

Choice model refinement from network data

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1 Introduction

This article 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 (Nagel and Flötteröd, forthcoming; Cascetta, 1989).

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 (Antoniou et al., 2007; Balakrishna, 2006; Vaze et al., 2009). 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 Flötteröd et al. (2011) is an exception; here, a tractable analytical approximation of a complete DTA microsimulation system is developed and exploited. That research

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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 article 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 article is structured as follows. Section 2 outlines MATSim, the DTA microsimulation deployed in this work. Section 3 develops the proposed calibration approach. Section 4 then presents a large-scale case study, which is based in parts on real and in parts on synthetic data. Finally, Section 5 discusses the results and indicates possibilities for further improvements.

2 Outline of deployed DTA microsimulation

The experiments reported in this article are conducted using the MATSim simulation software ("Multi-agent transport simulation toolkit", www.matsim.org). Since both its principles and its technical peculiarities are described in various other publications (e.g., Nagel and Flötteröd, forthcoming; Flötteröd et al., forthcoming; Raney and Nagel, 2006), this section constrains itself to a presentation of its core aspects. MATSim is agent-based in that it models the all-day travel behavior of individual decision-makers, which are denoted here by n = 1...N. The travel behavior of an agent is encoded in its travel plan, which comprises a complete trip sequence, including mode and departure time information for each trip. The choice set of agent n's travel plans is denoted by C_n . In its general design, MATSim allows this choice set to evolve in the course of a simulation. For the purposes of this study, however, the choice set is exogenously and a priori defined. Its construction is described in Subsection 4.1.

Agents select their travel plans in consideration of network congestion and the resulting travel times. MATSim uses a multinomial plan choice model (e.g., Ben-Akiva and Lerman, 1985) and a utility function of the following structure (Chary-

par and Nagel, 2005):

$$V(plan) = \sum_{\log l} V(l) + \sum_{\text{activity } a} V(a)$$
(1)

The utility V(a) of performing an activity a is positive and has the following functional form:

$$V(a) = \beta_{act} \cdot t^*(a) \cdot \ln t(a)$$
⁽²⁾

where $t(\alpha)$ is the actual duration of activity α , $t^*(\alpha)$ is its ideal (intended) duration, and β_{act} is the marginal utility of an activity at its typical duration. The (disutility) V(l) of traveling along a leg l is typically a linearly decreasing function of the travel time t(l) along that leg, with a mode-dependent slope. The concrete functional form for travel (dis)utility used in this article differs somewhat from the "usual" form; hence, it is only described together with the concrete case study in Subsection 4.1.

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, which are loaded on the network using a queueing simulation with spill-back (Cetin et al., 2003; Gawron, 1998). This mutual dependency is iteratively resolved, where an iteration can be intuitively thought of as a "simulated day": In every iteration, every agent n selects a travel plan from C_n to be executed in that day, and then the travel plans of all agents are executed jointly in the mobility simulation, generating network flows. Due to limited network capacities, congestion and delays occur. This information is observed by the agents and accounted for in the next iteration. Eventually, the system attains a stationary regime where travel demand (represented by plan choice distributions for all agents) and network supply (represented by time-dependent network conditions) are mutually consistent. These "equilibrated" or "relaxed" conditions constitute the solution of the DTA model system. Denote by Π_{ni} the probability that agent n selects plan i in stationary conditions. $\Pi = (\Pi_{ni})$ is the vector of stationary choice probabilities for the entire agent population.

3 Calibration approach

This section derives the proposed calibration approach. Subsection 3.1 develops an analytical approximation of the measurement equation that connects timedependent network flows and behavioral model parameters. It builds on earlier findings by Flötteröd et al. (2011). Subsection 3.2 then formulates a nonlinear least squares estimator and clarifies how this estimator is inserted into the iterative logic of the DTA simulation. Finally, Subsection 3.3 derives an approximation of the parameter covariance matrix for this estimator.

3.1 Analytical approximation of measurement equation

The calibration objective is to identify a vector β of behavioral model parameters, such as travel time coefficients or alternative specific constants for certain modes, given a vector of observed network flows $\mathbf{y} = (y_{ak})$, 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 \mathbf{y} to the parameters β . However, this effort is worthwhile because it allows to extract gradient information, which can be exploited to accelerate the calibration process and to analyze solution properties.

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

$$d_{ak} = \sum_{n=1}^{N} \sum_{i \in C_n} \mathbf{1}(i \sim ak) \Pi_{ni}$$
(3)

where $i \sim ak$ reads as "following travel plan i implies entering link a during time step k", and $\mathbf{1}(\cdot)$ is the indicator function. 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

$$q_{ak} = \alpha_{ak} d_{ak} + \beta_{ak} \tag{4}$$

is assumed, where α_{ak} and β_{ak} are real-valued coefficients. Assuming for now that these coefficients are known, (3) and (4) can be combined into a linear mapping of plan choice probabilities Π on link flows $\mathbf{q} = (q_{ak})$:

$$\mathbf{q} = \mathbf{L}\mathbf{\Pi} + \mathbf{b} \tag{5}$$

where the matrix $\mathbf{L} = (l_{ak,ni})$ consists of elements $l_{ak,ni} = \alpha_{ak} \mathbf{1}(i \sim ak)$ and the vector $\mathbf{b} = (\beta_{ak})$ is composed of the intercepts of model (4).

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

$$\Pi(\boldsymbol{\beta}) = \int \mathbf{P}(\mathbf{x}; \boldsymbol{\beta}) \pi(\mathbf{x}) d\mathbf{x}.$$
 (6)

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

$$\mathbf{q}(\boldsymbol{\beta}) = \mathbf{L}\mathbf{P}(\bar{\mathbf{x}};\boldsymbol{\beta}) + \mathbf{b}.$$
 (7)

This is the analytical approximation of the measurement equation used in this article. Given a behavioral model that yields choice probabilities that are differentiable with respect to the behavioral model parameters, its Jacobian can be written as

$$\frac{\partial \mathbf{q}(\boldsymbol{\beta})}{\partial \boldsymbol{\beta}} = \mathbf{L} \frac{\partial \mathbf{P}(\bar{\mathbf{x}}; \boldsymbol{\beta})}{\partial \boldsymbol{\beta}}.$$
(8)

3.2 Nonlinear least squares estimator

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

$$\min_{\boldsymbol{\beta}} Q(\boldsymbol{\beta}) = \frac{1}{2} (\mathbf{y} - \mathbf{q}(\boldsymbol{\beta}))^{\mathsf{T}} (\mathbf{y} - \mathbf{q}(\boldsymbol{\beta})) + \frac{1}{2} (\boldsymbol{\beta}^{0} - \boldsymbol{\beta})^{\mathsf{T}} \mathbf{W} (\boldsymbol{\beta}^{0} - \boldsymbol{\beta})$$

s.t. $\mathbf{q}(\boldsymbol{\beta}) = \mathbf{L} \mathbf{P}(\bar{\mathbf{x}}; \boldsymbol{\beta}) - \mathbf{b}$ (9)

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, β^0 is a vector of prior parameter estimates and $\mathbf{W} = (w_{ij})$ 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 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 Flötteröd et al. (2011), 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 in every iteration of the DTA microsimulation:

- 1. A parameter vector β is estimated, relying on a linearized network loading.
- 2. Using β , 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 Madsen et al. (2004) and exploiting the analytically available Jacobian (8). 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 (4). This is accomplished by (i) observing after step 2 of each iteration the current link demand d_{ak} according to (3), (ii) observing after step 3 the resulting link flow q_{ak} , and (iii) updating α_{ak} and β_{ak} for each link separately with a recursive regression step. This approach was already successfully deployed by Flötteröd et al. (2011) 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.

3.3 Parameter covariance analysis

The previous subsection proposes to computing 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:

$$E\{\beta\} \approx \bar{\beta} = \frac{1}{c_2 - c_1 + 1} \sum_{c=c_1}^{c_2} \beta^{(c)}.$$
 (10)

To analyze some properties of this estimator, all stochastic quantities of the DTA simulation that may possibly affect the parameter estimates β are summarized in a disturbance vector ε . The variance/covariance matrix VAR{ β } of the parameter estimates can then be decomposed as

$$VAR\{\beta\} = E\{\underbrace{VAR\{\beta \mid \varepsilon\}}_{1}\} + VAR\{\underbrace{E\{\beta \mid \varepsilon\}}_{2}\}.$$
(11)

Elements 1 through 4 of this expression are computed as follows.

1. The covariance VAR{ $\beta^{(c)} | \epsilon^{(c)}$ } of the parameter estimates $\beta^{(c)}$ within a single iteration c and given the stochasticity $\epsilon^{(c)}$ of that particular iteration is computed with a sandwich estimator (e.g., Greene, 2003)

$$VAR\{\beta^{(c)} \mid \varepsilon^{(c)}\} \approx A^{(c)}B^{(c)}A^{(c)}$$
(12)

where

$$A^{(c)} = \left(\frac{\partial^2 Q(\beta^{(c)})}{\partial \beta^2}\right)^{-1}$$
(13)

$$B^{(c)} = \sum_{\alpha k} \frac{\partial q_{\alpha k}(\beta^{(c)})}{\partial \beta} \frac{\partial q_{\alpha k}(\beta^{(c)})}{\partial \beta}^{\dagger} + \mathbf{W}.$$
(14)

The Hessian in (13) is numerically computed. The second addend in (14) results from the treatment of the prior parameter vector β^0 as a supplementary set of measurements, following the arguments of Spiess (1987). A more careful analysis of this covariance component is certainly desirable and possible (Greene, 2003).

- 2. $E\{\beta^{(c)} | \epsilon^{(c)}\} = \beta^{(c)}$ because $\beta^{(c)}$ results from the minimization of (9), which is deterministic for a given $\epsilon^{(c)}$.
- 3. The expectation $E{VAR{\beta | \epsilon}}$ is approximated using the arithmetic mean over many iterations in stationary conditions:

$$E\{VAR\{\beta \mid \epsilon\}\} \approx \frac{1}{c_2 - c_1 + 1} \sum_{c=c_1}^{c_2} A^{(c)} B^{(c)} A^{(c)}.$$
 (15)

4. The variance VAR{E{ $\beta \mid \epsilon$ }} is also approximated by an average over many iterations in stationary conditions:

VAR{E{
$$\beta \mid \epsilon$$
}} $\approx \frac{1}{c_2 - c_1 + 1} \sum_{c=c_1}^{c_2} (\beta^{(c)} - \bar{\beta})^2.$ (16)

The feasibility of approximations (15) and (16) depends on the ergodicity of the stochastic process implemented by the iterated simulation system (e.g., Ross, 2006). 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 4.

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.

4 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.

4.1 Scenario description

This case study considers the Greater Berlin area, with a network size of 24335 links and 11345 nodes. A synthetic population of 57688 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 (Kutter et al., 2002; Scheiner, 2005; Rümenapp and Steinmeyer, 2006). A more complete description can be found in Moyo O. and Nagel (2012). 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 (Grether et al., 2009; Rieser et al., 2009). 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 (1) is defined for the purposes of these experiments (other forms are possible and have been used) as

$$V(l) = \begin{cases} \beta_{travel,car} t(l) + \beta_{left} n_{left}(l) & \text{if } l \text{ is by } car \\ \beta_{travel,non-car} t(l) & \text{otherwise.} \end{cases}$$
(17)

Here, $\beta_{travel,car}$ is a negative coefficient for the travel time t(l) if leg l uses the car mode, β_{left} is a negative coefficient for the number of left-turns $n_{left}(l)$ in leg l, and $\beta_{travel,non-car}$ 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.

4.2 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 (17) is computed based on the following parameter values: $\beta_{travel,car} = -4.5 \text{ EUR/h}$, $\beta_{left} = -0.5 \text{ EUR}$, $\beta_{travel,non-car} = -3 \text{ EUR/h}$, and $\beta_{act} = 6.0 \text{ EUR/h}$. MATSim is then run with these parameters, using otherwise the configuration described in Subsection 4.1, 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 simulation. Hence, there are ten independent sensor data sets available, all of which are generated based on the same behavioral parameters, but being stochastically different due to the randomness of the MATSim simulation logic.

4.3 Calibration results

Ten experiments, each with one of the ten independently generated synthetic measurement data sets, are conducted. The simulation configuration of these experiments differs from the configuration in which the synthetic traffic counts were created in that "wrong" values for the in-car travel time and for left turns are used: $\beta^0_{travel,car} = -6.0$ EUR/h and $\beta^0_{left} = 0.0$ 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 $\boldsymbol{\beta} = (\beta_{travel,car}, \beta_{left})^T$ is calibrated, using the prior estimates $\boldsymbol{\beta}^0 = (\beta_{travel,car}^0, \beta_{left}^0)^T$ 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 stationary iterations, and the parameter covariance matrices are computed as described in Subsection 3.3, also over all stationary iterations. Figure 1 visualizes the results. 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 denotes the parameter estimate only of the last iteration of an experiment, without any averaging. The coordinate axes intersect at the true parameter values $(\beta_{tt}^*, \beta_{left}^*) = (-4.5, -0.5)$. Note the different scalings of the axes.

Overall, the parameter estimates are near the true values, but have a visible bias in that β_{tt} is underestimated by approximately 0.5 and β_{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



Figure 1: Estimated parameters and 95% confidence regions

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 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 (3)-(5) 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 (Flötteröd and Bierlaire, 2009), nonlinear network dynamics in general are known to be very difficult to account for when calibrating travel demand from traffic counts (Frederix, 2012). 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 (6) 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 Osorio (2010), where a structural analytical model is supplemented with a regressionbased approximation of the objective function, appears particularly applicable to this problem.

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