|^2 m + |L|\ell_a + \ell_b\right]$. The last element of the array $P\left[|M||L|^2\right]$ is set to 0, and is used to index pairs of activities that do not follow each other.

The decision variables are, for each day d and activity a:

- $\omega_{a,d} \in \{0, 1\}$: activity participation,
- $x_{a,d} \in \mathcal{T}$: start time,
- $\tau_{a,d} \in \mathcal{T}$: duration,
- $z_{ab,d} \in \{0, 1\}$: indicator variable of sequence of activities (a, b),
- $m_{a,d} \in M_{a,d}$: mode of transportation,
- $l_{a,d} \in L_{a,d}$: location,
- $\rho_{ab,d}$: travel time between a and b,
- $i_{ab,d} \in [0, |M||L|^2]$: index in travel time array P for (a, b).

where $\mathcal{T}$ is the (discrete) time domain, $M_{a,d}$ is the set of modes available for activity a on day d, and $L_{a,d}$ is the set of possible locations for activity a on day d.

The constraints are the same as those formulated for the multiday MIP (eqs. (4.5) to (4.22)), although simplified as, in CP, we can formulate some logical constraints (e.g. if-then, or) directly. The constraints related to the indexed travel time are the following:

$$z_{ab,d} \rightarrow i_{ab,d} = |L|^2 m + |L|\ell_a + \ell_b \qquad \forall a, b \in A, d \in T \tag{C.1}$$

$$\neg z_{ab,d} \rightarrow i_{ab,d} = |M||L|^2 \qquad \forall a, b \in A, d \in T \tag{C.2}$$

$$\text{ELEMENT}\left(i_{ab,d}, P, \rho_{ab,d}\right) \qquad \forall a, b \in A, d \in T \tag{C.3}$$

where ELEMENT(i, K, j) is an element constraint such that ELEMENT$(i, K, j) \Leftrightarrow j = K[i]$.

The CP model was implemented using Google OR-Tools CP-SAT solver (Google Developers, 2023).

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PhD candidate in the Transport and Mobility laboratory at Ecole Polytechnique Fédérale de Lausanne (EPFL). Developed OASIS, an open-source optimization-based activity-based model to simulate daily activity-travel schedules, succesfully implemented and used by research and industry partners (including Swiss Federal Railways). Experienced in teaching undergraduate and postgraduate courses in transportation and behavioral modeling, with supervision of several Master's theses.

Languages: French (Native), Italian (Fluent), English (Fluent), Spanish (Conversational), German (Basic)

Education

- **Ph.D. (Civil engineering) - EPFL (CH)** Sept.2019 – Oct.2023
  Thesis: OASIS : An integrated optimisation framework for activity scheduling
  Advisors: Prof. M. Bierlaire and Dr. T. Hillel
- **Master of Science (Civil engineering) - EPFL (CH)** Sept. 2016 – Feb. 2019
  Thesis: Digital and physical methods to monitor urban mobility: Case study of Pully
  Advisors: Prof. N. Geroliminis, Prof. P.-Y. Gilliéron
- **Bachelor of Science (Civil Engineering) - EPFL (CH)** Sept. 2013 – July 2016
  Thesis : Development of efficient one-way car-sharing schemes
  Advisor: Prof. N. Geroliminis

Research experience

- **Doctoral student - EPFL (CH)** 2019–present
  Transport and mobility laboratory (TRANSP-OR), Advisors: Prof. M. Bierlaire, Dr. T. Hillel
  - Development of an open-source activity scheduling simulator based on random utility maximization, simultaneously integrating all activity-travel choice dimensions (activity participation, scheduling, mode of transportation, location).
  - Successful collaboration with the Swiss Federal Railways to integrate OASIS within their long-term nationwide travel demand forecasting framework.
  - Successful academic collaborations (e.g., Prof. V. Kaufmann, Prof. K. Axhausen) to explore potential applications of OASIS.
  - This work resulted in publications in the Journal of Choice Modelling Transportation, Transportation Research Part C: Emerging Technologies, several conference talks, including IATBR (International Association of Travel Behaviour Research). This work was funded through an Innosuisse grant, a Cluster grant from EPFL's School of Architecture, Civil and Environmental Engineering, and a grant from the Swiss Federal Office of Energy.
- **Visiting researcher - University College London (UK)** Sep. 2022 – Jan. 2023
  Behaviour and Infrastructure Group (BIG)
  Dept. of Civil, Environmental and Geomatic Engineering
- **Graduate student - EPFL (CH)** 2019
  Advisors: Prof. N. Geroliminis, Prof. P-Y. Gilliéron
  - Collaborated with the telecom provider Swisscom to calibrate and validate their Mobility Insights tool for the town of Pully (CH).
  - Performed a cost-benefit analysis on behalf of the town of Pully for the installation of mobility sensors in the town center.
  - Developed a methodology to fuse data from physical (from sensors) and digital sources (from mobile traces).

◦ This work was awarded with the Citec Mobility Solutions Prize 2019, and VSS Swiss association of roads and transports professionals) prize 2019. It was published as an article in the monthly publication of VSS's *Strasse und Verkehr*.

Research grants

- **Swiss Federal Office of Energy** 2022–2025
  Project: eBike City
  - Grant value: 420 kCHF total (value to lab 30 kCHF)
  - Principal investigators: Prof. K. Axhausen (IVT-ETHZ), Prof. M. Bierlaire
  - Role: Researcher. Exploring the integration of OASIS into MATSim microsimulator for behaviorally realistic inputs and insights.
- **EPFL ENAC Cluster grant** 2020–2021
  Project: Activity scheduling an rhythmic style: multi-day modeling of mobility habits
  - Grant value: 70 kCHF total (value to lab 35 kCHF)
  - Principal investigators: J. Pougala, M.-E. Schultheiss (Laboratory of urban sociology, EPFL)
  - Role: Principal investigator. Proposal writing and submission, project management. The goal of the project was to develop a methodology to simulate multiple days of activities, integrating socio-economic characteristics and constraints.
- **Innosuisse** 2020–2022
  Project: Optimization of individual mobility plans to simulate future travel in Switzerland
  - Grant total: 586'915 CHF (value to lab 311'990 CHF)
  - Principal investigator: Prof. M. Bielaire (EPFL)
  - Role: Researcher. This project was a collaboration with the Swiss Federal Railways (SBB), to integrate OASIS into their long-term transport demand forecasting for Switzerland.

Institutional responsibilities

- **Civil engineering teaching commission - EPFL (CH)** Sept. 2019 - now
  PhD representative

Teaching activities

- **Introduction to transportation systems**: Bachelor course for engineers. Role: teaching assistant. Spring 2023.
- **Mathematical modeling of behavior**: Master course for mathematicians and engineers. Role: teaching assistant. Fall 2019, 2020, 2021, 2022.
- **Decision-aid methodologies in transportation**: Master course for engineers. Role: teaching assistant. Spring 2020, 2021, 2022.
- **Discrete Choice Analysis: Predicting Individual Behavior and Market Demand**: Industry and doctoral course, given by Prof. M. Bierlaire and Prof. M. Ben-Akiva. Role: lecturer and teaching assistant. Spring 2020, 2021, 2022, 2023
- **Project supervision**: Supervised 6 Master theses (MSc) and 9 Bachelor semester projects. 2019 - 2023

Conference, lectures and seminars

- **hEART 2023**: Speaker – *Zurich, (CH) – September 2023*
- **IATBR 2022**: Speaker – *Santiago de Chile (CL) – December 2022*
- **TUM Symposium on activity-based models, 2022**: Speaker – *Munich (DE) – September 2022*
- **mobil.TUM 2022**: Speaker – *Online – April 2022*
- **hEART 2020**: Speaker – *Lyon (FR) – April 2021*
- **Swiss Transport Research Conference**: Speaker – *Ascona (CH) – May 2019, 2020, Sept. 2021, May 2022, May 2023*

Prizes, awards, fellowships

- **hEART 2023 - Best paper award**: for the paper ”Modelling the impact of activity duration on utility-based scheduling decisions: a comparative analysis”.
- **EPFL’s Doctoral School of Civil and Environmental Engineering Mobility Award 2022**: funding for academic visit to external research institution.
- **ENAC Cluster Grants 2020**: Activity scheduling and rhythmic style: multi-day modeling of mobility habits . PI: M.E. Schultheiss, J. Pougala – *Sept.2020 - Sept.2021*
- **Innosuisse**: Optimization of individual mobility plans to simulate future travel in Switzerland. PI: Prof. M. Bierlaire – *Sept.2020 - March.2022*
- **VSS Foundation award**: for outstanding Master’s theses in the field of transportation – *Feb. 2020*
- **Citec Mobility Solutions award**: for outstanding Master’s theses in the field of mobility and transportation – *Oct. 2019*

Research output

- **Peer reviewed journal publications**:
  - Pougala J., Hillel T., Bierlaire M. (2023). OASIS: Optimisation-based Activity Scheduling with Integrated Simultaneous choice dimensions. Transportation Research Part C: Emerging Technologies, Volume 155
  - Pougala J., Hillel T., Bierlaire M. (2022). Capturing trade-offs between daily scheduling choices. Journal of Choice Modelling, Volume 43 (100354)
  - Manser P., Haering T., Hillel T., Pougala J., Krueger R., Bierlaire M. (2022). Estimating flexibility preferences to resolve temporal scheduling conflicts in activity-based modelling. Transportation
- **Conference proceedings**:
  - Pougala J., Hillel T., Bierlaire M. (2023) From one-day to multiday activity scheduling: extending the OASIS framework. Proceedings of the 23rd Swiss Transport Research Conference (STRC), 10-12 May, Ascona, Switzerland
  - Pougala J., Hillel T., Bierlaire M. (2022) Parameter estimation for activity-based models. Proceedings of the 22nd Swiss Transport Research Conference (STRC), 18-20 May, Ascona, Switzerlan
  - Salvadé N., Hillel T., Pougala J., Haering T., Bierlaire M. (2022) Representing location choice within activity-based models. Proceedings of the 22nd Swiss Transport Research Conference (STRC), 18-20 May, Ascona, Switzerland
  - Pougala J., Hillel T., Bierlaire M. (2021) Choice set generation for activity-based models. Proceedings of the 21st Swiss Transport Research Conference (STRC), 12-14 September, Ascona, Switzerland
  - Hillel T., Pougala J., Manser P., Luethi R., Scherr W., Bierlaire M. (2020) Modelling mobility tool availability at a household and individual level: A case study of Switzerland. Proceedings of the 9th Symposium of the European Association for Research in Transportation (HEART), 3-4 February 2021, Lyon, France
  - Pougala J., Hillel T., Bierlaire M. (2020) An optimization framework for daily activity schedules. Proceedings of the 9th Symposium of the European Association for Research in Transportation (HEART), 3-4 February 2021, Lyon, France
  - Pougala, J., Hillel, T., and Bierlaire, M. (2020). Scheduling of daily activities: an optimization approach. Proceedings of the 20th Swiss Transport Research Conference (STRC) 13-14 May, 2020.
- **Other publications**:
  - Pougala Janody. ”Observatoire de la mobilité à Pully: Un outil qui permet de quantifier la mobilité dans le centre-ville”. *Strasse und Verkehr*, VSS, July-Aug. 2020