PC-SPSA: Implementation assessment and exploration of different historical data-set generation methods for enhanced DTA model calibration

Moeid Qurashi*[1], Qing-Long Lu[2], Guido Cantelmo[1], and Constantinos Antoniou[3]

[1]Research Associate, Technical University of Munich, Germany
[2]Research Assistant, Technical University of Munich, Germany
[3]Full Professor, Technical University of Munich, Germany

SHORT SUMMARY

Calibrating DTA models is complex due to the involved undeterminedness, non-linearity, and dimensionality, restricting calibration approaches especially when calibrating larger networks. Simultaneous perturbation stochastic approximation (SPSA) has been proposed for the DTA model calibration, with encouraging results, for more than a decade with multiple variants trying to improve its application scalability on larger networks. Recently, PC-SPSA has been proposed, combining Principal Component Analysis (PCA) with SPSA to reduce the problem dimensions and non-linearity by limiting the search space in lower dimension space based on orthogonal Principal Components evaluated upon a set of historical estimates. In this paper, we further explore PC-SPSA implementation by assessing its sensitivity towards SPSA parameters definition, its performance in calibrating synthetic problems of different dimensions and non-linearity, and formulating multiple OD historical data–set generation methods for improved calibration (in case of non-existent or irrelevant historical estimates). The performance of each method is compared calibrating an urban network of Munich with similar PC-SPSA settings, depicting more correlated generation techniques perform better consistently than simplified ones.

Keywords: Model calibration, principal component analysis (PCA), simultaneous perturbation stochastic approximation (SPSA)

1 Introduction

Dynamic Traffic Assignment (DTA) model calibration is a long–hauled research topic, due to its complexity and non–linearity, which increases exponentially with the sizes of the network. Especially, the need to dynamically update a large set of DTA model parameters (route choice, link capacity, Origin–Destination flows), leveraging a much smaller set of available traffic measures (link counts, speeds), limits the application of the existing calibration approaches for larger networks (Marzano, Papola, & Simonelli, 2009). Due to its ability to deal with non–linear and stochastic systems, the Simultaneous Perturbation Stochastic Approximation (SPSA) (Spall, 1998) is one of the most popular algorithms for DTA model calibration (Balakrishna, Antoniou, Ben-Akiva, Koutsopoulos, & Wen, 2007). However, it has also been observed to reasonably fail in convergence with larger–scale problems, with many researchers proposing different variants to improve its applicability (Cantelmo, Cipriani, Gemma, & Nigro, 2014; Antoniou, Azevedo, Lu, Pereira, & Ben-Akiva, 2015; Lu, Xu, Antoniou, & Ben-Akiva, 2015; Tympakianaki, Koutsopoulos, & Jenelius, 2015). Recently, a novel approach named PC–SPSA has been proposed (Qurashi, Ma, Chaniotakis, & Antoniou, 2019). This approach combines Principal Component Analysis (PCA) (widely adopted for both offline and online calibration problems (Djukic, Van Lint, & Hoogendoorn, 2012; Prakash, Seshadri, Antoniou, Pereira, & Ben-Akiva, 2018)) with SPSA, limiting its search space within a lower dimensional space for faster and more efficient calibration. PCA, given a series of historical estimates, evaluates strong patterns and correlations, representing the variance present with a few orthogonal/uncorrelated Principal Components (PCs) in a low dimensional space. The unknown estimation variable (OD demand) is transformed into a few PC–scores, which are then estimated using SPSA. Qurashi et al., 2019 demonstrated the performance of PC–SPSA calibrating synthetic demand scenarios of a medium sized urban network, significantly improving upon previously defined SPSA (Balakrishna et al., 2007). Although being powerful and intuitive, PCA–based methods rely on the historical data–set to extrapolate estimation patterns.

Within this research, we aim to further explore and propose the implementation methods of PC–SPSA, e.g. assessing its sensitivity towards SPSA parameters and problem characteristics (dimensionality vs. non–linearity), exploring its implementation in different demand scenarios, proposing solutions for favorable/unfavorable (irrelevant or non–existing) historical estimates.

The remainder of the document is structured as follows. Section 2 briefly describes PCA implementation, SPSA and PC–SPSA. Then, Section 2.4 introduces the new probability functions that will be adopted to produce different historical data–sets for the PCA in unfavorable scenarios. Finally, in Section 3 the case study and their results are described, while conclusions are discussed in Section 4.

2 Methodology

In this section, we introduce our methodology for DTA calibration with PC–SPSA. The following table reports the most relevant notations.

Table 1: List of Symbols

D	Historical data matrix with dimensions $[n_d \times n_ij]$
x	Current/prior OD estimate
D_{ij}^t, x_{ij}^t	OD pair between zone i to j at time interval t
n_{ij}, n_t, n_d	Number of OD pairs, time intervals and historical days
δ_{rand}	Randomly generated number
δ_{od}	Normally distributed random vector of size equal to OD vector with $\mu = 0$ and $\sigma = 0.333$
δ_t	Normally distributed random vector of size equal to total time intervals with $\mu = 0$ and $\sigma = 0.333$
δ_d	Normally distributed random vector of size equal to total historical estimated (days) with $\mu = 0.5$ and $\sigma = 0.08325$
R_d, R_{od}, R_t	Factor/weight coefficients for days, OD and time interval based randomness values

2.1 PCA implementation

PCA is implemented as per Qurashi et al., 2019. Singular value decomposition (SVD) is applied to the historical data matrix D to evaluate its principal components (PCs) as:

$$D = U\Sigma V^T \tag{1}$$

where columns of the $n_{ij} \times n_{ij}$ unitary matrix V present orthogonal PCs, with their corresponding PC–scores stored in the rectangular–diagonal matrix Σ with dimension $n_d \times n_{ij}$. U is a $n_p \times n_p$ unitary matrix with orthogonal vectors. V is reduced to $\hat{V}$, where only the first few significant PCs n_v are retained:

$$\hat{V} = [\, v_1 \; v_2 \; v_3 \; \ldots \; v_{n_v} \,] \tag{2}$$

The new matrix $\hat{V}$ is then used to reduce our starting OD flows vector x into PC scores z of dimension $[n_v \times 1]$, as:

$$z = \hat{V}^T x \tag{3}$$

Furthermore, the OD vector can be approximated as:

$$x \approx \hat{V} z \tag{4}$$

2.2 Simultaneous perturbation stochastic approximation (SPSA)

As defined by Spall, 1998, SPSA randomly perturbs its set of estimation variables θ (equation 5) by a perturbation coefficient c_k and Δ (± 1 Bernoulli distribution random vector) to evaluate a random numerical gradient g (equation 6) and later minimize the estimation variables θ by the evaluated gradient and a minimization coefficient a_k (equation 7). The function $f(\theta)$ in equation 6 captures the error associated to a set of parameters θ.

$$\theta^{\pm} = \theta_k \pm c_k \Delta \tag{5}$$

$$g' = \frac{f(\theta^+) - f(\theta^-)}{2c_k} \left[\Delta_1 \ \Delta_2 \ . \ . \ \Delta_h\right]^T \tag{6}$$

$$\theta_{k+1} = \theta_k - a_k {g'}_k(\theta_k) \tag{7}$$

2.3 PC–SPSA

Within PC–SPSA, PC–scores vector z resulted from the implementation of PCA on the OD flows vector x are calibrated instead of the OD flows vector x itself, using a modified SPSA algorithm settings (as per Qurashi et al., 2019). The two modifications include: 1) Replacing the estimation variables θ from OD flows vector x to its PC-scores z, 2) Modified steps of perturbation and minimization from equation 5 and 7 to equation 8 and 9.

$$\text{Perturbation:} \qquad z^{\pm} = z_k \pm z_k \times c_k \Delta \tag{8}$$

$$\text{Minimization:} \qquad z_{k+1} = z_k - z_k \times a_k g' \tag{9}$$

2.4 Historical matrix estimation

PCA limits SPSA search space within the patterns/correlations captured by the estimated PCs in historical estimates. Although being powerful and intuitive, PCA–based methods need to rely on strong relevance of historical data–set with the targeted estimate, as if, the patterns of the target solution are not present within the variance of historical estimates, PC–SPSA will not be able to provide a good quality solution. This limits the applicability of PC–SPSA in scenarios of irrelevant or non–existing historical estimates. In such scenarios, possible generation methods of historical estimates with different correlations among time–dependent OD flows can follow three different dimensions.

- **Spatial correlation:** Spatial correlation among OD pairs presenting the spatial structure of the demand over the network.
- **Temporal correlation:** Temporal correlation of the OD flows i.e. fluctuation of the demand from one time interval to another.
- **Day to day correlation:** Mobility demand is correlated to the demand for activities. As such, it follows a structure and day to day variations are likely to occur.

Exploiting the three correlation dimensions that cover the possible user behaviors, historical estimates are generated using 6 different methods:

1. Spatial correlation:

$$D = \sum_{d=1}^{n_d} \sum_{t=1}^{n_t} D^t = \sum_{d=1}^{n_d} \sum_{t=1}^{n_t} (1 + R_{od}\delta_{od}) \times x^t \tag{10}$$

2. Temporal correlation:

$$D = \sum_{d=1}^{n_d} \sum_{ij=1}^{n_{ij}} D_{ij} = \sum_{d=1}^{n_d} \sum_{ij=1}^{n_{ij}} (1 + R_t\delta_t) \times x_{ij} \tag{11}$$

3. Spatial and temporal correlation:

$$D = \sum_{d=1}^{n_d} D = \sum_{d=1}^{n_d} (1 + R_{od}\delta_{od \times t}) \times x \tag{12}$$

4. Spatial and day-to-day correlation:

$$D = \sum_{t=1}^{n_t} D^t = \sum_{t=1}^{n_t} (1 + R_{od}\delta_{od \times d}) \times x^t \tag{13}$$

5. Temporal and day-to-day correlation:

$$D = \sum_{ij=1}^{n_{ij}} D_{ij} = \sum_{ij=1}^{n_{ij}} (1 + R_{od}\delta_{t \times d}) \times x_{ij} \tag{14}$$

6. Spatial, temporal and day-to-day correlation:

$$D = \sum_{d=1}^{n_d} D = \sum_{d=1}^{n_d} (1 + R_{od}\delta_d\delta_{od \times t}) \times x \tag{15}$$

Beyond capturing all possible correlations between variables (spatial, within-day temporal, day-to-day temporal), an additional value of these formulations is that the distributions δ_{od}, δ_t, and δ_d can be derived by other data sources, such as mobile phone network data and survey data. This lead to a framework that is more general - as does not depend on an historical database - and more flexible - as the structure of the PCs would reflect both OD flows as well as other spatial-temporal dynamics.

3 RESULTS AND DISCUSSION

3.1 Experimental setup

3.1.1 Network

The urban network of Munich city center (shown in Figure 1) is used to set up the calibration case study in the open–source traffic simulator DLR SUMO (Lopez et al., 2018). The network consists of 2605 edge links with 564 detector locations (area of 9.5×10.5 km) and the demand of the morning peak (between 7am and 10am) is represented in 15 min intervals with an OD matrix of [61×61] or 3721 OD pairs. The simulations are set up in the mesoscopic resolution with trip–based (one–shot) stochastic user route choice assignment.

3.1.2 Calibration scenario

The probability functions defined in Section 2.4 can be used for generating a series of scenarios, capturing (up to a certain extent) user behaviors and assessing how the model performs, when erroneous assumptions are made. The most appropriate and probable scenario that captures the user behavior is generated using the probability functions for spatial and temporal correlations, as per the guidelines from Antoniou et al., 2016, using equation 16 with x considered as true/target demand and X the initial demand.

$$X = (R_d + R_{od}\delta_{od \times t}) \times x \tag{16}$$

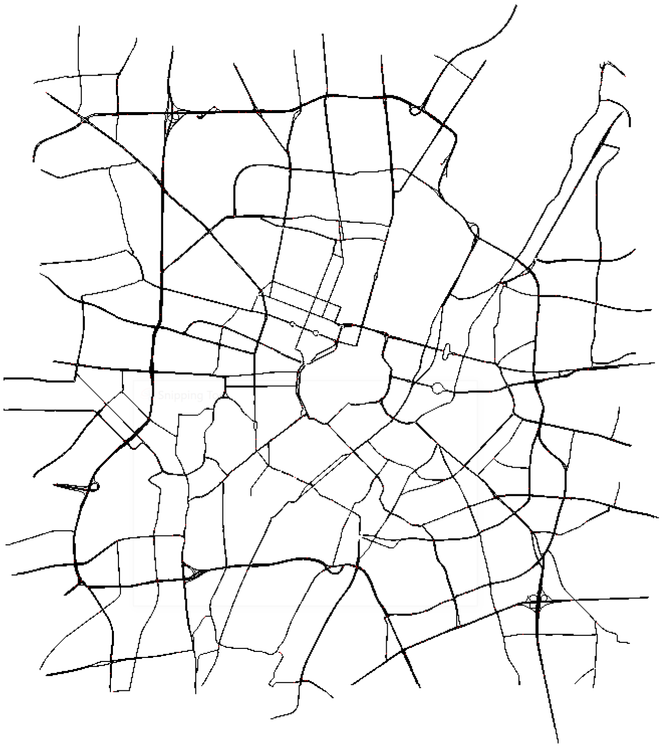

Figure 1: Network of Munich city center

3.2 Results

3.2.1 PC–SPSA parameters

Being a random search stochastic algorithm, SPSA requires appropriate pre–definition of its hyper–parameters, varying significantly for different problems (guidelines as per Spall, 1998). Without any universal set of SPSA parameters identified, they are defined mostly by trial–and–error methods during implementation. As shown in Qurashi et al., 2019, in PC–SPSA, these parameters are significantly less sensitive, due to two reasons: 1) they act as percentage change in perturbation and minimization (eq. 8 and 9), instead of absolute change (eq. 5 and 7 from SPSA); and 2) due to the faster rate of convergence with PC–SPSA and properties of PC scores (fewer estimation variables with even lesser being more significant). Figure 2 shows a simple sensitivity analysis result of the hyper–parameters c and a, calibrating one hour demand for the Munich network, evidently showing very similar convergence patterns with different values of both hyper–parameters.

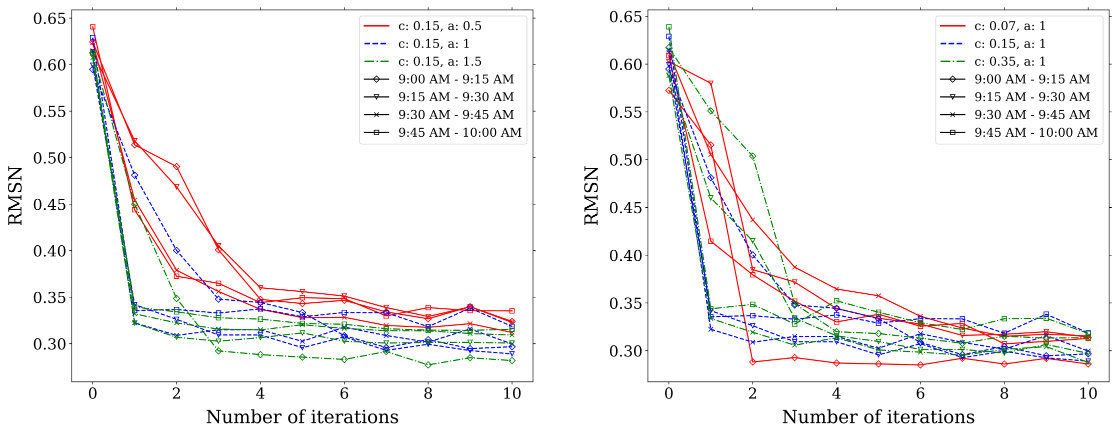

Figure 2: Comparison of using different hyper parameter values (c and a) for PC–SPSA

3.2.2 Problem dimensions vs. non–linearity

PC–SPSA improves on SPSA by improving its resilience against dimensionality (fewer estimation variables–PC scores) and non–linearity (orthogonal PCs) in DTA model calibration. Figure 3 shows convergence rate results of both SPSA and PC–SPSA for calibrating problems with dimensions varying from 20 to 90 OD zones (i.e. 20^2 to 90^2 OD pairs), mapped using non–linear synthetic functions to link counts.

Convergence results of all functions depict that the increase in problem dimension does not affect the convergence performance of PC–SPSA and results from all except Easom function show that PC–SPSA can also well cater for different amount of non–linearity with orthogonal PCs (also evident with Easom function results, showing similar performance for both PC–SPSA and SPSA due to its property of being flat with a single global minimum). SPSA performance in the simple non–linear and rastrigin functions deteriorates with an increase of the problem dimensions and for the eggholder function it is almost unable to converge due to either its complexity or inappropriate hyper–parameter settings.

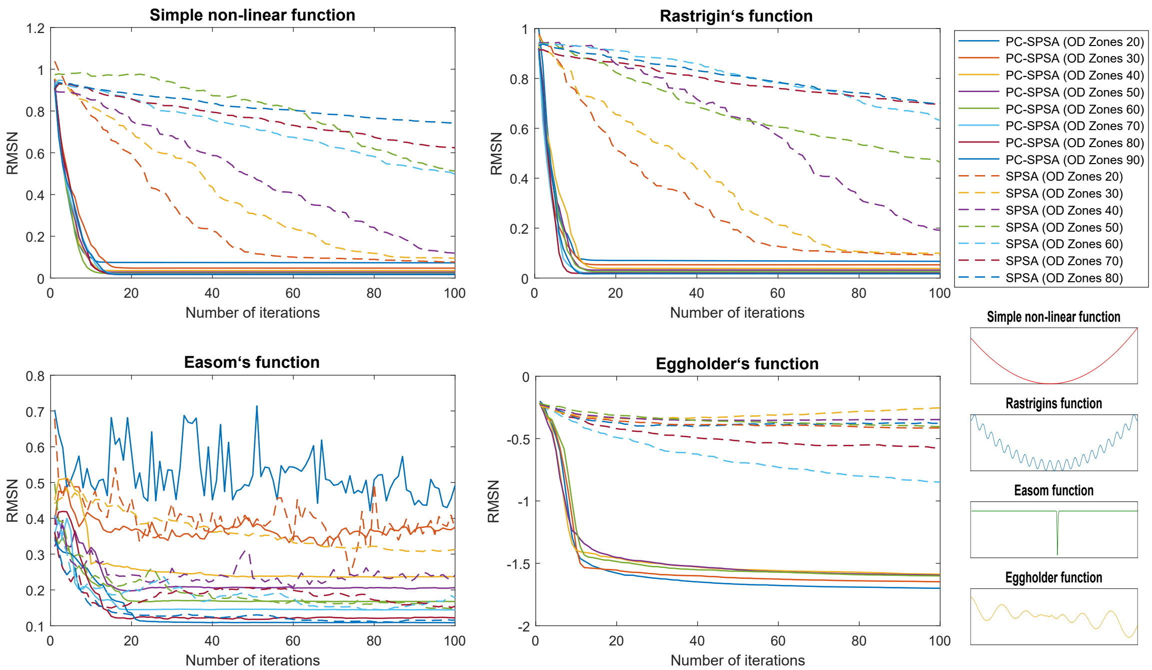

Figure 3: Non-linear synthetic functions with different dimensions

3.2.3 Historical matrix generation methods

The generated scenario is calibrated using 6 historical data matrices with PC–SPSA (methods showed in equations 10-15). Performance evaluation of such calibration techniques requires three major performance indicators, given as:

1. Best goodness–of–fit between calibrated and target OD matrix [Figure 4 (left)].
2. Best goodness–of–fit between observed and measured counts [Figure 4 (right)].
3. Best convergence performance over the required number of iterations for different time intervals [Figure 5].

For the first two performance indicators, method 6 (i.e. Equation 15, spatial, temporal and day to day correlation) and method 3 (i.e. Equation 12 spatial, temporal correlation) depict best performance for converging to the least RMSN (observed versus calibrated traffic counts) and best quality solution (calibrated OD matrix versus target OD matrix figure 4). It's also evident that methods 1 and 2 (historical data–set with single correlation either spatial or temporal, equation

10-11) are worst in performing consistently, getting good quality solution or lowest RMSN for traffic counts.

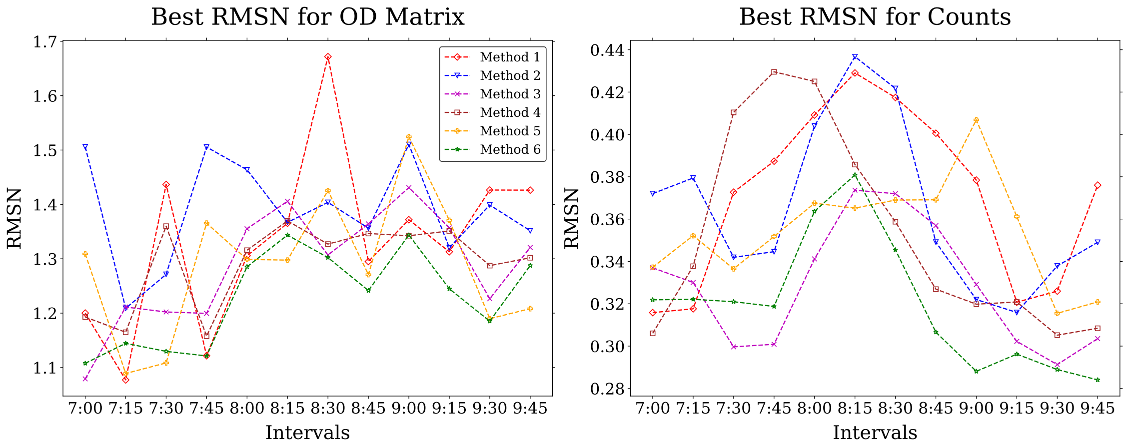

Figure 4: Comparison between all generation methods

Figure 5 depicts the convergence patterns for all 6 historical data–sets for two specific time intervals, confirming method 6 based historical data–set as the best for the third performance indicator (calibrating to the least RMSN error within the first few —3 or 4— iterations).

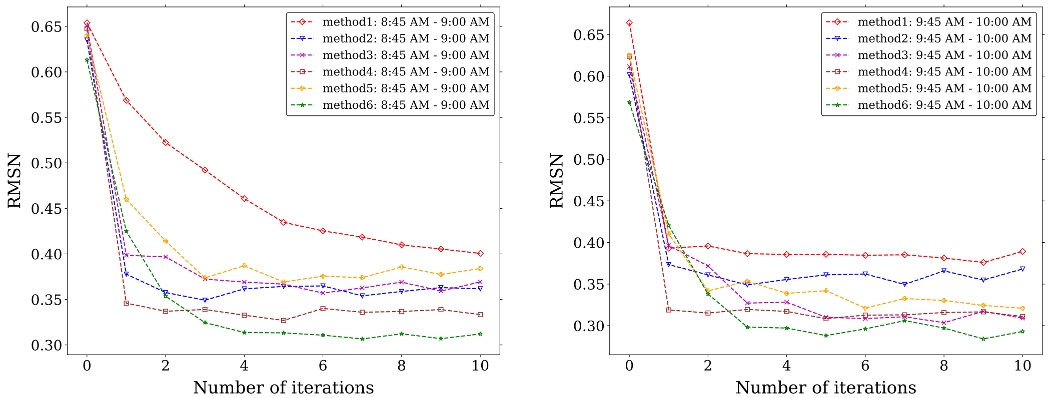

Figure 5: Comparison between generation methods for specific intervals

The results for method 3 and 6 evidently show that the combination of spatial and temporal correlation is crucial for scenarios created with similar technique but method 6, performing the best, also adds a day to day based correlation within the historical estimate providing somewhere more search space or variance for PC–SPSA to find a better solution and improve the overall calibration performance.

4 Conclusion

This paper explores the implementation of PC–SPSA by analyzing its stability/robustness against SPSA hyper–parameters definition and different problem characteristics, and proposing effective methods of historical data–set generation crucial for calibration performance for principal component analysis (PCA) based algorithms. Calibrating the network of Munich, PC–SPSA shows good stability against a range of values for different hyper–parameters. This is not usually the case for SPSA, which is more sensitive against appropriate definition of these parameters (section 3.2.1). Secondly, we used synthetic experiments and simplified functions to test PC–SPSA's resilience against dimensionality (network sizes) and non-linearity (multiple local minima, flat objective function) 3.2.2). Also in this case, the model shows resilience against the increase in problem dimensionality and different types of non–linear functions, due to its property of calibrating the problem in lower dimensional space based on orthogonal PCs.

Multiple historical data–set generation methods are proposed exploiting three different correlations among time dependent OD flows and are later analyzed with most probable demand calibration scenario (replicating realistic changes in OD demand). As per the results (section 3.2.3), historical estimates that are generated with more correlation (i.e. method 3 and 6) outperform other simplified techniques in terms of consistency, OD estimation quality, and minimum error, probably due to containing more correlated information than random variance.

Furthermore, in the MFTS2020 conference, we will include validation of historical matrix generation technique on a larger network of Munich city (with a network of 8689 links, 706 detector location and demand of OD matrix [73 × 73] or 5329 OD pairs) with different demand scenarios and also other network information e.g. travel times. Also, since the results proposed in this study are based on synthetic experiments, we aim to test PC–SPSA and its historical data–set generation methods using real traffic data from Munich to generate an assumption–free benchmark scenario i.e. the "true" network state is derived from real data, allowing us to validate our probability functions against real data.

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References

Antoniou, C., Azevedo, C. L., Lu, L., Pereira, F., & Ben-Akiva, M. (2015). W-SPSA in practice: Approximation of weight matrices and calibration of traffic simulation models. *Transportation Research Part C: Emerging Technologies*, *59*, 129–146.

Antoniou, C., Barceló, J., Breen, M., Bullejos, M., Casas, J., Cipriani, E., ... van Lint, H. (2016). Towards a generic benchmarking platform for origin-destination flows estimation/updating algorithms: Design, demonstration and validation. *Transportation Research Part C: Emerging Technologies*, *66*, 79–98.

Balakrishna, R., Antoniou, C., Ben-Akiva, M., Koutsopoulos, H. N., & Wen, Y. (2007). Calibration of microscopic traffic simulation models: Methods and application. *Transportation Research Record*, *1999*(1), 198–207.

Cantelmo, G., Cipriani, E., Gemma, A., & Nigro, M. (2014). An adaptive bi-level gradient procedure for the estimation of dynamic traffic demand. *IEEE Transactions on Intelligent Transportation Systems*, *15*(3), 1348–1361.

Djukic, T., Van Lint, J., & Hoogendoorn, S. (2012). Application of principal component analysis to predict dynamic origin–destination matrices. *Transportation research record*, *2283*(1), 81–89.

Lopez, P. A., Behrisch, M., Bieker-Walz, L., Erdmann, J., Flötteröd, Y.-P., Hilbrich, R., ... Wießner, E. (2018). Microscopic traffic simulation using sumo. In *The 21st IEEE International Conference on Intelligent Transportation Systems.* IEEE. Retrieved from <https://elib.dlr.de/124092/

Lu, L., Xu, Y., Antoniou, C., & Ben-Akiva, M. (2015). An enhanced spsa algorithm for the calibration of dynamic traffic assignment models. *Transportation Research Part C: Emerging Technologies*, *51*, 149–166.

Marzano, V., Papola, A., & Simonelli, F. (2009). Limits and perspectives of effective o–d matrix correction using traffic counts. *Transportation Research Part C: Emerging Technologies*, *17*(2), 120–132.

Prakash, A. A., Seshadri, R., Antoniou, C., Pereira, F. C., & Ben-Akiva, M. (2018). Improving scalability of generic online calibration for real-time dynamic traffic assignment systems. *Transportation Research Record*, *2672*(48), 79–92.

Qurashi, M., Ma, T., Chaniotakis, E., & Antoniou, C. (2019). PC-SPSA: Employing dimensionality reduction to limit SPSA search noise in DTA model calibration. *IEEE Transactions on Intelligent Transportation Systems*.

Spall, J. C. (1998). Implementation of the simultaneous perturbation algorithm for stochastic optimization. *IEEE Transactions on Aerospace and Electronic Systems*, *34*(3), 817–823.

Tympakianaki, A., Koutsopoulos, H. N., & Jenelius, E. (2015). c-SPSA: Cluster-wise simultaneous perturbation stochastic approximation algorithm and its application to dynamic origin–destination matrix estimation. *Transportation Research Part C: Emerging Technologies*, *55*, 231–245.