Transportation Research Part C 155 (2023) 104291

Contents lists available at ScienceDirect

Transportation Research Part C

journal homepage: www.elsevier.com/locate/trc

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

Janody Pougala [a,*], Tim Hillel [b], Michel Bierlaire [a]

[a] École Polytechnique Fédérale de Lausanne (EPFL), School of Architecture, Civil and Environmental Engineering (ENAC), Transport and Mobility Laboratory, Switzerland

[b] University College London (UCL), Department of Civil, Environmental and Geomatic Engineering, United Kingdom

ARTICLE INFO

Keywords:
Activity-based modelling
Discrete choice modelling
Parameter estimation
Choice set generation
Maximum likelihood estimation
Simulation

ABSTRACT

Activity-based models offer the potential of a far deeper understanding of daily mobility behaviour than trip-based models. However, activity-based models used both in research and practice have often relied on applying sequential choice models between subsequent choices, oversimplifying the scheduling process. In this paper we introduce OASIS, an integrated framework to simulate activity schedules by considering all choice dimensions simultaneously. We present a methodology for the estimation of the parameters of an activity-based model from historic data, allowing for the generation of 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 from a Swiss nationwide travel survey, and evaluating the output of the OASIS model against realised schedules from the data. 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 that are consistent with behavioural theory. This work opens the way for future developments of activity-based models, where a great deal of constraints can be explicitly included in the modelling framework, and all choice dimensions are handled simultaneously.

1. Introduction

Activity-based models have been the focus of increasing research efforts in a variety of domains, including transport research, energy demand, and epidemiology. In transportation, they provide a behaviourally realistic alternative to traditional trip-based models and aggregate analyses.

In previous work (Pougala et al., 2022) we have introduced an activity-based model to simultaneously estimate choices of activity participation, scheduling, travel mode and location. The model is utility-based and uses mixed-integer optimisation to simulate realisations of feasible activity schedules. The major benefit of the simultaneous approach over traditional sequential approaches (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.

* Corresponding author.
E-mail address: janody.pougala@epfl.ch (J. Pougala).

https://doi.org/10.1016/j.trc.2023.104291
Received 4 November 2022; Received in revised form 21 June 2023; Accepted 7 August 2023
Available online 1 September 2023

A significant limitation and challenge of the simultaneous approach is the estimation of stable and significant parameters. In Pougala et al. (2022), the parameters are not estimated, instead a set of accepted values from the literature are used to illustrate the principles of the framework. Parameter estimation is generally a challenging task in activity-based models, due to the size of the problem, the complexity of the structure 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 also 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 paper, 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. 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 Swiss Mobility and Transport Microcensus (BfS and ARE, 2017).

The integration of simultaneous activity scheduling simulation and the parameter estimation from OASIS (Optimisation-based Activity Scheduling with Integrated Simultaneous choice dimensions): a flexible activity-based framework able to accommodate the requirements and context-specific constraints of different application domains, and thus provide tailored behavioural insights.

The main contributions of this research are:

1. The formulation of an integrated framework of simultaneous activity-travel simulation, as opposed to sequential. As the framework is built upon first principles, it provides more flexibility than conventional models, and does not require changes to the fundamental methodology to accommodate different scenarios.
2. A methodology to efficiently sample unchosen daily schedules. Enumeration is especially challenging in the activity-travel context, because of the combinatorial nature of the solution space. Traditionally, the choice set is either considered given (e.g. Bowman and Ben-Akiva, 2001), or requires rules or constraints (often based on expert knowledge to be defined). The method we propose generalises this procedure.
3. 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.

2. Relevant literature

Activity-based models 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:

1. 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;
2. models tend to suffer from biases due to unrealistic aggregations in time, space, and within the population; and
3. space and time constraints are usually not included.

The early works of Hägerstraand (1970) and Chapin (1974) established the fundamental assumption of activity-based models, 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. Rasouli and Timmermans (2014) and Axhausen (2000) provide in-depth reviews of the state of research and practice in activity-based modelling.

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 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...) and combinatorial. The full set of solutions cannot be enumerated or fully observed by the modeller or the decision maker. 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 therefore two main issues to address: generating a choice set for the purpose of parameter estimation, and formulating a tractable model specification which is able to capture multidimensional correlations.

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

Both deterministic and stochastic models exist for the generation of spatio-temporal choice sets (Pagliara and Timmermans, 2009) for the purpose of 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). Danalet and Bierlaire (2015) adapt and apply the methodology proposed by Flötteröd and Bierlaire (2013) to sample alternatives in an activity-based context. The alternatives are activity schedules (defined as paths in a spatiotemporal network). They establish that importance sampling with the Metropolis–Hastings algorithm provides a better model fit than random sampling. However, these methods are not straightforward to apply to activity-based models because of their multidimensionality, 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 the uncertainty associated with it. Deterministic choice sets are used in early activity-based models

Several methods are adopted for the estimation of utility parameters, including heuristics (e.g. Recker et al. (2008) and Allahviranloo and Axhausen (2018) use a genetic algorithm to estimate the parameters of their respective utility-based activity-based models) and maximum likelihood estimation using discrete models (e.g. Nijland et al., 2009; Arentze et al., 2011; Xu et al., 2017). Nijland et al. (2009) estimate the parameters of Arentze and Timmermans's need-based activity-based model, 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 properly capture the randomness and unobserved factors in the need-building process, Arentze et al. (2011) also estimate the parameters of the need-based model, but with an error components mixed logit model. The set-up 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 model explicitly 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 Household Activity Pattern Problem (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 of the model performance using edit distance as an error measure, as opposed to a case where the priorities are equal. As they calibrate their model parameters by confronting their simulated and observed patterns, their methodology cannot provide insights on unchosen activity 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, and 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 full choice set. In addition, the methodology to generate choice sets creates endogeneity and is biased towards alternatives with 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.

In this paper, we propose a parameter estimation procedure for the simultaneous activity-based model presented in Pougala et al. (2022). The model simulates daily schedules of activities for a given individual by maximising the utility they gain from participating to activities. The output is a distribution of schedules conditional on the distribution of the random error terms. The first iteration of the model demonstrated the ability of the approach to generate realistic activity schedules while explicitly accounting for scheduling trade-offs. However, the parameters of the utility function were not estimated, and we used instead values from the literature. The methodology we present here is based on Maximum Likelihood Estimation (MLE). Similarly to other state-of-the-art approaches, we take advantage of the theoretical robustness and flexibility of discrete choice models for this task, but applied to a framework where all of the activity-travel choices are considered simultaneously. This allows to capture trade-offs and interrelations between choices, but with the added cost of complex solution spaces and combinatorial choice sets. We apply here a methodology for choice set generation using the Metropolis–Hastings algorithm, based on the works of Flötteröd and Bierlaire (2013) and Danalet and Bierlaire (2015).

Table 1 summarises the papers described in this section, and the methodologies developed or applied by the authors for the generation of individual choice sets and for the estimation of parameters.

3. Methodology

We present a methodology to estimate the parameters of an activity-based model where all scheduling choice dimensions (activity participation, timing decisions, mode, location, etc.) are considered simultaneously within a mixed integer optimisation

Table 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. (2011)	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
Current paper	Simultaneous ABM	Metropolis–Hastings sampling	Logit model

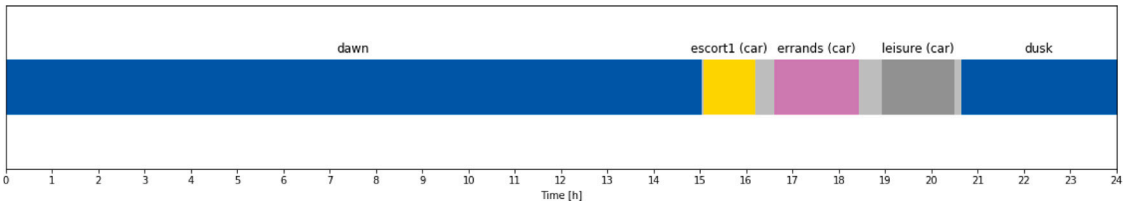


Fig. 1. Example of a daily schedule. The light gray patches between activities indicate travel. *Dawn* and *dusk* are the first and last *home* activities of the day.

framework. The estimation process consists of two elements: (i) choice set generation, and (ii) discrete choice parameter estimation. The model, presented in Section 3.1, 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. This procedure is explained in Section 3.2. The likelihood function, as defined by Train (2009), requires an enumeration of the alternatives of the choice set. We present a methodology to generate an appropriate choice set in Section 3.3.

3.1. Scheduling framework

We use the same definition of a schedule as Pougala et al. (2022): it is 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 next 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".

Fig. 1 shows an example of schedule for one person, which includes 3 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 preferences of the individual 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 (Pougala et al., 2022), and a utility specification originally proposed for the scoring of activity schedules in the MATSim microsimulator (Feil, 2010), where the utility for activity duration is assumed to have a S-shape.

3.1.1. Utility specification with linear penalties

As defined in Pougala et al. (2022), 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:

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

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 activity (e.g. resource availability at the level of the household).
2. The utility $U_a^{\text{participation}}$ associated with the participation of the activity a, irrespective of its starting time and duration.

$$U_a^{\text{participation}} = \gamma_a + \beta_{\text{cost}} c_a + \varepsilon_{\text{participation}}, \tag{2}$$

where γ_a and β_{cost} are unknown parameters to be estimated from data, and $\varepsilon_p articipation$ is an error term.

3. The utility $U_a^{\text{start time}}$, which captures the perceived penalty created by deviations from the preferred starting time.

$$U_a^{\text{start time}} = \theta_a^{\text{early}} \max(0, x_a^* - x_a) + \theta_a^{\text{late}} \max(0, x_a - x_a^*) + \varepsilon_{\text{start time}}, \tag{3}$$

Table 2
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)	$\varepsilon_{\text{travel}}$	–	

where $\theta_a^{\text{early}} \leq 0$ and $\theta_a^{\text{late}} \leq 0$ are unknown parameters to be estimated from data, and $\varepsilon_{\text{start time}}$ is an error term. The first (resp. second) term captures the disutility of starting the activity earlier (resp. later) than the preferred starting time.

4. The utility U_a^{duration} associated with duration. This term captures the perceived penalty created by deviations from the preferred duration.

$$U_a^{\text{duration}} = \theta_a^{\text{short}} \max(0, \tau_a^* - \tau_a) + \theta_a^{\text{long}} \max(0, \tau_a - \tau_a^*) + \varepsilon_{\text{duration}} \tag{4}$$

where $\theta_a^{\text{short}} \leq 0$ and $\theta_a^{\text{long}} \leq 0$ are unknown parameters to be estimated from data, and $\varepsilon_{\text{duration}}$ is an error term. 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 $U_{\text{travel}}^{a,b}$ associated with the trip from ℓ_a to ℓ_b. irrespective of the travel time. This term is composed of the penalty associated with the travel time ρ_{ab}, and other travel variables (including variables such as cost, level of service, etc.) Here, we illustrate the framework with a specification involving travel cost. It also includes an error term, capturing the unobserved variables.

$$U_{a,b}^{\text{travel}} = \beta_{t,\text{time}} \rho_{ab} + \beta_{t,\text{cost}} c_t + \varepsilon_{\text{travel}} \tag{5}$$

where $\beta_{t,\text{time}}$ and $\beta_{t,\text{cost}}$ are unknown parameters to be estimated from data, and $\varepsilon_{\text{travel}}$ is an error term.

The schedules generated by the simulator must be *feasible*, according to a set of constraints defined at the level of the individual or the household by the modeller. For example, a schedule is feasible if:

- it does not exceed the maximum (time or cost) budget,
- each activity starts when the trip following the previous activity is finished,
- trips using mode m are only made if and when m is available,
- each activity meets its respective requirements (e.g. participation of other members of the household, feasible time windows, follows/precedes another activity)
- ...

The parameters involved in the utility function are summarised in Table 2. Indices S, a, and n denote respectively a schedule, an activity and an individual. The *Estimated* column indicates which parameters are estimated in the current study, with results presented in Section 4. 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.

3.1.2. 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. (7)). 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 as the duration where the utility reaches its maximum. The parameters involved in the utility function are summarised in Table 3. Indices S, a and n denote respectively a schedule, an activity and an individual. The *Estimated* column indicates which parameters are estimated in the current study, with results presented in Section 4.

$$U_S = \sum_{a=0}^{A-1} (U_a^{\text{act}} + U^{\text{travel}}) \tag{6}$$

Table 3
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	

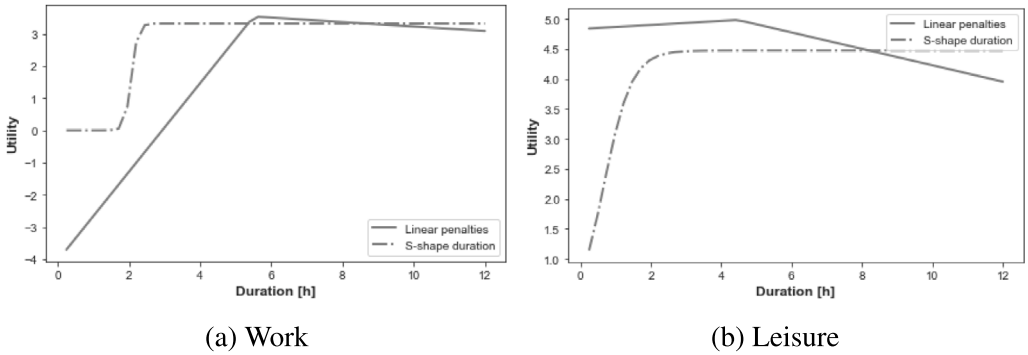


Fig. 2. Effect of duration on utility for the tested specifications.

$$U_a^{\text{act}} = U_a^{\min} + \frac{U_a^{\max} - U_a^{\min}}{(1 + \zeta_a \exp \beta_a \left[\alpha_a - \tau_a\right])^{1/\zeta_a}} \tag{7}$$

Fig. 2 illustrates the utilities of *work* and *leisure* for both specifications and different values of duration.

3.2. Parameter estimation

The scheduling process can be considered as a discrete choice model where the alternatives are full daily schedules, each associated with a utility.

In principle, maximum likelihood estimation requires 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 actually necessary in the activity-travel context, where the full choice set C_n of alternatives is combinatorial and characterised by complex constraints. For each individual n in the sample, we consider a sample 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):

$$P_{in} = P_n(i|\tilde{C}_n) = \frac{e^{\mu V_{in} + \ln P_n(\tilde{C}_n|i)}}{\sum_{j \in \tilde{C}_n} e^{\mu V_{jn} + \ln P_n(\tilde{C}_n|j)}} \tag{8}$$

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 used to generate the choice set.

Each component of the utility function (Eqs. (2)–(5)) is associated with a random term. This defines a mixed logit model with error components, by creating correlations between alternatives which share 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 that there is no correlation between alternatives. This assumption is adopted in the case study presented in Section 4.

3.3. Choice set generation

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 (8). 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 high probability of being chosen, to represent a choice set that the individual would actually 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

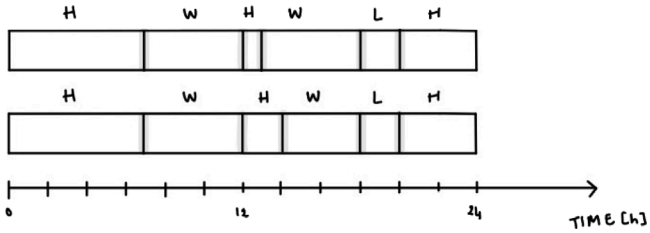


Fig. 3. Example of neighbouring schedules. The schedules differ in the duration of the time spent at home during lunch time.

strategy to build the choice set must therefore 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 Metropolis–Hastings algorithm (Flötteröd and Bierlaire, 2013; Danalet and Bierlaire, 2015) is a good strategy to achieve this objective, while keeping tractable probabilities to derive the sample correction for the likelihood function.

The Metropolis–Hastings algorithm (Hastings, 1970) is a Markov Chain Monte-Carlo method used to generate samples from a multidimensional distribution, using a predefined acceptance/rejection rule. The procedure is summarised in algorithm 1 (see Gelman et al., 1995).

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

Choose starting point X_0 from starting distribution $p(X_0)$
for $t = 1, 2, \ldots$ **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 (Eq. (1)).

3.3.1. Generation of a candidate point

We define X_t the state(or point) at time t. X_t is a 24 h 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). 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 ν, at the start of a block, indicating the position of the operator changes. In this context, each block corresponds to the temporal magnitude of the change.

Each operator must generate a feasible schedule, as defined in Section 3.1. In addition, the following conditions must be satisfied by the algorithm:

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

$$Q(X_t|X_{t-1}) > 0 \qquad \forall X_t, X_{t-1} \tag{9}$$

  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 Metropolis–Hastings 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.

$$Q(X_t|X_{t-1}) > 0 \qquad \forall X_t, X_{t-1} \tag{10}$$

$$Q(X_{t-1}|X_t) > 0 \qquad \forall X_t, X_{t-1} \tag{11}$$

  Defining single change operators enables to derive tractable probabilities.

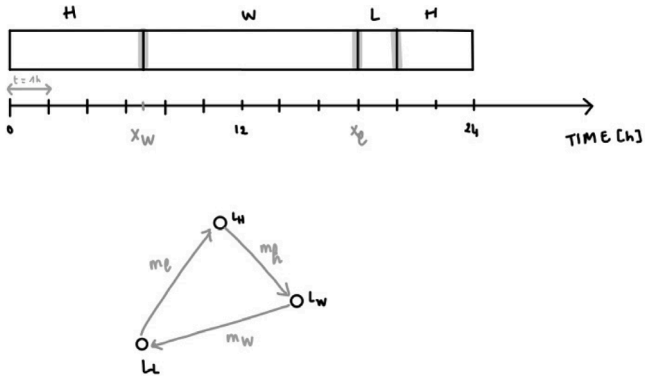


Fig. 4. Initial schedule.

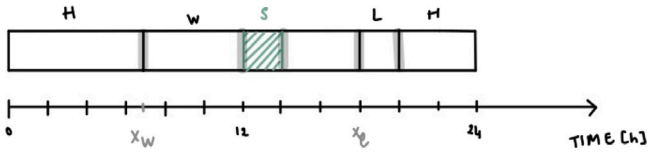


Fig. 5. Change applied by the *assign* operator.

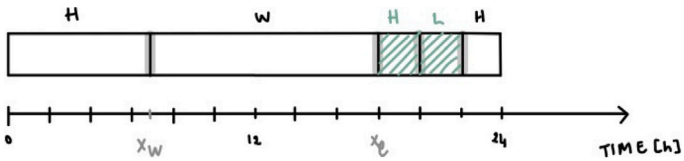


Fig. 6. Change applied by the *swap* operator.

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 Fig. 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.

Anchor The anchor operator ω_{anchor} adds an anchor node v in the schedule. This change does not affect the activity sequence, but allows to change 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 anchor node.

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

Fig. 5 illustrates an example of modification applied by the *assign* operator on the initial schedule.

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

Fig. 6 illustrates an example of modification applied by the *swap* operator on the initial schedule.

Inflate/deflate The *inflate/deflate* operator $\omega_{\text{inf/def}}$ allows to perform a shift of the schedule by randomly inflating the duration (i.e. adding one block of length δ) of the activity i at position v 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 start time of the activity, while maintaining its duration. This operator modifies durations without generating infeasible schedules (e.g. schedules with a total duration that is different than the time budget). In order to ensure the validity constraint that the schedule must start and end at home, the first and last time block of the schedule cannot be modified.

Fig. 7 illustrates an example of modification applied by the *inflate/deflate* operator on the initial schedule.

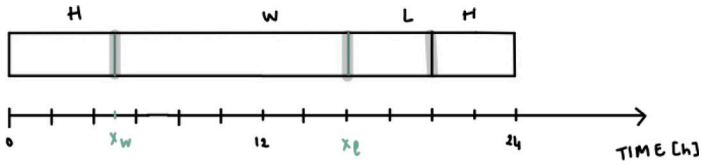


Fig. 7. Change applied by the *inflate/deflate* operator.

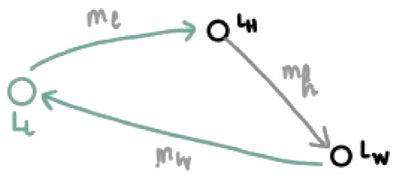


Fig. 8. Change applied by the *location* operator.

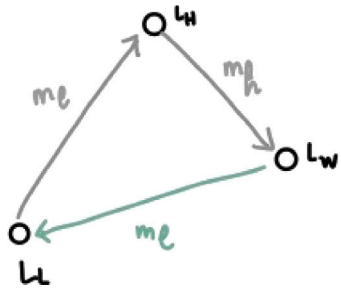


Fig. 9. Change applied by the *mode* operator.

Location The *location* operator ω_{loc} changes the location ℓ_i of a randomly selected activity i at position v, 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 as compared to the available time budget is absorbed by the time at home. For this reason, and to remain compliant with validity constraints, the resulting change cannot go over 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 selection of a location 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.

Fig. 8 illustrates an example of modification applied by the *location* operator on the initial schedule.

Mode Similarly to the *location* operator, the *mode* operator ω_{mode} changes the mode m of the outbound trip of a randomly selected activity i at position v. 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 as compared to the available time budget is absorbed by the time at home. For this reason, and to remain compliant with validity constraints, the resulting change cannot go over the time budget by more than the minimum time at home (i.e. 2δ). The selection of a mode must therefore be done according to a distribution $P_m(\rho)$ which is conditional on the travel times ρ. We assume that this distribution is exogenous to the choice-set generation algorithm. As the last home activity is not linked to an outbound trip, it cannot be selected for a mode change.

Fig. 9 illustrates an example of modification applied by the *mode* operator on the initial schedule.

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 $\delta = 15$ min). This change does not affect the activity sequence, but allows to change 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.

Fig. 10 illustrates an example of modification applied by the *block* operator on the previously introduced 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 $n \in 2, \dots, N_{op}$, 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

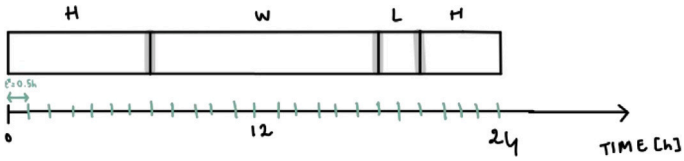


Fig. 10. Change applied by the *block* operator.

Table 4
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}
Swap	Activity participation, Time	Swaps the activities of two adjacent blocks	P_{swap}
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}
Block	–	Modifies time discretisation of the schedule	P_{block}
Meta-operator	All	Combines two or more operators	P_{meta}

them "on the fly"' during the random walk 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 4. As previously mentioned, this list is not exhaustive: other operators can be created or combined to fit the requirements of the intended applications, or simply to improve the performance of the MH algorithm.

More details on the operators and the derivations of the transition probabilities can be found in Pougala et al. (2021).

3.3.2 *Acceptance of candidate points*

The target distribution of the MH algorithm is the schedule utility function (Eq. (1)), conditional on the distribution of the error terms, and with unknown parameters to be estimated. The acceptance probability is defined by:

$$\alpha(X_{t-1}, X^*) = \min\left(\frac{p(X^*)q(X_{t-1}, X^*)}{p(X_{t-1})q(X^*, X_{t-1})}\right) \tag{12}$$

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:

$$p(X_t) = \tilde{U_S}(X_t) \tag{13}$$

where $\tilde{U_S}$ is a schedule utility function with the same specification as the target (Eq. (1)) 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

$t \leftarrow 0$, initialise state with random schedule $X_t \leftarrow S_0$
Initialise utility function with random parameters $\tilde{U_S}$
for $t = 1, 2, \ldots$ **do**
  Choose operator ω with probability P_ω
  $X^*, q(X_t, X^*) \leftarrow$ **ApplyChange**(ω, X_t)
  function ApplyChange(ω, state X)
    return new state X', transition probability q(X, X')
  Compute target weight $p(X^*) = U_S(\tilde{X}^*)$
  Compute acceptance probability $\alpha(X_t, X^*) = \min\left(\frac{p(X^*)q(X_t|X^*)}{p(X_t)q(X^*|X_t)}\right)$
  With probability $\alpha(X_t, X^*)$, $X_{t+1} \leftarrow X^*$, else $X_{t+1} \leftarrow X_t$

Following Ben-Akiva and Lerman (1985), we define for each individual n the alternative specific corrective term for a choice set C_n of size $J + 1$ with $\tilde{J}$ unique alternatives (Eq. (14)). Each alternative j is sampled from the target distribution of the

Metropolis–Hastings algorithm with probability q_{jn}, such that $q_{jn} = 0$ if $j \notin C_n$.

$$q(C_n|i_n) = \frac{1}{q_{in}} \prod_{j \in C_n} \left(\sum_{j \in C_n} q_{jn} \right)^{J+1-\bar{J}} \tag{14}$$

4 Empirical investigation

The objective of the empirical investigation is to apply the methodology on a real-life case study to illustrate the parameter estimation procedure. We use the Mobility and Transport Microcensus (MTMC), a Swiss nationwide survey gathering insights on the mobility behaviours of local residents (BfS and ARE, 2017). Respondents provide their socio-economic characteristics (e.g. age, gender, income) and those of the other members of their household. 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. For illustration purposes, we focus on the sample of full-time students residing in Lausanne (236 individuals).

We start by generating the choice sets of daily schedules for each individual in the sample. Each choice set is composed of 10 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 (Eq. (14)) to be added to the utility function.

4.1 Choice sets

For each person in the train dataset, we generate a choice set of 10 alternatives (including the observed schedules) randomly (Section 4.1.1), using the clustering method developed by Allahviranloo et al. (2014), (Section 4.1.2), and following the methodology presented in Section 3.3.

4.1.1 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 with the travel time between both location,
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 time remaining.

Assuming that every alternative generated this way has equal probability of being selected, the sampling correction term in Eq. (8) cancels out.

4.1.2 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 develop 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 individual n by drawing patterns from non-chosen patterns.[1]

With this method, the choice set is composed of real activity patterns from the dataset.

4.1.3 OASIS generation

The initial state X_0 of the random walk is the observed schedule. We implement 6 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 (Eq. (1)), 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 a number of iterations n_{iter}. We discard $n_{\text{warm-up}}$ of these iterations to sample from a stabilised distribution. To create the choice set, we draw 9 alternatives by only keeping 1 out of n_{skip} schedules. The experimental set-up is summarised in Table 5.

[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 equal probability of being chosen.

Table 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

Table 6
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)

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

4.2 Model specification

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

Following the definition of Pougala et al. (2022), travel is not considered as 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 Eq. (1),
- The scheduling preferences (desired start time and durations) are derived from the dataset. For each activity, we fit a distribution (either normal or log normal) across the student population. The calibrated parameters are reported in Table 6. For each person, we draw values of desired start times and durations from these distributions.
- For the S-shaped utility function Eq. (7), 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 7 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 Eq. (1).
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 Eq. (15):

$$\begin{aligned} U_S^{\text{act. sp.}} &= \gamma_a + \sum_a [\theta_a^{\text{early}} \max(0, x_a^* - x_a) + \theta_a^{\text{late}} \max(0, x_a - x_a^*) \\ &+ \theta_a^{\text{short}} \max(0, \tau_a^* - \tau_a) + \theta_a^{\text{long}} \max(0, \tau_a - \tau_a^*)] + \varepsilon_S \end{aligned} \tag{15}$$

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 Eq. (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 Eq. (16):

$$\begin{aligned} U_S^{\text{flex}} &= \gamma_a + \sum_f \lambda_f^a [\theta_f^{\text{early}} \max(0, x_a^* - x_a) + \theta_f^{\text{late}} \max(0, x_a - x_a^*) \\ &+ \theta_f^{\text{short}} \max(0, \tau_a^* - \tau_a) + \theta_f^{\text{long}} \max(0, \tau_a - \tau_a^*)] + \varepsilon_S \end{aligned} \tag{16}$$

with f a category of flexibility $f \in \{\text{Flexible, Not Flexible}\}$. 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 considered not flexible, while leisure, shopping and home are considered flexible.

Table 7
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		✓	✓		✓	✓

Table 8
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

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 Eq. (15).
6. **Model 3 - OASIS with MATSim scoring function:** An activity-specific S-shaped utility for duration, with a choice set generated using Algorithm 2. The utility function is given by Eq. (6).

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

- Benchmark 1: this model serves as benchmark for the improvement of estimating the parameters instead of fixed values.
- Benchmark 2 and 3: these models serve as benchmark 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 withe observed distribution from the dataset.

4.2.1 Parameters

Benchmark 1: Literature parameters The parameters from the literature were used in the first implementation of the framework, as described in Pougala et al. (2022). Values from the departure time choice literature (e.g. ratios from Small, 1982) were used to derive the parameters defined in Table 8. 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 behind this is that, all else being equal, there is no inherent preference to perform any activity (home included). Any effect of this nature is therefore fully included in the random term of the schedule ϵ_S.

Benchmark 2: Random choice set The home activity is used as a reference, such that $\gamma_{\text{home}} = 0$. The magnitudes and signs of the other constants are relative to the baseline behaviour which is staying at home. The estimated parameters are summarised in Table 9. 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 value of the parameter 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 in the observed schedule. Interestingly, for *work*, the duration parameters are not significant, and the start time deviations are penalised symmetrically.

Table 9
Estimation results for the Random choice set model on the student population.

	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[a]
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[a]
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[a]
7	$\theta^{\text{early}}_{\text{leisure}}$	0.0779	0.103	0.757	0.449[a]
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.[a]
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[a]
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[a]
20	$\theta^{\text{short}}_{\text{work}}$	0.968	0.857	1.13	0.258[a]

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

[a] Indicates parameters that are not statistically significant based on their p-value.

Benchmark 3: Empirical choice set The home activity is used as a reference, such that $\gamma_{\text{home}} = 0$. The magnitudes and signs of the other constants are relative to the baseline behaviour which is staying at home. The estimated parameters are summarised in Table 10.

Similarly to the random choice set, many parameters result 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 counter intuitive result, as it implies that individuals reward scheduling work for shorter durations than preferred. This indicates that either the preferred duration (mean of the corresponding cluster), or the choice set is not appropriate (e.g. every alternative except for the chosen one has a long work duration). In order to correct for this, an additional step after the choice set generation is required to ensure not only the mathematical feasibility of the sampled schedules but also their concordance with individual-specific constraints, as suggested by Xu et al. (2017).

Model 1: OASIS with flexibility-level parameters The home activity is used as a reference, such that $\gamma_{\text{home}} = 0$. The magnitudes and signs of the other constants are relative to the baseline behaviour which is staying at home. The estimated parameters are summarised in Table 11. 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, for non flexible activities, being early seems to be more negatively perceived than being late. The duration penalties are symmetrical.

Model 2: OASIS with activity-specific parameters We consider both activity-specific constants and schedule deviation penalties. For all parameters, the home activity is set as a reference, 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), which are summarised in Table 12.

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 have a more negative impact on the utility function; in particular, 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 constraining activity for students, in the sense that it is less likely to trigger trade-offs in the scheduling process than the other activities.

Table 10
Estimation results for the empirical choice set model on the student population.

	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[a]
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[a]
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[a]
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[a]
15	$\theta^{\text{short}}_{\text{shopping}}$	5.90	3.37	1.75	0.0798[a]
16	γ_{work}	1.90	1.60	1.19	0.235[a]
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[a]
20	$\theta^{\text{short}}_{\text{work}}$	3.69	0.784	4.71	2.49e−06

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

[a] Indicates parameters that are not statistically significant based on their p-value.

Table 11
Estimation results for OASIS flexibility-level model on student population.

	Parameter	Param. estimate	Rob. std err	Rob. t-stat	Rob. p-value
1	$\theta^{\text{early}}_{\text{F}}$	−0.175	0.12	−1.46	0.145[a]
2	$\theta^{\text{late}}_{\text{F}}$	−0.333	0.14	−2.38	0.0171
3	$\theta^{\text{long}}_{\text{F}}$	−0.105	0.0722	−1.45	0.146[a]
4	$\theta^{\text{short}}_{\text{F}}$	−0.114	0.194	−0.585	0.559[a]
5	$\theta^{\text{early}}_{\text{NF}}$	−1.14	0.367	−3.10	0.00191
6	$\theta^{\text{late}}_{\text{NF}}$	−0.829	0.229	−3.61	0.0003
7	$\theta^{\text{long}}_{\text{NF}}$	−1.20	0.393	−3.05	0.00231
8	$\theta^{\text{long}}_{\text{NF}}$	−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 [s]

[a] Indicates parameters that are not statistically significant based on their p-value.

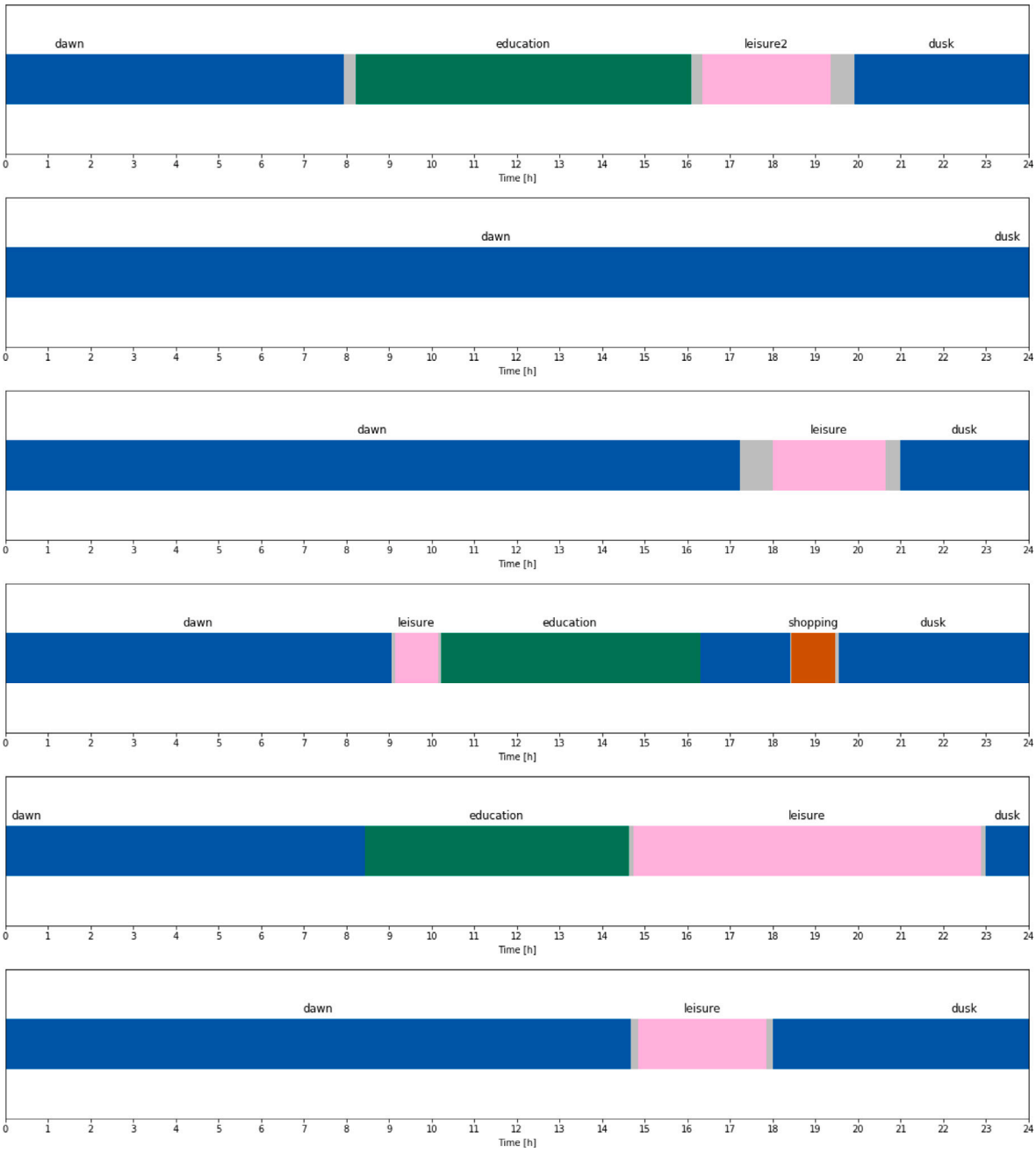


Fig. 11. Examples of simulated schedules (Model 2).

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.

Fig. 11 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 translates the fact that the duration at home is the remaining budget time after having performed out-of-home activities. The estimated parameters are summarised in Table 13.

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

Table 12
Estimation results for OASIS activity-specific model on student population.

	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[a]
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[a]
10	$\theta^{\text{short}}_{\text{leisure}}$	−0.101	0.149	−0.682	0.495[a]
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[a]
15	$\theta^{\text{short}}_{\text{shopping}}$	−1.81	1.73	−1.04	0.297[a]
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 [s]

[a] Indicates parameters that are not statistically significant based on their p-value.

For *education* and *work*, the α parameter (inflection point) is around 2 h, 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. 12(a)) 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 to 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.

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 stronger satiation effect for this activity as compared to *education*, which is expected

4.3 Simulation results

Using the parameters described in the previous section, we simulate schedules for the test dataset. The simulation procedure is described in detail in Pougala et al. (2022): 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 statistic between the original and simulated distributions for a quantitative evaluation of the goodness-of-fit of these distributions.

4.3.1 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 proportion of scheduled activity types. These statistics are derived exclusively for schedules which contain at least one activity out-of-home. It is worth noting that all models generate significantly more fully-at-home days (about 5 times more than what is observed in the MTMC data).

The results are summarised in Tables 14 and 15 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

Table 13
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 [s]

Table 14
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

Table 15
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

the average total time, but the proportions across activities are not as well captured. For example, the average durations spent in education are underestimated by about 1 h, while the time spent in leisure is overestimated (by 2 h in the case of the activity-specific model).

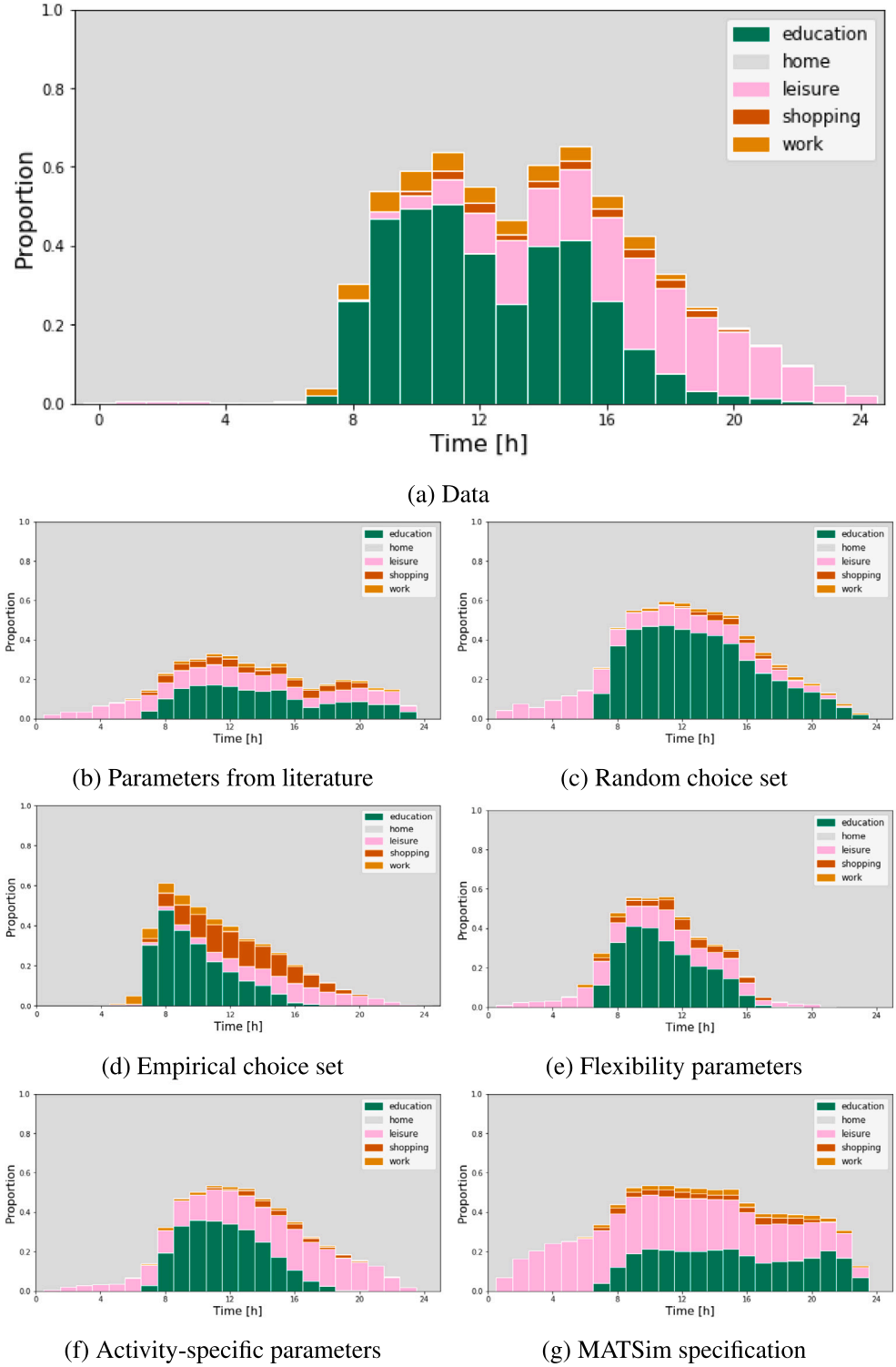
Regarding the proportion of scheduled activities (Table 15) Model 2 (OASIS with activity-specific parameters) significantly underestimates the frequency of each activity. This is likely due to the approximation of the desired start times, which are computed for only one instance of the activity, and do not properly account for bimodality or asymmetry in timing preferences (e.g. different desired start times for doing work in the morning or in the afternoon). This point in discussed further in Section 4.3.5. On the other hand, the MATSim specification seems to provide more realistic results.

4.3.2 Time of day participation

Fig. 12(a) shows the typical distribution of activities in the course of a day, for schedules including at least one activity out of home. The height of each bar represents the proportion of the sample that is participating in each activity at a given moment of time. 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 h (50%). The proportion decreases at lunch time (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*.

Figs. 12(b) to 12(g) show the distributions for out-of-home schedules[2] resulting from the simulator framework with the 5 mentioned configurations: with parameters from the literature (Fig. 12(b)), activity-specific parameters with random (Fig. 12(c)) and empirical choice set (Fig. 12(d)), OASIS generic (Fig. 12(e)), and activity-specific (Fig. 12(f)) model, and MATSim function

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



(a) Data

(b) Parameters from literature

(c) Random choice set

(d) Empirical choice set

(e) Flexibility parameters

(f) Activity-specific parameters

(g) MATSim specification

Fig. 12. Time of day activity frequency. The height of the bars is the proportion of people participating in each activity at a given moment.

(Fig. 12(g)). All configurations, with the exception of the MATSim specification, are able to capture the importance of *education* relative to the other activities in the schedule. However, as mentioned in the previous section, for all models, the majority of 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 11:00 peak. This discrepancy is likely due to the assumption of a 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 share of education. On the other hand, with the OASIS activity-specific parameters, the activity is overrepresented during the night (midnight to 7:00), as compared to the other simulated activities, and the leisure observations in the data for this time period. The rest of day, the profile is similar to the real one.

For the *shopping* activity, it 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 10).

For the MATSim specification, we notice that the time of day activity frequency is not properly 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 due to the fact that start time is not included in the specification. This result supports the assumption that the satiation effect for activity duration is different depending on the time of day.

4.3.3 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. 13), and respective Kolmogorov–Smirnov (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).

With the exception of *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 properly captured by either of the estimated models. This is likely due to the approximation of desired times to a 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.

4.3.4 Duration

Similarly, we compare the simulated durations per activity and model, by visualising the kernel density estimations of each model (Fig. 14) and computing their respective KS statistic.

For all activities, the model with parameters from the literature tends to generate short activities ($\tau_a \leq 2$ h) more frequently, and in smaller proportions activities with a duration of about 8 h (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, although there is a non negligible number of schedules with very long shopping activities (8 h), which is not close to what was observed nor particularly realistic. This limitation is also reflected by the high value of the KS statistic.

4.3.5 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 shown to provide results fitting the observed distribution better.

As shown by the comparison of benchmark 2 (model with random choice set) with models 1–3, the parameters obtained with the Metropolis–Hastings algorithm yield simulation results that are 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 is contains meaningful (or high probability) alternatives. In addition, the comparison of 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, a significant number of alternatives is required to achieve results that are consistent and comparable with the observed data, as illustrated by Fig. 15. For the Metropolis–Hastings choice set, a low number of alternatives already yields 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, but 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 have a significant impact on 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

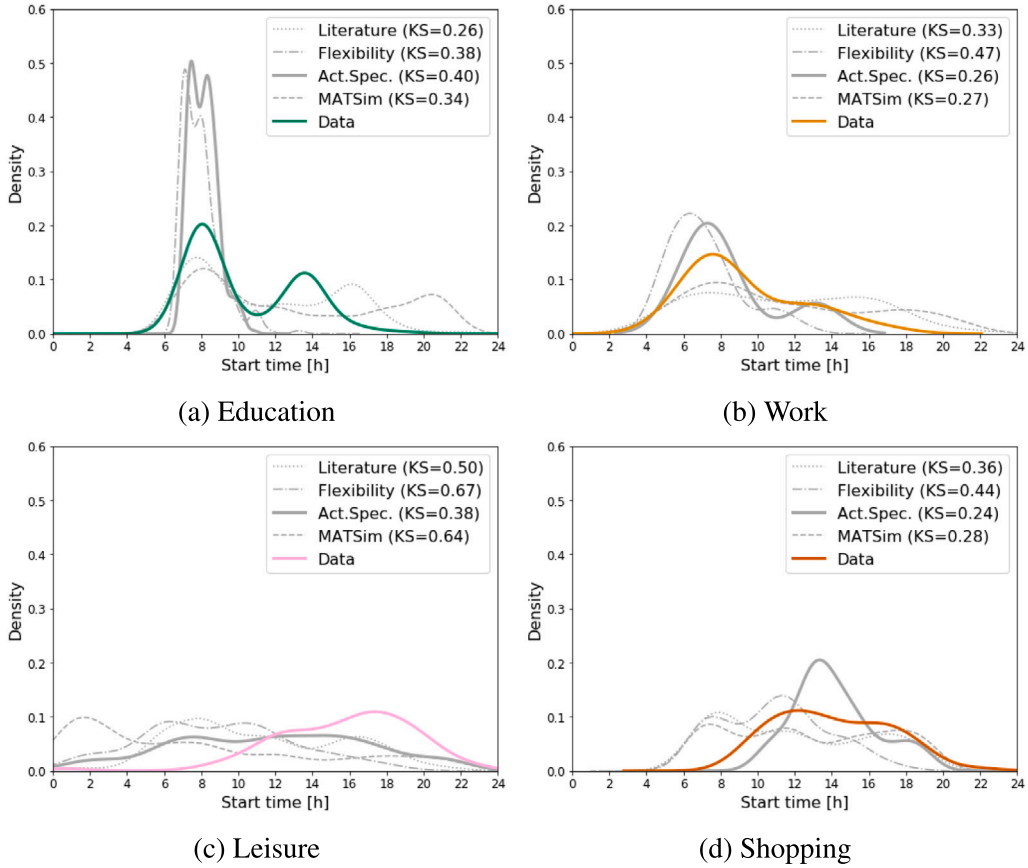


Fig. 13. Simulated start times, per model and activity.

and reflective of the observations. This change requires to reconsider 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 actually 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 who clearly impact the scheduling decisions (and specifically, the decision to travel out of home). More complex specifications must be investigated, starting with mixed logit models which relax the IIA assumption.

5 Conclusion and future work

We have presented a procedure to estimate the parameters of the OASIS framework, which includes the optimisation-based simulator introduced in Pougala et al. (2022). The estimation process includes: (i) the generation of a choice set for parameter estimation, with a sufficiently high 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 on a simple case: a time-dependent and linear-in-parameters utility function, and a small dataset. The resulting parameters are statistically significant and behaviourally interpretable, even with a relatively small number of 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 a state-of-the-art utility specification, used within the MATSim microsimulator. The utility function has a more behavioural realistic assumption for the impact of duration on the schedule utility than the linear specification used so far in OASIS. Another advantage is that the S-shape of the function does not require the explicit definition of the desired duration. However, the impact of start time is clearly significant based on our analyses, and should therefore be included in the specification.

In this paper, we have focused on demonstrating the feasibility and added value of the methodology. This is a necessary foundation for the framework to be able to solve problems of higher complexity, including social interactions or multi-day behaviour.

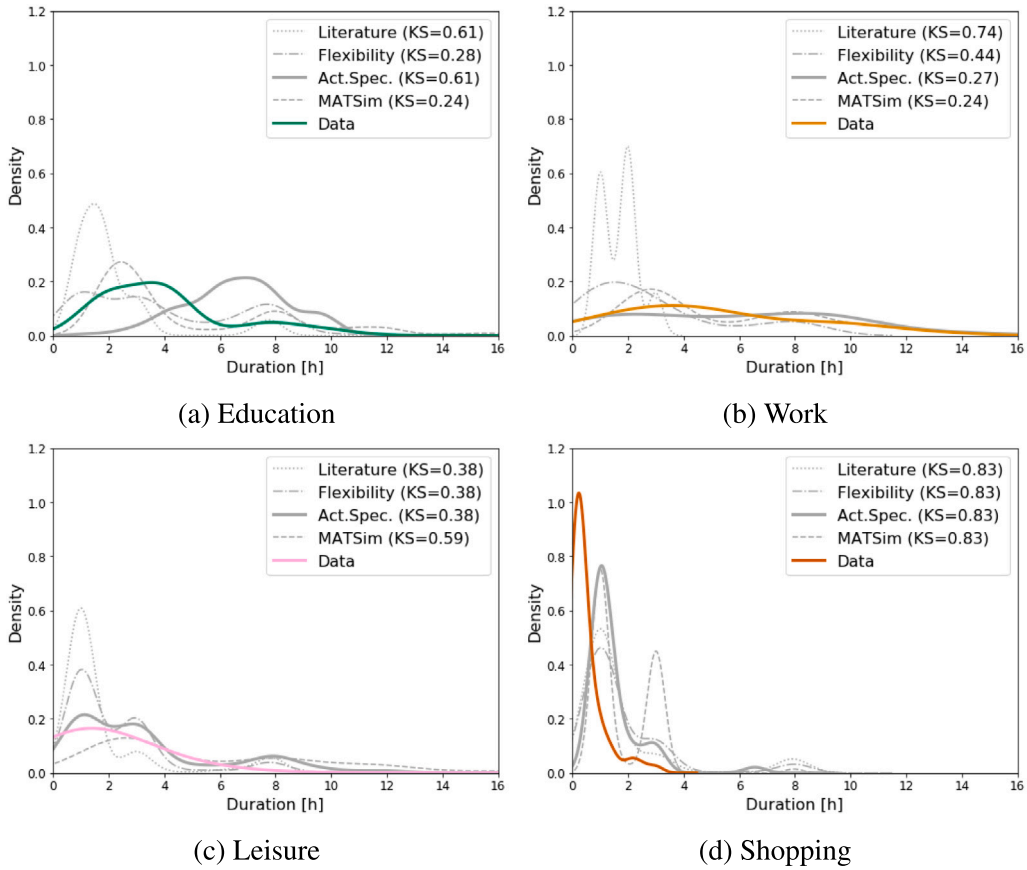


Fig. 14. Simulated durations, per model and activity.

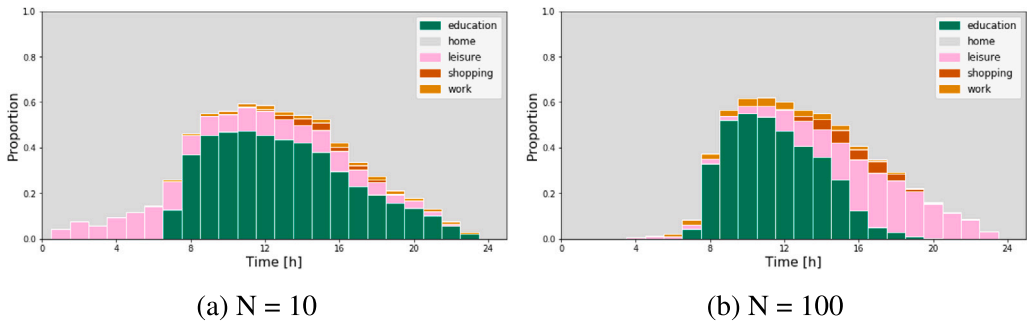


Fig. 15. Impact of choice set size on time of day distribution for random choice set model.

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 the estimation of 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 on how both dimensions interact and affect the schedule utilities.

We have performed the estimations on small samples, both in terms of observations and alternatives in the choice set. Our results show that we were able to estimate significant parameters with the Metropolis–Hastings algorithm, whereas the random choice set requires a greater number of alternatives in order to properly inform the estimation process. The next steps is to find the optimal number of alternatives N^* to sample with the OASIS methodology in order to obtain the best trade-off between estimation quality and computational efficiency.

Regarding validation, we will investigate in future work a multidimensional distance metric to compare observed and simulated schedules, similarly 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 to evaluate the estimation quality against known control variables.

Regardless, the results of this paper 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 important contribution of the OASIS framework is that the methodology remains the same for any change of context-specific constraints and features or change in utility specification. 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. 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 therefore develop flexible and tailored models for a variety of applications to integrate in the framework in a straightforward way. The parameters can then be estimated, even with limited data, with positive impact on the realism the resulting simulations.

Supplementary materials

The source code for OASIS is available at: https://github.com/transp-or/oasis.

CRediT authorship contribution statement

Janody Pougala: Conceptualization, Methodology, Software, Formal analysis, Investigation, Data curation, Writing – original draft, Visualization. **Tim Hillel:** Conceptualization, Methodology, Investigation, Writing – review & editing, Supervision, Project administration, Funding acquisition. **Michel Bierlaire:** Conceptualization, Methodology, Writing – review & editing, Supervision, Project administration.

Acknowledgments

This work is supported by an Interdisciplinary Cluster Grant from EPFL's School of Architecture, Civil and Environmental Engineering (ENAC). This work was further supported by research funding from the Accenture Turing Strategic Partnership on Digital Twins.

References

Allahviranloo, M., Axhausen, K., 2018. An optimization model to measure utility of joint and solo activities. Transp. Res. B.
Allahviranloo, M., Regue, R., Recker, W., 2014. Pattern clustering and activity inference. In: Transportation Research Board 93rd Annual Meeting.
Arentze, T., Ettema, D., Timmermans, H., 2011. Estimating a model of dynamic activity generation based on one-day observations: Method and results. Transp. Res. B 45 (2), 447–460.
Arentze, T., Timmermans, H., 2000. Albatross: A Learning Based Transportation Oriented Simulation System. Technische Universiteit Eindhoven / EIRASS.
Arentze, T.A., Timmermans, H.J., 2009. A need-based model of multi-day, multi-person activity generation. Transp. Res. B.
Axhausen, K.W., 2000. Activity-based modelling: Research directions and possibilities. Arbeitsberichte Verk.- Raumplan. 48.
Ben-Akiva, M.E., Lerman, S.R., 1985. Discrete Choice Analysis: Theory and Application to Travel Demand, Vol. 9. MIT Press, Cambridge, MA, USA.
BfS and ARE, 2017. Population's transport behaviour 2015. key results of the mobility and transport microcensus. Neuchâtel, Berne, p. 16.
Bierlaire, M., 2020. A Short Introduction to PandasBiogeme.
Bierlaire, M., Krueger, R., 2020. Sampling and Discrete Choice. Technical Report TRANSP-OR 201109, Transport and Mobility Laboratory, Ecole Polytechnique Fédérale de Lausanne, Lausanne, Switzerland.
Bowman, J.L., Ben-Akiva, M.E., 2001. Activity-based disaggregate travel demand model system with activity schedules. Transp. Res. A 35 (1), 1–28.
Castiglione, J., Bradley, M., Gliebe, J., 2014. Activity-Based Travel Demand Models: A Primer. Transportation Research Board, Washington, D.C..
Chapin, F.S., 1974. Human Activity Patterns in the City: Things People Do in Time and in Space, Vol. 13. Wiley-Interscience.
Charypar, D., Nagel, K., 2005. Generating complete all-day activity plans with genetic algorithms. Transportation 32 (4), 369–397.
Chen, S., Prakash, A.A., De Azevedo, C.L., Ben-Akiva, M., 2020. Formulation and solution approach for calibrating activity-based travel demand model-system via microsimulation. Transp. Res. C 119, 102650.
Chow, J.Y., Recker, W.W., 2012. Inverse optimization with endogenous arrival time constraints to calibrate the household activity pattern problem. Transp. Res. B 46 (3), 463–479.
Danalet, A., Bierlaire, M., 2015. Importance sampling for activity path choice. In: 15th Swiss Transport Research Conference.
Feil, M., 2010. Choosing the Daily Schedule: Expanding Activity-Based Travel Demand Modeling (Ph.D. thesis). ETH Zürich.
Flötteröd, G., Bierlaire, M., 2013. Metropolis–Hastings sampling of paths. Transp. Res. B 48, 53–66.
Frejinger, E., Bierlaire, M., Ben-Akiva, M., 2009. Sampling of alternatives for route choice modeling. Transp. Res. B 43 (10), 984–994.
Gelman, A., Carlin, J.B., Stern, H.S., Rubin, D.B., 1995. Bayesian Data Analysis. Chapman and Hall/CRC.
Guevara, C., Ben-Akiva, M., 2013. Sampling of alternatives in Logit Mixture models. Transp. Res. B 58, 185–198.
Hägerstraand, T., 1970. What about people in regional science? Pap. Reg. Sci..
Hastings, W.K., 1970. Monte Carlo sampling methods using Markov chains and their applications.
Joh, C.-H., Arentze, T., Hofman, F., Timmermans, H., 2002. Activity pattern similarity: a multidimensional sequence alignment method. Transp. Res. B 36 (5), 385–403.
Joh, C.H., Arentze, T.A., Timmermans, H.J., 2005. A utility-based analysis of activity time allocation decisions underlying segmented daily activity-travel patterns. Environ. Plan. A.

Nijland, L., Arentze, T., Timmermans, H., 2009. Estimating the parameters of a dynamic need-based activity generation model. In: 12th International Conference on Travel Behaviour Research (IATBR 2009), December 13-18, 2009, Jaipur, India.
Pagliara, F., Timmermans, H., 2009. Choice set generation in spatial contexts: a review. Transp. Lett. 1 (3), 181–196.
Pougala, J., Hillel, T., 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., Bierlaire, M., 2022. Capturing trade-offs between daily scheduling choices. J. Choice Model. 43, 100354.
Rasouli, S., Timmermans, H., 2014. Activity-based models of travel demand: promises, progress and prospects. Int. J. Urban Sci. 18 (1), 31–60.
Recker, W.W., 1995. The household activity pattern problem: general formulation and solution. Transp. Res. B 29 (1), 61–77.
Recker, W., Duan, J., Wang, H., 2008. Development of an estimation procedure for an activity-based travel demand model. Comput.-Aided Civ. Infrastruct. Eng. 23 (7), 483–501.
Regue, R., Allahviranloo, M., Recker, W., 2015. Understanding household priorities when scheduling activities. In: Proceedings of the 94th Annual Meeting of the Transportation Research Board in Washington DC, Vol. 3.
Small, K.A., 1982. The scheduling of consumer activities: work trips. Amer. Econ. Rev..
Train, K., 2009. Discrete Choice Methods with Simulation, second ed. Cambridge University Press, Cambridge.
Vovsha, P., Bradley, M., Bowman, J., 2005. Activity-based travel forecasting models in the United States: progress since 1995 and prospects for the future. In: EIRASS Conference on Progress in Activity-Based Analysis.
Xu, Z., Kang, J.E., Chen, R., 2017. A random utility based estimation framework for the household activity pattern problem. Transp. Res. Procedia 23, 809–826.