Adding a comprehensive Calibration Methodology to an Agent-Based Transportation Simulation

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Abstract

Simulation represents the operation of a process or system in reality over time. [9] Therefore the more realistic the imitation is, the more useful/sensible the simulation is. Simulation of transportation systems is an important area of discipline in Traffic Engineering and Transportation Planning today. MATSim [78] is a fully disaggregate (agent-based) transportation simulation that can be used to simulate large-scale scenarios in a relatively short time. This dissertation describes some different ways to make MATSim more realistic or MATSim simulation results more sensible.

At first, measures were taken to improve this microscopic model of traffic in the Zurich region in Switzerland on the supply and demand side. Improvements to the network (supply side) were realized by using data from the open source project “OpenStreetMap”. Improvements to the demand (demand side) were completed by adding missing demand e.g. through traffic. Other improvements were achieved by adding choice dimensions: besides the usual route choice, the simulated travelers could adjust their activity timing and their mode choice, which improved the results, in spite of the already relatively good initial data availability for the Zurich region. It is concluded that public data sources will eventually remove some of the data problems for large scale systems, and that the additional adaptive capability of MATSim may help to make it more realistic.

Further, the travel behavior in simulation was calibrated from aggregate measurements of traffic flows in the real case of the metropolitan area of Zurich, for which a novel calibration technique that adjusts all choice dimensions\(^1\) at once from traffic counts was applied. Meanwhile cross-validation results were obtained and competitive with any state-of-the-art four-step model. That means, a more realistic (on the aggregate traffic flow level) travel behavior can be simulated by MATSim.

The usefulness of the above mentioned results for further demand analysis purposes was also elaborates. However the results are useful only for short-term prediction, because this approach encounters problems when anything in the system that is presumably related to the structural changes of traffic volumes on some roads. Thereby, a calibration of “higher level” behavioral parameter would be useful.

At last, the aforementioned calibration system has been extended to the refinement of behavioral parameter using observations of time-dependent network flows.

\(^1\) all-day travel behavior including route choice, departure time choice, and mode choice.
to the greatest possible extent and pursues an analytical approach instead. In a nut-shell, the resulting findings are as follows:

1. It is possible to calibrate behavioral model parameters and their covariance matrices using network flows in a computationally very efficient manner, however

2. the approach needs further refinement to deliver reliable estimates. The various sources of imprecision in the current approach are therefore analyzed and possibilities to overcome them are discussed.

In conclusion, some progress has been made in refinement of the behavioral choice parameter i.e. allowing making more realistic decisions of agents (choice model) in MATSim.
Zusammenfassung


Ferner wurde das Verkehrsverhalten in der Simulation aufgrund aggregierter Messungen der Verkehrsflüsse in der realen Fall des Metropolitanraum Zürichs kalibriert, wofür eine neuartige Kalibrierungstechnik angewendet wurde, die alle Wahl-Dimensionen auf einmal auf die Reproduktion der Verkehrszählungen orientiert verstellen kann. Inzwischen ergaben sich Resultate der Kreuzvalidierung und die sind konkurrenzfähig mit irgendeinem State-of-the-art Vier-Stufen-Modell. Das heißt, dass realistischeres (auf der aggregierten Ebene des Verkehrslusses) Verkehrsverhalten durch MATSim simuliert werden kann.

24-Stunden-Verkehrsverhalten inkl. Routenwahl, Abfahrtszeit-Wahl und Verkehrsmittelwahl.
Die Nützlichkeit der oben erhaltenen Resultate für den Zweck der weiteren Nachfrageanalyse wurde auch ausführlich erläutert. Aber die Resultate sind nur für kurzfristige Vorhersage nützlich, weil die Probleme mit diesem Ansatz entstehen, wenn sich etwas im System ändert, was vermutlich mit der strukturellen Änderung des Verkehrsaufkommens zusammenhängt. Daher würde eine Kalibrierung der Verhaltensparameter auf der “höheren” Ebene sinnvoll sein.

Endlich hat sich das oben genannte Kalibrierungssystem auf die Verfeinerung der Verhaltensparameter unter Verwendung der Beobachtungen der zeitabhängigen Verkehrsaufkommen erweitert. Methodisch verzichtet sie auf den Einsatz von Black-Box-Optimierung / Kalibrierung Techniken so weit wie möglich, und verfolgt einen analytischen Ansatz. Kurz gesagt, sind die daraus resultierenden Erkenntnisse, dass

1. sowohl es möglich ist, Parameter im Verhaltensmodell und deren Kovarianzmatrizen mit der Anwendung der Verkehrsflüsse im Netzwerk auf rechnerisch sehr effiziente Weise zu kalibrieren, als auch, dass

2. der Ansatz muss sich weiter verfeinern lassen, um verlässliche Schätzungen zu liefern. Die verschiedenen Ursachen von Ungenauigkeiten im aktuellen Ansatz wurden deshalb analysiert und ihrer Überwindungsmöglichkeiten wurden diskutiert.

Dies bedeutet, dass bemerkenswerter Fortschritt bei der Verfeinerung von Verhaltenswahlparametern geschafft wurde, d.h. eine realistischere Entscheidungstreffung der Agenten (Wahl-Modell) in der MATSim wird verwirklicht.

Agentenbasierte Transportsimulation, Zustandsschätzung, Kalibrierung des Verkehrsverhaltens, Parameterschätzung
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Chapter 1

Introduction

The emergence of the city marked the beginning of civilization. Along with the development of civilization, the trip mode of the human is changing and developing. Progress in means of travel and even transport system makes the people able to endure a longer commute, i.e. living farther from workplace, and consequently, the progress makes further expansion of city possible. City expansion and the increase in city residents challenge the entire transportation system to offer better service for citizens. It follows that city is inextricably related to traffic, in other words, the two always are in a co-evolution.

The process of urbanization is very fast. Already over 50% of the global population are urban dwellers, and forecasts now show that two-thirds of humanity will live in cities within two decades from now. This means it is our obligation to map out better plans for our cities, and to seriously consider climate change in cities.\(^1\)

The increasing city population inevitably puts pressure on existing city transport infrastructure, and is a challenge for traffic planning and management. Nowadays, because of the increase in city population, traffic congestion is growing in many regions of the world, which becomes an unavoidable and difficult challenge for effective traffic management, since it is also very difficult, to build new road infrastructure in most of those regions, where the urban area for building is nearly exhausted, i.e. the expansion of the city is approaching the limit. On the other hand, unlimited expansion of the city, at least that of infrastructure, will inevitably cause a rapid increase in the cost of governance.

At the same time, the role of transport in climate change cannot be ignored. Due

\(^1\)First Announcement: The Sixth Session of the World Urban Forum
to the fact that it consumes a high percentage of carbon-based fuels, it is increasingly becoming a prominent sector for CO2 emission reduction.[57]

Therefore, rational, efficient and environmentally friendly utilization of present infrastructure has been the main objective of traffic planning for a long time, in order to fulfill the rising demand for transportation. Thereby, the importance of traffic management and planning, e.g. traffic control has become increasingly prominent.

To achieve the above-mentioned purpose it can be taken to predict and control, this is to say, that to evaluate the current and/or short-term predicted traffic conditions, and then consider taking measures. This requires good basic data and very realistic models.

The quality of essential data has a direct effect on the evaluation of traffic state. Recent advances in the field of communication, sensing and computation was used to better collect real-time data of traffic, eventually to record some information of the traffic state, e.g. inductive loop detectors, video cameras, overhead TrafficEye, cell phone movement, Global Positioning System (GPS), toll collection devices, floating car data (FCD) and so on. Nevertheless, these types of traffic measurement data show less information about the traffic state, because even if the identical traffic measurement data were collected, there could be several different corresponding traffic states. Consequently, it is essential to use good state estimation methods to decipher the traffic state.

Recently, there has been a common approval about modeling urban transportation systems with microscopic computer simulation systems that represent individual traveler and their travel plans as software objects. That means they make it possible to represent traffic highly realistically, because they possess discretionarily fine-grained model structure, which is also an important advantage over the conventional computer-based traffic system simulations. On the other hand, the latter i.e. traditional macroscopic static assignment models traffic as static streams, this means that it does not have temporal dynamics, which impedes representation of detailed traffic state, e.g. modeling of queue spill-back, or tolls [8], [10]. Therefore, this thesis also uses an agent-Based DTA microsimulator (MATSim [78]^2), whose models are also stochastic.

The structural correctness of the transportation modeling with microscopic computer simulation systems is of utmost importance for representing traffic highly re-

---

^2see some detailed description in Chapter 2
alistically. Generally, the models cannot provide completely correct representation of reality. Even if they were really able to do it, they would generate a different dynamic trajectory of traffic state than reality because of that stochasticity. As a result, it is necessary to calibrate the modeling by e.g. comparing its output and the measures from the real world.

However, more modeling, data, and calibration are indispensable to the aforementioned advantages of microscopic computer simulation systems.

This thesis describes the implementation of a method (cadyts[38]) applied to calibrate the travel behavior of individual motorists and its choice parameter from measures of aggregate traffic flows obtained at a limited set of network locations. It provides a helpful basis for traffic state reproduction and finding meaningful parameter sets that shape travel behavior during the simulations. In other words, knowing how people would travel enables the traffic managers to forecast and possibly reduce congestion.

1.1 Definition of Problem Domain

In this section, the work scope of this dissertation is outlined and some terminology is introduced.

The notion of "calibration" in the title refers to the following issues:

- Improvement of network and demand for traffic simulations, i.e. reduction of uncertainty or errors in essential data as well as adding more choice dimensions for simulated agents.

- Adjustment of travel behavior or transport demand from measures, i.e. reduction of uncertainty of the outputs of traffic simulation;

- Estimation of parameters in a structurally predefined model based on real data, i.e. reduction of uncertainty of the inputs of traffic simulation.

1.1.1 Traffic Assignment

Traffic assignment models are central components of comprehensive transportation system models because their outputs describe the state of the system (or the mean
state and its variation). Assignment model outputs successively are inputs for design and/or evaluation of transportation projects. [27]

Traffic assignment consists in assigning trips between origins and destinations to links constituting connecting routes in transportation networks. [35] Traffic assignment models simulate the interaction between traffic demand and supply on a transportation network. These (demand-supply interaction) models allow the calculation of performance measures and user flows for each supply element (network link), resulting from origin-destination (O-D) demand flows, path choice behavior, and the mutual interactions between supply and demand, i.e. on the one hand, traffic demand flows themselves are usually influenced by path costs in choice dimensions (route, mode, destination, etc.); On the other hand, link and path performance measures and costs generally depend on flows as a result of congestion. Consequently, there is a circular dependency among demand, flows, and costs, which traffic assignment models represent. [27]

Traffic assignment models are usually classified into two categories: static and dynamic traffic assignments. [65]

**Static Traffic Assignment**

As the fourth and final step of the traditional urban transportation planning process, the static traffic assignment determines traffic (flows) loadings on arcs and paths of the road network in a steady state setting based on the assumption that traffic demand, link volumes, and link costs (e.g. travel time) are time-invariant during the period of analysis, and that travelers choose routes with minimum travel costs resulting in an (quasi-)equilibrium³. [112, 65, 56]

**Dynamic Traffic Assignment (DTA)**

Dynamic traffic assignment concerns traffic loading problems in a dynamic setting, i.e. it deals with time-varying flows based on the standard static assignment assump-

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³Not all static traffic assignment models result in equilibriums, e.g. all-or-nothing assignment never generates an equilibrium, an equilibrium can be resembled by using the incremental assignment with many increments. Capacity restraint assignment attempts to approximate an equilibrium solution by iterating between all-or-nothing traffic loadings and recalculating link travel times based on a congestion function that reflects link capacity, an optimum social equilibrium can be achieved by using system optimum assignment. [102, 110]
tions and nonstationary network conditions as well as drivers’ behavior. However, DTA models require path delay operators which express the delay on a given path caused by the traffic conditions confronted along the path considering the time of departure from the origin of the path. At present, MATSim used in this thesis is a DTA models which offers a universal solution for general networks. DTA models may be helpful to forecast the varying of congestion levels in time, which is essentially useful for traffic control and management in both the near-real time and deliberate planning contexts. [65, 56, 90] Such a formulation also exists: “dynamic user equilibrium”. As an extended first Wardrop’s principle of equilibrium, it may be defined as the state of equilibrium that no driver can reduce his generalized travel cost by shifting route or departure time, where generalized travel cost includes, schedule delay in addition in to costs generally considered. The stochastic version “Dynamic stochastic equilibrium” may be similarly defined in terms of perceived generalized travel cost. The existence of such equilibrium in complex networks has not been proven theoretically, and even if the existence of its uniqueness also remains open. [102, 110] Dynamic traffic assignment models are more data intensive and more complicated, while static traffic assignment models can be well solved by modern numerical schemes.

1.1.2 State estimation

In control theory, a state estimation is a system that models a real system so as to prepare to estimate its internal state given measurements of the input and output of the real system, and it is typically a mathematical model realized by means of computer. In most practical cases, the physical state of the system cannot be directly observed. Instead, the effects of the internal state are indirectly observed by analyzing measurements the system outputs. For an observable system, using the state estimation could fully reconstruct the system state from its output measurements. [107]

1.1.3 Parameter estimation

Parameter estimation consists in estimating the values of parameters based on measured/empirical data containing random constituents. In the estimation theory, it is assumed that the value of the relevant parameters describing an underlying physical
setting affects the distribution of the measured data. An estimator tries to decrypt the unknown parameters using the measurements. [62, 113, 104]

1.1.4 Optimization

Optimization includes finding “best available” values of some objective functions given a defined domain, and possibly selecting a best element (with regard to some criteria) from some set of available alternatives. [106, 109]

1.2 State of the Art

This subsection is a condensed version of the comprehensive literature review given in [42].

In the following literature, the calibration of both DTA simulators and disaggregate demand models has been mentioned a dozen times. However, we have not found any work that estimates individual-level travel behavior or its choice parameters within a DTA simulator from aggregate sensor data, and can be applied on practical level. All the approaches mentioned later on do not deal with this problem. [37, 42]

1.2.1 Origin-destination (OD) matrix estimation

OD matrix estimation is the most frequently used method for demand calibration from traffic counts. An OD matrix models the demand in a given time interval as flows from origin to destination in a traffic system. Several different methods were proposed to solve OD matrix estimation problems. [42]

A time-dependent OD matrix constitutes a mapping of origin, destination, and departure time on demand levels, this is to say it implements destination choice and departure time choice on an aggregate level. Route choice is indirectly realized through some modeling assumptions of the DTA system. Path flow estimators (PFEs) manage the obstacle. [42]

1.2.2 Path flow estimators (PFEs)

There have been several generations of PFEs [42]:

Assignment mapping of demand on link flows

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<td>Entropy maximization and information minimization [114]</td>
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<td>Bayesian estimation [73]</td>
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<td>Generalized least squares [11, 19, 25]</td>
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<td>Maximum likelihood estimation [108]</td>
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Static linear assignment

Static Nonlinear assignment mappings

Incorporated by a bilevel-approach that iterates between the nonlinear assignment and a linearized estimation problem [74, 121, 122] until a fixed point of this mutual mapping is reached [21, 29].

Quasi dynamic assignment (e.g. OD matrices in subsequent time slices)

Combined estimation [28]

Table 1.1: Methods to solve OD matrix estimation problems.

- seminal version - a macroscopic one-step network observer that estimates static path flows from link volume measurements based on a multinomial logit SUE (stochastic user equilibrium) modeling assumption in a congested network ([13, 14]). The estimation problem is transformed into one of smooth optimization solved iteratively.

- enhanced version - by multiple user classes and a simple analytical queuing model to represent traffic flow dynamics ([54, 12])

- nonstochastic user equilibrium version - [103, 55]

- further advanced version - [82, 83]

PFEs also serve as OD matrix estimators since an OD flow is the sum of the path flows between its OD pair.

The underlying modeling assumptions of all PFEs and OD matrix estimators determine their restriction [42]:

- PFEs only consider static demand per time slice and rely on particular assumptions about route choice behavior.
- Time-dependent OD matrix estimators represent demand correlations across subsequent time slices in a simplified and aggregate way, e.g., by auto-regressive processes or polynomial trends ([3, 123]).

These approaches neglect many aspects of real travel behavior resulting from highly individual activity patterns and likewise complex constraints ([16, 66, 67, 116]). That means, it is still impossible to handle those aspects by applying a PFE or an OD matrix estimator to a fully microscopic DTA simulator, while microscopic modeling approach makes progress in this context. [42]

### 1.2.3 Estimation of individual behavior

The Calibration of a mobility simulation from aggregate sensor data has been widely advanced, e.g. [33, 34, 36, 64, 69, 88, 89]. However, these approaches do not realize a calibration of the behavioral simulation component [42].

Random utility models (RUMs) capture travel behavior at the individual level, and there have been some sophisticated calibration procedures for this class of models [15, 20, 111]. However, these procedures require a mathematical link between observations and model parameters. In this case, this link is realized through a DTA microsimulator. We do not know any work that calibrates a RUM in such context. [42]

Moreover, no systematic research about behavioral state estimation for multi-agent traffic simulation has been found.

### 1.2.4 Behavior parameter estimation

The increased availability of detailed network measure data actuated recent efforts to calibrate behavioral model parameters (and also network supply parameters) jointly with the OD flows representing travel demand levels [1, 5, 115]. However, these approaches can be referred to black box optimization that, by design, exploits

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4Here, the travel behavior results from the demand for mobility across a network. Various aspects (e.g. route, departure time, mode choice) can be modeled as long as a representation for all the travelers itself is found [50, 79]

5The last footnote

6The Author has also tried some direct-search methods e.g. Nelder-Mead method (downhill simplex method) to solve this problem, but they generally take too long to obtain some representable results, i.e. man always has to start the total tests repeatedly with new parameters calculated by e.g.
problem structure at most in terms of a numerical linearization. [45]

1.3 Thesis Contribution and Outline

1.3.1 Conceptual Outline

In this section, the resulting architecture of the estimation/calibration is outlined.

This thesis focuses on travel behavior estimation and refinement of its choice parameters that follow a simple technical logic in spite of complicated mathematical derivation, such that the employed agent-based transport simulation (MATSim) structure is unchanged during the estimation. Cadyts, which estimates disaggregate demand models of DTA simulators from traffic counts and vehicle re-identification data [40], is embedded in the most primary component elements of MATSim (Fig. 1.1, 1.2, 1.3), and compares the simulated traffic flows of MATSim simulation with stationary count data in reality. This comparison makes the agents in simulation change their "plans" by changing their evaluation of each plan in their memories (choice set) or changing the way they evaluate plans (parameters in utility function), so that the resulting traveling behavior of the agents in simulation is closer to reality. What is more,

- for behavioral calibration: the utility of plans that improve the measurement reproduction is increased; the utility of plans that impair the measurement reproduction is decreased;

- for calibration of behavioral choice model parameters: the parameters that can better reproduce the measurement are pursued.

1.3.2 Methodological Contribution

Current and/or predicted traffic state is indispensable to almost all available traffic planning and management tools, new methods for state estimation of coarse grained systems could be helpful in this field. This thesis contributes to 2 fields:

- This thesis implements a novel approach to the fully disaggregate estimation of motorist behavior with a multi-agent transport simulation. The basis of

Nelder-Mead method.
Figure 1.1: Core structure of MATSim simulation. Replanning: in each iteration each agents receives a new plan; Scoring: for each plan, a score can be calculated that reflects how well the plan performed during the simulation; Execution (network loading): the plans of all agents are simultaneously executed in a simulation of the physical system.

Figure 1.2: Travel behavior estimation with cadyts, (a) simulated traffic volumes, (b) utility modification for each Plan
this approach is a combination of prior knowledge about the driver behavior with available measurements into posterior estimates of the behavior, so that arbitrary behavioral aspects ranging from single route choice to plan selection for a whole day can be estimated in a fully disaggregate manner, agent by agent.

- An approach for behavioral choice parameter estimation is carried out here as well, it is composed of an analytical approximation of the measurement equation that connects time-dependent network flows and behavioral model parameters and a nonlinear least squares estimator. The contribution of this approach is the following:

1. it demonstrates it is possible to computationally efficiently calibrate behavioral model parameters and their covariance matrices using network flows, but also that

2. the approach needs further refinement to deliver reliable estimates.

1.3.3 Structure of Thesis

The remaining part of this dissertation is organized as follows: Chapter 2 introduces MATSim (MultiAgent Transport Simulation), an open-source, agent-based simulation framework. The design of the framework is presented in detail, as it builds
the technical base for the integration of cadyts in MATSim. Chapter 3 generates a base case for microscopic, behavior-based (or agent-based) transport modeling as a precondition of an effectual calibration for transportation simulation. In this base case, the improvement of network for MATSim simulation and adding some choice dimensions are demonstrated. Chapter 4 focuses on the travel behavior estimation problem. The next chapter (Chapter 5) describes a way to estimate the travel behavioral parameter, which adopts a gradient method for this numerical optimization problem. Chapter 6 presents a naive approach of travel behavioral parameter estimation that is also based on the achievement presented in Chapter 4. The last chapter (Chapter 7) concludes the thesis, giving suggestions as to possible further research and summarizing the key findings of this work.
Chapter 2

Introduction of MATSim

Some of the following sections are excerpts from some papers [32, 43, 45] of the author in the past few years, and modified to integrate them into this dissertation.

The MATSim (“Multi-agent transport simulation toolkit” [93]) transport microsimulation is used for the purposes of this study. The MATSim web site provides a wealth of supplementary material that goes beyond the necessarily brief introduction given here.

Our simulation is constructed around the notion of agents that make independent decisions about their actions. Each traveler of the real system is modeled as an individual agent in our simulation. The overall approach consists of two important pieces mutually coupled:

- On the demand side, each agent independently generates a so-called plan, which encodes its intentions during a certain time period, typically a day. The plan is an output of an activity-based model that comprises but is not constrained to route choice, and its generation depends on the network conditions expected by the agent.

- On the supply side, all agents’ plans are simultaneously executed in the simulation of the physical system. This is also called the traffic flow simulation or mobility simulation. The outcome of the traffic flow simulation (e.g. congestion) depends on the planning decisions made by the decision-making modules\(^1\). However, those modules can base their decisions on the output of the traffic flow simulation (e.g. knowledge of congestion) using feedback from

\(^1\)see sec. 2.1.
the multi-agent simulation structure [61, 22].

The mutual coupling of demand and supply is iteratively resolved, which can be seen as a mechanism that allows agents to learn.

In our implementation, the system iterates between plans generation and traffic flow simulation, i.e. this sets up an iteration\(^2\) cycle which runs the traffic flow simulation with specific plans for the agents, then uses the planning modules to update the plans (replanning). These changed plans are again fed into the traffic flow simulation, etc. until consistency between modules is reached. These “equilibrated” or “relaxed” conditions constitute the solution of the DTA model system.

The feedback cycle is controlled by the agent database, which also keeps track of multiple plans generated by each agent, and scores the performance of each plan, allowing agents to reuse those plans at will. The repetition of the iteration cycle coupled with the agent database enables the agents to learn how to improve their plans over many iterations. Agents normally choose the plan with the highest score, sometimes re-evaluate plans with bad scores, and sometimes obtain new plans by modifying copies of existing plans [80].

This circle continues until the system has reached a relaxed state. At this point, there is no quantitative measure of when the system is “relaxed”; we just allow the cycle to continue until the outcome seems stable.

The simulation approach is the same as in many of our previous papers (e.g. [93]). The following sections constitute a shortened and simplified description of key elements.

### 2.1 Choice set generation

A plan contains the itinerary of activities the agent wants to perform during the day, plus the intervening trip legs the agent must take to travel between activities. An agent’s plan details the order, type, location, duration and other time constraints of each activity, and the mode, route and expected departure and travel times of each leg.

A specification of the plan choice set for every agent before the iterations is computationally extremely cumbersome because of the sheer number of possible

\(^2\)an iteration can be intuitively thought of as a “simulated day”
alternatives [16]. Such an approach also is conceptually questionable because the accessibility measures that affect the inclusion of a plan in the choice set are an outcome of the iterations, and hence they are a priori unknown. Therefore, the choice set is continuously updated during the iterations, i.e. MATSim allows this choice set to evolve in the course of a simulation. Speaking in the technical terms of MATSim, a plan can be modified by various modules. This thesis will make use of the following modules, e.g.:

- **Activity Times Generator:** This module is called to change the timing of an agent’s plan. At this point, a simple approach is used which applies a random “mutation” to the duration attributes of the agent’s activities. Although this approach is not very sophisticated, it is sufficient in order to obtain useful results. This is consistent with our overall assumption that, to a certain extent, simple modules can be used in conjunction with a large number of learning iterations (e.g. [81]). In every iteration, there is a certain e.g. 10% chance that this module is used to generate a new plan in chapter 3 and 4.

- **Router:** The router is implemented as a time-dependent Dijkstra algorithm that calculates link travel times from the output of the traffic flow simulation. The link travel times are encoded in 15 minute time bins, so they can be used as the weights of the links in the network graph. In every iteration, there is a certain e.g. 10% chance that this module is used to generate a new plan.

- **Mode choice** is simulated by giving every agent both at least one “car” and at least one “non-car” plan in its choice set.

These modules are used in the following way. In every iteration, each agent selects one plan or generates a new plan for execution. With a 10% probability, one plan is uniformly selected and a copy of it is created, the activity time generator is applied to this copy, and then the modified copy is executed. Likewise, there is a 10% probability to uniformly select a plan and to create a copy of it, the router is applied to the copy before the copy is executed. With the remaining 80% probability, no plan-changing module is used, and an existing plan is selected for execution according to the choice model described in the next section. The concrete 10% probability values ensure a stable yet relatively fast convergence of the iterated simulation; they are chosen based on experience. At most one module is applied at once to a plan.
The choice set generation can be turned off after a pre-specified number of iterations such that the agents select from a stable choice set using the utility-based choice model described next. This choice model is also applied during the choice set generation in order to drive the system towards a plausible state from the very beginning.

2.2 Choice

In order to compare plans, it is necessary to assign a quantitative score to the performance of each plan. In principle, arbitrary scoring schemes can be used. In this work, a simple utility-based approach is used. The elements of our approach are as follows:

- The total score of a plan is computed as the sum of individual contributions consisting of positive contributions for performing an activity and negative contributions for travelling.

- A logarithmic form is used for the positive utility earned by performing an activity $i$, which has the following form:

$$U_{\text{perf},i}(t_{\text{perf},i}) = \beta_{\text{perf}} \cdot t_{\ast,i} \cdot \ln\left(\frac{t_{\text{perf},i}}{t_{0,i}}\right)$$  \hspace{1cm} (2.1)

where $t_{\text{perf},i}$ is the actual performed duration of the activity $i$, $t_{\ast,i}$ is the "typical" duration of activity $i$, and $\beta_{\text{perf}}$ is the marginal utility of an activity at its typical duration. These durations are sampled from empirical distributions that are extracted from census data (e.g. [101]). $\beta_{\text{perf}}$ is the same for all activities, since in equilibrium all activities at their typical duration need to have the same marginal utility. $t_{0,i}$ is set to $t_{\ast,i}e^{-\frac{100}{t_{\ast,i}}}$. This has the (intended) consequence that all activities have the same utility contribution at their typical duration [78]. $t_{0,i}$ shifts the curve vertically and has, as long as activities cannot be dropped or inserted, little effect.\footnote{There is the well-intentioned rule implemented in MATSim that activities whose score according to the above rule becomes negative should receive score zero, since an agent could always do “nothing” instead. Unfortunately, this means that $t_{0,i}$ now has an effect, since it determines at which duration this rule kicks in. With the simulations reported here, the time pressure should never be so large that this effect is triggered.} Concrete values for the parame-
ters are given later in the description of the some case studies in some related sections.

- The (dis)utility of traveling along a leg \( l \) is assumed as linear in the travel time with different valuations of the time for different transport modes. Concrete parameter values are given later on.

The total utility of a plan \( i \) can thus be written as

\[
V(i) = \sum_{a \in i} V_{perf}(a) + \sum_{l \in i} V_{travel}(l).
\]  

(2.2)

It is important to note that the score thus takes into account the complete daily plan. More details can be found in [31, 93].

The plan choice is modeled with a multinomial logit model (which clearly calls for enhancements in the future) [15]. However, as stated before, it may happen that an agent receives a newly generated plan from one of the aforementioned plan generation modules, which then is chosen for execution without further evaluation. This is necessary because the utility of a plan is determined from its execution, and hence it is not available for newly generated plans.

Summarizing, the probability \( P_n(i) \) that agent \( n \) chooses plan \( i \) is

\[
P_n(i) \begin{cases} 
1 & \text{if } i \text{ is newly generated} \\ 
\sim \exp(V(i)) & \text{otherwise},
\end{cases}
\]  

(2.3)

where the normalization of the logit model is omitted for notational simplicity.

### 2.3 Traffic flow simulation

The traffic flow simulation executes all agents’ plans simultaneously on the network, and provides output describing what happened to each individual agent during the execution of its plan. The actually implemented time structure of a travel plan depends on the congestion in the network, which may induce delays. The congestion is in turn a consequence of the travel plans selected by the entire agent population. The traffic flow simulation is implemented as a queue simulation, which means that each street (link) is represented as a FIFO (first-in first-out) queue with 3 restrictions [51, 30]:
• Each agent has to remain for a certain time on the link, corresponding to the free speed travel time.

• The outflow rate of a link is constrained by its flow capacity.

• A link storage capacity is defined which limits the number of agents on the link. If it is filled up, no more agents can enter this link, and spillback may occur due to limited network capacities.

2.4 Controller

MATSim is composed of many different building blocks (Fig. 2.1) pieced together by the so-called “Controller”\(^4\), which ensures the handling of the correct data at the right time by the right module and the running of complete simulations with multiple iterations, and can be viewed as the center of MATSim.\(^94\)

In the Controller, there are 8 different extension points\(^5\), where additional functionalities could be modularly added (Fig. 2.1) at the right timings and places. This feature makes it easier to embed cadys in MATSim (Fig. 1.2 and 1.3) to calibrate travel behavior or its choice parameters. These extension points are:

• “Startup: Describes that the simulation starts up and that extensions should load any additional data they may require to function properly.

• Iteration Starts: Informs extensions that a new iteration starts. This may be used to reset internal data structures.

• Before Plans Execution: There are some modules that analyze the exact plans that are fed into the traffic flow simulation.

• After Plans Execution: Some modules may pre-process the outcome of the plans execution, resulting in additional outcome that is relevant for the scoring.

\(^4\)“Likely based on some misunderstanding, MATSim uses the wrong spelling ‘Controller’ instead of the correct ‘Controller’ since its beginning. In order to be consistent with the software, I use the wrong spelling knowingly in this thesis.”

\(^5\)The extension points are implemented as EventListener (an interface in Java - http://docs.oracle.com/javase/6/docs/api/java/util/EventListener.html)
• Scoring: Tells modules that the plans execution is over and no more events will be issued, so that the scoring can take place.

• Iteration Ends: Makes it possible for modules to write out analysis data that was collected during the iteration.

• Replanning: Informs the modules that now is the time to do replanning.

• Shutdown: Tells event listeners that the simulation is about to end, enabling extensions to write out final data or analysis results.” [94]

In the interim, Scoring and Replanning also both are realized by this "extension point" mechanism.

Figure 2.1: Main structure of the MATSim Controller [97]
Chapter 3

Manual Calibration of Simulation Scenario

The work reported in this chapter was presented as “Improving a large-scale agent-based simulation scenario” ([32]) as a working paper of Berlin Institute of Technology Transport Systems Planning and Transport Telematic. Most of the following sections are excerpts from the presented paper modified to integrate them into this dissertation, most of the experiments in the sections are also newly executed, in order to adapt them to the different setting of experiments in the next chapter (Chapter 4).

This chapter presents a case study performed with MATSim. This case study reports some of the measures that were taken to improve a fully microscopic model of traffic in the Zurich region in Switzerland. Improvements to the network were possible when considering data from the open source project “OpenStreetMap”. Other improvements were achieved by adding choice dimensions: besides the usual route choice, the simulated travelers can adjust their activity timing, and their mode choice. Addition of both choice dimensions improved the results, in spite of the already relatively good initial data availability for the Zurich region. We conclude that public data sources will eventually remove some of the data problems for large scale systems, and that the additional adaptive capability of microscopic, behavior-based models may help to make the models more realistic.
3.1 Introduction

Many cities or regions invest considerable resources into their transport modeling. There are many examples; some of the ones with publications in the academic world are San Francisco [60], Portland [23], New York [117], Chicago [24], Eastern Denmark [84], or Switzerland [71]. In all these cases, it seems that either considerable resources are necessary, or the model building process proceeds over many years, with the corresponding experience accumulating incrementally.

The situation is no different for microscopic, behavior-based (or agent-based) transport models: Similar amounts of work are necessary to obtain access to data sources, to merge these data sources, and to gain experience with the strengths and weaknesses of the data sets, in particular vis-a-vis the models. This paper reports the results of such an exercise undertaken for the metropolitan region of Zurich in Switzerland. While Refs. [6] and [75] describe the demand generation and report some initial results for the whole of Switzerland, this paper concentrates on the region of Zurich and on making the traffic flows more realistic.

Three different types of modifications will be considered:

- Adaptations of the network, where the open source project openstreetmap (www.openstreetmap.org) turned out to be very helpful;

- adaptations of the demand, where the inclusion of long-distance traffic turned out to be beneficial;

- and finally, and most importantly, integrating time adaptation and mode choice as additional adaptive choice dimensions. Thus, these are no longer fixated in the upstream demand generation, but are adapted in an iterative procedure in the same way routes are adapted in dynamic traffic assignment.

It is, in our view, a very positive effect that making additional choice dimensions adaptive makes the base case more realistic. Presumably, the adaptive agents find better ways to adjust to the particularities of the system than the more aggregated upstream methods. This was in spite of the comparatively good initial data availability for the Zurich region.

What is quite different between the approach described here and many other approaches including those mentioned earlier is that at this point the approach described here does not formally calibrate parameters (as could for example be done
with BIOGEME [18]. Instead, parameters are usually set to plausible values, and then emergent properties of the model (such as hourly traffic flows) are compared to real world data. This has to do with the fact that calibrating agent properties based on simulation-based emergent effects is not straightforward. Also, it is so far our experience that insight into the model behavior is also a successful strategy to build a more realistic model. Nevertheless, Refs. [37, 47] indicate that it is possible to develop concepts to calibrate agent-based travel behavior models. This will be the subject of future work.

This chapter is structured as follows. First, the simulation structure is explained. This is, except for the mode choice, similar to earlier expositions of the same material. Then, the scenario setup is reported, which contains a short summary of the demand generation process and lists the scenario-specific simulation parameters. Next, the validation methodology is presented, which essentially consists of time-dependent relative error when compared to real world counting stations. A longer section on “improvements” discusses the three elements mentioned above: network modifications, demand modifications, and additional choice dimensions. The paper is finished with a discussion and a conclusion.

### 3.2 Scenario Setup

The network initially used is a Swiss regional planning network [118] which includes the major European transit corridors and covers the area of Switzerland. It consists of 24180 nodes and 60492 links with attributes (flow capacity, free speed, number of lanes, . . . ) suitable for static traffic assignment, but not for our dynamic agent-based simulation.

An initial demand was prepared that consists of all travelers within Switzerland. The demand generation process is described in more details in Refs. [6, 75]. The following paragraphs give a short summary of the most important points for better understanding of the following improvements.

All travelers have complete daily activity patterns based on microcensus [101] information. Such activity patterns can include activities of type home, work, education, shopping, and leisure. The typical durations for those activities are derived from the microcensus data and are specified individually for each member of the synthetic population. Based on further data, an initial mode choice was calculated
with the restriction, that each agent can only use one transport mode for a plan.

The initial demand used for the simulations (referred to as “demand version 1” in the following) is based on the aforementioned demand of whole Switzerland, but consists only of all agents driving a car who, as part of their routing, are at least once inside an imaginary boundary around Zurich during their day. The boundary is defined as a circle with a radius of 30 kilometers (≈ 18.6 miles) and with its center at “Bellevue”, a central place in the city of Zurich. In order to obtain a higher computational speed, a random 10% sample was chosen for simulation, which consists of 61480 agents. Network capacities are scaled accordingly, resulting in realistic congestion patterns despite of the reduced number of travelers.

The “default” strategy setup uses time adaptation and route adaptation. This means that in each iteration of the simulation, 10% of the agents adapt routes, while another 10% of the agents adapt activity times. The remaining 80% of the agents can select another plan among the plans in their plans collection. All modifications are reported with respect to this default strategy setup.

<table>
<thead>
<tr>
<th>Activity type</th>
<th>Opening time</th>
<th>Closing Time</th>
</tr>
</thead>
<tbody>
<tr>
<td>Home</td>
<td>00:00</td>
<td>24:00</td>
</tr>
<tr>
<td>Work</td>
<td>07:00</td>
<td>18:00</td>
</tr>
<tr>
<td>Education</td>
<td>07:00</td>
<td>18:00</td>
</tr>
<tr>
<td>Shop</td>
<td>08:00</td>
<td>20:00</td>
</tr>
<tr>
<td>Leisure</td>
<td>00:00</td>
<td>24:00</td>
</tr>
</tbody>
</table>

Table 3.1: Activity opening and closing times used in the scenario.

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\beta_{perf}$</td>
<td>6 Euro/h</td>
</tr>
<tr>
<td>$\beta_{car}$</td>
<td>-6 Euro/h</td>
</tr>
<tr>
<td>$\beta_{non-car}$</td>
<td>-3 Euro/h</td>
</tr>
<tr>
<td># (existing plans)</td>
<td>4</td>
</tr>
</tbody>
</table>

Table 3.2: Behavioral parameters used in the scenario.

Activity locations were given opening and closing times in order to keep the agents within some timely limit. The opening and closing times are classified by activity type, i.e. the opening and closing times are distinguished for home, work,
education, shop and leisure activities. There is not yet any distinction based on
the location of an activity. Table 3.1 summarizes the opening and closing times
available to perform activities. Table 3.2 shows the behavioral parameters used in
the scenario. The denotation of $\beta_{per}$ can be found in section 2.2. Here, $\beta_{car}$ is a
negative coefficient for the travel time of traveling along a leg $l$, if leg $l$ uses the car
mode; and $\beta_{non-car}$ is a negative coefficient for the time spent traveling with a
mode different from car.

All simulations described in this paper are run for 500 iterations to retrieve a
relaxed state\(^1\), in which the initial plans are adapted to the traffic conditions. If
not otherwise specified, time and route adaptation are enabled, each for 10% of the
agents in every iteration.

### 3.3 Validation methodology

Modifications to network and travel demand only make sense if they help to increase
the accuracy of the simulation results. This means that some kind of measurement
must exist to determine the quality of the simulation. For the Zurich region, hourly
data from 161 traffic counting stations is available. This data is used to compare the
traffic volumes from the simulation to real-world values. Different statistical values
can be calculated, like mean relative error. Fig. 3.1 shows two examples of standard
reports that MATSim can automatically generate.

The model improvements described in this paper are all done to minimize the
mean relative error (red curve in Fig. 3.1(b)). No formal decision was taken of how
to weigh the different hours; instead, the graphs are interpreted visually.

The mean relative error for every sensor and every hour is calculated as:

$$\frac{\text{Simulated traffic volume} - \text{Real traffic volume}}{\text{Real traffic volume}}$$

Averages for a given hour are obtained by averaging over all sensors. In the ex-
ample shown in Fig. 3.1(b), the simulation deviates strongly from the reality during
the night hours, i.e. from midnight until 06:00 am\(^2\). However, during daytime, i.e.

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\(^1\)In this state, the average utility of all the executed plans is held in a very stable level since
numerous iterations.

\(^2\)There could be many reasons for the lack of night traffic, e.g. the cross-night traffic is not
simulated.
Comparing traffic volumes from the simulated (Y-axis) to real-world values (X-axis) for one hour.

(b) Hourly mean relative error over time of day

Figure 3.1: Realism of the base case. 161 traffic counting stations provide real traffic counts for the Zurich area.
from 06:00 am until late evening, the hourly mean relative error is around 30%.

3.4 Improvements

Two possible improvements are better network data and better travel demand. Both parts are essential for a realistic scenario. Additionally, it turns out that adding choice dimensions improves the quality of the simulation as well.

3.4.1 Network Improvements

The link capacities in the original network (“network version 1”) are quite undifferentiated for most of the non-freeways (see Fig. 3.2(a)). The reason for this is most probably that the original network data is meant for Swiss-wide national analysis, and therefore a secondary network with a capacity that is approximately correct in the average is sufficient. Clearly, since we are interested in a better resolution at the urban scale, this is not sufficient.

To correct this problem, all links within a circle with radius 4 kilometers ($\approx 2.5$ miles) around the center of Zurich are modified as follows:

- links corresponding to primary roads in OpenStreetMap (see Fig. 3.2(c)) get a capacity of at least 2000 vehicles per hour. If the original capacity is higher than that, the capacity is not changed.

- links corresponding to secondary roads in OpenStreetMap keep their original capacity (usually between 1000 and 2000 veh/h).

- all other links get a capacity of at most 600 veh/h. If the original capacity is lower, it is not changed.

- a few single links are manually adjusted based on local knowledge.

Fig. 3.2(b) shows the overview of the capacity of the links in this updated network (“version 2”). Comparing the mean relative errors from simulations with the two networks and the default strategy setup, one can see that the simulation with the adjusted network (version 2) has clearly a smaller mean relative error after 6am than the initial network (version 1) has (see Fig. 3.3), with the mean relative error being now constantly below 50% during the daytime. Fig. 3.4(a) and Fig. 3.4(b) show the
Figure 3.2: Link capacities in the original and modified network
geographical places where the counting stations are located on the network. The symbols and colors visualize the direct comparison of simulation volumes to the real-world volumes for one specific hour. This allows relating under- or overestimated links to geographical characteristics. In Fig. 3.4(a) one can recognize that on most counting stations in the city center the traffic flows are overestimated by the simulation (symbolized with +), while outside the city center the traffic volumes on many links are underestimated (symbolized with -). Red symbols depict a strong deviation between simulated and real traffic volumes, while green symbols stand for no or only a small difference. Comparing the number of red symbols in both figures, one can see that their number is highly reduced in the network version 2, also proving the effectiveness of the network modifications. -All runs in this paper, with the exception of the run used for Fig. 3.2(a), are done with the improved network (“network version 2”).

As a side remark, runs with a network that is entirely based on physical characteristics\(^3\) plus time-of-day dependent green splits on intersections seems to perform even better (M. Balmer, personal communication).

\(^3\)e.g. link capacity calculation is based on the simple physical size i.e. the number of lanes and head time gap (e.g. 2 seconds) and does not depend on the green time of traffic light on intersections, and some other local knowledge.
Figure 3.4: Locations of counting stations and comparison quality for the hour from 8am to 9am. Red symbols show a strong deviation of simulation volumes to counts, green symbols a good correlation. (Background-map: google earth)
3.4.2 Demand Improvements

As described in the section “Scenario Setup” (Sec. 3.2), the original travel demand (“demand version 1”) consists of agents traveling within the boundaries of Switzerland. When comparing the traffic volumes from the simulation with real-world data, one can observe that counting stations with too low volumes in the simulations are located especially along freeways, but only rarely in the city center or on smaller roads.

Further analysis resulted in the knowledge that a not to be underrated part of traffic on the freeways comes from abroad. Because of the short distance to neighboring countries (e.g. the border to Germany is less than 25 kilometers / 15 miles north of Zurich) it is not uncommon for people to live abroad but work in the Zurich area, or live in Zurich with its high cultural offers and work abroad. Those people are not part of the initial demand, as at least one of their activity locations lies outside Switzerland.

In addition, some of the intereuropean routes connecting Germany with Italy also pass through the greater area of Zurich. This leads to additional traffic not yet accommodated in the initial demand. Both cases could be solved by adding

![Error plots of the simulations with different travel demands](image)

Figure 3.5: Error plots of the simulations with different travel demands

“boarder-crossing traffic” (sometimes also referred as “through” traffic) [119]. Taking a 10% sample of all through traffic traveling with cars in the area of Zurich
added 5759 agents to the demand. Running the simulation with this extended de-
mand (“version 2”) on network version 2 resulted in a clear improvement of the
quality of the simulation, as Fig. 3.5 shows.

3.4.3 Improvements by adding choice dimensions

While network and demand are essential for realistic scenarios, the capabilities of
the simulation itself also have a big influence on the quality of the results. To
demonstrate that, the currently best case (network version 2, with modified capac-
ities according to OpenStreetMap, and demand version 2, which includes through
traffic) were run with different simulation features switched on or off:

- Route choice only, i.e. no mode choice, no time adaption. 10% of the agents
can adapt their route in every iteration.

- Route choice and departure time choice, i.e. no mode choice.

- Route choice, departure time choice and mode choice.

The first two cases, route-choice only and route- and time-choice, use the demand
version 2, consisting of private car traffic within Switzerland and through traffic, as
described in the section before. In these cases, the initial mode choice was used to
determine which agents where driving a car and which ones not, and this remains
fixed during the runs. In the third case where mode-choice is added, the initial mode
choice is ignored. Instead, all agents from within Switzerland (= “demand version
1”; thus mode-choice is not allowed for the agents added by the through traffic) are
given two plans, one where “car” is set as transport mode, and another one where
“non-car” is set as transport mode. In all other aspects, the two plans are identical
and identical to the plans in the original demand. This allows the agents to choose
between the two transport modes, effectively adding mode choice to the scenario.
Since now all agents are simulated and not only those with the initial mode choice
set to “car”, the number of simulated agents increases to 187484. Fig. 3.6 shows
the quality of the different setups after 500 iterations. The more choice dimensions
are available, the smaller is the mean relative error (red) for the time range from 8
am to 8 pm. For some other time segments, e.g. from 5 am to 6 am and from 8 pm
to 9 pm, the mean relative error deviates from this tendency. This depends on the
Figure 3.6: Error plots of the simulations with different replanning strategies

setting of activity opening and closing times (see Tab. 3.1); for a discussion of this see the “discussion” section.

It should be noted that the improvement from the red line to the orange line in Fig. 3.6 occurs in spite of the fact that the initial demand is rather good, since the available data is rather detailed. The simulation is still able to improve the quality by determining its own time and mode choices. This could be explained with the fuzziness created by aggregations and extrapolations to apply the initial mode choice, while in the simulation the particular characteristics of the daily plan and the particular traffic characteristics of the car mode are automatically included.4

It can be noted that in the case with route, time and mode choice, the mean relative error for the day hours is around 30%, sometimes a bit lower, sometimes a bit higher. While this may still be quite a big error in traditional, static traffic analysis applications, it is amongst the best results we know for dynamic traffic simulations, also because it is not only valid for the rush hours, but along a big part

4e.g. micro census can contain errors. After the application of time choice, the distribution of the departure time could be more approximate to that in the reality. The micro census generally records the daily journey on a typical travel day; some untypical days are not recorded. In fact, not all the typical travel days of all the people who completed the questionnaires happen on the same day. With the mode choice employed in this section, some traffic on the "typical day" is not executed with car mode, so that not each car-traveling happens on the same day.
3.5 Discussion

It was stated in the introduction that we are not aware of a currently existing practically feasible method to calibrate large scale models that use microscopic, behavior-based particles (= agents). Accordingly, the work presented above proceeds by heuristically adjusting different elements of the simulation. Still, we believe that the adjustments made in this paper can be defended: The improvement of the network was based on additional, and verifiably better input data; the improvement of the demand was based on demand that was clearly not covered by the existing demand generation; and it is in our view a good omen for the microscopic method that opening up the choice dimensions made the model better and not worse.

We also believe that the facility opening times, encoded in Tab. 3.1, are defensible although the particular values might still be improved. In reality not all facilities open at the same time. Finding better values here should be done in future work.

An arguably more sensitive issue is the scoring function (utility function) which drives the adaptation of the agents. The assumption of the existence of a utility function in itself is already a strong statement ([105, 76]), and this is important to state since the microscopic behavior-based approach could, in theory, also be based on alternative principles (see some of the chapters in [2]). If, however, we accept the utility function, it is instructive to look at its elements. As long as the synthetic travelers cannot drop activities, the following parameters are important:

- The typical duration, $t_{s,i}$, of each activity type.
- The slope of the utility function at its typical duration, for each activity type.
- The curvature of the utility function at its typical duration, for each activity type.

In consequence, at first glance it seems that there are three free parameters per activity type. Fortunately, this number can be reduced by the following arguments:

- In order to be optimal, the activity durations need to be selected such that all slopes (= marginal utilities) are the same, at least in the absence of constraints such as opening times or other influences such as strongly variable travel
times. This implies that one can, as a first approximation, set all slopes at the typical duration to the same value. This ends up being the marginal utility of leisure time [59], which can be estimated, because leisure has not the strict constraints due to opening and closing time.

- By the same argument, it should be possible to estimate “typical durations” of activity times from time use surveys: If marginal utilities are the same, then the typical durations need to be set such that the typical durations from time use surveys are recovered. - In our current work, the typical durations are directly taken from actual durations from time use surveys in Switzerland (see [101]).

The curvature at the typical durations remains as the most problematic parameter. This parameter determines the flexibility of an activity: a large curvature means that the marginal utility increases strongly when the activity duration is reduced, implying that time should rather be saved some-where else. For the time being, however, our choice of a function of type $A \ln(t/t_0)$ has the con-sequence that, after the slope at the typical duration has been set to the correct value as indicated above, no additional free parameter is left and, in consequence, there is nothing to calibrate.

### 3.6 Conclusion

A microscopic, behavior-based (“agent-based”) traffic simulation model is applied to the region of Zurich in Switzerland. The model is validated against hourly traffic counts of 161 counting stations. Not surprisingly, better demand data and better network data leads to better results. What is a bit more surprising is that the network improvements were informed by the freely available openstreetmap data, nourishing some hope that important network data for traffic modeling may eventually become available through this internationally available and standardized data source.

However, the most important result is that adding choice dimensions to the simulation (from “route choice only” to “route and time choice” and finally to “route, time, and mode choice”) makes the results more realistic. Our interpretation is that the locally optimizing agents are able to pick up local particularities of the urban system that are missed by more aggregate methods.
This is, in our view, a good omen for the microscopic, behavior-based methods which have always made the claim that, in the end, they might be more parsimonious than other methods.
Chapter 4

Travel Behavioral Calibration

The work reported in this chapter was presented as “Behavioral calibration and analysis of a large-scale travel microsimulation” ([43]). Most of the following sections are excerpts from the presented paper and the other 2 papers [46, 44] of the author in the past few years, modified to integrate them into this dissertation.

This chapter reports on the calibration and analysis of a fully disaggregate (agent-based) transport simulation for the metropolitan area of Zurich. The agent-based simulation goes beyond traditional transport models in that it equilibrates not only route choice but all-day travel behavior, including departure time choice and mode choice. This work shows that the application of a novel calibration technique that adjusts all choice dimensions at once from traffic counts yields cross-validation results that are competitive with any state-of-the-art four-step model, and elaborates on the usefulness of the obtained results for further demand analysis purposes in a real-world scenario.

4.1 Introduction

The well-known four-step process, consisting of trip generation, trip distribution (= destination choice), mode choice, and route assignment, has been the modeling tool in urban transportation planning for many decades [85]. However, the four-step process, at least in its traditional form, has many problems with modern issues, such as time-dependent effects, more complicated decisions that depend on the individual, or spatial effects at the micro (neighborhood) scale [116].

An alternative is to use a microscopic approach, where every traveler is mod-
eled individually. One way to achieve this is to start with the synthetic population and then work the way “down” towards the network assignment. This typically results in activity-based demand models [ABDM, e.g. 17, 23, 60, 91], which sometimes do and sometimes do not include the mode choice, but typically end with time-dependent origin-destination (OD) matrices, which are then fed to a separate route assignment package. The assignment package computes a (typically dynamic) route equilibrium and feeds the result back as time-dependent zone-to-zone travel impedances. When feedback is implemented, then the activity-based demand model recomputes some or all of its choices based on those travel impedances [70].

This type of coupling between the ABDM and the traffic assignment leaves room for improvement [7, 96]. In particular, it can be argued that route choice is also a behavioral aspect, and in consequence the decision to include route choice into the assignment model rather than into the demand model is arbitrary. Problems immediately show up if one attempts to base a route choice model in a toll situation on demographic characteristics – the demographic characteristics, albeit present in the ABDM, are no longer available at the level of the assignment. Similarly, in all types of intelligent transport system (ITS) simulations, any modification of the individuals’ decisions beyond route choice becomes awkward or impossible to implement.

An alternative is to split the assignment into a route choice model and a network loading model and to add the route choice to the ABDM, which leaves the network loading as the sole non-behavioral model component. If it is implemented as a microscopic or mesoscopic traffic flow simulation, then the integrity of the simulated travelers can be maintained throughout the entire modeling process. This has the following advantages:

- Both the route choice and the network loading can be related to the characteristics of the synthetic person. For example, toll avoidance can be based on income, or emission calculations can be based on the type of vehicle (computed in an upstream car-ownership model).

- Additional choice dimensions besides route choice can be included in the iterative procedure of assignment [87, 124, 80].

- The fully disaggregate approach enables an ex post analysis of arbitrary demand segments. This is an important advantage over any simulation based on
OD matrices, where the aggregation is done prior to the simulation.

This implies that, at least in principle, all choice dimensions of the ABDM can react to the network conditions, but it also requires to build models of this feedback for all affected choice dimensions. While, for example, route choice only looks at the generalized cost of the trip, departure time choice also includes schedule delay cost, mode choice compares the generalized costs between different modes, location choice includes the attractiveness of the possible destinations, etc. This brings along a vast increase in modeling opportunities, but it also requires substantially more modeling efforts.

In this chapter, we report on how such an approach can be implemented, calibrated, and analyzed, using the metropolitan area of Zurich as an example (as a sub-region of an “all-of-Switzerland” scenario [75]). In previous work [46, 42], the results of the calibrated simulation are compared to 161 counting stations in the Zurich metropolitan area. Despite of the vastly increased scope of the model when compared to a four-step approach, we are able to reproduce traffic counts with an error of 10% to 15% throughout the entire analysis period. Qualitatively, these results are competitive with any state-of-the-art four-step model, but they come along with entirely new modeling perspectives. While the previously published results aimed at an illustration of the deployed calibration method, this work gives a detailed analysis of the real-world scenario and the calibration results, and it elaborates on the usefulness of these results for further demand analysis purposes. Specifically, we investigate how certain characteristic numbers generated by the calibration can be behaviorally interpreted, and how this interpretation facilitates a further trip generation/attraction analysis and the identification of over-/underestimated demand segments.

The quality of the presented real-world results is to a large extent due to new methodological advances on the calibration side: Until recently, the four-step-process was ahead of our approach in this regard because its simple mathematical structure allowed for the development of a broad variety of (more or less automated) demand calibration procedures. In this chapter, however, we deploy a novel methodology for the calibration of demand microsimulations from network conditions such as traffic counts. The theory for this was developed over the last couple of years [42, 37].

The remainder of this chapter is organized as follows. Section 4.2 introduces the deployed calibration system. The field study is described in Section 4.3. Section
4.4 details the mechanisms through which the calibration takes effect and elaborates on the further demand analysis opportunities this brings along. Finally, Section 4.5 summarizes the chapter and indicates future research opportunities.

4.2 Calibration system

Chapter 2 describes a simulation that predicts the performance of a transportation system through an iterative process that couples complex behavioral and physical models. Notably, some aspects of the simulation are what one may call “procedurally modeled” in that there is no explicit mathematical specification of the respective sub-model but rather a sequence of processing steps that build the model output.

This lack of a comprehensive mathematical perspective on the simulation and its outputs has, until recently, rendered the calibration of the system a task based on intuition and, unfortunately, the arbitrariness this brings along. This section outlines the Cadyts (“Calibration of dynamic traffic simulations”, see [40, 38]) calibration tool. Because it allows to calibrate arbitrary choice dimensions from traffic counts in a fully disaggregate manner, it lends itself to an application in the Zurich case study.\(^1\)

4.2.1 Basic functioning

Cadyts makes no assumptions about the form of the plan choice distribution or about the choice dimensions it represents. It combines the prior choice distribution \(P_n(i)\) with the available traffic counts \(y\) into a posterior choice distribution \(P_n(i|y)\) in a Bayesian manner. The resulting posterior distribution is, essentially, of the following form [42]:

\[
P_n(i|y) \sim \exp \left( \frac{\partial \mathcal{L}(y)}{\partial P_n(i)} \right) \cdot P_n(i) \tag{4.1}
\]

where \(\mathcal{L}(y)\) is the log-likelihood function of the sensor data \(y\).

Some intuition into the workings of this quite general formulation can be obtained by adopting a simplified perspective where congestion is assumed to be light

---

\(^1\)Cadyts is not constrained to the MATSim microsimulation but is designed to be compatible with a wide variety of transport simulation systems.
and the traffic counts are independently and normally distributed. In this setting, the above formula simplifies into\(^2\)

\[
P_n(i|y) \sim \prod_{ak \in i} \exp \left( \frac{y_a(k) - q_a(k)}{\sigma_a^2(k)} \right) \cdot P_n(i)
\]

(4.2)

where \(y_a(k)\) is the available traffic count on link \(a\) in simulation time step \(k\), \(q_a(k)\) is its simulated counterpart, and \(\sigma_a^2(k)\) is the variance of the respective traffic count. The product runs over all links \(a\) and time steps \(k\) that (i) are contained in plan \(i\) in that the plan schedules to cross that link in the given time step and (ii) are equipped with a sensor. (The calibration functions with arbitrary sensor configurations.)

Intuitively, this works like a controller that steers the agents towards a reasonable fulfillment of the measurements: For any sensor-equipped link, the according \(\exp(\cdot)\) factor is larger than one if the measured flow is higher than the simulated flow such that the choice probabilities of plans that cross this link are scaled up. Vice versa, if the measured flow is lower than the simulated flow, the according factor is smaller than one such that plans that cross this link are penalized.

What is described here is a calibration of the individual-level choice distributions in the agent population that does not change the parameters of the choice model that generates the prior choice probabilities \(P_n(i)\). On the one hand, this is a quite general result in that it is \textit{independent} of the specification of the choice model. On the other hand, this also implies that, without further modifications, rather an improved picture of the current status quo is obtained than stable parameter estimates that could be used for forecast and scenario analysis. Subsection 4.2.3 continues the discussion of this topic in the context of a concrete application to the MATSim simulation system, which is described next.

\(^2\)The probability of a measurement \(y_a(k)\) would be \(p(y_a(k)) \sim \exp[-(y_a(k) - q_a(k))^2/(2\sigma_a^2(k))]\). Because of independence, the probability of a measurement set \(y\) would be the product of this, i.e., \(p(y) \sim \prod_{ak} \exp[-(y_a(k) - q_a(k))^2/(2\sigma_a^2(k))]\). From there, \(\frac{\partial \ln p(y)}{\partial P_n(i)} = \frac{\partial \ln p(y)}{\partial P_n(i)} \sim \sum_{ak \in i} \frac{y_a(k) - q_a(k)}{\sigma_a^2(k)}\), where the sum now goes over all \(ak\) that are used by plan \(i\); since plan choice probabilities translate in uncongested conditions on average into vehicle counts on links contained in the respective plans, the derivative of \(q_a(k)\) with respect to \(P_n(i)\) is one if \(ak \in i\) and zero otherwise.
4.2.2 Application to MATSim

Apart from the immediate execution of newly generated plans, the behavioral model of MATSim is of the multinomial logit form \( P_n(i) \sim \exp(V(i)) \). Substituting this into the posterior choice model (4.1) yields

\[
P_n(i|y) \sim \exp \left( V(i) + \frac{\partial \mathcal{L}(y)}{\partial P_n(i)} \right)
\]

That is, an implementation of the posterior choice distribution requires nothing but to add a plan-specific utility correction to every considered plan.

For independently distributed traffic count errors with \( \mathcal{L}(y) = \sum a_k \mathcal{L}(y_a(k)) \), an assumption that is maintained in the following, the above can be written as

\[
P_n(i|y) \sim \exp \left( V(i) + \sum_{a_k \in i} \frac{\partial \mathcal{L}(y_a(k))}{\partial P_n(i)} \right) =: \exp \left( V(i) + \sum_{a_k \in i} \Delta V_a(k) \right).
\]

Here, the plan-specific utility corrections are composed of link- and time-additive correction terms \( \Delta V_a(k) \). These terms are computed per sensor location and -time, but independently of which plan they affect. The utility correction of a full plan results from summing up all \( V_a(k) \) that are covered by the respective plan.

Returning to the intuitive example given in the previous subsection, the correction terms would be of the form \( \Delta V_a(k) = (y_a(k) - q_a(k))/\sigma_a^2(k) \). Again, the functioning of the calibration can be interpreted as a controller in that the utility of plans that improve the measurement reproduction is increased and the utility of plans that impair the measurement reproduction is decreased.

In congested conditions, the computation of the derivatives in (4.4) is more involved. [42] detail this logic based on [41], which essentially relies on a linear regression of the actual flow across a sensor against the number of vehicles that intend to cross that sensor.

As described in Chapter 2, MATSim functions in two phases, where the first phase builds the choice sets and the second phase simulates the choices based on fixed choice sets. Important from a calibration perspective, plans that are newly generated during the first phase are immediately chosen for execution in the mobility simulation in order to assess their performance. The utility-driven estimator (4.4) is applied in either phase in the following way:

- During the first phase, a newly generated plan is always selected. If no new plan is generated, then an available plan is selected according to (4.4).
• During the second phase, no new plans are generated and the calibrated choice distribution (4.4) is always employed.

This means that the calibration takes full effect only after the choice set generation is turned off.

Finally, it should be mentioned that Cadyts introduces in the setting described above an almost negligible computational overhead over a plain simulation of the same scenario. The respective performance measures can be found in [42].

4.2.3 Scope of the calibration

Subsection 4.2.2 describes how the simulated travel behavior in MATSim is adjusted to traffic counts through additive modifications of the utility functions, assuming a logit choice model. This approach can be applied more generally for every multivariate extreme value (MEV) choice model because every such model can be phrased in logit form [with a term involving the generating function added to the utility; see, e.g., 15]. This approach is equivalent to the calibration of an alternative specific constant (ASC) of every single alternative of every traveler.

Adopting this perspective, the calibrated simulation system still solves the original fixed-point problem of attaining consistency between the demand model and the supply model, however, based on calibrated ASCs. The more general formulation (4.1) does not even require a utility-driven demand model; in this case, it is legitimate to state that the calibrated simulation system deviates from the fixed point formulation of the original demand/supply model in a way that leads to greater consistency with the sensor data.

As described so far, the approach does not calibrate structural model parameters beyond ASCs. For that purpose, one could start by adopting a two-stage approach: In the first stage, Cadyts identifies changes to the utility function values that improve consistency with the traffic counts. In the second stage, these utility changes are then exploited in order to conclude about possible improvements of further structural model parameters. The remainder of this chapter, in particular sec. 4.4, exemplifies various opportunities along these lines.

However, although the ex post analysis of the utility corrections provided by Cadyts is an insight- and useful exercise, it clearly is desirable to adopt a one-stage approach where structural model parameters are calibrated directly. This opportu-
nity is explored in chapter 5, some theoretical results are by now available that show the feasibility of a direct parameter estimation of choice model coefficients beyond ASCs [39]. The reminder of this subsection briefly outlines this concept.

The original Cadyts approach (4.1) results from the maximization of a posterior entropy function that essentially represents the plausibility of the simulated travel behavior of all agents given the measurements. Mathematically, this approach can be directly rephrased as a parameter estimation problem by maximizing the posterior entropy function with respect to its structural parameters. An implementation of this approach has already been made available [40], however, its experimental investigations are still ongoing (see chapter 5 and chapter 6). An apparently highly relevant issue in this context is the consistent treatment of sampled choice sets: While it is well-known in discrete choice theory that this sampling needs to be corrected for when estimating choice model parameters [15], a consistent correction of this type in the context of path flow or OD matrix estimation appears to have not yet been discussed in the literature.

### 4.3 Zurich field study

This section describes a real-world case study for the city of Zurich, this scenario is just that in chapter 3. The setting of the test case is presented and some selected calibration results from a previous study are recalled [42, 46]. The utility offsets obtained from this calibration are analyzed in the next Section 4.4. This novel analysis shows that the utility corrections, which originally result from a formal solution of the calibration problem, have not only an intuitive meaning but also enable further demand analyses and calibrations.

Table 4.1 shows the parameters used in the scenario. There is not yet any distinction based on the location of an activity.

For calibration purposes, traffic counts from 161 inductive loop sensor stations are available. This data is used in the following way. First, the scenario is simulated with MATSim alone, without using the traffic counts. The results of this “base case” simulation are then compared to the traffic counts. Second, MATSim is run jointly with the calibration in different settings that use one subset of the traffic counts for calibration and the remaining counts for validation. Table 4.2 gives an overview of the results, which are described below.
Table 4.1: Simulation parameters.

<table>
<thead>
<tr>
<th>parameter</th>
<th>value</th>
</tr>
</thead>
<tbody>
<tr>
<td>total number of iterations</td>
<td>500</td>
</tr>
<tr>
<td>iterations for choice set generation</td>
<td>300</td>
</tr>
<tr>
<td>min. / avg. / max. home duration</td>
<td>0.5 / 14.7 / 23.0</td>
</tr>
<tr>
<td>min. / avg. / max. work duration</td>
<td>0.5 / 6.1 / 20.0</td>
</tr>
<tr>
<td>min. / avg. / max. education duration</td>
<td>0.5 / 5.8 / 20.0</td>
</tr>
<tr>
<td>min. / avg. / max. shop duration</td>
<td>0.5 / 1.7 / 12.0</td>
</tr>
<tr>
<td>min. / avg. / max. leisure duration</td>
<td>0.5 / 2.6 / 20.0</td>
</tr>
</tbody>
</table>

Table 4.2: Simulation and estimation results.

<table>
<thead>
<tr>
<th></th>
<th>reproduction MWSE</th>
<th>validation MWSE</th>
</tr>
</thead>
<tbody>
<tr>
<td>plain simulation</td>
<td>103.6</td>
<td>103.6</td>
</tr>
<tr>
<td>calibrated simulation</td>
<td>20.9</td>
<td>75.1</td>
</tr>
<tr>
<td>relative difference</td>
<td>- 80 %</td>
<td>- 28 %</td>
</tr>
</tbody>
</table>
The first data column of Table 4.2 ("reproduction MWSE") compares the measurement data fit of a plain simulation without calibration to that of a simulation where the calibration uses all available measurements at once. The MWSE ("mean weighted square error") shown here is the average quadratic deviation between simulated and observed counts at all sensor stations and in all time steps. All terms in this sum are weighted with one over two times the measured value; this corresponds to the assumption of independently normally distributed measurements with variances equal to the measurements. Table 4.2 shows that the reproduction MWSE is reduced by 80% through the calibration, which indicates an excellent adjustment to the data.

The second data column of Table 4.2 shows cross-validation results that were obtained by (i) splitting the sensors in ten disjoint subsets, (ii) running ten calibrations based on the data from nine subsets each, and (iii) comparing each calibration result to the unused sensor data set. A global improvement of almost 30% is obtained.

We stress that the fact that the validation improvement of 28% is lower than the reproduction improvement of 80% is not a sign of overfitting: The calibration adjusts directly only the behavior of those agents that may travel across sensors. The behavior of all other agents is implicitly changed through interactions with the immediately adjusted agents in the network (congestion feedback). Having a lower validation improvement than reproduction improvement indicates that the number of sensor locations is insufficient to "reach" the entire agent population in the calibration – some agents travel simply too far away from the sensors to be meaningfully adjusted. (The same observation holds for OD matrix estimators, which adjust only those OD flows directly that go across sensors.) In summary, rather than pulling only the simulated flows at the sensor locations towards the measurements while ignoring everything else, the calibration pulls the whole system towards a more realistic state.

4.4 Analysis of plan utility offsets

The ability of the Cadyts calibration system to adjust simulated behavior at the level of individual travelers enables an analysis at the fully disaggregate level. This section demonstrates how the utility corrections generated by Cadyts can be used for the further analysis of virtually arbitrary demand segments. The important ad-
Figure 4.1: Spatial layout of the link-based utility offsets at 8 am–9 am. Red: Counts are too high, negative utility offsets try to discourage traffic. Green: Counts are too low, positive utility offsets try to encourage additional traffic. Width corresponds to the magnitude of the utility offset.

Vantage of this approach over what one could do based on OD matrices is that the definition of a demand segment can be made after the simulation/calibration is conducted. This flexibility inevitably gets lost in any approach that aggregates the demand prior to the simulation/calibration.

4.4.1 Direct inspection of utility offsets

One can plot the link- and time-additive correction terms $\Delta V_a(k)$ from (4.4); results look like in Figure 4.1. From such plots, investigated over all hourly time slices, one obtains the following insights:

- Cadyts compensates for overall bias; i.e., it adjusts the rhythm of daily demand to the counts: Figure 4.2 shows the average hourly bias (simulated minus measured counts) over all sensors before the calibration, the average effect of the calibration over all sensor links (all other links have zero utility offsets), and the hourly bias after the calibration. Clearly, the calibration
counteracts the bias: The utility corrections are the more positive (i.e., encouraging traffic) the more negative the bias is (i.e., the simulated counts are lower than the measured counts).

In contrast to other approaches, demand is not considered as fully elastic, but it can be moved between time slices. This is possible only because in MATSim travelers possess different plans with different time structures and Cadyts is designed to take advantage of that feature. However, if the demand was elastic, e.g., in that there was a “stay-at-home” plan, then this elasticity would be exploited by Cadyts as well.

- Cadyts compensates for a directional bias; i.e., it reduces regular commuting and increases reverse commuting\(^3\). This is already visible in Figure 4.1, but it will become more evident in the subsequent analysis.

- Cadyts attempts to compensate for a systematic over-prediction in an east-west corridor at the lake (blue circle in Figure 4.1). This feature is visible across all time slots. It is, presumably, a network error in the sense that the links possess too much capacity in the simulation.

  This is likely to bias the demand estimation results in that the demand is adjusted in an attempt to correct for a supply error. This type of error can be avoided by jointly estimating the demand side and the supply side of the simulation; this is an important topic of future research.

- As a tendency, the corrective signal is the stronger the lower the density of counting stations. This is plausible since with a high density of counting stations several counting stations can collaborate to correct traffic into the desired direction.

### 4.4.2 Trip generation/attraction maps

Equation (4.4) maps the link-based utility corrections on all-day travel plans. This allows analyzing the effect of the calibration on arbitrary demand segments (by

\(^3\)A reverse commute is a round trip, regularly taken, from a metropolitan area to a suburban one in the morning (e.g. going to work), and returning in the evening (e.g. coming home from work) [92]
Figure 4.2: Mean counts bias and utility correction as a function of time. The counts bias is computed as the mean value of simulated minus measured counts at all sensor locations.

classifying only the respective subsets of the population) or on arbitrary demand dimensions (e.g., only route choice between two certain regions within a certain time interval). In the following, we analyze the utility corrections that persist after the convergence of the calibrated simulation.

We first adopt a trip-based perspective in that we extract from the agent-based demand model only the trips that fall into the morning rush hour. For each trip, we compute the utility correction according to (4.4). We then plot the resulting information in two ways on a map of Zurich, cf. Figures 4.3 and 4.4.

Both plots are generated by putting a 1 km times 1 km grid over the analysis region. In Figure 4.3, the colors of the cells represent the average utility corrections of all trips starting between 8 am and 9 am in the respective cell, whereas in Figure 4.4 this color corresponds to the average utility correction of all trips ending between 8 am and 9 am in the respective cell. Figure 4.3 (trip generation) shows positive trip utility offsets for trips originating in the city center, and negative trip utility offsets for trips originating in the surroundings. This can be interpreted as having not enough trip generation between 8 am and 9 am in the city center, and having too much trip generation in the surroundings.
Figure 4.3: Spatial distribution of utility corrections for trips generated between 8 am and 9 am. Only grid cells with at least 50 generated trips are shown.

Figure 4.4: Spatial distribution of utility corrections for trips attracted between 8 am and 9 am. Only grid cells with at least 50 attracted trips are shown.
Figure 4.5: Spatial distribution of utility corrections for all-day travel plans that have each at least one trip generated between 8 am and 9 am. Only grid cells with at least 50 generated trips are shown.

Figure 4.6: Spatial distribution of utility corrections for all-day travel plans, which have each at least one trip attracted between 8 am and 9 am. Only grid cells with at least 50 attracted trips are shown.
Figure 4.4 (trip attraction) shows negative trip utility offsets for trips arriving in most of the center, while a small area has positive offsets. This area contains the historical city center, the train station, and important parts of two universities. Offsets in some of the far-away surroundings are positive again. This can be interpreted as having too many trips arriving in most of the city center, while there are not enough arrivals in the indicated small area. At the same time, there are not enough arrivals in parts of the surroundings. However, the following analysis shows that the trip-based results described so far need to be taken with great care.

Now we turn to the exploitation of a feature that is unavailable in a purely trip-based (OD matrix driven) traffic simulation: We analyze the all-day utility offsets of the all-day plans that correspond to the previously described trips.

Figure 4.5 shows the plan-based counterpart of Figure 4.3, i.e., the utility offsets of the entire plans that contain a trip that starts between 8 am and 9 am in the depicted grid cells. One observes a qualitatively similar pattern with a somewhat higher overall level of the corrections, which results from the fact that the corrections are now summed up along a whole day (and not just one hour). Overall, the plan-based perspective confirms the trip-based analysis.

Figure 4.6 shows the plan-based counterpart of Figure 4.4, i.e., the utility offsets of the entire plans that contain a trip that ends between 8 am and 9 am in the depicted grid cells. Here, a striking difference between the plan-based and the trip-based perspective can be observed. Most importantly, the negative utility offsets in the trip-based perspective that discourage travel towards the city center turn into positive utility offsets in the plan-based perspective that encourage travel. Also, the slightly negative trip utility offsets in the city surroundings turn into mostly clearly positive values in the plan based perspective. This difference is explained in the following.

The analysis of all-day plans instead of separate trips allows accounting for the dynamical constraints that guide real travel: Behaviorally, it is well known that travelers choose between trip sequences and not between individual trips. Physically, the mass conservation of persons and vehicles must be accounted for. A first conclusion of the comparison between Figures 4.4 and 4.6 is that the negligence of these constraints can lead to drastic misinterpretations.

Regarding the concrete values shown in Figures 4.4 and 4.6, one can conclude that the trips ending in the city center between 8 am and 9 am are not the result of
an overall demand surplus, but only the result of a demand mis-allocation, possibly due to imprecise destination or departure time choice modeling (see below): the calibration actually encourages *plans* that end in the city center between 8 am and 9 am, which is consistent with the general demand underestimation in the simulation as shown in Figure 4.2.

The completely different picture in the trip-based perspective may be due to (i) errors in the choice model specification and (ii) errors in the attributes fed into the choice model.

- Choice model specification errors are very likely to be present in the given scenario: The simple multinomial logit plan choice model ignores correlation across alternatives. The choice model coefficients are not estimated from data but inferred on a trial-and-error basis. (As mentioned before, the work in chapter 5 and chapter 6 indicates that the latter error source can be removed in that the calibration also adjusts choice model parameters [39]).

- Errors in the attributes fed into the choice models are likely to exist as well. Perhaps most noteworthy is the assumption of identical opening and closing times for all facility types, cf. Table 4.1. This is likely to result in an unrealistic morning peak concentration that would be smoothed out by more distributed starting times of, in particular, the work activity.

The analysis given here already demonstrates clearly that (i) utility offsets computed from traffic counts can be used for an insightful spatio-temporal demand analysis and that (ii) the new approach of calibrating a fully disaggregate demand of individual travelers can lead to completely different (and structurally far more meaningful) results than what an estimation of independent OD matrices per time slice suggests.

### 4.4.3 Identification of underestimated demand segments

This subsection presents an exemplary analysis of how the utility corrections generated by Cadyts can be used to identify demand segments that are likely to be corrupted by modeling errors.

For this, we analyze the travel demand by purpose, where we distinguish trips that head for work, education, shopping, leisure or home, or belong to the “border-crossing” demand segment. Figure 4.7 shows histograms of the offsets by purpose,
Figure 4.7: Histogram of trip utility offsets by purpose

with a uniform histogram bin size of 0.25 and accounting only for such trips that cross a sensor at least once (all other trips would do nothing but add a peak at a zero utility correction to the histogram). The histograms reveal a striking difference between the trips for border-crossing and all other travel purposes. While all other trips are quite symmetrically centered around an almost zero utility offset, the border-crossing trips are much more widely scattered around a mean of approximately +10 utility units.

This means that Cadyts strongly encourages border-crossing traffic but is on average almost indifferent with respect to the other demand segments. This indicates that the border-crossing demand is substantially underestimated in the synthetic population of the Zurich scenario. This observation motivated a re-examination of the demand modeling of this scenario, which indeed revealed an inconsistency: The initial demand contains, statistically, all trips generated by persons living in Switzerland, plus all trips generated by vehicles crossing the borders of Switzerland. As a result, all border-crossing traffic by Swiss drivers is, statistically, counted twice, while non-border-crossing traffic by non-Swiss drivers is missing. It is plausible to assume that, 50 km away from the border, the second segment is larger than the first, and that the second segment mostly comprises of through traffic, which looks somewhat similar to the border-crossing traffic. Here, the calibration has revealed
a structural incompleteness in the demand modeling that should be corrected for in future work.

The wide histogram scatter of the utility corrections for border-crossing traffic can in part be explained with the relatively low total number of border-crossing travelers simulated, which naturally leads to a higher variability in the histogram. However, the wide scatter of utility values may also indicate that a further disaggregation of this demand segment is necessary. This is quite plausible given the above observation that the initial demand modeling in some sense compensates for one demand segment through another. We leave the further analysis of these details to future studies.

In summary, this section demonstrates that the utility corrections computed by Cadyts for every single synthetic traveler can be utilized for an ex post analysis of the simulation system in various ways. It needs to be stressed again that the manual/visual inspection conducted here has by no means pushed this approach to its limits: A logical next step is to utilize the utility corrections not only for the calibration of the plan choice patterns in a given population but also for an adjustment of the size of the different demand segments within that population.

4.5 Discussion and Summary

A standard question in conjunction with calibration is in how far the results are useful for prediction. Based on the results of the last sections, one can argue that the results are useful for short-term prediction: both in a real-time setting or for a short-term policy measure, the link offsets could be frozen and then used in the prediction. As discussed in [37], care needs to be taken that the offsets are only used for choice and not for choice set generation, i.e., not for routing.

Clearly, this approach runs into problems when anything in the system that is presumably related to the link offsets changes. A simple example would be the addition of a lane to such a link. For such situations, a calibration of “higher level” behavioral parameters is necessary and is investigated in chapter 5 and chapter 6.

Apart from the calibration of utility functions, an analysis of the utility offsets reveals further calibration opportunities. Since the plan-specific utility offsets can be interpreted as encouragements (when positive) or discouragements (when negative) of the respective travel behavior, the total levels of arbitrary demand segments can
be analyzed in hindsight. While this chapter only indicates this opportunity through the analysis of selected demand segments in a single scenario, it appears feasible to develop a calibration method that also corrects such inconsistencies in a statistically consistent manner.

In summary, this chapter demonstrates that a fully disaggregate transport microsimulation that represents travel demand at the level of individual persons can be applied to the realistic simulation of large metropolitan systems. The agent-based simulation goes beyond traditional transport models in that it equilibrates not only route choice but all-day travel behavior, including departure time choice and mode choice. A novel calibration method is applied to the calibration of the microscopic travel demand from traffic counts. The method does not only generate a clear improvement in measurement and validation data fit, it also adjusts the demand in a behaviorally interpretable way. It does so by computing utility corrections to which the utility-driven travel demand simulator reacts with more realistic behavior. A detailed analysis of these utility corrections clarifies their behavioral interpretation, shows ways in which they can be applied for demand analysis, and indicates possibilities for their further exploitation in the automatic calibration of disaggregate travel demand models.
Chapter 5

Calibration of Travel Behavioral Parameters

The work reported in this chapter was presented as "Choice model refinement from network data" [45]. Most of the following sections are excerpts from the presented paper, modified to integrate them into this dissertation.

This chapter considers the problem of refining the parameters of disaggregate travel demand models using observations of time-dependent network flows. The measurement function that links the behavioral model parameters to the network flows is given through an iterated DTA (dynamic traffic assignment) microsimulation. The challenging aspect of this configuration is that the measurement equation is not given in closed form but is the result of a complex simulation process, in the course of which disaggregate models of travel behavior and of network flows are repeatedly evaluated until a state of consistency between demand and supply is attained [80, 26].

The increased availability of detailed network surveillance data triggered recent efforts to calibrate behavioral model parameters (and also network supply parameters) jointly with the origin/destination flows representing travel demand levels [1, 5, 115]. These approaches, however, resort to black box optimization techniques that, by design, exploit problem structure at most in terms of a numerical linearization. The approach of [42] is an exception; here, a tractable analytical approximation of a complete DTA microsimulation system is developed and exploited. That research demonstrated that the calibration of individual-level route choice, departure time choice, and mode choice probabilities for a region as large as the Greater
Zurich area is possible with (i) an improvement in measurement fit of up to 80% and (ii) a computational overhead of as small as 10% over a plain simulation.

Motivated by those results, the present chapter moves on to the calibration of choice model parameters from network flows. Methodologically, it abstains from deploying black-box optimization/calibration techniques to the greatest possible extent and pursues an analytical approach instead. In a nutshell, the resulting findings are that (i) it is possible to calibrate behavioral model parameters and their covariance matrices using network flows in a computationally very efficient manner, but also that (ii) the approach needs further refinement to deliver reliable estimates. The various sources of imprecision in the current approach are therefore analyzed and possibilities to overcome them are discussed.

The remainder of this chapter is structured as follows. Section 5.1 develops the proposed calibration approach. Section 5.2 then presents a large-scale case study, which is based in parts on real and in parts on synthetic data. Finally, Section 5.3 discusses the results and indicates possibilities for further improvements.

## 5.1 Calibration approach

This section derives the proposed calibration approach. Subsection 5.1.1 develops an analytical approximation of the measurement equation that connects time-dependent network flows and behavioral model parameters. It builds on earlier findings by [42]. Subsection 5.1.2 then formulates a nonlinear least squares estimator and clarifies how this estimator is inserted into the iterative logic of the DTA simulation. Finally, Subsection 5.1.3 derives an approximation of the parameter covariance matrix for this estimator.

### 5.1.1 Analytical approximation of measurement equation

The calibration objective is to identify a vector $\beta$ of behavioral model parameters, such as travel time coefficients or alternative specific constants for certain modes, given a vector of observed network flows $y = (y_{ak})$, where $y_{ak}$ is the measured flow on link $a$ in time interval $k$. Given the complexity of the iterated DTA simulation, it is technically quite challenging to analytically link the measurements $y$ to the parameters $\beta$. However, this effort is worthwhile because it allows extracting
gradient information, which can be exploited to accelerate the calibration process and to analyze solution properties.

To achieve this goal, the link demand \( d = (d_{ak}) \) is defined through

\[
d_{ak} = \sum_{n=1}^{N} \sum_{i \in C_n} 1(i \sim ak) \Pi_{ni}
\]

where \( i \sim ak \) reads as “following travel plan \( i \) implies entering link \( a \) during time step \( k \)”, and \( 1(\cdot) \) is the indicator function. \( \Pi_{ni} \) denotes the choice probability that agent \( n \) chooses plan \( i \) from its plan choice set. That is, \( d_{ak} \) represents the expected number of travelers intending to enter link \( a \) in time step \( k \). The simplifying assumption is made that the flow \( q_{ak} \) across a link \( a \) in time step \( k \) is a function of its link demand \( d_{ak} \) only. Specifically, a linear relationship

\[
q_{ak} = \alpha_{ak}d_{ak} + \beta_{ak}
\]

is assumed, where \( \alpha_{ak} \) and \( \beta_{ak} \) are real-valued coefficients. Assuming for now that these coefficients are known, (5.1) and (5.2) can be combined into a linear mapping of plan choice probabilities \( \Pi \) on link flows \( q = (q_{ak}) \):

\[
q = L\Pi + b
\]

where the matrix \( L = (l_{ak,ni}) \) consists of elements \( l_{ak,ni} = \alpha_{ak}1(i \sim ak) \) and the vector \( b = (\beta_{ak}) \) is composed of the intercepts of model (5.2).

It remains to link the stationary choice probabilities \( \Pi \) to the behavioral model parameters \( \beta \). For this, let \( x \) denote the vector of all network attributes that affect the agents’ plan choice behavior, and denote by \( \pi(x) \) its stationary distribution. Further, let \( P_n(i | x; \beta) \) be agent \( n \)’s behavioral model, defining the probability of selecting plan \( i \in C_n \) given network attributes \( x \) and behavioral model parameters \( \beta \). Letting \( P(x; \beta) = (P_n(i | x; \beta)) \), the stationary plan choice distribution can then be written as

\[
\Pi(\beta) = \int P(x; \beta)\pi(x)dx.
\]

Assuming that the agents base their decisions on average network conditions \( \bar{x} \), such that \( \pi(x) \) collapses into a singleton \( \pi(x) = \delta(x - \bar{x}) \), one obtains \( \Pi(\beta) = P(\bar{x}; \beta) \), and hence

\[
q(\beta) = LP(\bar{x}; \beta) + b.
\]
This is the analytical approximation of the measurement equation used in this chapter. Given a behavioral model that yields choice probabilities that are differentiable with respect to the behavioral model parameters, its Jacobian can be written as

\[
\frac{\partial q(\beta)}{\partial \beta} = L \frac{\partial P(\bar{x}; \beta)}{\partial \beta}.
\]  

(5.6)

5.1.2 Nonlinear least squares estimator

Relying on the approximations of the previous subsection, a nonlinear ordinary least squares estimator can now be stated:

\[
\min_{\beta} Q(\beta) = \frac{1}{2} (y - q(\beta))^T (y - q(\beta)) + \frac{1}{2} (\beta^0 - \beta)^T W (\beta^0 - \beta)
\]

s.t. \( q(\beta) = LP(\bar{x}; \beta) + b \)  

(5.7)

The first term in the objective function \( Q(\beta) \) measures the deviation between observed and simulated flows. Given the limited amount of information that can be extracted from aggregate network flows, this objective function can (and should if possible) be enriched with a priori obtained behavioral parameter estimates. They are represented by the second term and could result from, e.g., a previous survey. Here, \( \beta^0 \) is a vector of prior parameter estimates and \( W = (w_{ij}) \) is a positive definite diagonal weighting matrix. Superscript \( T \) denotes the transpose.

It remains to ensure consistency between the behavioral parameters, which are estimated subject to a particular linearization of the network loading, and the network loading, which is linearized given the travel demand resulting from a particular choice of the behavioral parameters. A very similar problem is encountered in the field of origin/destination matrix estimation. Again following [42], the iterative nature of the underlying DTA simulation can be exploited in ensuring this consistency in a computationally efficient manner. Instead of iterating between (i) a parameter calibration given a linearization of equilibrated network conditions and (ii) a complete network equilibration given an updated parameter set, the parameter calibration is inserted into the iterative (day-to-day) loop of the DTA simulation system.

Specifically, the following sequence of operations takes place every iteration of MATSim:

1. A parameter vector \( \beta \) is estimated, relying on a linearized network loading.
2. Using $\beta$, the choice model of every agent is evaluated, and a selected plan is obtained.

3. All agents are loaded on the network according to their selected travel plans.

4. The linear approximation (parameters $L$ and $b$) of the network loading is updated.

Step 1 is solved with the Levenberg-Marquardt method, using an implementation following [72] and exploiting the analytically available Jacobian (5.6). Steps 2 and 3 correspond to the plain DTA simulation logic and are sometimes also referred to as “demand simulation”, followed by “supply simulation”. Step 4 requires to compute for every sensor-equipped link and every time step the coefficients of model (5.2). This is accomplished by (i) observing after step 2 of each iteration the current link demand $d_{ak}$ according to (5.1), (ii) observing after step 3 the resulting link flow $q_{ak}$, and (iii) updating $\alpha_{ak}$ and $\beta_{ak}$ for each link separately with a recursive regression step. This approach was already successfully deployed by [42] in the estimation of choice distributions (but not of the underlying parameters) from traffic counts.

Due to the stochastic fluctuations of the DTA simulation even in stationary conditions, this approach yields one parameter estimate $\beta^{(c)}$ per iteration $c$. The relevance and proper interpretation of this is clarified in the next subsection.

### 5.1.3 Parameter covariance analysis

The previous subsection proposes to compute one parameter vector $\beta^{(c)}$ per (stationary) iteration $c$ of the stochastic DTA microsimulation. These estimates will in general be different due to the stochasticity of the simulation. The expected value of these stochastic estimation results in stationary conditions is proposed as a point estimator of the behavioral model parameters:

$$
E\{\beta\} \approx \bar{\beta} = \frac{1}{c_2 - c_1 + 1} \sum_{c=c_1}^{c_2} \beta^{(c)}.
$$  \hspace{1cm} (5.8)

To analyze some properties of this estimator, all stochastic quantities of the DTA simulation that may possibly affect the parameter estimates $\beta$ are summarized in a disturbance vector $\epsilon$. According to the "Law of total variance" [120], the variance/covariance matrix $\text{VAR}\{\beta\}$ of the parameter estimates can then be decom-
posed as
\[
\text{VAR}\{\beta\} = \text{E}\{\text{VAR}\{\beta \mid \varepsilon\}\} + \text{VAR}\{\text{E}\{\beta \mid \varepsilon\}\}. \tag{5.9}
\]

Elements 3 and 4 are the "unexplained" and the "explained component of the variance", elements 1 through 4 of this expression are computed as follows.

1. The covariance \(\text{VAR}\{\beta^{(c)} \mid \varepsilon^{(c)}\}\) of the parameter estimates \(\beta^{(c)}\) within a single iteration \(c\) and given the stochasticity \(\varepsilon^{(c)}\) of that particular iteration is computed with a sandwich estimator [e.g., 52]
\[
\text{VAR}\{\beta^{(c)} \mid \varepsilon^{(c)}\} \approx A^{(c)} B^{(c)} A^{(c)} \tag{5.10}
\]

where
\[
A^{(c)} = \left(\frac{\partial^2 Q(\beta^{(c)})}{\partial \beta^2}\right)^{-1} \tag{5.11}
\]

\[
B^{(c)} = \sum_{ak} \frac{\partial q_{ak} (\beta^{(c)})}{\partial \beta} \frac{\partial q_{ak} (\beta^{(c)})}{\partial \beta}^T + W. \tag{5.12}
\]

The Hessian in (5.11) is numerically computed. The second addend in (5.12) results from the treatment of the prior parameter vector \(\beta^0\) as a supplementary set of measurements, following the arguments of [108]. A more careful analysis of this covariance component is certainly desirable and possible [52].

2. \(\text{E}\{\beta^{(c)} \mid \varepsilon^{(c)}\} = \beta^{(c)}\) because \(\beta^{(c)}\) results from the minimization of (5.7), which is deterministic for a given \(\varepsilon^{(c)}\).

3. The expectation \(\text{E}\{\text{VAR}\{\beta \mid \varepsilon\}\}\) is approximated using the arithmetic mean over many iterations in stationary conditions:
\[
\text{E}\{\text{VAR}\{\beta \mid \varepsilon\}\} \approx \frac{1}{c_2 - c_1 + 1} \sum_{c=c_1}^{c_2} A^{(c)} B^{(c)} A^{(c)}. \tag{5.13}
\]

4. The variance \(\text{VAR}\{\text{E}\{\beta \mid \varepsilon\}\}\) is also approximated by an average over many iterations in stationary conditions:
\[
\text{VAR}\{\text{E}\{\beta \mid \varepsilon\}\} \approx \frac{1}{c_2 - c_1} \sum_{c=c_1}^{c_2} (\beta^{(c)} - \bar{\beta})^2. \tag{5.14}
\]
The feasibility of approximations (5.13) and (5.14) depends on the ergodicity of the stochastic process implemented by the iterated simulation system (e.g. [98]). One possibility to establish this property is to (i) assume fixed choice sets and (ii) give every travel plan a strictly positive probability to be selected. This is the case for the experiments presented in Section 5.2.

In summary, these developments make available an analytical approximation of the covariance matrix of the estimated parameters, which accounts for simulation stochasticity and can be efficiently computed. It does, however, also rely on various approximations, the effect of which is investigated in the following case study.

5.2 Case study

This section presents a large case-study the purpose of which is to demonstrate the feasibility of the proposed calibration approach. It is based in large parts on real data, but replaces unobserved quantities by simulated ones, in order to assess the performance of the calibration.

5.2.1 Scenario description

This case study considers the Greater Berlin area, with a network size of 24,335 links and 11,345 nodes. A synthetic population of 57,688 travelers is simulated. This constitutes a 2% sample of the Berlin population, limited to individuals whose travel behavior is reflected in the MATSim model system. Network capacities are scaled accordingly, resulting in realistic congestion patterns despite of the reduced number of travelers.

All synthetic travelers have complete daily activity patterns, including typical durations, based on a household survey from 1998 also used in other studies [68, 100, 99]. A more complete description can be found in [77]. Such activity patterns can include activities of type home, work, education, shopping, leisure, holiday / journey, business, multiple, other, see a doctor. The elements of a single agent’s plan choice set differ in their routes and modes. The choice of a plan hence implies the choice of an all-day mode and route sequence, with all other behavioral dimensions fixed. For simplicity, a physical network simulation of public transport is replaced by a “teleportation mode” that moves travelers on public transport trips.
at half the speed of a car in uncongested conditions [53, 95].

Every agent is given an exogenously created plan choice set. This choice set is constructed based on a different MATSim simulation of the same Berlin scenario, where an incremental choice set generation mechanism is used. The resulting choice set consists, per agent, of the following elements: (i) The last selected plan in the simulation. This constitutes a behaviorally plausible reference alternative. (ii) A plan where the routes of all car-legs are replaced by the fastest route given the travel times obtained in the last iteration of the simulation. (iii) A plan where for all car-legs routes with a reduced number of left-turns are generated. (iv) A variation of plan (i) with randomly varied mode choice. The mere purpose of this choice set generation is to obtain a strong simulation response to variations in the behavioral parameters; otherwise, it clearly is of little behavioral relevance.

The utility contribution of a leg \( l \) to the all-day plan utility (2.2) is defined for the purposes of these experiments (other forms are possible and have been used) as

\[
V(l) = \begin{cases} 
    \beta_{car} t(l) + \beta_{left} n_{left}(l) & \text{if } l \text{ is by car} \\
    \beta_{non-car} t(l) & \text{otherwise.}
\end{cases} 
\]  

(5.15)

Here, \( \beta_{car} \) is a negative coefficient for the travel time \( t(l) \) if leg \( l \) uses the car mode, \( \beta_{left} \) is a negative coefficient for the number of left-turns \( n_{left}(l) \) in leg \( l \), and \( \beta_{non-car} \) is a negative coefficient for the time spent traveling with a mode different from car. Again, the illustrative purpose of this behavioral model specification needs to be stressed.

### 5.2.2 Generation of synthetic traffic counts

Although real hourly traffic counts from 346 sensor stations in Berlin are available, this explorative study does not exploit this data but constrains itself to the generation of synthetic traffic counts. Through this, the calibration results can be compared to a synthetic ground truth, which would not be available if real data was used. The synthetic traffic counts are generated as follows.

A synthetic reality is assumed, where the leg utility (5.15) is computed based on the following parameter values: \( \beta_{car} = -4.5 \text{ EUR/h} \), \( \beta_{left} = -0.5 \text{ EUR} \), \( \beta_{non-car} = -3 \text{ EUR/h} \), and \( \beta_{act} = 6.0 \text{ EUR/h} \). MATSim is then run with these parameters, using otherwise the configuration described in Subsection 5.2.1, including the fact that the choice set for every agent is fixed. Once the iterations have reached stationary
conditions, the simulation is stopped and the simulated hourly traffic flows of the
last iteration are extracted at all sensor locations, resulting in a set of synthetic traffic
counts.

This process is repeated ten times, using different random seeds in the simula-
tion. Hence, there are ten independent sensor data sets available, all of which are
generated based on the same behavioral parameters, but being stochastically differ-
ent due to the randomness of the MATSim simulation logic.

5.2.3 Calibration results

Ten experiments, each with one of the ten independently generated synthetic mea-
surement data sets, are conducted. The simulation configuration of these exper-
iments differs from the configuration in which the synthetic traffic counts were cre-
at in that “wrong” values for the in-car travel time and for left turns are used:

\[ \beta_{\text{car}}^0 = -6.0 \text{ EUR/h} \quad \text{and} \quad \beta_{\text{left}}^0 = 0.0 \text{ EUR/h}. \]

The calibration, which is now inserted into the simulation loop, then adjusts these parameters according to the synthetic traffic counts. All other simulation parameters are the same as in the generation of the synthetic measurements.

Overall, a two-dimensional parameter vector \( \beta = (\beta_{\text{car}}, \beta_{\text{left}})^T \) is calibrated, us-
ing the prior estimates \( \beta^0 = (\beta_{\text{car}}^0, \beta_{\text{left}}^0)^T \) and a prior weight matrix \( \mathbf{W} = \begin{pmatrix} 0.25 & 0 \\ 0 & 0.25 \end{pmatrix} \).

Since the hourly traffic counts, which are in the order of hundreds or thousands, have
uniform weights of one, the prior parameter weights have a very low effect on the
 calibration results. They are used to keep the Levenberg-Marquardt method from
generating trial parameters that are extremely far off a reasonable value range and
hence avoid numerical problems in the evaluation of the choice probabilities and
their derivatives.

All experiments are run well beyond stationarity. For every experiment, the
ultimately estimated parameters are computed as average values over all station-
ary iterations, and the parameter covariance matrices are computed as described in
Subsection 5.1.3, also over all stationary iterations. Figure 5.1 visualizes the re-
sults. Each dot represents the final parameter estimates of one experiment. It is
located in the center of an ellipse representing the 95% confidence region, which
is computed from the corresponding parameter covariance matrix. Each cross de-
notes the parameter estimate only of the last iteration of an experiment, without any
averaging. The coordinate axes intersect at the true parameter values \((\beta^*_\text{car}, \beta^*_\text{left}) = (-4.5, -0.5)\). Note the different scalings of the axes. Overall, the parameter estimates are near the true values, but have a visible bias in that \(\beta_{\text{car}}\) is underestimated by approximately 0.5 and \(\beta_{\text{left}}\) is overestimated by approximately 0.04. The 95% confidence regions have an order of magnitude that roughly corresponds to the distribution of the estimated parameters, but they vary quite significantly between experiments. Clearly, these results are yet too unreliable to be operationally useful. They are, however, in the right order of magnitude. The one-shot estimates (crosses), which incorporate the simulation noise of the last iteration, are within the range predicted by the covariance matrices. Also, the number of iterations until stationarity is only in the order of \(10^2\). This suggests that further refinements of the proposed method will eventually yield both reliable and efficiently computable results. The following section discusses this in greater detail.
5.3 Discussion and outlook

A method to calibrate behavioral model parameters from network flow observations was presented. Different from the few other approaches to the same problem, an analytical approximation of the problem is derived and used in the calibration. Overall, the method yields estimation results of plausible order of magnitudes. In its current form, however, it fails to provide a precision that would be necessary for its deployment in practical applications. Fortunately, the various approximations made during the derivation of the method are well-understood, such that systematic efforts to improve upon them are possible.

The analytical measurement equation is only an approximation, and this affects both the estimates of the parameters and their covariance matrices: The linearization of then network loading (5.1)-(5.3) assumes that the flow across a link is not affected by flows across adjacent links. This neglects spillback effects. While improved linearizations that capture link flow interactions are possible and have been demonstrated for single intersections [41], nonlinear network dynamics in general are known to be very difficult to account for when calibrating travel demand from traffic counts [49]. In addition to this, the recursive regression based on which the linear model coefficients are updated maintains limited fluctuations even as the calibrated simulation attains stationarity, adding to the imprecision of the linearization. Further, the simplification of (5.4) based on the assumption that agents select their travel plans only in consideration of average network conditions is not perfectly correct. In MATSim, agents smooth their perceived network experiences with a recursive first order filter, but this filter maintains some variability even in stationary conditions.

Operational consideration may render an exact reformulation of the above approximations infeasible. Rather than switching back to a black-box calibration approach, the proposed method should then be supplemented with less analytical and more “sampling-based” techniques. This combination would exploit the analytical approach in quickly finding good approximate solutions, which could then be refined using alternative techniques. The meta-model approach of [86], where a structural analytical model is supplemented with a regression-based approximation of the objective function, appears particularly applicable to this problem.
Chapter 6

A simplified Parameter Estimation

This chapter introduces a simplified method of parameter estimation based on some of the Intermediate results in Chapter 4.

6.1 Theory

Chapter 4 demonstrated that each plan in plan choice set of each agent can get a utility correction ($\sum_{ak \in i} \Delta V_a(k)$ in Equation 4.4) from “cadyt” which reflects the fit between the daily traffic plan in reality and in simulation and also influences the plan choice of each agent as an alternative specific constant (ASC) appended to the score of the corresponding plan. This is to say, to some extent, these utility corrections give the agents an “operational guideline”, by means of which they can better reproduce the real traffic situations (s. Chapter 4). A utility correction sometimes could equal zero which could mean:

1. no count stations are passed in the daily journey of this agent, or

2. every link utility offset acquired from the count stations that an agent pass in its daily journey equals zero, or

3. such link utility offsets counteract each other in the last possibility.

Certainly, Number 2 and 3 occur very infrequently in real cases. The ideal state is that number 2 occurs in the case of all the agents in Network, i.e. the real counts were perfectly reproduced. The objective of this chapter is to adjust the parameters that are able to influence the plan choice to realize a better reproduction of traffic
counts in reality through multiagent simulation, in other words, to minimize the absolute values of all the plan utility corrections and eventually link utility offsets.

As described in the last paragraph, it is pursued to minimize the absolute values of all the plan utility corrections through adjustment of some parameters, i.e. to make the utility corrections needless as far as possible. The approach proposed here should be able to supersede the effect of plan utility corrections as ASCs by adjustment of relevant parameters, e.g. behavior parameters in scoring function in MATSim, which directly influence plan scores/utilities, so that the so-called ASC is not an additive component of the plan score any more in this chapter. In brief, the plan score calculation for one plan in Chapter 4 has the following form:

\[ S = \sum_p \beta_p A_p + \Delta S \]  

(6.1)

where \( S \) denotes score/utility of a plan, \( p \) is index of behavior parameter \( \beta_p \) in MATSim scoring function, \( A_p \) is the attribute value corresponding to \( \beta_p \), \( \Delta S \) denotes the aforementioned plan utility correction. In other words, the plan score calculation for one plan in this Chapter can be written as:

\[ S = \sum_p \beta'_p A_p \]  

(6.2)

where \( \beta'_p \) denotes the behavior parameter after adjustment.

Substituting the right side of Eq. 6.2 for the \( S \) in Eq. 6.1 yields

\[ \sum_p \Delta \beta_p A_p = \Delta S \]  

(6.3)

where \( \Delta \beta_p \) denotes the difference between the adjusted parameters and the original parameters i.e. \( (\beta'_p - \beta_p) \). In every iteration of MATSim simulation, the plan utility offset \( \Delta S \) can be generated by cadyts, the attributes, which are necessary for plan score calculation, can also eventually be obtained from the scoring calculation in MATSim, so the \( \Delta \beta_p \) and \( \beta'_p \) apparently could be straightforwardly\(^1\) calculated for this plan. Nevertheless, this calculated \( \Delta \beta_p \) and \( \beta'_p \) can only work for this plan. What is pursued in this chapter, is a set of behavior parameters that works for all the plans of all agents. So it is necessary to generalize about Eq. 6.3 for all the population.

\(^1\)Certainly, Equation 6.3 may have innumerable solutions, if \( p > 1, p \in N \).
What is meant here is, a unified parameter set. This object can be realized through solving a system of linear equations that can be written as:

\[
\begin{bmatrix}
  a_{11} & \cdots & a_{1n} \\
  \vdots & \ddots & \vdots \\
  a_{m1} & \cdots & a_{mn}
\end{bmatrix}
\begin{bmatrix}
  \Delta \beta_1 \\
  \vdots \\
  \Delta \beta_n
\end{bmatrix}
=
\begin{bmatrix}
  \Delta s_1 \\
  \vdots \\
  \Delta s_m
\end{bmatrix}
\] (6.4)

and also in matrix notation as:

\[
A \Delta \beta = \Delta S
\] (6.5)

where \(a_{ij}\) denotes the attribute value that corresponds to the to be adjusted parameter \(\beta_j\) for plan \(i\). \(A\) denotes the matrix constituted by all the \(a_{ij}\). Because of a total of \(n\) parameters to be adjusted, there also are \(n\) differences between the adjusted parameters and the original parameters i.e. \(\Delta \beta_j\), their corresponding vector is denoted by \(\Delta \beta\). \(\Delta s_i\) denotes utility correction for plan \(i\), its corresponding vector is \(\Delta S\). In our real study cases, there are often hundreds of thousands of agents, each agent has several plans in its plan choice set. However, the number of behavioral parameters in the scoring function in MATSim is much lower than the number of agents or plans by comparison. That is, this system of linear equations has much more equations than unknowns which has no solutions i.e. this is an overdetermined system, which has no accurate solutions. Nevertheless, it is worth to solve the approximate solution for the system. That is why the objective of this chapter is rather to find the set of approximated behavior parameters \(\{\Delta \beta_j\}\) which “best” fits the equations.

The method of least squares is often used to find an approximate solution of overdetermined systems in the sense of solving a quadratic minimization problem, and, in the context of this chapter, it has the following form:

\[
\begin{bmatrix}
  \hat{\Delta \beta}_1 \\
  \vdots \\
  \hat{\Delta \beta}_n
\end{bmatrix}
= \arg \min_{\Delta \beta} \sum_{i=1}^{m} \left| \Delta s_i - \sum_{j=1}^{n} a_{ij} \Delta \beta_j \right|^2,
\] (6.6)

with a new numbering of all the plans in choice sets of all the agents from 1 to \(m\). Certainly, it is unnecessary to account for all the plans of the travel demand, e.g. some plan \(i\) has zero attributes corresponding to the parameters to be adjusted (\(\forall j : a_{ij} = 0\)) or zero plan utility corrections (\(\Delta S_i = 0\)). So, the advantage of this approach that it is not necessary that every agent has a choice set of equal size.

Certainly, some of the equations might be linearly dependent which happens fairly rare, but it does not change the fact that this system has no solutions.
and also can be written in matrix notation as:

$$\Delta \hat{\beta} = \argmin_{\Delta \beta} \| \Delta S - A \Delta \beta \|^2,$$  \hspace{1cm} (6.7)

where \(\Delta \hat{\beta}_j\) or \(\Delta \hat{\beta}\) denotes the approximate solution. The \(\| \Delta S - A \Delta \beta \|^2\) is the so-called objective function of the minimization problem, whose unique solution can be given by solving the following normal equations:

$$(A^T A) \Delta \hat{\beta} = A^T \Delta S,$$  \hspace{1cm} (6.8)

where the \(A^T\) denotes the matrix transpose of \(A\). The algebraic solution of the normal equations (Eq. 6.8) can be written as:

$$\Delta \hat{\beta} = (A^T A)^{-1} A^T \Delta S = A^+ \Delta S,$$  \hspace{1cm} (6.9)

where \(A^+\) denotes the Moore-Penrose pseudoinverse of \(A\). This equation (Eq. 6.9) works in many applications and also is used here because of its simpleness and straightforwardness, although it is not computationally efficient enough. Then the approximate new behavior parameters can be straightforwardly calculated:

$$\hat{\beta}' = \beta + \Delta \hat{\beta}$$  \hspace{1cm} (6.10)

### 6.2 Implementation

In this section the implementation of the theory of sec. 6.1 in MATSim simulation is introduced.

At first, it is explained how to implement it in one iteration. The total calculation in sec. 6.1 should take place after “iteration starts” (the marked point 2 in Fig. 2.1) and before “replanning” (the marked point 7 in Fig. 2.1), so that it is possible to calculate the new parameter set and prepare for the next round of “replanning” there. For the calculation the following 3 Terms are indispensable:

- The prior behavior parameter set \(\{\beta_j\}\) (\(\beta\)), which was calculated and used during the “scoring” in the last iteration and can be read from configuration in MATSim in “iteration starts” i.e. at the beginning of the iteration.

- As described above, the plan utility offsets \(\{\Delta S_i\}\) (\(\Delta S\)) can be generated by cadyts in the last iteration anywhere after “execution (mobsim)” (s. Fig. 2.1), thus cadyts has got enough information about the traffic situation (e.g. traffic volumes on the links, where count stations are installed) to calculate \(\Delta S\);
• the attributes \( \{a_{ij}\} (A) \) can also be obtained during the “scoring” (the market point 5 in Fig. 2.1).

The \( A^+ \) in Eq. 6.9 is solved by means of EJML (efficient-java-matrix-library\(^4\), version 0.18) whose codes were also written in Java.

Considering the stochasticity in MATSim (e.g. logit choice by replanning), the behavior parameter adjustment was carried out every iteration, i.e. the parameters were continuously revised every iteration. In principle, the traffic flows in every iteration are pulled in the direction of “better” counts reproduction, i.e. the absolute value of the most \( \Delta S_i \)'s should gradually decrease, at least during the first iterations, and all the \( \{\Delta \hat{\beta}_j\} \) approach toward zero, i.e. \( \hat{\beta}' \) is increasingly close to the “best” value of \( \beta \) with that the “best” counts reproduction can be achieved.

6.3 Small case study

The method of traffic behavior parameter adjustment in sec. 6.1 is applied in 2 small scenarios that have the same network and initial synthetic population, and different measurement and Scoring configuration. (sec. 6.3.1).

6.3.1 Scenario description

Network

This network (Fig. 6.1) is derived from MATSim equil example\(^5\), but there are only 2 parallel routes for “car”. The capacity and the length of link 19 are scaled up by about 20% and those of link 11 are scaled down by about 20% (Tab. 6.1). Moreover, link 2 has a freespeed that is half as fast as the others. Consequently, the route 2-11 (link Id) is the shortest one, and the route 10-19 is the fastest one in empty network.

Synthetic Population

In this small Scenario, there are only 100 agents. Each agent has only 3 (home(link 1)-work(link 20)-home) plans, 2 of them have different routes and can be performed

\(^4\)http://code.google.com/p/efficient-java-matrix-library/
\(^5\)http://matsim.svn.sourceforge.net/viewvc/matsim/matsim/trunk/examples/equil/network.xml
Table 6.1: Properties of the links in the network (Fig. 6.1).
only by car. By the rest one, agents use teleported public transit\(^6\) to cover the way to work, and drive for the way homewards.

The initial population for the next parameter calibration simulation is extracted from a steady (or at least relaxed) network condition of some iteration in a MATSim simulation that has parameter set \(\beta_{\text{car}} = -6.0\) and \(\beta_{\text{left}} = 0.0\)\(^7\) in the scoring function described in sec. 5.2.1 to estimate/adjust, and during that no plan innovation occurred i.e. every agent in the synthetic population has a fixed plan choice set and chooses its plan for the next iteration only according to logit choice model.

**Stationary measurement data**

The traffic volumes in a steady (or at least relaxed) network condition by one iteration of a MATSim simulation with different parameter set (e.g. in this section \(\beta_{\text{car}} = -4.5\) and \(\beta_{\text{left}} = -0.5\)) in MATSim scoring function than that for synthetic population generation are extracted to create synthetic counts for the following parameter calibration simulations, so that it is convenient to verify, whether the proposed calibration method does work.

**Scoring and Parameter adjustment setting**

The scoring function in this scenario is the same as that in sec. 5.2.1. Here, 2 behavior parameters are adjusted, their initial values and expectation for the parameter adjustment are listed in Tab. 6.2.

<table>
<thead>
<tr>
<th>Parameter to be adjusted</th>
<th>(\beta_{\text{car}}) [utils/h]</th>
<th>(\beta_{\text{left}}) [utils/left turn]</th>
</tr>
</thead>
<tbody>
<tr>
<td>Initial value</td>
<td>-6.0</td>
<td>-0.0</td>
</tr>
<tr>
<td>Expectation</td>
<td>-4.5</td>
<td>-0.5</td>
</tr>
</tbody>
</table>

Table 6.2: Initial values and expectations of parameters to be adjusted

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\(\beta_{\text{car}}\):\(^6\)public transport route with a “teleportation mode” that moves travelers on public transport trips at the fixed speed of 25 km/h. The length for public transport trip is estimated by multiplying beeline distance between origin and destination of this trip with a so called “beelineDistanceFactor” (here the default value 1.3 was used), in order to approximately express the (teleported) public transport trip length.

\(\beta_{\text{left}}\):\(^7\)represents penalty for a turning left, which some people do not like.
6.3.2 Results and analysis

Tab. 6.3 shows that the result of the parameter adjustment with the approach proposed in this chapter was not or only slightly influenced by \( \text{minStddev}^8 \), be that as it may, the larger the \( \text{minStddev} \) is, the more consistently the curves look.

<table>
<thead>
<tr>
<th>( \text{minStddev} )</th>
<th>( \beta_{\text{car}} ) [utils/h]</th>
<th>( \beta_{\text{left}} ) [utils/left turn]</th>
</tr>
</thead>
<tbody>
<tr>
<td>20</td>
<td>-4.46</td>
<td>-0.49</td>
</tr>
<tr>
<td>50, 100</td>
<td>-4.48</td>
<td>-0.50</td>
</tr>
</tbody>
</table>

Table 6.3: Adjusted behavior parameter: average values of the last 1000 iterations of some of the tests with different \( \text{minStddev} \).

Table 6.4: the log-likelihood values of MATSim simulations in the search space of different parameter settings (\( \beta_{\text{car}} \) and \( \beta_{\text{left}} \))

The adjusted parameter values agree with the expectation proved by the observation of the so-called log-likelihood values in search space (s. Tab. 6.4).

Comparison with the approach in Chapter 5

In this section, the approach proposed in Chapter 5 is applied to this scenario. Although in this approach a common standard deviation is used, the results of experiments are still worthy of analysis, because the traffic counts are not very large, if the \( \text{minStddev} \geq 25 \), the effect of utility offset are the same as when using common standard deviation (= \( \text{minStddev} \)). The results in Fig. 6.3 shows that the calibrated parameter curves have stabilized before the 1000th iteration, which is much earlier

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8 \( \text{minStddev} \) is a strictly positive real number that defines the smallest allowed standard deviation [48], the larger this parameter in cadyts is, the more count data with small count value are attenuated.
Figure 6.2: The adjusted behavior parameters $\hat{\beta}'$ from simulations with different $\text{minStddev}$ over iterations.
Figure 6.3: The calibrated behavior parameters in the small case.
than those in Fig. 6.2, although the converged values in Fig. 6.3 are not so plausible as those in Fig. 6.2, however they have met the general precision requirement of MATSim simulation.⁹

### 6.4 Real case study

This section presents a large case-study the purpose of which is to demonstrate the feasibility of the proposed calibration approach. The scenario in sec. 5.2.1 is directly adopted.

#### 6.4.1 Calibration results

The results of 10 simulations with 10 different synthetic traffic counts in sec. 5.2.3 are shown in the Fig. 5.1. Because of some unknown problems of the experiment environment, many simulations in this section were not run long enough. So only results of 4 simulations are shown here. Despite 7000 iterations, these curves in Fig. 6.4 can not convince us of their convergence, this means, this calibration method proposed in this chapter would find the best solution very slowly, if it could find the best one.

On the other hand, the calibrated values of $\beta_{car}$ stand between approx. -6.8 and -8.0, which are too far from the expectations.

### 6.5 Discussion

The method proposed in this chapter is just a simple least squared method:

- It is independent between all the iterations. This means, there is not direct correlation between iterations executed with respect to the process of param-

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⁹There is no concrete precision requirement for these parameters in MATSim. Nevertheless, the investigation of estimations carried out with other models shows the magnitude of variation of the estimated parameters, e.g. we investigate $\beta_{car}$, in MATSim $VTTS = \beta_{perf} - \beta_{car}$, VTTS is the abbreviation of the valuation of travel time savings. In [4] the estimated VTTS in Switzerland vary widely (from 10 to 100 CHF/h), and also are strongly dependent on travel distance, destination, income of traveler, and means of transportation. In this case in this chapter, the "true" value of $VTTS = 6 - (-4.5) = 10.5$, the estimated values are ca. 10.5 and 10.7, whose variation magnitude is much smaller than the results in [4].
Figure 6.4: The calibrated behavior parameters in the Berlin scenario.
eter estimation or optimization, which is decelerated by the randomness or uncertainty in MATSim simulation.

- This method does not include recursive algorithms and therefore, does not fast converge.
- This method also does not belong to descend method, thus an explicit direction to a minimum point as well does not exist.

Meanwhile, the method proposed in chapter 5 includes recursive algorithm and also implicitly has descend method.

On the other hand, the method proposed in this chapter tries to compensate the plan utility offset by adjusting parameters, which also can be seen as a linearization of network loading given the travel demand resulting from a particular choice of the behavioral parameters, and which just is a simplification of the estimation calculation and not sufficient for the parameter calibration. The plan utility offset is derived from normal distribution, and the first term of the objective function 5.7 in chapter 5 also realizes the same effect. So the effect of the second term of it can not be represented in the method proposed in this chapter. This means, the method proposed in this chapter takes into account only the deviation between observed and simulated flows, a priori obtained behavioral parameter estimates are not considered, which is the reason why the method proposed in this chapter works much better by the small synthetic case (sec. 6.3) than by the real case (sec. 6.4), whose result is so far away from the expectation. Because the small scenario is so simple, that there really is no correlation between $\beta_{\text{car}}$ and $\beta_{\text{left}}$, and the real scenario is completely the opposite.

### 6.6 Summary

At this stage, it is already possible to obtain an accurate enough estimate of parameters for traffic counts reproduction in small and simple scenario with the approach proposed in this chapter. For more complicated real cases, the method described in chapter 5 is a better choice. With the approach in chapter 5, the parameter est-

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10 if the estimated parameters do not strongly correlate with each other. For some parameter sets that contain parameters that closely correlate with each other, using none of the above-mentioned 2 approaches can obtain acceptable results.
timation much faster converges at much better results than the calibration with the relative simple approach in this chapter, especially by some real scenarios.
Chapter 7

Summary and Outlook

7.1 Summary

This dissertation presents concepts and implementation for making a fully disaggregate transport microsimulation (MATSim) more realistic in terms of simulated traffic flows.

MATSim was applied to the real study case in the region of Zurich in Switzerland and was validated against hourly traffic counts of 159 counting stations. The network improved by using the freely available openstreetmap data and adding choice dimensions (from “route choice only” to “route and time choice” and finally to “route, time, and mode choice”) to the agents lead to better/more realistic simulation results. Therefore it can be so interpreted, that the agents optimizing locally are able to collect local characteristics of the urban system, which are often disregarded by more aggregate methods.

Subsequently, a novel calibration method was applied to the calibration of the microscopic travel demand from traffic counts. The method:

- significantly improved simulation results in measurement and validation data fit,
- moreover, it regulated the demand in a behaviorally interpretable way, which is realized by computing and adding a utility corrections term to the systematic utility of every evaluated alternative/Plan in choice set, so that the simulated agents behave more realistically. A detailed analysis of these utility corrections:
  - clarifies their interpretation with respect to travel behavior;
• shows ways of their application to demand analysis;

• indicates possibilities for their further exploitation in the automatic calibration of disaggregate travel demand models.

As has been noted (Sec. 4.5), this aforementioned calibration method has its limitations, e.g. anything in the system that is presumably related to the link offsets is not allowed to be changed. Therefore, the capability of Cadyts has been expanded into behavioral model parameter calibration from network flow observations. Overall, the method can yield estimation results of plausible order of magnitudes which might not be precise enough in practical applications. Despite all this, some progress has been made in refinement of behavioral choice parameter.

7.2 Outlook

In Chapter 3, flow capacities of network links were roughly modified according to the road classification in OpenStreetMap, in order to adapt the network for the traffic simulation at the urban scale. However, this capacity modification could be finer, e.g. link flow capacity could be proportional to fraction of period when the light is green on the corresponding intersection at the end of the link, if the traffic signal-timing plan were available. This would make the transport microsimulation more realistic.

In this dissertation, all the calibration/estimation investigations are based on aggregate traffic flow measurements. In fact, any aggregate measurement that is a function of the state of a link or a turning move can be used directly in the cadyts-calibration.[37] This means sensor data sources and types could be applied to these traffic state calibrations, e.g. FCD, because it also records travel time/speed of links.

Location choice, in particular “secondary” activity location choice, is also configurable in MATSim simulation [58], which can also directly be calibrated with the same logic of calibration as in Chapter 4.

Because of a fixed choice set size in MATSim in consideration of computing power limits, it is impossible to save all the possible routes/plans in choice set, we can only try to keep the most representative routes/plans. The existing state of (route) choice set for the research in this dissertation is as follows:
• In Chapter 4, the plan choice sets of agents are built during the first phase of the simulation, by which the need of diversity of routes is not well met, because sometimes the (over)optimizing of agents could lead to similarity between alternatives in choice sets.

• In addition to this, due to all kinds of limiting factors (e.g. the restriction of the computer hardware resources), the plan choice sets in Section 5.2.1 were exogenously generated, so that it is easier to obtain a strong simulation response to variations in the behavioral parameters. Thus, these choice sets might not be realistic or at least not representative.

In reality, each driver/traveler has his own taste, i.e. his own criterion for route choice or generalized travel cost calculation, which certainly also depends on timing or occasion, e.g. route with the fewest (sharp) turns, the most comfortable route (e.g. with the least bumpings), the shortest route, the fastest route, route with the least fuel consumption, the most economical route (e.g. depending on toll), route with the most main roads fraction, route with the best landscape, the safest route and so on. Although some of them can still not be taken into account by MATSim, better choice set (primarily better car-route) generation algorithms are required, which can generate route choice sets with enough diversity and representativeness. The amelioration of route choice sets directly influence at least the quality of the results of travel behavioral calibration, therefore it is worth the effort to create better (route) choice set, which contains many enough meaningful, representative routes.

On the other side, the current standard version of scoring function in MATSim focuses on (dis)utility of traveling and performing activities, in an extended version the personal economic situation of agents has also been included [63], this means, there are too few parameters to estimate. Moreover, when more than 1 parameter is estimated at a time, these parameters should not correlate too strongly, otherwise it is also very difficult to distinguish between their traffic effects. On the other hand, the current scoring function can not interpret some traffic phenomena (e.g. someone chooses a slower route just because of the scenery along the way) in detail. Therefore, it is worth adding new parameters to the scoring function in MATSim, e.g. parameters for driving experiences: angel of turning, number of turns/intersections, driving speed, number of brakings and so on, even though some of them are very difficult to measure.
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