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## A metamodel simulation-based optimization approach for the efficient calibration of stochastic traffic simulators

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### Abstract

This work considers the calibration of stochastic microscopic traffic simulators. It formulates the calibration problem as a simulation-based optimization (SO) problem, and uses metamodel SO ideas. The main idea is to embed within the calibration algorithm an analytical problem-specific description of how the calibration parameters are related to the simulation-based objective function. Preliminary results on a toy network are presented. Ongoing work applies these ideas to the calibration of a Berlin metropolitan area network.

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*Keywords:* calibration; stochastic microscopic simulation; simulation-based optimization

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### 1. Introduction

There is extensive research in the field of transportation engineering that studies the problem of calibration of simulation-based traffic models. Traditional approaches based on well-established statistical frameworks and standard numerical procedures (e.g., Buisson et al. 2012) typically involve strong model assumptions (e.g., continuity, differentiability, normality or ergodicity of model outputs), which are typically violated by detailed traffic simulators. Hence, the calibration community has mostly focused on the use of black-box (i.e., general purpose) optimization algorithms. For a survey, see Balakrishna (2006). Such algorithms impose little to no requirements on the underlying problem, and hence have often been used by the broader optimization community to

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address highly complex and intractable optimization problems. Nonetheless, the generality of these algorithms is also their main drawback: they do not exploit the structure of the underlying problem. Optimization algorithms that exploit the rich structure of transportation problems have great potential to have good short-term numerical performance. Existing black-box algorithms used for calibration problems lack good numerical performance and require large computational efforts (e.g., numerous simulation runs) in order to identify points with good performance.

Cascetta and Nguyen (1988) provide a classical overview of calibration literature for origin-destination (OD) matrices. Cascetta et al. (1993) extended the static calibration problem to a dynamic setting, leading to abundant literature in the field of calibration. Unlike OD matrix estimators, which calibrate aggregate demand flows, path flow estimators (PFEs) attempt to calibrate the underlying route choice, cf. the seminal PFE work of Bell et al. (1997). See Flötteröd (2008) or Buisson et al. (2012) for a comprehensive survey in this field.

The increased availability of detailed surveillance data triggered recent efforts to calibrate demand and supply parameters jointly (e.g., Balakrishna 2006, Antoniou et al. 2007, Vaze et al. 2009). Nonetheless, the most common approach is to resort to general-purpose black-box optimization algorithms that exploit problem structure at most in terms of a numerical linearization: e.g., simulated annealing (Kirkpatrick et al. 1983), simultaneous perturbation stochastic approximation (SPSA) (Spall 1992), genetic algorithms (Holland 1975), unscented Kalman filters (Julier and Uhlmann 1997), and particle filters (Arulampalam et al. 2002). See Antoniou (2004), Balakrishna (2006) for two representative monographs and Ben-Akiva et al. (2012) for a comprehensive literature review.

Typical traffic micro-simulations capture travel demand in terms of time-dependent origin/destination (OD) matrices, from which they sample individual trip makers. Usually, a probabilistic route choice model is then applied to select a route for each trip maker, and a mesoscopic or microscopic traffic flow model is used to propagate the trip makers' vehicles through the network. If the route choice model is congestion-dependent, then route choice and traffic flow simulation are iterated until a stochastic fixed point of mutual consistency is attained (Barcelo 2010).

Microscopic simulations enable detailed representations of reality, and as such they are built around data-intensive model systems. This renders the automatic calibration of micro-simulations a difficult and practically relevant problem. A largely unresolved methodological challenge in this context is the formulation of tractable measurement equations that link available surveillance data from the real transport system to the model parameters one wishes to calibrate.

In this paper, we propose a general methodology for the calibration of stochastic traffic simulation models. As explained in the following, the approach sets itself apart from the existing literature in that it combines response information from a complex traffic micro-simulation with information from a tractable analytical traffic model. More specifically, this work formulates the calibration problem as a simulation-based optimization (SO) problem. Metamodel ideas are used to embed information about the underlying problem structure within the calibration algorithm. The metamodel is then embedded within the computationally efficient SO algorithm proposed by Osorio (2010).

## 2. Methodology

### 2.1. Formal problem statement

To make the proposal concrete, we focus in the following on the calibration of travel demand parameters from network flows. Each OD pair  $n = 1 \dots N$  is connected by one or more routes. The set routes in OD pair  $n$  is denoted by  $C_n$ . The total travel demand within OD pair  $i$  is written as  $d_n$ . The probability that a traveler in OD pair  $n$  selects a route  $i \in C_n$  is written as  $P_n(i | \mathbf{x}, \boldsymbol{\theta})$  where  $\mathbf{x}$  represents the network attributes (in particular, travel times) that characterize the alternative routes and  $\boldsymbol{\theta}$  is a vector of coefficients (to be estimated) that guide the choice process.

Let  $\delta_{i,t}^{a,k}(\mathbf{x})$  be one if a traveler having departed on route  $i$  in time interval  $t$  enters link  $a$  in time interval  $k$ , and zero otherwise. This parameter depends in the presence of congestion on the travel times contained in  $\mathbf{x}$ . The flow (in vehicles) across link  $a$  in time step  $k$  can then be written as

$$q_{a,k} = \sum_{n=1}^N d_n \sum_{i \in C_n} \delta_{i,t}^{a,k}(\mathbf{x}) P_n(i | \mathbf{x}, \boldsymbol{\theta}) \quad (1)$$

Since the network travel times contained in  $\mathbf{x}$  depend in turn on the network flows defined here, this equation is circular and can in general only be solved iteratively. In a traffic microsimulation, these iterations can be interpreted as a learning process over subsequent days, where in each day all trip makers select a route according to the most recent network conditions  $\mathbf{x}$ , followed by a simulation of the corresponding vehicle flows through the network, which in turn yields updated network conditions.

Let  $y_{a,k}$  be the number of vehicles counted in reality on link  $a$  in time step  $k$ . A natural non-linear least squares formulation of the calibration problem is then to minimize the following objective function:

$$Q(\boldsymbol{\theta}) = \sum_{a,k} (y_{a,k} - q_{a,k})^2, \quad (2)$$

where  $q_{a,k} = q_{a,k}(\boldsymbol{\theta})$  due to (1). The difficulty of this problem is owed to the complexity of constraint (1), which is not available in closed form but is represented only procedurally through the traffic microsimulation.

This project proposes to solve Problem (2) by embedding structural information that *analytically* approximates the main components of (1). Developing an analytical approximation of the main components of (1) is a challenging problem because the approximated mapping involves the highly nonlinear and stochastic *network loading map* of path flows on network conditions, comprising in the micro-simulation context all difficulties that come along with real traffic flow dynamics in urban networks (including, e.g., multi-lane flows, spill-back, flow interactions in complex intersections). The recent doctoral dissertation of Frederix (2012) makes clear that this is anything but a solved problem.

The goal of this paper is to derive an analytical and computationally efficient approximation of (1). We then embed this information within a simulation-based calibration algorithm. We expect this analytical information to significantly enhance the computational efficiency of the calibration algorithm, and ultimately to allow us to efficiently solve high-dimensional calibration problems.

## 2.2. Metamodel formulation

To start off, we focus on the calibration of a single route choice parameter. We assume an analytical closed-form expression for the corresponding route choice model is given,  $P_n(i | \mathbf{x}, \boldsymbol{\theta})$ . We propose to derive an analytical approximation of the System of Equations (1).

The main idea is to derive an analytical approximation that combines information from the simulator (i.e., this is the traditional approach) with information from an analytical macroscopic and computationally efficient traffic model. Ideas along these lines have been used to efficiently address large-scale urban traffic management problems while using inefficient yet detailed microsimulators (Osorio and Chong 2014, Osorio and Nanduri 2014, Chen et al. 2012). This combination will be formulated based on metamodel (also called surrogate model) ideas from the field of simulation-based optimization (SO), as in Osorio and Bierlaire (2013).

A metamodel is an analytical approximation of the simulation-based objective function (2). Metamodel SO techniques iterate over two main steps. Firstly, the metamodel is constructed based on a sample of simulated observations. Secondly, it is used to perform optimization and derive a trial point (i.e., a route choice parameter value). The performance of the trial point can be evaluated by the simulator, which leads to new observations. As new observations become available the accuracy of the metamodel can be improved (Step 1), leading ultimately to better trial points (Step 2). In this paper, we use the general metamodel SO framework of Osorio and Bierlaire (2013), which uses the derivative-free trust region algorithm of Conn et al. (2009).

We propose an analytical approximation of the expected link flow for link  $a$ , denoted  $q_{a,k}$  in Equation (2). We first consider a time-independent approximation, and hence have for a given link  $a$  the same approximation for all time-steps  $k$ . We denote this approximation  $q_a$ , and refer to it as the (link-specific) metamodel. It is given by:

$$q_a(\theta; \beta_i) = \beta_{i,0} \lambda_a(\theta) + \beta_{i,1} + \beta_{i,2} \theta, \quad (3)$$

where  $\theta$  is the route choice model parameter,  $\lambda_i(\theta)$  is the expected flow of link  $i$  as approximated by the analytical traffic model, and  $\beta$  is a vector of metamodel parameters. These parameters are fit by solving a least squares problem that minimizes the distance between simulated link flows and metamodel predictions. For parameter estimation details, see Osorio and Bierlaire (2013). The metamodel formulation (Equation (3)) can be interpreted as a scaled approximation provided by the analytical traffic model and an additive correction term that is linear in  $\theta$ .

### 2.3. Analytical traffic model

We now describe how the analytical approximation of the expected link flow (denoted  $\lambda_a(\theta)$  in Equation (3)) is obtained. We build upon the analytical traffic model used in Osorio and Bierlaire (2013), which is based on a finite (space) capacity representation of an urban road network. The formulation is based on the general queueing-theoretic ideas in Osorio and Bierlaire (2009) and urban traffic ideas in Osorio (2010, Chap. 4).

There has been a recently renewed interest in the use of queueing network ideas to describe vehicular traffic. The work of Osorio and Flötteröd (2014) and Osorio et al. (2011) has proposed a stochastic formulation of Newell's simplified kinematic wave model (Newell 1993, Yperman et al. 2007). Here, the goal is to derive an analytical, differentiable, and computationally tractable urban traffic model such that calibration problems for large-scale networks can be addressed.

The analytical traffic model used in Osorio and Bierlaire (2013) is indeed analytical, differentiable and computationally tractable. Nonetheless, for the purpose of calibration, its main limitation is that it assumes exogenous assignment. In this work, we use a formulation that allows for endogenous assignment.

Note that the use of a finite (space) capacity queueing network representation of a road network allows for the finite length of roads to be accounted for. Hence, the spatial propagation of congestion is accounted for (e.g., vehicular spillbacks). This is done through the queueing notion of blocking. Describing the spatial propagation of congestion is particularly important when calibrating models of congested urban networks.

We first briefly present the formulation of the model of Osorio (2010, Chap. 4). We then present its extension to account for endogenous assignment. The model of Osorio (2010) considers a general road network. In this paper, we limit the formulation to single-lane roads. This formulation can be readily extended to multi-lane roads. Each road is modeled as a finite (space) capacity  $M/M/1/\ell$  queue.

The finite space capacity  $\ell$  captures the finite length of each road. It is given by:

$$\ell_i = \lfloor (l_i + d_2) / (d_1 + d_2) \rfloor, \quad (4)$$

where  $l_i$  is the length of lane  $i$  in meters,  $d_1$  is the average vehicle length (set to 4 meters), and  $d_2$  is the minimal inter-vehicle distance (set to 1 meter). The fraction is rounded down to the nearest integer.

For a given queue  $i$ , the following notation is used.

$\gamma_i$	external arrival rate;
$\lambda_i$	total arrival rate;
$\mu_i$	service rate;
$\tilde{\mu}_i$	unblocking rate;
$\hat{\mu}_i$	effective service rate;
$\rho_i$	traffic intensity;
$P_i^f$	probability of being blocked after service at queue $i$ ;

$\ell_i$	space capacity;
$N_i$	number of vehicles in queue $i$ ;
$P(N_i = \ell_i)$	probability of queue $i$ being full;
$p_{ij}$	transition probability from queue $i$ to queue $j$ ;
$D_i$	set of downstream queues from queue $i$

For a given road network represented as a queueing network, the marginal queue-length distributions of each queue are obtained by simultaneously solving for all queues the following system of equations.

$$\lambda_i = \gamma_i + \frac{\sum_j p_{ji} \lambda_j P(N_j < \ell_j)}{P(N_i < \ell_i)} \tag{5}$$

$$\frac{1}{\hat{\mu}_i} = \frac{1}{\mu_i} + P_i^f \frac{1}{\tilde{\mu}_i} \tag{6}$$

$$\frac{1}{\tilde{\mu}_i} = \sum_{j \in D_i} \frac{\lambda_j P(N_j < \ell_j)}{\lambda_i P(N_i < \ell_i) \hat{\mu}_j} \tag{7}$$

$$P(N_i = \ell_i) = \frac{1 - \rho_i}{1 - \rho_i^{\ell_i + 1}} \rho_i^{\ell_i} \tag{8}$$

$$P_i^f = \sum_j p_{ij} P(N_j = \ell_j) \tag{9}$$

$$\rho_i = \frac{\lambda_i}{\hat{\mu}_i} \tag{10}$$

For details regarding this formulation, we refer the reader to Osorio (2010, Chap. 4).

In order to account for endogenous assignment, the model is complemented by the following assignment equations.

$d_s$	demand for OD pair $s$ ;
$c_t$	travel cost of path $t$ ;
$y_t$	flow on path $t$ ;
$r_{it}$	proportion of flow on path $t$ that goes through queue $i$ ;
$a_{it}$	indicates whether path $t$ contains queue $i$ ;
$a_{it}^*$	indicates whether the first link of path $t$ is link $i$ ;
$l_{st}$	probability that a vehicle travelling the OD pair $s$ takes path $t$ ;

$E[T_i]$	travel cost of queue $i$ ;
$E[N_i]$	number of vehicles in queue $i$ ;
$l(i)$	length of road $i$ ;
$v(i)$	maximum speed of road $i$ ;
$\theta$	route choice model parameter;
$P_s$	set of paths of OD pair $s$ ;
$S$	set of OD pairs;
$Q$	set of queue indices;
$T$	set of paths indices;
$G_{ij}$	set of paths that consecutively go through queues $i$ and $j$ ;
$H_i$	set of paths that go through queue $i$ ;

$$p_{ij} = \frac{\sum_{t \in G_{ij}} y_t}{\sum_{t \in H_i} y_t} \quad \forall i \in Q, \forall j \in Q \quad (11)$$

$$y_t = \sum_{s \in S} d_s l_{st} \quad \forall t \in T \quad (12)$$

$$l_{st} = \frac{e^{-\theta c_t}}{\sum_{j \in P_s} e^{-\theta c_j}} \quad \forall s \in S, \forall t \in P_s \quad (13)$$

$$c_t = \sum_{i \in Q} r_{ti} E[T_i] \quad \forall t \in T \quad (14)$$

$$r_{ti} = \frac{a_{ti}}{\sum_{j \in Q} a_{tj} z_{ij}} \quad \forall t \in T, \forall i \in Q \quad (15)$$

$$E[T_i] = \frac{E[N_i]}{\lambda_i P(N_i < \ell_i)} + \frac{l(i)}{v(i)} \quad \forall i \in Q \quad (16)$$

$$E[N_i] = \frac{\rho_i}{1 - \rho_i} - \frac{(\ell_i + 1) \rho_i^{\ell_i + 1}}{1 - \rho_i^{\ell_i + 1}} \quad \forall i \in Q \quad (17)$$

$$\gamma_i = \sum_{t \in T} a_{ti}^* y_t \quad \forall i \in Q \quad (18)$$

The indicator variables are defined as follows.

$$a_{ii} = \begin{cases} 1 & \text{if queue (i.e., link) } i \text{ is part of path } t, \\ 0 & \text{otherwise.} \end{cases} \quad (19)$$

$$a_{ii}^* = \begin{cases} 1 & \text{if queue (i.e., link) } i \text{ is the first link of path } t, \\ 0 & \text{otherwise.} \end{cases} \quad (20)$$

The goal of these equations is to provide an analytical description of how the turning probabilities  $p_{ij}$  are related to the calibration parameter  $\theta$ . This allows for endogenous turning probabilities, i.e., endogenous assignment. The above system of equations is based on the use of a multinomial logit route choice model (Equation (13)), with link costs defined by expected link travel time (Equation (16)). The expected travel time is expressed as the sum of delay (first term on the right-hand side) and free-flow travel time (second term on the right-hand side). The delay term is based on the use of Little's law (Little 2011, 1961) for a finite (space) capacity queue. The expression for the expected number of vehicles in a queue (Equation (17)) is derived in detail in Appendix A of Osorio and Chong (2014). Since the assignment is now considered endogenous, the external arrivals to a queue,  $\gamma_i$ , are also endogenous. Equation (18) gives their expression as a function of expected path flows.

In summary, the analytical traffic model used to approximate the expected link flows  $\lambda_i(\theta)$  of Equation (3) are obtained by evaluating the system of nonlinear differentiable equations (5)-(18).

### 3. Case study

To illustrate the performance of this approach, we consider a small toy network displayed in Fig. 1. Each link in the network consists of a single lane and is modeled by a single queue. The network has one origin-destination pair, nodes 1 and 5 respectively. There are two routes that connect the pair, a route to the north (through nodes 1, 2, 3, 5) and a route to the south (through nodes 1, 2, 4, 5). The northern route has a shorter free flow travel time, yet faces delay at a signalized intersection at node 3, whereas the southern route is entirely unsignalized and free of bottlenecks. The “true” link counts are simulation-based.

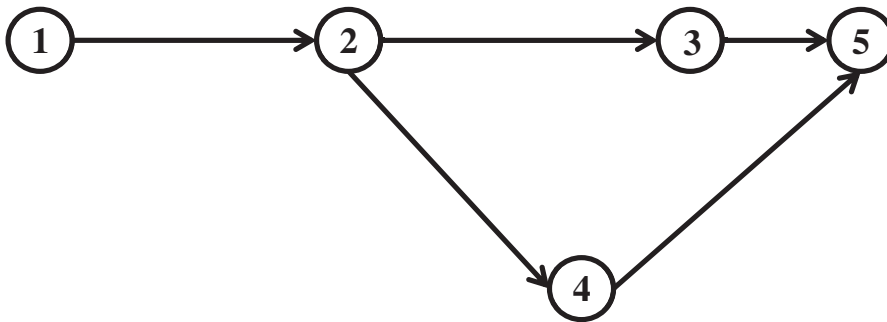


Fig. 1. Network topology.

We compare the performance of the proposed approach with the metamodel formulation as given in Equation (3) to that of a metamodel that does not resort to the use of the analytical traffic model. In other words, following the notation of Equation (3), the benchmark metamodel is formulated as:

$$q_a(\theta; \beta_i) = \beta_{i,1} + \beta_{i,2}\theta. \quad (21)$$



This benchmark metamodel approximates the expected flow of a given link as a polynomial that is linear in the calibration parameter  $\theta$ .

We run the simulation-based optimization (SO) algorithm allowing for a maximum of 50 different  $\theta$  values to be evaluated. Note that all algorithmic details are identical for the proposed approach and the benchmark approach, the only difference is the metamodel formulation.

In the figures of this section the proposed metamodel is denoted  $m$  while the benchmark metamodel is denoted  $\phi$ . Fig. 2 considers a scenario where the true value of the calibration demand parameter value is:  $\theta^* = -42$ . The SO algorithm is initialized with  $\theta_0 = -57$ . For each metamodel, the SO algorithm is run 5 times, allowing each time for a maximum of 50 values of  $\theta$  to be simulated. The x-axis displays the algorithm's iteration, while the y-axis displays the current iterate (i.e., current  $\theta$  value proposed as a solution by the algorithm). A method with good performance is one where the current iterate is near the true value (-42) within very few iterations. The results that correspond to the proposed approach are depicted by solid lines; those of the benchmark approach are depicted by dashed lines.

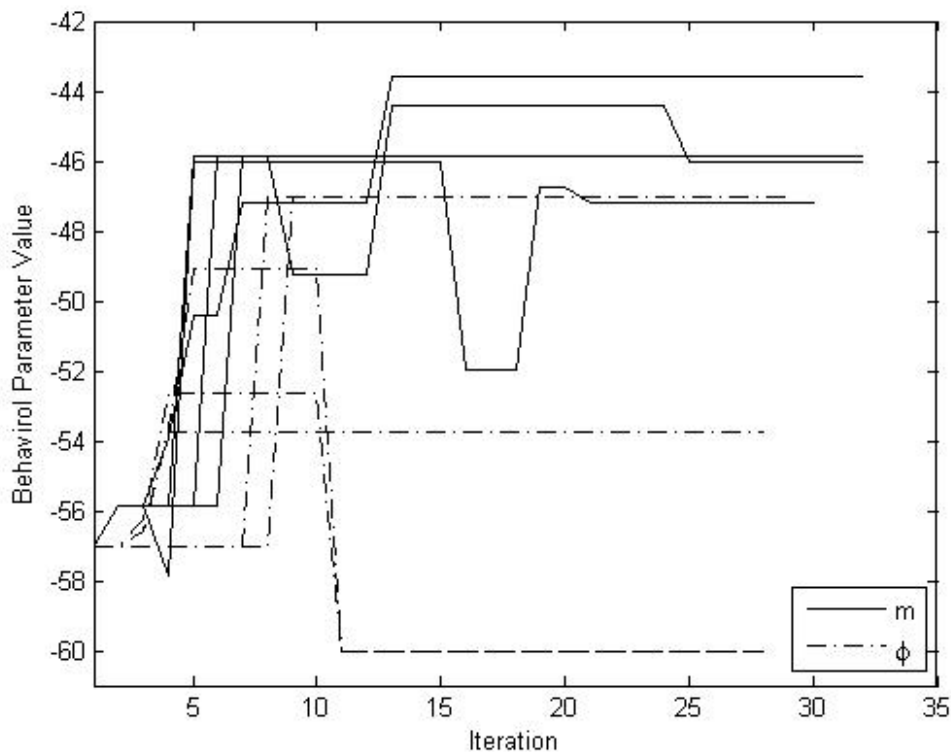


Fig. 2. Initial point  $\theta_0 = -57$ , optimal point  $\theta^* = -42$ . Simulated calibration parameter values across algorithmic iterations.

Note that for each metamodel, we run the algorithm 5 times. The figure displays 5 lines for each method. Consider iteration 25, the line with a y-value of 45.8 consists of 2 overlapping solid lines. The dashed line with y-value -47 consists of 2 overlapping dashed lines. The dashed line with y-value -60 consists of 2 overlapping dashed lines.

Fig. 2 shows that after iteration 25 all solutions derived by the proposed approach are within the range  $[-43, -47]$ . Only 2 of the 5 solutions proposed by the benchmark approach are within this range.

Similar results are obtained when initializing the SO algorithm with a  $\theta_0 = -10$ . These are displayed in Fig.3.

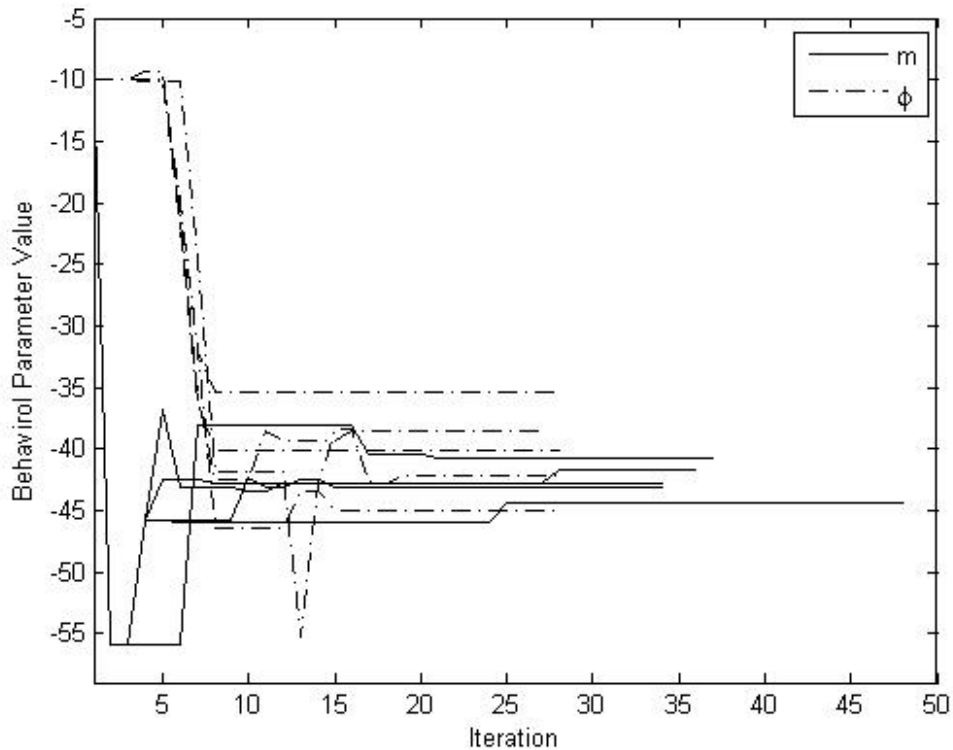


Fig. 3. Initial point  $\theta_0 = -10$ , optimal point  $\theta^* = -42$ . Simulated calibration parameter values across algorithmic iterations..

Again, as of iteration 25, all 5 solutions derived by the proposed approach are within 10% of the true  $\theta$  value, whereas only 3 out of the 5 solutions proposed by the benchmark approach are within this range.

#### 4. Conclusion

In this paper, we propose to embed analytical problem-specific information within calibration algorithms such as to enhance their computational efficiency. We propose a metamodel approach, and use a metamodel that embeds information from an analytical differentiable traffic model. The latter provides an analytical description of how the calibration parameter (a route choice parameter) is related to the calibration objective function (expected link flows). The performance of the approach is compared to that of a similar metamodel approach that does not embed analytical traffic model information. Preliminary results on a toy network are presented. Ongoing work applies these ideas to the calibration of a Berlin metropolitan area network.

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