Destination choice modeling with spatially distributed constraints

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Abstract: Destination choice models are a key component of any transport and land-use model. Applications in agent-based models allow for destination choice on an individual level including personal variables, like trip purpose, or situational variables. Commonly applied methodologies stem from econometrics, discrete choice theory and utility maximization using either revealed or stated preference data. This paper presents a framework to integrate cross-section flows between distinct geographic areas, which can be obtained from cordon surveys or mobile phone data. Proposed optimization methodology—based on extended shadow price theory—accommodates these complementary data sources as spatially distributed constraints, in addition to the destination capacity constraints such as workplaces.

The new generic and robust optimization methodology accounts for constraints as observed on cross-section flows and destination capacities while maintaining econometric choice model theory. As a proof of concept, the suggested methodology is successfully applied in a real-case, agent-based application covering the tri-national Basel region with about 2 million residents, and a large set of $2 \cdot 10^4$ distinct destination alternatives. Due to different wage levels in all three countries and other reasons, the region's cross-border commuter flows are highly asymmetric. Including data on cross-border flows obtained from a cordon survey, the choice model's mean deviation declines by 20% and more on a cross-section level and even more so on a choice alternative level, compared to calculations ignoring shadow prices. Moreover, multiple scenario calculations show considerable improvements in planning and forecasting applications. The results demonstrate the suitability and relevance of the proposed approach to optimize destination choice models with limited destination capacities in geographical regions usually characterized by travel demand asymmetries.

Keywords: Destination, choice, model, shadow, prices, transport

1   Introduction

Destination choice models are key components of both aggregated travel demand flow models and disaggregate, activity-based models. Destination choice models assign either aggregated demand flows or individuals with their distinct characteristics to destination locations where they perform their activi-

ties, and therefore affect trip patterns of individuals, households and firms. Depending on trip purpose, either singly or doubly constrained trip distribution models are applied as part of aggregated travel demand models to describe travel flows between different locations for different trip purposes (Ortuzar & Willumsen, 2011). Doubly constrained models ensure that information on the number of both generated and attracted trips can be taken into account. In this way, that when describing the distribution of work or education trips it can be ensured that only as many trips end in a specific destination as jobs or education opportunities are actually available. However, as such modelling approaches describe aggregated flows, individual-specific information such as car availability or profession type can only be taken into account if the trip distribution model is segmented for specific groups which increases the modelling and computation burden substantially, especially at detailed and large-scale models.

Disaggregated destination choice models on the other hand can flexibly include alternative specific and person specific variables (e.g., generalized utilities) and situational variables, as weather or weekdays, to a lesser extent. However, constraints at destinations, such as the number of available workplaces at a specific zone, have so far only rarely be considered in the application of disaggregated destination choice models. At the same time, disaggregated activity-based models generally would allow to not only take into account hard constraints, such as the number of jobs in a certain work sector within a specific area, but also time-dependent factors such as the overcrowding of certain facilities such as shopping centers or leisure facilities as soft constraints.

Additionally, constraints can affect entire cross-section flows, e.g., between geographic areas. In case of subdivided geographic areas with border lines, destination choice is affected by potential cross-section impedance, different wage levels, language barriers or capacity restrictions at border lines. These aspects are both key in planning and often addressed with manual travel demand corrections. Impedance factors are often unknown or difficult to determine quantitatively in parameter estimation, but still needed to be included in the choice model application. Destination choice models are therefore unlike matrix fitting models like the gravity model, which fit the entire travel demand flows according to the marginal totals.

In this paper we propose and investigate the applicability of a new approach that allows to account for hard constraints both with regards to the distribution of work and education trips as well as cross-section flows. The proposed approach is applicable in the context of large-scale aggregated models such as national models, or activity-based travel demand models as described in comprehensive overviews in Vovsha et al. (2004) and Rasouli and Timmermans (2014); examples are DaySim (Bradley et al., 2010), ActivitySim (ActivitySim, 2019), SimMobility (Adnan et al., 2016) or CEMDAP (Bhat et al., 2004). We refrain from also addressing soft and time-dependent constraints in this paper as such constrains refer to short term choices which are covered by different modelling approaches in separate stages of the activity-based travel demand modelling process.

To this end, the following two research questions are addressed in this paper: (1) Given the travel census data availability, can we increase destination choice model quality by adding complementary data and constraints such as empirical cross-section flow data or destination capacity data, to address these spatially distributed constraints? Assuming constraints on both cross-sections and destination alternatives, the proposed methodology should then aim to optimize any origin-destination relation and underlying individual choices, which are approximated to the empirically given exogenous constraints. (2) Is it possible to implement such a methodology with spatially distributed constraints within destination choice models, also in large-scale applications with > 10,000 potential destinations, like currently running destination choice models at authorities and in planning practice, and in a robust manner (e.g., sufficient convergence)? And as part of an integration or application, how can we deal with parameter values in scenarios and forecast calculations that might include adaptions with regards to a proposed methodology?

The below introduced methodology and destination choice model are part of a real-case activity-and agent-based travel demand model, coupled with a multimodal transport simulation MATSim (Horni et al., 2016). This paper proposes a destination choice model assigning workers to corresponding workplaces and focuses specifically on commuters; however, also students of three different age groups are successfully assigned to school locations taking into account the respective education level (primary, secondary and tertiary level mirror the educational system) with an identical methodology. While focusing on an encompassing destination choice model in Vitins et al. (2016), this paper focuses on generalized theory for spatially distributed constraints in destination choice, and applicability in a large-scale case study (tri-national Basel agglomeration) with 20,000 potential destinations. Due to the different wage levels in the three countries and different spoken languages, the region's cross-border commuter flows are highly asymmetric. This paper additionally includes multiple scenario calculations for planning and forecasting applications, showing its potential and robustness for a variety of cases.

2   Literature review

2.1   Utility-based models and alternative methods

Destination choice on an individual level builds on the idea of individuals having a choice among distinct destination alternatives, as described in micro-econometric choice theory (e.g., Ben-Akiva,1973; McFadden, 1974). Micro-econometric utility maximization theory assumes different utilities among choice alternatives, and decisions depending on individuals' utility maximization. (1a) represents the general logit formula with utility u for person k and alternative i. (1b) describes multinomial logit (MNL) assumptions with deterministic components of commonly linear β coefficients, (transformed) attributes X and error term ε iid extreme value. (1a) and (1b) are refined for segmented, non-linear, generalized utility functions, or complemented shadow prices as shown in this paper.

$$p_{i,k} = \frac{e^{u_{i,k}}}{\sum_{j \in J} e^{u_{j,k}}} \tag{1a}$$

And for MNL with:

$$u_{i,k} = \beta_{0,i,k} + \sum_{n} \beta_n X_{i,k,n} + \varepsilon_{i,k} \tag{1b}$$

(1a) and (1b) have been applied and advanced in numerous destination choice models, including relaxation of above independence and error distribution assumptions of error term ε, or alternative-specific effects of β related to the attributes (Adler & Ben-Akiva, 1976; Ben-Akiva & Lerman, 1985; Ben-Akiva, 1973; Fotheringham, 1986; Waddell, 1993). However, discrete choice models as described in (1a) and (1b) ignore consideration of other individuals' choices; destination choice models often exclude mutual decisions in existing literature, unlike e.g., market models which simulate entire market behavior (as mentioned below as alterative approach). Such choice models are specifically relevant to prevent overcrowding at constrained cross-sections or at favored alternatives; this paper builds on to these ideas as described below.

Gravity models have provided an alternative approach to choice modeling, and have been applied widely since the early years of transport modeling. Origin – destination flows are fitted with a matrix-fitting method (e.g., Deming & Stephan, 1940; Pukelsheim, 2013; Rich & Mulalic, 2012), and therefore are capable of restricting flows on both cross-sections and specific origins and destinations. Even though Anas (1983) showed consistency of the logit model of joint origin-destination choice, and

a doubly constrained gravity model, above mentioned utility-based choice models have further evolved in transportation theory and are mostly preferred in applications; and recent developments have reproduced more detailed behavioral characteristics.

Market models are additional, alternative methods applied for destination choice and model individual choices under market constraints (Hackney et al., 2013; Hurtubia et al., 2010). Hedonic price models are often coupled with utility-based choice models, and iterative procedures avoid over- and undercrowding (e.g., Kockelman, 2011; Zhou & Kockelman, 2011). Market models mirror and integrate interaction between individuals, and therefore they differ from choice modeling of isolated individuals in a static environment. It remains unclear how market models are also applicable in transportation modeling since auction behavior possibly diverges from transport-related behaviors.

2.2   Capacity constraints and shadow prices

Shadow prices serve as impedance for attractive alternatives with limited capacity, and therefore offer a generic approach for constraint choice models. Shadow prices reflect alternatives' constraints as explained in the following example based on micro-economics and productivity optimization. In an imperfect or inefficient market situation, demand possibly exceeds supply due to distributional effects; then, shadow price implementation allows market model extension (Bhattacharyya et al., 2019). In economics, shadow prices are used to estimate the unknown costs of a certain good or alternative. A price $p > 0$ can be assumed as well as a stock of X with sold units x where $0 \leq x \leq X$, and the objective max(px). Customers buying units x optimize their utility u, with respect to their time and budget limits, resulting in at least two dependent optimization problems. Any resource is considered a constraint (e.g. time, units), if the number that customers would like to use exceeds availability. In linear programming, shadow prices are associated with constraints, and define how much the optimal value of the objective would increase per unit increase in the amount of resources available, or how much individuals are willing to pay. They are equal in most cases to the solution of the dual variables of a given constrained linear program (Wagner, 1975).

In destination choice, shadow prices can be assigned to constrain capacities of alternatives and are therefore regarded as additional impedance for persons destination choice. Shadow prices account for the capacity and scarcity constraints of these alternatives, and mirror the marginal utility of relaxing capacity constraints. Vitins et al. (2016) estimated primary destination choice on the entire Singapore city-state, including generalized utility and log(alternative capacity).Results showed that quality of the model (ρ^2) increased considerably due to consideration of constrained capacities at destinations, and applied shadow price methodology. In comparison, the current paper adds to the generalized theory for spatially distributed constraints in destination choice, and applicability in a Basel case study with multiple scenarios presented in the result section. The literature in the field of transportation modeling includes additional applications of shadow prices (e.g., Beckmann & Wallace, 1969; de Palma et al., 2007), and few applications in behavioral choice models (Gupta et al., 2014; Spiess, 1966); however detailed methodology and references lack in literature for primary destination choice models.

Additional challenges as spatial correlation are tackled in choice model estimation due to unobserved spatially distributed and demographic attributes (Bhat & Guo, 2004; Sener et al., 2011). As an example, Bernardin et al. (2017) improved travel demand estimation at state border crossings through utility function adaption, and compared results with expanded cell phone data based on traffic shares and population within districts, before and after calibration. Large alternative sets are also challenging in destination choice modeling due to required computational resources, and sampling techniques are discussed widely (Lee & Waddell, 2010: McFadden, 1978), also for geographic purposes (Kwan & Hong,

1998; Lee & Waddell, 2010; Thill, 1992). Frejinger et al. (2009) and Nerella and Bhat (2004) found that a large number of observations are needed to achieve reasonable model parameter values. Nerella and Bhat (2004) suggested drawing 1⁄8 from the full choice set size as a minimum and 1⁄4 as a desirable sample share—in the case of their MNL models, and non-MNL models are even more demanding about required sample size.

3 Data sources for basel case study application

3.1 Case study area and population

The considered case study area covers 5,460 km² (85 km long and 91 km wide) with 1.96 million inhabitants as of 2015. Basel as the main city lies in the corner of three nations: Switzerland, Germany, France; therefore, this region is often called the tri-national region. Population and workplaces are defined for 20,645 spatial zone units as indicated in Figure 1(a). In an inner area around Basel, the zones are generated based on hectare raster cells with a 100m side length. The zone length in the outer core area amounts 200m, while the remaining area is covered by zones representing municipal borders. The population distribution is displayed in Figure 6(a) focusing on Basel city, and workplace distribution in Figure 6(b) (placed in "Results" section for later outcome comparison). Data is provided from BfS (2019) for Switzerland and complemented for German and French areas based on Bau- und Verkehrsdepartement Basel-Stadt (2015), BfS (2019). A synthetic population is defined in an initial step of the real-case activity- and agent-based travel demand model Basel and is based on a Bayesian network approach (Sun & Erath, 2015).

Table 1 provides an overview of the required data and variables for the destination choice model of the Basel region, including survey data described below. Complementary model and data information is provided in Vitins et al. (2021) for the entire activity-based travel demand model and all modeling steps, beside the destination choice model.

Table 1. Required data for the destination choice model of the Basel region, including regions of Switzerland, Germany and France

	Variables:		Granularity:

Synthetic population:	- Age
	- Gender
	- Home location
	- Part-time worker
	- Citizenship
		- Household size
		- Car license
		- Car ownership
		- Public transport
		  season ticket type
			- Address level
			- Alternatively:
			  zones

Choice alternatives	- Travel time
	- Parking search time
	- Gas, parking, car costs
	- Access, in-vehicle time
		- Ticket costs
		- Vehicle interchange
		  impedance
		- Service frequency
			- Destinations /origin desti-
			  nation pairs

Constraints:			
Cross-section flows:	- Travel flows between defined geographic regions		- National borders
Destination capacities:	- Workplaces and educational opportunities		- Destination zones

3.2   Survey data

3.2.1   Workplace survey data

A workplace survey data is derived from BfS (2019) for Switzerland and from Bau- und Verkehrsdepartement Basel-Stadt (2015) for France and Germany. Data is standardized for the study area based on former studies and projects within the Basel region. Workplace survey data serves as a destination capacity constraint in the proposed destination choice methodology.
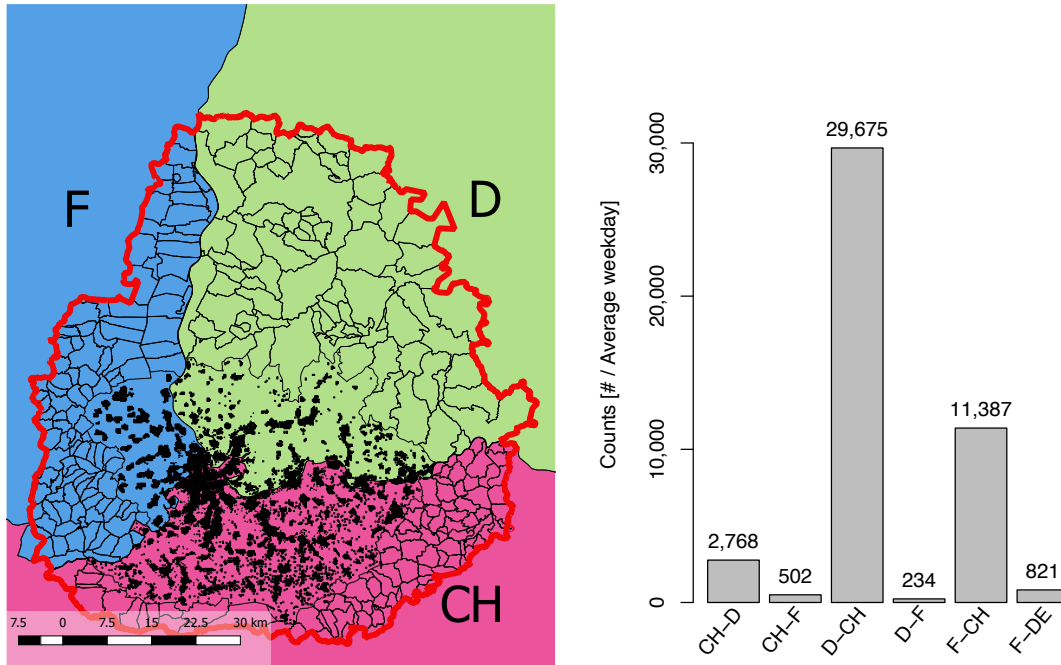
(a) Model region with perimeter border, zones, and country borders between France (F), Germany (D) and Switzerland (CH).

(b) Empirical cross-section flows between regions for home-based commuting trips.

Figure 1. Model overview and considered commuters cross-section flows

Source: Bau- und Verkehrsdepartement Basel-Stadt (2015)

3.2.2   Cross-border flows

The cross-border flow data is derived from a cordon line survey conducted in 2010 (Bau- und Verkehrsdepartement Basel-Stadt, 2015) for specific trip purposes, as displayed in Figure 1(b). The flow differences are considerable and are accounted for in the proposed choice model approach. The cross-border flows are available for an inner region indicated in Figure 1(a) with small raster cells. An identical perceived behavior is assumed for remaining flows and border impedance. The main motivation of this research is to optimize a destination choice model application with empirical and also asymmetric flows, to improve model results.

3.2.3   Travel distance distributions

The travel distances are derived from census data of the Swiss Mobility and Transport Microcensus (MTMC) (Swiss Federal Statistical Office (BFS), 2017) conducted in 2015 by the Federal Office for Statistics of Switzerland (further referred to as "MZMV 2015"). The resulting travel distances of this paper, based on the destination choice model, are compared against census data for validation purposes (see in "Results" section). The census includes data of 57,090 interviewed persons and their households provides a substantial sample for travel behavior evaluation. The households were selected systematically from within Switzerland, with higher densities in larger cities and agglomeration regions. Additionally, the resulting travel distances of this paper are compared against a commuter flow evaluation conducted originally for the whole of Switzerland in 2011 (BfS, 2019), where commuter flows were derived from population and workplace registers.

3.3   Available destination choice model of Basel region

This paper proposes and applies a shadow price methodology and therefore relies on an already existing destination choice model which is available and applied in the transport model of the Basel Region (Bau- und Verkehrsdepartement Basel-Stadt, 2015). Choice model parameter fitting and estimation are omitted for the destination choice model in this paper (see also Chapter 4 for detailed methodology explanations). The model parameters of the already existing destination choice model were estimated as an MNL model separately for individual trip purposes, namely commuting, educational, shopping, leisure and service trips. The existing model includes a logsum formulation for the generalized cost calculation, based on four transport modes, namely car, public transport (pt), bicycle and pedestrian modes. The following variables and corresponding parameters are available for the generalized cost calculation: For *car, travel times, distance, estimated parking search time, gas costs, parking* and *car costs* are considered in the model. For pt, *in-vehicle time, access time, ticket costs, vehicle interchange, service frequency, season card availability* were used. Travel time is used for bicycle and pedestrian trips, calculated with average travel speeds. Parameter values are further used for utility (u) calculation, mentioned as β parameters in Section 4.1. From a scientific perspective, different variables possibly allow model quality improvement, e.g., season card availability can lead to an endogenous bias; also, the utility formulae can be replaced with a more comprehensive generalized utility approach. The existing model is limited regarding these aspects but still valuable from an application point of view, and suitable for the following shadow price methodology and application.

4   Methodology

The proposed methodology focuses on destination choice for transport demand estimation, and therefore refers to agents travelling to destinations for activity execution. Two generic constraints, namely for destination capacities and cross-section flows, are added in proposed methodology.

Destination constraints are relevant in destination choice models because capacity is potentially exceeded when applying a choice model on each agent without knowing the decisions of other agents. Since destinations are potentially constrained in their capacities, e.g., at workplaces, we assume that workplace numbers serve as an upper limit, or are exactly known. Technically, workplace constraints are defined as a one-dimensional constraint (array), whereas each array value refers to only one specific destination. In the two-dimensional case for cross-section flows, we refer to exogenous information on cross-sections, such as counts, between defined geographic regions. The counts can be available between

two regions separated by a mountain range or political border. Then, the cross-section counts serve as constraint when assigning specific destinations to certain agents. One- or two-dimensional constraints are therefore independent of each other, and can be considered alone or jointly in destination choice models. Figure 2 depicts both categories of spatially distributed constraints; the x and y axes represent destinations and origins, such as workplaces and home locations. The proposed methodology offers a
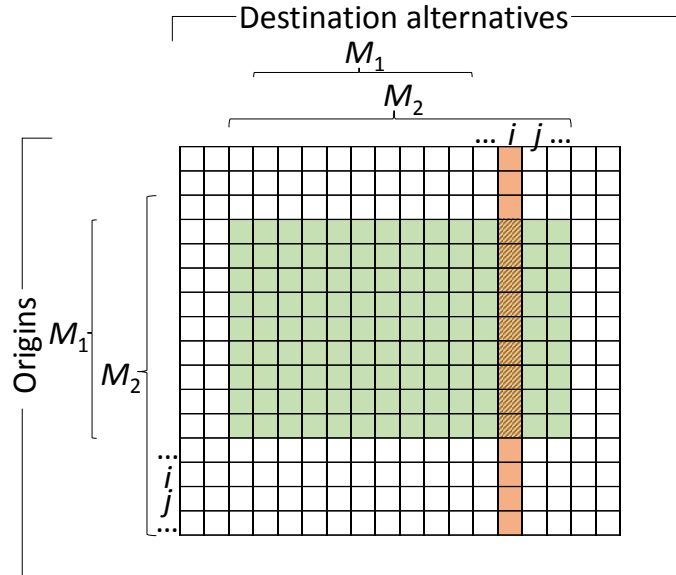

Figure 2. One-dimensional destination constraint (orange) i and two-dimensional cross-section constraint M_1–M_2 (green)

broad application potential for one- and / or two-dimensional constraints as showed in Figure 2, e.g., considered capacity constraint at transit vehicles in route or departure time choice. Unlike Vitins et al. (2016), this paper focusses on two-dimensional constraints and a detailed case study application and scenario calculations. Due to additional, more generic constraints, the methodology is adapted and rewritten in the following based on new formulae and content.

4.1   Shadow price calculations for destination choice models

The following methodology aims at refining existing model approaches for destination choice intransport models, and starts with the same premises as MNL choice models (1a), however, thefollowing modifications are added:

1. The shadow prices are defined and calculated as dis-utility added to the destinations dueto capacity restrictions. So, the shadow prices are positive, and are negatively perceived by choice makers.
2. On the one hand, it is assumed to be impossible to assign more workers to designated workplaces than indicated in the workplace survey data. On the other hand, we assume certain vacant workplaces. Therefore, an assignment balance is defined with a certain upper restriction (ceiling constraint).
3. The cross-section flows are exogenous values; in the following it is assumed that they match with modeled flows (exact approximation).
4. All exogenous constraints need to allow a feasible solution.
5. The choice model parameters for the utility calculations are given as input parameters, and therefore estimated beforehand (e.g., with Biogeme (Bierlaire, 2019)).

Starting with above MNL model (1a), the probability $p_{i,j}$ of choosing alternative destination j and travel demand $g_{i,j}$ are defined as:

$$g_{i,j,k} = P_{i,k} \cdot p_{i,j,k} = P_{i,k} \cdot \frac{e^{u_{i,j,k}}}{\sum_j e^{u_{i,j,k}}} \tag{2}$$

whereas $u_{i,j,k}$ equals the deterministic utility of alternative j. $P_{i,k}$ is the number of individuals commuting from origin i (a building or a zone), and k is a specific person or person group with a potentially person-specific utility. It can be shown that the following convex minimization problem (3a) is equivalent to (2) and its probability-based notation, by applying the Karush-Kuhn-Tucker conditions (Horst, 1979):

$$\text{Min} \sum_{i,j,k} g_{i,j,k}\big(ln(g_{i,j,k}) - 1 - u_{i,j,k}\big) \tag{3a}$$

subject to:

$$\sum_j g_{i,j,k} = P_{i,k} \ \text{ for all } k. \tag{3b}$$

The capacity restrictions of destination zones (3d) are added as additional constraints to the optimization problem above ((3a),(3b)). Moreover, two-dimensional matrix restrictions are also added (3e) where we define all geographic subregions for origin – destination cross-section flows with $M = \{M_1, M_2, ...M_m\}$ where $\{i, j\} \in M_m$ for both origin and destination subregions (see Figure 2 for a schema visualization). The known cross-section flow values are defined in $B = \{B_{M_1,M_1}, B_{M_1,M_2}, ...\}$ and added as additional constraints in (3e). The definition of the in-/equality of these constraints depends on available input data, and the in/equality is due to known upper limit, lower limit, or exact approximation of a given cross-section flow. (Here, probability constraints might be added alternatively in future research (e.g., Prekopa, 1970).)

k is omitted in the following (3c) for improved readability; however, individual variables can be re-added for completeness in generalized utility functions. The shadow prices are calculated for each destination alternatives and cross-section, but are insensitive for k meaning that every person experiences the same shadow price.

$$g_{i,j} = \sum_k g_{i,j,k} \tag{3c}$$

$$\sum_i g_{i,j} \le C_j \tag{3d}$$

$$\sum_{i \in M_1, j \in M_2} g_{i,j} = B_{M_1,M_2} \tag{3e}$$

The total number of employees should not exceed the total number of workplaces available (3f), or the above problem becomes unsolvable. This requirement is assumed as given beforehand. Here, it is important to know that employees are assigned to workplaces. However, the proposed methodology is also applicable if the constraint (3f) is violated, resulting in oversaturated destinations. The defined set

of cross section flow constraints needs to be compatible and inclusive (e.g., for M_1 see (3g)). The cross-section initialization of B-values can be incomplete, meaning that not all possible cross-section flows of M are needed for the proposed methodology.

$$\sum_i P_i \leq \sum_j C_j \tag{3f}$$

$$\sum_m B_{M_1,M_m} \leq \sum_{i \in M_1} P_i \tag{3g}$$

In practical model applications, an inequation of capacity constraints as in (3f) means that the sum of workers is lower or equal to the sum of workplaces available. Here, two aspects complicate practical applications: First, workers traveling from outside the model perimeter are ignored in the model, and their workplaces should be subtracted as is often done in destination choice models. Second, part-time workers can be considered with appropriate adaptions to part-time shares.

We introduce the Lagrange function in (4) with vectors λ_1, λ_2, and matrix λ_3 added as Lagrange multipliers, to reduce equality and inequality constraints. λ_1 has length i, λ_2 has length j, λ_3 has length $\leq i \times j$. λ_2 is constraint to ≥ 0 due to the inequality of (3d):

$$L(g_{i,j}, \lambda_1, \lambda_2, \lambda_3)$$

$$= \sum_{i,j}(g_{i,j} \cdot ln(g_{i,j}) - g_{i,j} - u_{i,j} \cdot g_{i,j}) + \lambda_1\left(\sum_j g_{i,j} - P\right) + \lambda_2\left(\sum_i g_{i,j} - C\right)$$

$$+ \lambda_3\left(\sum_{i \in M_1, j \in M_2} g_{i,j} - B\right)$$

$$\tag{4}$$

Now, the optimality conditions of (4) are ($\lambda_2 \geq 0$):

$$g_{i,j} = e^{-\lambda_{1,i}-\lambda_{2,j}-\lambda_{3,i \in M_1, j \in M_2}-u_{i,j}} \text{ for all } i, j. \tag{5}$$

and

$$\sum_j e^{-\lambda_{1,i}-\lambda_{2,j}-\lambda_{3,i,j}-u_{i,j}} = P_i \text{ for all } i. \tag{6a}$$

$$\sum_i e^{-\lambda_{1,i}-\lambda_{2,j}-\lambda_{3,i,j}-u_{i,j}} \leq C_j \text{ for all } j. \tag{6b}$$

$$\sum_{i \in M_1, j \in M_2} e^{-\lambda_{1,i}-\lambda_{2,j}-\lambda_{3,i,j}-u_{i,j}} = B_{M_1,M_2} \text{ for all defined } M_n, M_o \text{ pairs.} \tag{6c}$$

Unlike (3a) – (3e), the dual problem (6a) – (6c) comes without constraints; λ_1, λ_2 and λ_3 can be determined by solving (6a) – (6c).

For efficiency, all variables in (6a) – (6c) are transformed: $\alpha = e^{-\lambda_1}$, $\gamma = e^{-\lambda_2}$, $\zeta = e^{-\lambda_3}$
$U_{i,j} = e^{-u_{i,j}}$, where α, γ, ζ, $U > 0$ and $\gamma < 1$:

$$\alpha_i \cdot \sum_j \gamma_j \zeta_{i,j} U_{i,j} = P_i \tag{7a}$$

$$\gamma_j \cdot \sum_i \alpha_i \zeta_{i,j} U_{i,j} \leq C_j \tag{7b}$$

$$\zeta_{i,j} \cdot \sum_{i \in M_1, j \in M_2} \alpha_i \gamma_j U_{i,j} = B_{M_1,M_2} \tag{7c}$$

4.2 Efficient algorithm to determine shadow prices on one and two dimensional constraints

Based on the above formulae, the following set of unknown parameter values is given: α, γ, ζ, whereas the utility u is assumed as given (including β parameters). The problem is a non-linear equation system with linear equality and inequality constraints, and the parameters to be fitted with empirical data. The utility parameters are established and fitted based on a maximum likelihood method once at the start. Assuming a generalized logit model, it can be estimated with known methods (Ben-Akiva & Lerman, 1985; McFadden, 1974). Ignoring the constraints, the maximum likelihood method can be applied with various algorithms for unconstraint nonlinear optimization since it is strictly concave; and algorithm mainly differ in convergence speed and memory. The utility then mirrors unconstrained choice behavior.

After estimating utility, γ and ζ values are approximated iteratively with Algorithm 1. The threshold t_1 defines the allowed capacity excess at given destinations. For example, $t_1 = -2$ means that the capacity can be exceeded by a maximum of 2 individuals. t_2 defines the allowed cross-section flow deviation, and also serves as a threshold and breakup criterion. Algorithm 1 approximates a balanced situation within an adequate number of iterations, where all commuters are assigned to a workplace and where defined cross-section flows are approximated to empirical values. The shadow prices λ_2, λ_3 can be viewed as additional utilities for all individuals, to respect capacity constraints and cross-section flows. λ_2 reflects the spatial development potential of underdeveloped alternatives. λ_3 includes the shadow prices on a specific relation between M_x and M_y.

Algorithm 1 efficiently approximates a balanced situation, where all the commuters find a designated working location under the given cross-section constraints. The proposed Algorithm 1 is similar to a gradient projection methodology (e.g. Haftka & Gürdar, 1992). It starts with a solution where γ and ζ are set to 1 (all shadow prices are then 0). This is the stage which is calculated in regular destination choice models, and shadow prices are ignored at this stage. Therefore, the proposed algorithm can be also seen as a calibration step after a "regular" application of a choice model. Generally, the algorithm assumes that active constraints in the nth iteration are also active at iteration $n + 1$. Subsequently, the vectors γ and ζ are redefined after intermediate results when necessary. The equality condition of the cross-section impedance (3e) leads to a continuous recalculation of the cross-section shadow prices in each iteration n when values are over- and underestimated compared to the given constraints. In the case

of the destination capacities, β are recalculated when the inequality is violated and destinations are oversaturated in iteration n.

4.3   Data balancing considerations

The proposed algorithm is capable of dealing with unequal total sums (e.g., in the case of part-time workers), and still allows convergence. If the entire capacity sum of all destinations is

Algorithm 1. Shadow price calculation for one and two dimensional constraints

$n \leftarrow 0$

$\gamma_n \leftarrow 1$

$\zeta_n \leftarrow 1$

while $C - \sum_i g_i < t_1$ **and** $B_{M_x,M_y} - \mathrm{abs}\left(\sum_{i\in M_x, j\in M_y}\right) < t_2$ **do**

   1. Calculate $g_{i,j,n}$ for each pair i, j based on (5) and (7a):

$$g_{i,j,n} \quad \leftarrow \quad \frac{P_i \cdot \gamma_n \cdot \zeta_n \cdot U_{i,j}}{\sum_j \gamma_n \zeta_n U_{i,j}} \tag{8}$$

   2a. One dimensional case: Recalculate γ parameters based on (5) and (7b):

$$\gamma_{n+1,j} \quad \leftarrow \quad \min\left(\frac{C_j \cdot \gamma_n}{\sum_i g_{i,j,n}}, 1\right) \tag{9}$$

   2b. Two dimensional case: Recalculate ζ parameters based on (5) and (7c):

$$\zeta_{n+1,i,j} \quad \leftarrow \quad \frac{B_{M_1,M_2} \cdot \zeta_n}{\sum_{i\in M_1, j\in M_2} g_{i,j,n}} \tag{10}$$

   2c. One and two dimensional cases: Recalculate γ and ζ parameters based on (5),(7b) and

   (7c):

$$\gamma_{n+1,j} \quad \leftarrow \quad \min\left(\frac{C_j \cdot \gamma_n}{\sum_i g_{i,j,n}}, 1\right) \tag{(9)}$$

$$\zeta_{n+1,i,j} \quad \leftarrow \quad \frac{B_{M_1,M_2} \cdot \zeta_n}{\sum_{i\in M_1, j\in M_2} g_{i,j,n}} \tag{(10)}$$

   3. $n \leftarrow n + 1$

end while

Shadow prices for destination alternatives: $\lambda_2 \quad \leftarrow \quad -\log(\gamma)$

Shadow prices for cross section flows: $\lambda_3 \quad \leftarrow \quad -\log(\zeta)$

Terminate.

too low, certain destinations are preferred by individuals and overfilled where individuals require the least utility. If the entire capacity sum of all destinations is larger than the sum of workers, destinations are assigned first where again individuals require the least utility.

5 Results

5.1 Algorithm 1 convergence characteristics

5.1.1 Global convergence behavior

Convergence takes place over multiple iterations with decreasing deviations at given constraints, as defined in (3d), (3e). For visualization purposes, Figure 3(a) shows the absolute median and mean differences of all assigned workplaces relative to the available workplaces, for iterations $n = \{0...14\}$. The results of iteration 0 can be seen as initial solution before applying Algorithm 1, and therefore can serve as a reference. Figure 3(a) depicts decreasing deviations at workplace capacities at increasing iteration numbers $\{0...14\}$, in line with Algorithm 1 theory. Second, the mean cross-section flow differences converge towards a minimum, as expected from theory (median is ignored because of the low numbers of 6 examined cross-section flows). Figure 3(b) refers to the single cross section flows instead of mean values and show even larger deviation between the calculated cross-section flows and counts, however, flows converge again over iterations and approximate observed counts. Figure 3(c) compares the cross section flow values calculated with the choice model (iteration 0) against results after iteration 15 (Algorithm 1) and against count values. As expected, Algorithm 1 minimizes deviation, and the flow values approximate empirical values.

As a benchmark, convergence behavior is approximated with an exponential function for comparability with potential future applications. The workplace capacity constraint optimization at destinations is separately optimized and evaluated from cross-section flow optimization to facilitate future comparison (see case 2a and 2b in Algorithm 1 and also Figure 7(a) and Figure 7(b) later on). Regarding workplace capacity constraint optimization, an exponential approximation of $e^{-0.129}$ is achieved in the Basel application, where the cross-section flow optimization is approximated with $e^{-0.013}$.

Algorithm 1 takes about 2.5 hours to calculate 15 iterations on a 2.6 GHz Intel Core i7 processor with a 15 GB memory. Iteration 0 uses about 1.5 hours of total calculation time due to the initial, encompassing utility calculation. The definition of the cut-off criteria for Algorithm 1 is subject to the underlying application. In the current application, 15 iterations were defined as cut-off criteria based on achieved results and convergence behavior. Larger deviations occur before iteration 10 (Figure 3(a)), however, minor deviations remain after iteration 10 especially at specific cross-section flows (Figure 3(b)). It is assumed that the convergence behavior varies between case studies and applications, and a general cut-off criteria definition for Algorithm 1 requires more application experience.

5.1.2 Detailed workplace saturation evaluation

Figures 4(a) and 4(b) depict the workplace saturation at iteration 0 and 15, respectively, when considering continuous flows $g_{i,j,n}$ (8), e.g., for aggregated model applications. Over- and under-saturated workplaces can be found in iteration 0 (Figure 4(a)) whereas workplaces are almost completely saturated in iteration 15 (Figures 4(b)). As expected, oversaturation is minimized as a result of shadow prices assigned to overcrowded destinations (ceiling condition in (3d)). Figures 4(c) and 4(d) depict workplace saturation at iteration 0 and 15, respectively, after applying the choice probabilities on the Basel synthetic population and its discrete agents. As expected, Figures 4(c) and 4(d) show similarities to above Figures
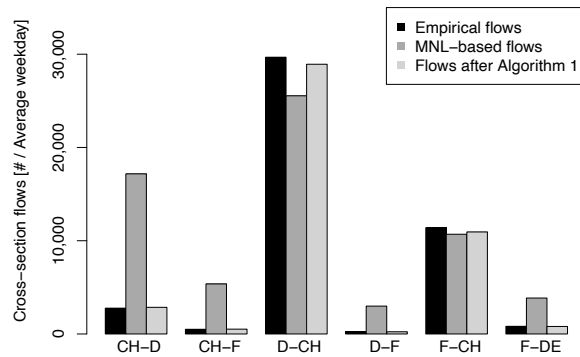
4(a) and 4(b). As in Figures 4(c) and 4(d), it is clear that Algorithm 1 still allows oversaturation
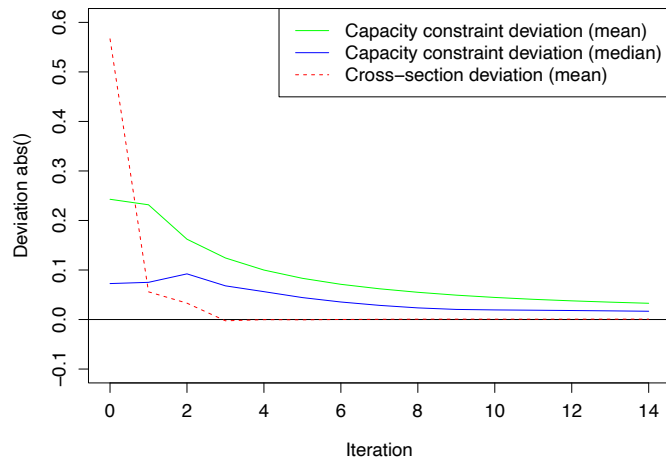
(a) Destination constraints and cross-section flow constraint optimization.
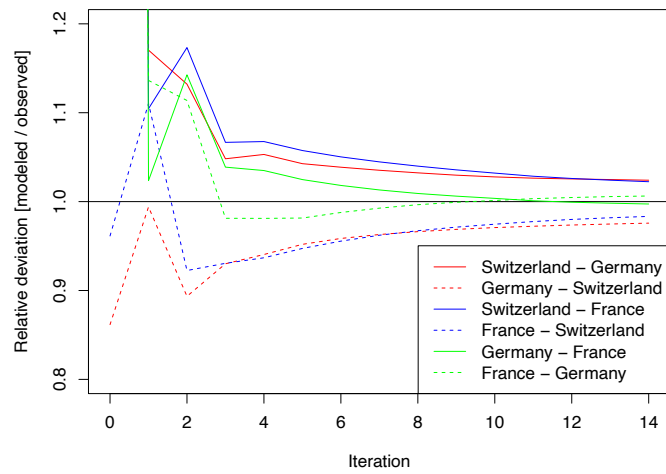
(b) Convergence behavior of Algorithm 1 for cross-section flows, compared to counts.

(c) Comparison of empirical flows, and calculated flows with both MNL and consecutive Algorithm 1 application.

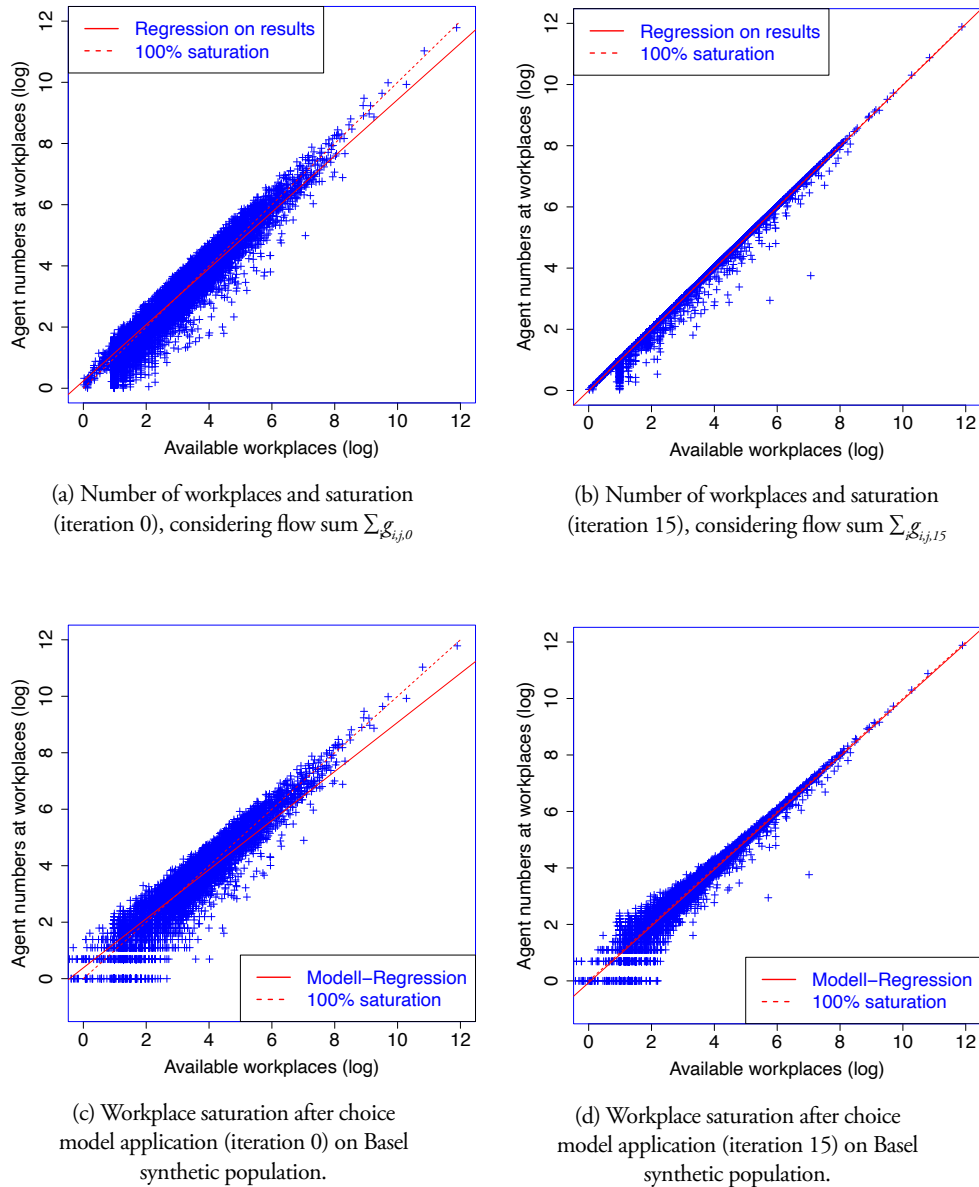**Figure 3.** Algorithm 1 convergence behavior and cross-section flows

(a) Number of workplaces and saturation
(iteration 0), considering flow sum $\sum_g g_{i,j,0}$

(b) Number of workplaces and saturation
(iteration 15), considering flow sum $\sum_g g_{i,j,15}$

(c) Workplace saturation after choice
model application (iteration 0) on Basel
synthetic population.

(d) Workplace saturation after choice
model application (iteration 15) on Basel
synthetic population.

Figure 4. Regression with workplace capacities and workplace saturation

at iteration 15 due to its probability-based methodology, which means that it never guarantees an exact 100% saturation. Overall, the applied Algorithm 1 is applicable in both cases of considering flows, and discrete applications, respectively, making Algorithm 1 an attractive methodology for both continuous flow models and discrete agent-based modeling.

5.1.3   Trip length distributions

Figure 5 shows the cumulative distance distributions for iteration 0 and 15, and the potential distributional changes due to the Algorithm 1 application. All distance calculations include network routing calculations in equilibrium conditions. Figure 5 shows two reference distance distributions. First reference distance distribution includes trips from the MTMC; second reference distance distribution represents

the selected and encompassing commuting trip distribution (see Section 3.2.3 for further information). Figure 5(a) shows the distance distribution of all commuters before applying Algorithm 1. At this stage, the destination alternatives are potentially overcrowded, and cross-section flows potentially differ from observed counts. Figure 5(b) shows cumulative distance distribution after applying Algorithm 1 for 15 iterations, including cross-section flow balancing, and shadow prices calculations at destinations. Figures 5(a) and 5(b) both show that before and after applying Algorithm 1, overall travel distributions mirror the reference data provided from alternative sources. Distance distributions slightly increase after applying Algorithm 1 especially between 5 km and 20 km travel distances, because of reassigning agents to different locations. However, effects on travel distance distribution are minor, and the overall fit most likely satisfies modeling needs.

5.2   Spatial shadow price distribution and interpretation

This section shows main findings in spatial shadow price distribution, in comparison with population and workplace distribution. The spatial evaluations foster model understanding and provide insights into land use development and planning. Figure 6(a) shows the spatial distribution of the Basel population, Figure 6(b) workplaces and 6(c) shadow price (λ_2 = -log(γ)) distribution for the destination alternatives. Shadow price distribution in Figure 6(c) depicts a centralistic pattern. Shadow prices are higher at the outskirts and average in the city center, due to low workplace density at the outskirts, and due to higher accessibility in the city center.
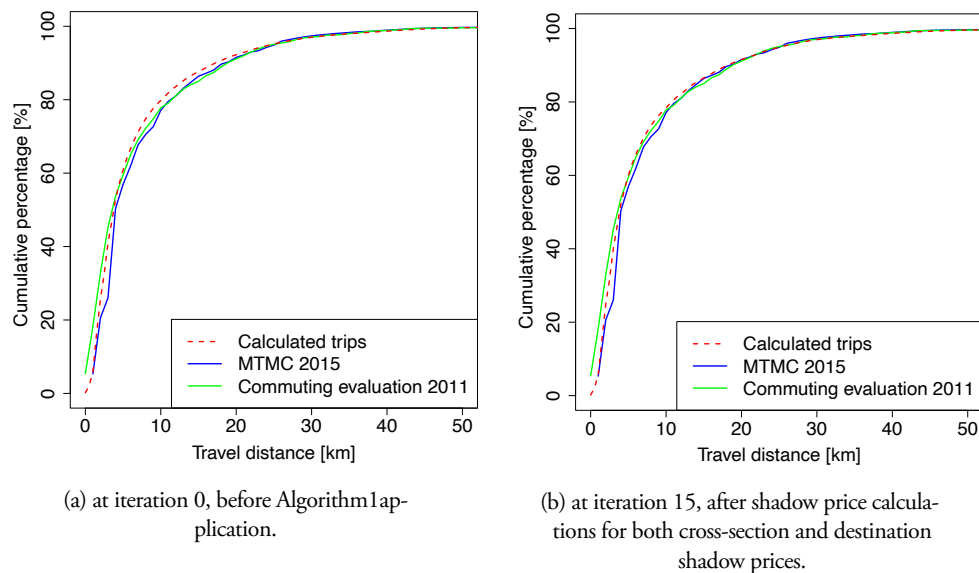

(a) at iteration 0, before Algorithm1ap-
plication.

(b) at iteration 15, after shadow price calcula-
tions for both cross-section and destination
shadow prices.

Figure 5. The cumulative car travel distance distribution for commuters of the entire synthetic population within Swiss perimeter area, in comparison with reference distributions

A belt around the city center has low shadow prices due to relatively high workplace density. Additional clusters with high shadow prices are calculated in the south-east and north-east of the city center due to lower workplace density.

Compared to independent census data (Swiss Federal Statistical Office (BFS), 2017) sampled for the identical geographic region, the Algorithm 1 application was capable of improving destination alternative choice by 4.4% compared to the reference census data. This result can serve as an additional

indicator for goodness of fit improvement, beside minimized constraint violation when applying Algorithm 1 as described above. However, further model parameter estimation and discrete choice model design are omitted in this paper, as this paper emphasizes the Algorithm 1 methodology and highlights convergence characteristics, constraint integration and scenario applications. Further research is required on detailed choice parameter estimation and further statistical goodness of fit evaluation (see Section 6).

For planning purposes, shadow prices can improve model accuracy and scenario calculations (see below), but also unveil regional and local clusters with over- and undersaturated workplaces. This is especially useful for planning under sparse land availability and high costs. Shadow prices therefore unveil such spatial clusters in a quantitative manner. Compared to accessibility measures, shadow prices also include demand patterns and their closeness. High accessibility does not necessarily mean high attractiveness if competition is also high. Shadow prices cope with these circumstances and considers demand and supply.

5.3 Algorithm adaption, forecasts and scenarios

Multiple applications are described in this section. First, Algorithm 1 is adapted and independently applied for capacity constraint and cross-section flow optimization. Second and third, results are shown of forecasts and infrastructure scenarios.

5.3.1 Independent capacity constraint and cross-section flow optimization

Algorithm 1 is adaptive for consideration of only (a) cross-section flow, or (b) destination capacity constraints. Both cases are calculated and results are shown in Figures 7(a) and 7(b).

(a) Figure 7(a) shows cross-section flow optimization with Algorithm 1, while ignoring capacity constraints at destinations. Capacity constraints at destinations are exceeded also at increasing iteration numbers.

(b) Figure 7(b) shows capacity constraint optimization at destinations, while ignoring cross-section constraints. The cross-section flows deviate from counts also at increasing iteration numbers.
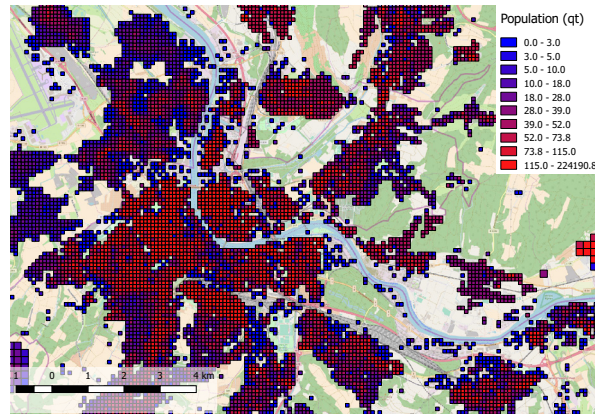
(a) Population distribution
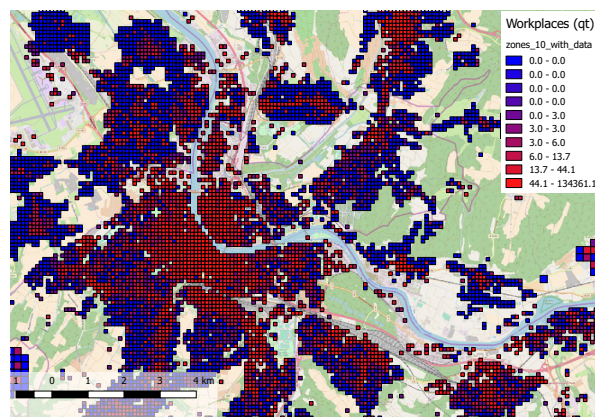
(b) Workplace distribution
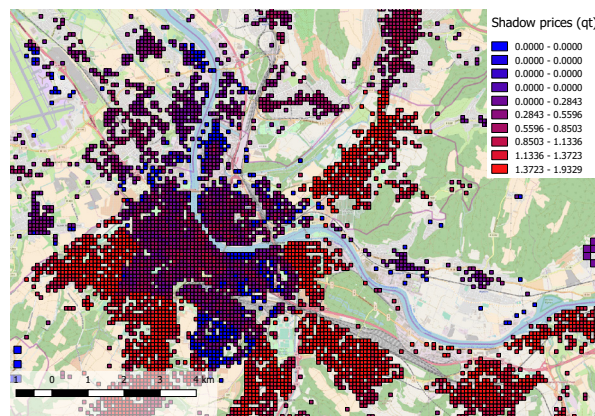
(c) Shadow prices λ_2 distribution after iteration 15

Figure 6. Basel population, workplace and shadow prices distributions for workplaces

5.3.2   Forecast capabilities and scenarios

Proposed forecast scenarios consider population and workplace growth, where Algorithm 1 can be applied similarly with adapted alternatives' capacities. However, cross-section counts remain unknown for

forecasts and scenarios. For this reason, two solutions (c) and (d) are proposed for improved forecasts and destination choice calculations.

(c) Calculated cross-section impedance (γ values), based on current and empirical cross-section counts, are reapplied to forecast destination choice calculation, and γ values remain constant for scenario calculations. Most probably, cross-section flows deviate from empirical flows due to implemented growth conditions in population and workplace forecasts. Figure 7(c) depicts the average deviation of workplace capacities and cross-section flows, of a forecast scenario with a global 20% population and workplace growth, and shows deviation for cross-section flows as supposed above. (All subfigures in Figure 7 are also comparable to reference evaluation in Figure 3(a).)

(d) Cross-section counts are assumed to be known, which means that count values are assumed to remain or grow accordingly (e.g., by 20%). Figure 7(d) shows convergence behavior with remaining cross-section counts as in original data. As expected, Algorithm 1 optimizes destination choice behavior and matches modeled flows with counts.

5.3.3 Scenario applications

As an example, Figure 8 depicts shadow price changes between two scenarios differing in infrastructure supply, namely a fictitious road link connecting two city neighborhoods. Changed infrastructure then affects travel times and destination choice behavior. Figure 8 depicts city neighborhood clusters changing in their shadow prices depending on the new link and its impact.
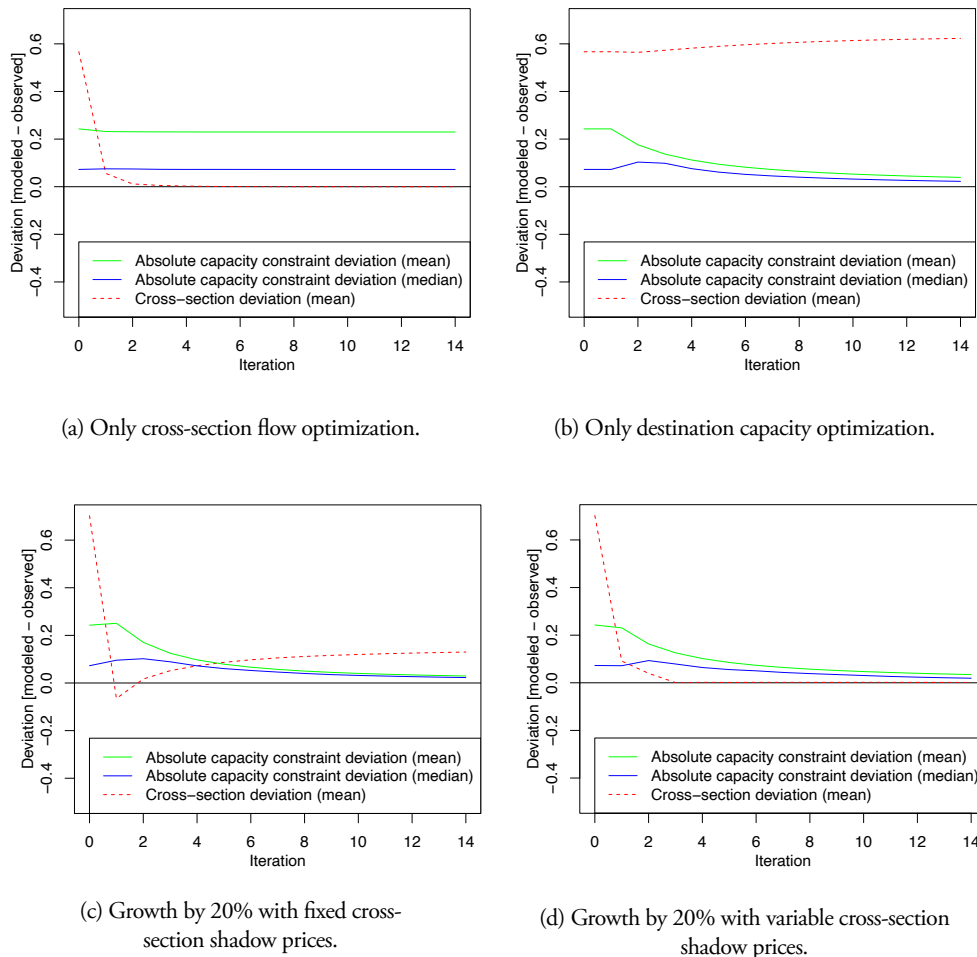

(a) Only cross-section flow optimization.

(b) Only destination capacity optimization.

(c) Growth by 20% with fixed cross-section shadow prices.

(d) Growth by 20% with variable cross-section shadow prices.

Figure 7. Global convergence behavior of Algorithm 1 over 15 iterations, differing in considered spatial constraints

It shows a systematic change in values summarized in spatially aggregated clusters.

5.3.4   Further algorithm modification

Unlike gravity models, proposed Algorithm 1 allows workplace numbers which are lower than capacity at a given destination. To further mirror the gravity model approach, inequality constraint (3f) is replaced by an equality constraint (11), which means that attractiveness of undersaturated workplaces is increased by adapting γ values, and additional commuters are attracted at these workplaces.
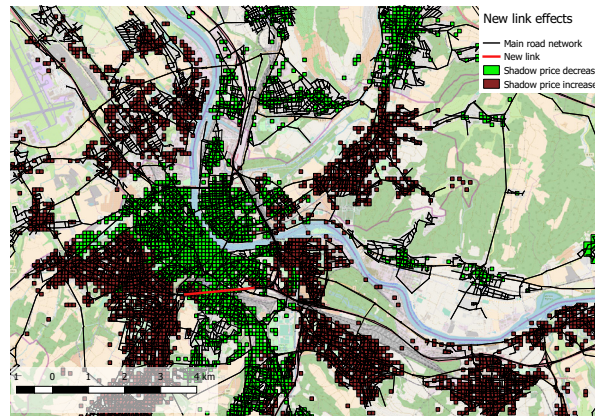

Figure 8. Clustering of shadow price changes when adding new infrastructure, here a road link
Source: Assumptions differing from and incomparable with any other planned study.

$$\sum_i P_i = \sum_j C_j \tag{11}$$

Replacing (3f) with (11) leads to faster convergence behavior of the marginals compared to the inequality constraint due to more efficient γ values adaption, with precise assignment results already at iteration 15 (Figure 9). Exceedance might still occur, however, it is worth to verify such an algorithm modification in scenario applications since exceedance is only minimal in the current Basel case study.
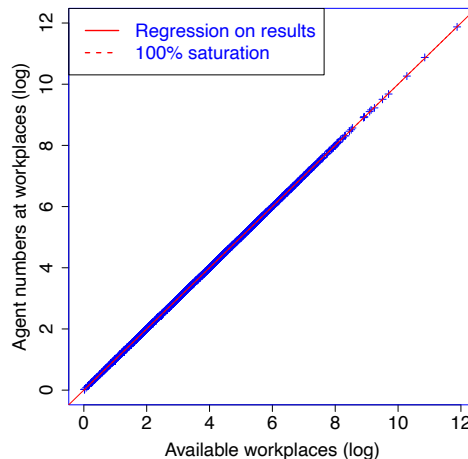

Figure 9. Effects of replacing inequation with equation on capacity constraints (iteration 15)

6 Discussion and outlook

Two generic types of spatially distributed constraints are successfully integrated in a new and robust algorithm to improve destination choice modeling, namely capacity constraints at destinations, and cross-section counts e.g., from counts at borders or bridges. The proposed Algorithm 1 is successfully applied in a detailed, large-scale model covering a 2 Mio. inhabitants area and 20,000 destination alternatives. Results show that the applied methodology improves destination choice on a cross-section level as well as on single choice alternatives. On cross-sections, precision improvements (mean relative deviation) are as high as 20% and more compared to without Algorithm 1. Regarding choice alternatives and destination capacities, the proposed methodology avoids over-saturations at favorable locations and therefore considerably improves destination choice. Both methodologies for cross-section flows and destination capacities are applicable separately or simultaneously in destination choice calculations. According to our calculations and results, the travel distance distribution of all trips only slightly changes when applying the proposed methodology, compared to empirical reference sample distributions.

The proposed methodology serves as a robust solution for macroscopic transport models and agent-based simulations, still maintaining choice heterogeneity especially relevant for agent-based simulations. It therefore can be efficiently implemented in large-scale agent-based models as shown in the Basel case study. Moreover, the proposed methodology allows forecast and scenario calculations with necessary parameter choice (constant or variable impedance for cross-section flows) as demonstrated and evaluated in this paper. For land use planning purposes, shadow prices support future spatial development of underdeveloped - or unused, valuable -destination alternatives.

Still, additional research might be of interest especially on the following five topics: (1) There is a presumption that the statistical model fit improves during Algorithm 1 iterations, in contrast to ignoring capacity constraints. Therefore Algorithm 1 might improve the overall model prediction; this needs to be verified on cross-section flow calculations with a more comprehensive generalized utility model and in other model applications. A similar model fit improvement was demonstrated in Vitins et al. (2016), where ρ^2 increases from $\rho^2 = 0.115$ to $\rho^2 = 0.168$ for destination choice. (2) So far it is assumed that choice model parameters are estimated prior to shadow price calculations since they mirror individual behavior without constraints per se. Especially when parameters are estimated with RP data, parameter estimation should already include shadow price effects; this integration of shadow price theory should be considered in future research. (3) Perimeter border effects might occur in model applications, similar to the perimeter effects occurring in other transport models. The effects of persons from areas outside the model perimeter might affect calculations and results; especially areas easily accessible from outside of the model perimeter with relatively high transport demand exchange and flows. These external effects are challenging to capture quantitatively, and future studies might reveal the quantitative extents of these effects. (4) Algorithm 1 still allows reduced under- or over-saturated alternatives after many iterations, depending on the case study and probability calculations. Convergence might be compared with future applications and optimized based on the mentioned benchmark results. A final assignment of the remaining agents at over-saturated alternatives can lead to a guaranteed assignment of every agent to the remaining available workplaces. (5) Future models might include additional variables and underlying data to estimate more parameters with underlying choice model methodology. Improvements in choice model parameters can account for different economic sections and job types (industry, chemistry, etc.), in combination with a detailed destination choice model including generalized utilities to consider economic sections, as proposed in Vitins et al. (2016). Moreover, it is necessary to adapt existing methods such as mixed multinomial logit models (MMNL), which also increase model accuracy. Combinations of MMNL and other model categories together with the proposed method in this paper are missing so far and would be part of future and interesting research.

Various other planning tasks are potentially tackable with the proposed methodology: Vehicle occupancy constraint will be additionally interesting for research and suitable for shadow prices, coupled with mode and route choice, for dense cities with frequently overloaded public transport lines and services. Battery charging stations for e-mobility or general parking choice might profit from the proposed methodology, along with transportation modeling. As applied in land use models, primary location choice can be considered with proposed methodology for households and firm locations. Spatial economics (as mentioned above) might profit, and as might probably other constraint resource distribution, in a wider sense.

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Author contribution

Basil J. Vitins: Methodology Design, Study Conception, Mathematical Derivation, Result Calculations. Original draft. Basil J. Vitins and Alexander Erath: Data pre-processing, Review and Editing, Management.

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