

1 Modified bi-level framework for dynamic OD demand estimation in  
2 the congested networks

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1 **ABSTRACT**

2 This paper presents a modified bi-level optimization framework to solve the high-dimensionality of a non-  
3 linear OD estimation problem that is frequently found in congested networks. The upper-level is formulated  
4 as a generalized least square function of OD demand and traffic counts. The framework is modified by  
5 adding a recursive step to account explicitly the impact of OD demand variation on traffic observations,  
6 leading to improvement of the optimization function performance. The recursive step involves evaluation  
7 of the marginal effects for the subset of significant OD pairs whose variation leads to large changes in  
8 link flow proportions and traffic flows. Furthermore, to overcome the extra computational requirement, an  
9 heuristic method for obtaining a reduced set of OD pairs in the evaluation of marginal effects is proposed.  
10 In this way, the number of optimization function evaluations is reduced allowing the modeller to control  
11 the trade-off between simplicity of the model and the level of realism for large-scale, congested networks.  
12 A conventional bi-level optimization solutions approach is used in the performance assessment study. All  
13 the OD demand estimation approaches are implemented in a mesoscopic traffic simulation tool, Aimsun,  
14 to perform the traffic network loading on a large-scale network: the Vitoria urban network with 3249 OD  
15 pairs, 389 detectors, and 600km road network. The results demonstrate the applicability of the proposed  
16 solution approach to efficiently obtain dynamic OD demand estimates for large-scale, congested networks  
17 within computationally short periods.

## 1 INTRODUCTION

2 This paper focuses on the efficient estimation of OD matrices for congested networks, which are essential  
3 inputs for dynamic traffic management and Dynamic Traffic Assignment (DTA) applications. The absence  
4 of reliable OD matrices, especially in the peak hours, limits the potential for DTA deployment to analyse and  
5 alleviate traffic congestion as part of Intelligent Transportation System (ITS) measures. In order to remedy  
6 this problem a number of solutions are being examined and developed as part of the EU Horizon2020 SETA  
7 project which aims to examine the impact of multiple dynamic data sources, many of which, are sourced  
8 through telematics or mobile phones.

9 The OD estimation problem itself is computationally intensive due to the complexity of the demand  
10 estimation problem, the approaches, and the fact that dynamic OD matrices for real-life transport networks  
11 typically constitute high dimensional data structures. One of the problems with estimating OD demand is  
12 that, in many cases, development and availability of emerging technologies for their direct observation is  
13 still in the early stages. Thus, OD trips have to be inferred from alternative, available traffic observations  
14 (e.g. link traffic counts, speeds). From a modelling point of view, the key difference between the OD  
15 demand estimation approaches, is how the relationship between OD demand and any available traffic data is  
16 defined, calculated and re-calculated throughout the estimation process. Therefore, an exact description of  
17 this relationship leads to an accurate description of traffic state reality in the network, but to more complexity  
18 as well.

19 Initial efforts in research and practice have defined this relationship as linear with the assumption  
20 that variations in OD demand do not impose changes in all the traffic flow observations. However, the linear  
21 relationship may be invalid when congestion builds up in the network, resulting in a non-linear relationship  
22 between OD flows and link traffic observations. Consequently, the existence of non-linearity may lead  
23 to non-optimal solutions. In the past decades, researchers have attempted to develop new methods and  
24 techniques to capture the relationship and effects of OD demand variation on traffic observations. These  
25 methods can be categorized into three fundamental alternatives used to express this relationship: analytical  
26 derivation, simulation-based, and numerical-based approximation.

27 **Analytical derivation:** Dynamic link-flow proportions, expressed in the assignment matrix form,  
28 are typically used to express the weights between OD flows and link traffic counts. Theoretically, these link-  
29 flow proportions can be analytically derived using network topology, path choice set, current route choice  
30 model and equilibrium travel times (1). However, it is recognised that the complexity of the problem at hand  
31 can quickly lead to intractable situations (1).

32 **Simulation-based approximation:** The relationship between demand flows and traffic observa-  
33 tions (e.g. link traffic counts, speeds, density) is uncovered by using traffic simulation without the direct  
34 derivation of the assignment matrix. The most studied method is the Simultaneous Perturbation Stochastic  
35 Approximation (SPSA) method (2), (3), (4), (5), (6), (7) which allows one to approximate a descent gradient  
36 direction with significantly lower computational resources than through the explicit derivation. However,  
37 due to the stochasticity of the simulation model, for each perturbation of the SPSA or W-SPSA where  
38 gradient needs to be determined, the DTA has to be replicated  $R$  times, leading to  $2R$  runs (7).

39 **Numerical approximation:** Recent studies by ((8), (9), (10)) rely on linear approximation of the  
40 assignment matrix, which explicitly accounts for congestion effects. This definition requires the computa-  
41 tion of the marginal effects of demand flow change on the link-flow proportions at the current solution of  
42 each iteration. It is possible to use the finite differences approach to numerically approximate the Jacobian  
43 matrix by using a traffic simulation, but it would be required in every iteration of the gradient solution to  
44 perturb each element in the OD demand vector, one at a time, leading to  $2RDK$  runs, where  $D$  the number  
45 of OD pairs in the network and  $K$  the number of time intervals for the simulation period. In their studies  
46 relationship between demand flows and link traffic counts has been examined.

47 Given the high computational costs involved in evaluating marginal effects of OD demand changes  
48 on traffic observations, there is a need for heuristic approaches and algorithms that can identify solutions

1 with a good performance at a low computational cost. To overcome the computational overhead, a number  
 2 of authors have proposed **heuristic-based approaches**. Toledo and Kolechkina (2013) neglected the effect  
 3 of changes in one OD pair over the other OD pairs in the assignment matrix. Frederix, Viti and Tampre  
 4 (2013) implemented space decomposition of the network in the congested and non-congested sub-networks,  
 5 where derivatives were computed only for the congested area. Shafiei et al. (2017) reduced computation  
 6 costs through iterations progress and computing derivatives on OD pairs whose flows have a higher tendency  
 7 to vary during the dynamic OD demand estimation process. However, their approach requires in the second  
 8 iteration step evaluation of the derivatives for all the OD pairs that still leads to *3DK* simulation runs and  
 9 high computational costs. Note that three simulation evaluations per each OD pair within one iteration  
 10 step are required to compute the numerical derivatives of the first Taylor approximation. Also, all these  
 11 approaches rely on strong heuristic assumptions such as ignoring the effect of OD demand changes outside of  
 12 congested area as shown in Djukic et.al (2017) ((11)) or have been tested on relatively small or medium sized  
 13 networks. Further research is therefore necessary to develop approaches to solve nonlinear OD estimation  
 14 problems that will guarantee reliability and computational efficiency in the large-scale networks.

15 Here we extend the previous work by proposing a modified bi-level optimization solution approach  
 16 to estimate dynamic OD demand for large-scale, congested networks that accounts for relationship approx-  
 17 imation between traffic counts and OD flows. This relationship has been computed for the subset of the OD  
 18 pairs when performance of the objective function has been deteriorated. The subset of the most important  
 19 OD pairs in the network has been identified based on the highest variation in the link flows obtained with  
 20 demand derived in two consecutive iteration steps. Reducing the problem dimensionality through selection  
 21 of the most significant OD pairs replaces the conventional approach of computing derivatives for all OD  
 22 pairs, whether through all the iteration steps or in the initial step as proposed in (10). The importance of this  
 23 approach lies in the possibility to capture the most important effects of congestion, and not only at congested  
 24 links, by relaxing assumption of constant link-flow proportions without loss of accuracy and considerable  
 25 decrease in model dimensionality and computational complexity. In addition, model formulation and solu-  
 26 tion is not limited only to link traffic counts. For example, other traffic observations can be added in traffic  
 27 measurements vector as well as in function for the selection of the most important OD pairs.

28 The paper is organized as follows. In the first Section, we summarize the main challenges in defin-  
 29 ing the non-linear relationship between traffic observations and OD demand. In the second Section, we  
 30 present the modified bi-level optimization framework with an additional recursive step to overcome the di-  
 31 vergence of the optimization function performance. Next, we explore the properties of reducing the number  
 32 of optimization function evaluations by defining the subset of significant OD pairs whose variation leads  
 33 to large changes in link-flow proportions and traffic flows. Subsequently, we demonstrate the performance  
 34 of the proposed OD estimation model on a large-scale network, Vitoria, Spain. The paper closes with a  
 35 discussion on further research perspectives of the OD demand estimation model.

## 36 THE PROBLEM FORMULATION

37 This section describes the most critical issue in OD matrix estimation, whether static or dynamic, the re-  
 38 lationship (mapping) of the observed traffic condition data with unobserved OD flows. This relationship  
 39 is often accomplished by means of an assignment matrix. In the dynamic problem, the assignment matrix  
 40 depends on link and path travel times and traveller route choice fractions - all of which are time-varying,  
 41 and the result of dynamic network loading models and route choice models. These dynamics are reflected  
 42 in travel times between each origin and destination trips on a network, influenced by traffic link flow. While  
 43 a vast body of literature has been developed in this area over the past two decades, this section focuses on  
 44 some of the efforts that highlight the basic dimensions of the problem.

45 The general OD estimation problem is to find an estimate of OD demand by effectively utilizing  
 46 traffic and demand observations. Let  $\Omega \subseteq N \times N$  be set of all  $n$  OD pairs in the network, and  $L' \subseteq L$   
 47 be the set of  $l$  links where traffic data observations are available. The time horizon under consideration is

1 discretised into  $R$  time intervals of equal duration, indexed by  $r = 1, 2, \dots, R$ . The OD matrix,  $\mathbf{x} = \{x_{nr}\}$ ,  
 2 defines the demand for each OD pair  $n \in N$  with departure time interval  $r \in R$ . Prior information on the  
 3 OD matrix is defined as vector,  $\tilde{\mathbf{x}} = \{\tilde{x}_{nr}\}$ . The vector  $\tilde{\mathbf{y}} = \{\tilde{y}_{lt}\}$  defines traffic flow observations for time  
 4 interval  $t = 1, 2, \dots, T$ , for each link in  $L'$ . It is also assumed that  $T$  and  $R$  describe the same length of time  
 5 interval, but their decomposition to time intervals can be different.

The dynamic OD estimation problem can be formulated as a constraint optimization problem (12)  
 as:

$$\min_{x \geq 0} Z(\mathbf{x}) = \alpha f(\mathbf{x}, \tilde{\mathbf{x}}) + (1 - \alpha) f(\mathbf{y}, \tilde{\mathbf{y}}) \quad (1)$$

6 Regardless of the function  $f$  used, the purpose is to obtain an OD demand that yields OD flows and  
 7 traffic data as closely as possible to their observed values. When solving the OD problem in Eq. (1) the  
 8 relationship between traffic observations and OD demand has to be defined, implicitly or explicitly. Most  
 9 dynamic OD demand estimation methods, define this relationship implicitly by the traffic assignment model  
 10 that can be expressed as:

$$\hat{\mathbf{y}}_t = \sum_{h=r-k}^r A_t^h \mathbf{x}_h \quad (2)$$

11 There are two main drawbacks of relationship defined in Eq (2):

1. *Separability of traffic count observations*: it assumes that the traffic flow observed at the link  $l$   
 during time interval  $t$  can always and only be changed by changing one of the OD flows that passes link  
 $l$  when  $\mathbf{x}_h$  is assigned in the network. This assumption of separability is incompatible with some typical  
 phenomena in congested networks, such as congestion spillback between links and time lags due to the  
 delay during congestion. In these cases, it is very likely that increasing an OD flow will cause delays to  
 other flows that do not pass that time-space interval, hereby altering the amount of flow passing the link in  
 the considered time interval. This issue has been addressed in past studies ((13), (14), (15)). Frederix, Viti  
 and Tampre (9) suggested using a Taylor approximation to specify the linear approximation of Eq. (2) using  
 a non-separable response function, given by

$$\hat{\mathbf{y}}_t = \sum_{h=r-k}^r A_t^h(\mathbf{x}_0) \mathbf{x}_r + \sum_{h=r-k'}^r (\mathbf{x}_h - \mathbf{x}_{0h}) \left[ \sum_{h'=r-k'}^r \frac{d(A_t^{h'}(\mathbf{x}_{h'}))}{d\mathbf{x}_h} \mathbf{x}_{0h'} \right] \quad (3)$$

12 2. *Limited only to one data source*: formulation of relationship by assignment matrix in Eq. (2)  
 13 and Eq. (3) restricts dynamic OD demand estimation problem to the use of traffic count data only, which  
 14 can potentially over-fit to counts at the expense of traffic dynamics. Relationships between traffic condition  
 15 data, such as speeds and densities, and OD flows are expected to be non-linear and approximations similar  
 16 to the assignment matrix cannot be justified (16). This issue has been addressed in the past studies ((16),  
 17 (4), (6), (7)) who proposed use of traffic simulation models to capture the nonlinear relationship between  
 18 OD flows and traffic observations instead of the assignment matrix.

19 Although presented solutions significantly contributed to quality improvement of dynamic OD demand  
 20 estimates, they still share a common challenge to overcome high computational costs. A complicating  
 21 factor in utilizing these methods for estimation or prediction purposes, is that OD matrices are very large  
 22 data structures, that grows rapidly in large networks. Even in case where high-dimensional OD flows can be  
 23 reduced (see e.g. (17) and this is not entirely unlikely, there are serious methodological difficulties in finding  
 24 optimal solutions (e.g. getting stuck in local minima, slow convergence, high number of simulation runs,  
 25 etc.), aside from the computational and memory requirements for such a procedure on the basis of thousands  
 26 (to millions) of traffic observations. For example, computing the exact Jacobian vector in the second term  
 27 of Eq. (3) with respect to changes in OD flows for each OD pair remains intractable even when an efficient,  
 28 well calibrated, DTA model is used.

## 1 METHODOLOGY

2 Algorithms proposed in literature to solve the problem given in Eq. (1) that incorporate computation of the  
 3 marginal effects of demand changes on traffic observations, lead to high computational costs for medium- or  
 4 large-scale networks. In this situation, dimensionality reduction of simulation runs required to capture these  
 5 effects is necessary, leading to improve computational performance. In order to overcome problems related  
 6 to the dimensionality of OD demand problem we propose the following heuristic approach. First of all, we  
 7 propose the use of Eq. (3) to capture marginal effects with respect to changes in OD flows, rather than using  
 8 a more conventional approach with linear assignment proportions given by Eq. (2). Secondly, we propose  
 9 to use Eq. (3) on the subset of the OD pairs whose variation in demand creates the divergence of the cost  
 10 function given by the objective function defined in Eq. (1). Lastly, we suggest using an initial OD matrix that  
 11 produces similar congestion patterns as those observed in reality, i.e. that allows one to start with the correct  
 12 traffic regime. It is convenient to start the presentation of the proposed solution approach with reference  
 13 to the idea of OD demand estimation problem formulation as bi-level optimization framework. Then, we  
 14 provide modified bi-level optimization framework with recursive step to account the marginal effects of OD  
 15 demand on the link-flow proportions.

### 16 Conventional OD model formulation in bi-level optimization framework

17 Dynamic OD demand estimation problem can be defined as a bi-level optimization framework. The main  
 18 advantage of using the bi-level formulation is the ability to capture network congestion effects in the dynamic  
 19 OD demand estimation problem, as the traffic assignment model can be defined as an optimization problem  
 20 in itself. The upper level is formulated as an ordinary least square (OLS) problem, which estimates the  
 21 dynamic OD demand based on the given link-flow proportions. Assuming that errors are independently  
 22 and identically normally distributed, the objective function aims to minimize the square distance between  
 23 estimated and observed traffic flows, and the estimated and prior OD demand matrix, defined in Eq. (4) as  
 24 follows:

$$\min_{x \geq 0} Z(x) = \alpha \|x - \tilde{x}\|^2 + \|(A(x)x - \tilde{y})\|^2 \quad (4)$$

subject to

$$y = DTA(x) \quad (5)$$

25 Here we assume that the entire set of link traffic counts for the analysis period,  $L' \times T$ , is used to simul-  
 26 taneously estimate the OD demand for all time intervals,  $N \times R$ . The link-flow proportions are, in turn,  
 27 generated from the dynamic traffic network loading problem at the lower level, which can be solved through  
 28 a simulation-based DTA procedure (in this case, Aimsun software (18)).

29 In general terms, all dynamic OD demand estimation methods defined as a bi-level optimization  
 30 problem aim to find the most probable OD matrix by iteratively solving problems defined at upper and  
 lower-level. The iterative solution algorithm is given as follows:

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**Algorithm 1** The conventional bi-level optimization algorithm

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**Step 1. Initialization.** Initiate prior OD demand matrix, set  $k = 0$ .

**Step 2. Assignment.** Assign the demand to the network to obtain assignment matrix,  $A_k^h$  and estimated link  
 traffic counts on the links with traffic observations, by Eq. (2) or Eq. (3).

**Step 3. Convergence test.** Check objective function value convergence. If objective function value has  
 converged, stop and accept the current demand. Otherwise, proceed to step 4.

**Step 4. Update OD demand.** Estimate OD demand with link flows obtained from DTA, as given by Eq.  
 (2). Go to step 2,  $k = k + 1$ .

**End**

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1           When non-separability of traffic observations is considered, as was shown in the previous section,  
 2 Eq.(3) has to be applied in Step 2 to capture the marginal effects of the demand variation on the changes  
 3 in traffic flow observations. The traffic assignment relationship given in Eq.(3) can be solved by computing  
 4 the numerical derivatives using a finite or central differences method of the traffic link flows with respect to  
 5 changes in all OD pairs. This requires perturbing each OD pair in the OD demand two times, one at the time,  
 6 resulting in  $2NR$  traffic simulation runs and objective function evaluations per iteration step. It is obvious  
 7 that such an approach will result in computationally expensive tasks, that have to be overcome.

### 8 **Modified bi-level optimization framework**

9 The bi-level optimization framework presented in the previous section is modified to meet the following  
 10 requirements for congested, large-scale networks:

- 11           • Relax assumption on link-flow proportions derived from DTA by computing the marginal effects  
 12 of the demand deviations on link flows given by Eq.(3);
- 13           • Reduce the number of OD variables in Eq.(3) through the inclusion of only those OD pairs whose  
 14 change in demand values cause significant deviations in the link flows;
- 15           • Keep the computational costs lower.

16 These requirements are implemented through the following modified iterative solution algorithm with re-  
 17 cursive step:

---

#### **Algorithm 2** The modified bi-level optimization algorithm

---

**Step 1. Initialization.** Initiate prior OD demand matrix, set  $k = 0$ ,  $I' = \emptyset$ .

**Step 2. Assignment.** Assign the demand to the network to obtain assignment matrix,  $A_k^h$  and estimated link  
 traffic counts on the links with traffic observations, by Eq.(2) or Eq.(3).

**Step 3. Convergence test.** Check objective function value convergence. If objective function value has  
 converged, stop and accept the current demand. Otherwise, proceed to step 4.

**Step 4. OF performance test.** Check performance of the objective function value. If objective function  
 decreases proceed to step 5. Otherwise, proceed to step 6,  $k = k - 1$ .

**Step 5. Update OD demand.** Estimate OD demand with link flows obtained from DTA, as given by Eq.(2).  
 Otherwise, proceed to step 2,  $k = k + 1$ .

**Step 6. Select OD pairs.** Determine OD pairs whose variation has a considerable impact on link flow  
 variation in the previous iteration and insert them in  $I'$ .

**Step 7. Update assignment.** Update the link-flow proportions in the assignment matrix  $A_{k-1}$ , with values  
 obtained from Equation (3) for the selected OD pairs in  $I'$ .

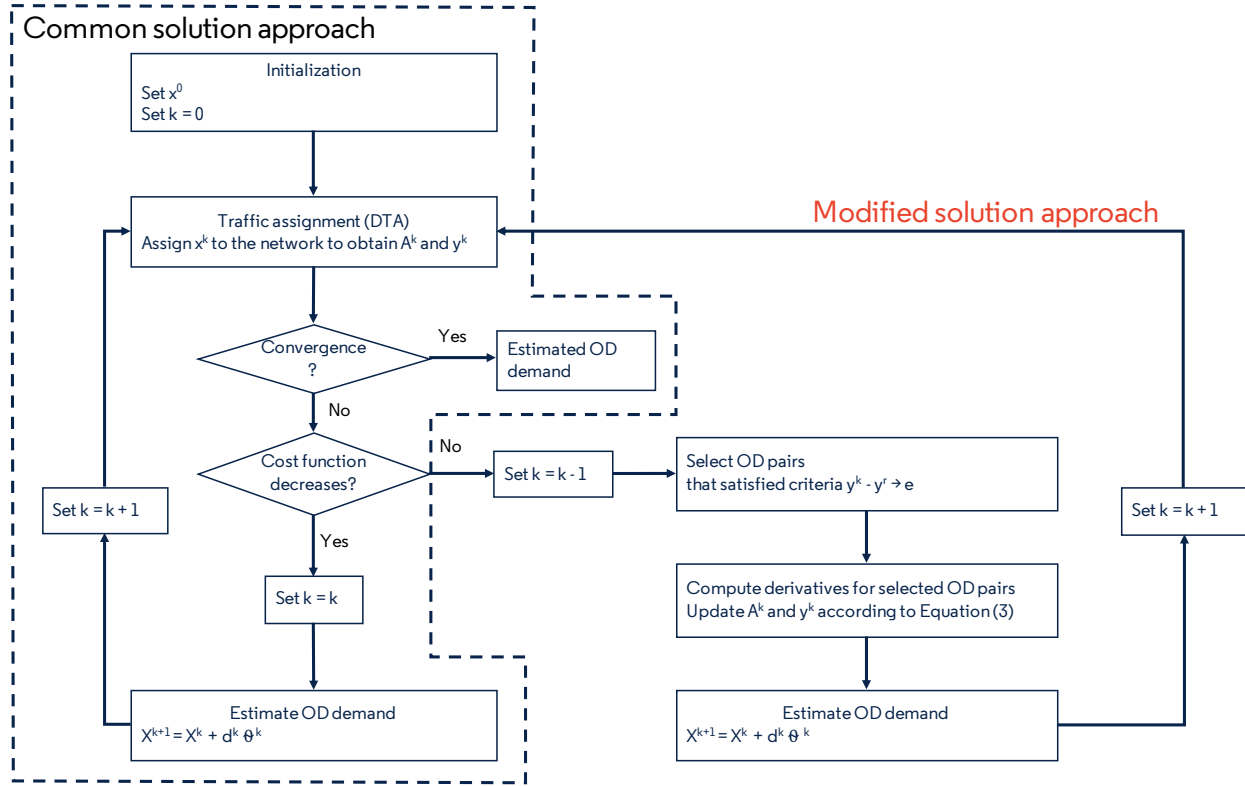
**Step 8. Update OD demand.** Estimate OD demand with link flows obtained from Eq.(3). Go to step 2,  
 $k = k + 1$ .

**End**

---

18           The common and modified bi-level optimization framework with inputs and outputs for OD demand  
 19 estimation is illustrated in Figure 1.





**FIGURE 1 Generic algorithm based on the proposed modified bi-level solution framework.**

1 Note that the proposed solution algorithm in Steps 6 and 7 uses a demand with one iteration step  
 2 latency because the updated demand at iteration step  $k$  caused the increase of the objective function value.  
 3 Therefore, following the modified bi-level framework, Step 8 denotes correction of the state variable for  
 4 iteration  $k$ , using the information from the link-flow proportions and link flows for iteration  $k = k - 1$ ,  
 5 obtained in Steps 6 and 7. In Step 6, we analyse the change in the link flows obtained with demand assigned  
 6 in iteration step  $k$  and  $k = k - 1$ , and determine the link flows with the highest variation. Using the  
 7 information from the link flow proportions matrix, we can identify which OD flows are crossing these links  
 8 with the highest flow variation and set them in  $I'$ . Then, in Step 7 the elements of the link-flow proportion  
 9 matrix are corrected for these OD pairs using the Eq.(3). The upper-level problem in Steps 5 and 8 is  
 10 solved using the gradient decent method. The OD demand estimation results are evaluated in Step 3 against  
 11 termination criteria and the procedure would continue if termination criteria is not met. Finally, the Steps 6-8  
 12 reflect our corrected knowledge on the OD demand state at iteration  $k = k - 1$  to improve the performance  
 13 of the solution algorithm.

#### 14 Method for solving the upper-level problem

15 Let  $x_k$  be the demand at iteration step  $k$ , and  $A_k$  and  $y_k$  the assignment matrix and simulated traffic counts  
 16 given by this demand. As an approximation to the OD estimation objective function given in Eq. (4) that  
 17 we want to minimize, we consider the following auxiliary objective function:

$$Z_k(x) = \|\tilde{y} - y_k - A_k(x - x_k)\|^2 + \alpha \|x - \tilde{x}\|^2 \quad (6)$$

18 There are different types of exact and heuristic methods proposed in the literature that can be em-  
 19 ployed to solve the optimization problem defined in Eq. (6) with non-negative variable constraints. At every



1 outer iteration step, the gradient descent method is selected to minimize the objective function defined in  
 2 Eq. (6), which uses the gradient as search direction:

$$d = -\nabla Z_k \quad (7)$$

3 where

$$\nabla Z_k(x) = 2\alpha(x - \tilde{x})^2 + 2(A_k^T A_k x - A_k^T \tilde{y} + A_k^T y_k - A_k^T A_k x_k) \quad (8)$$

4 To perform this gradient method, we start at  $x = x_k$  and we perform  $M$  gradient steps, the direction  
 5 being given by the latter Eq. (8). At internal step  $m \leq M$ , let us denote the estimated demand by  $\mathbf{x}_k^m$ .  
 6 After determining the search direction, which is given by  $\nabla Z(\mathbf{x}_k^m)$ , the optimal step length,  $\theta^m$  needs to be  
 7 obtained in each internal iteration step. The following criterion is used to compute the step size:

$$\theta^m = \min_{\theta^m} Z(\mathbf{x}_k^m - \theta^m \nabla Z(\mathbf{x}_k^m)) \quad (9)$$

8 The exact line search procedure proposed by Cauchy (1847) (19) is used to compute the step size.  
 9 In the case where  $Z$  is a quadratic function, the optimal step can be computed analytically. In this case, the  
 10 optimal step size is computed using the following expression:

$$\theta^m = \frac{\|\nabla Z(\mathbf{x}_k^m)\|^2}{\|\nabla Z(\mathbf{x}_k^m)\|^2 + \|A_k \nabla Z(\mathbf{x}_k^m)\|^2} \quad (10)$$

## 11 NUMERICAL EXPERIMENT DESIGN

12 In this section, we will first describe the input data used, e.g. historical OD demand generation and the DTA  
 13 traffic assignment procedure. We consider three assessment scenarios in terms of link-flow proportions  
 14 derivation (i.e. with and without computation of marginal effects). Numerical experiments are performed  
 15 on a large-scale network, (Vitoria, Basque Country, Spain) with real data to evaluate the performance of the  
 16 proposed approach.

### 17 DTA with mesoscopic simulation model

18 In the experiments, we use the mesoscopic event-based demand and supply models in Aimsun, each synthe-  
 19 sizing microscopic and macroscopic modelling concept. The travel demand in Aimsun is represented by dy-  
 20 namic OD demand matrices. Vehicle generation is performed for each OD pair separately with arrival times  
 21 that follow an exponential distribution. The iterative interaction between demand and supply models allows  
 22 the system to update the set of routes and the travel times after each iteration leading to robust estimation  
 23 and prediction of traffic conditions in the network. For this study, a route choice set will be pre-computed  
 24 in Aimsun and used as fixed for all the simulation runs in performance analysis. In this way, dependence of  
 25 re-routing effects on the changes in the OD demand is ignored. Here we focus on investigating the effects  
 26 of travel time variation and congestion spill-back on traffic observations in the network.

### 27 Network and traffic data

28 The proposed OD estimation approach is evaluated for the large-scale network in Vitoria, consisting of  
 29 57 zones, 3249 OD pairs (57 x 57) with 2800 intersections and 389 detectors, presented as black dots in  
 30 Figure 2. This network is available in the mesoscopic version of the Aimsun traffic simulation model for  
 31 the reproduction of traffic propagation over the network. The true OD demand is available for this network,  
 32 which allows analysts to assess the performance of the proposed method. The true assignment matrix and  
 33 traffic counts on detectors are derived from the assignment of true OD matrix in Aimsun for the evening  
 34 period from 19:00 to 20:00 reflecting a congested state of the network. The simulation period is divided into

- 1 15 minute time intervals with an additional warm-up time interval,  $R = 5$ . The link flows resulting from the  
 2 assignment of the true OD demand are used to obtain the real traffic count data per observation time interval.



**FIGURE 2 The Vitoria network, Basque Country, Spain**

- 3 The historical OD demand flows are derived by adding a uniform normal component in the range  
 4 of  $\pm 40\%$  to the real OD demand to produce uncertainty in the historical demand and congestion in the  
 5 network.

#### 6 **Assessment scenario**

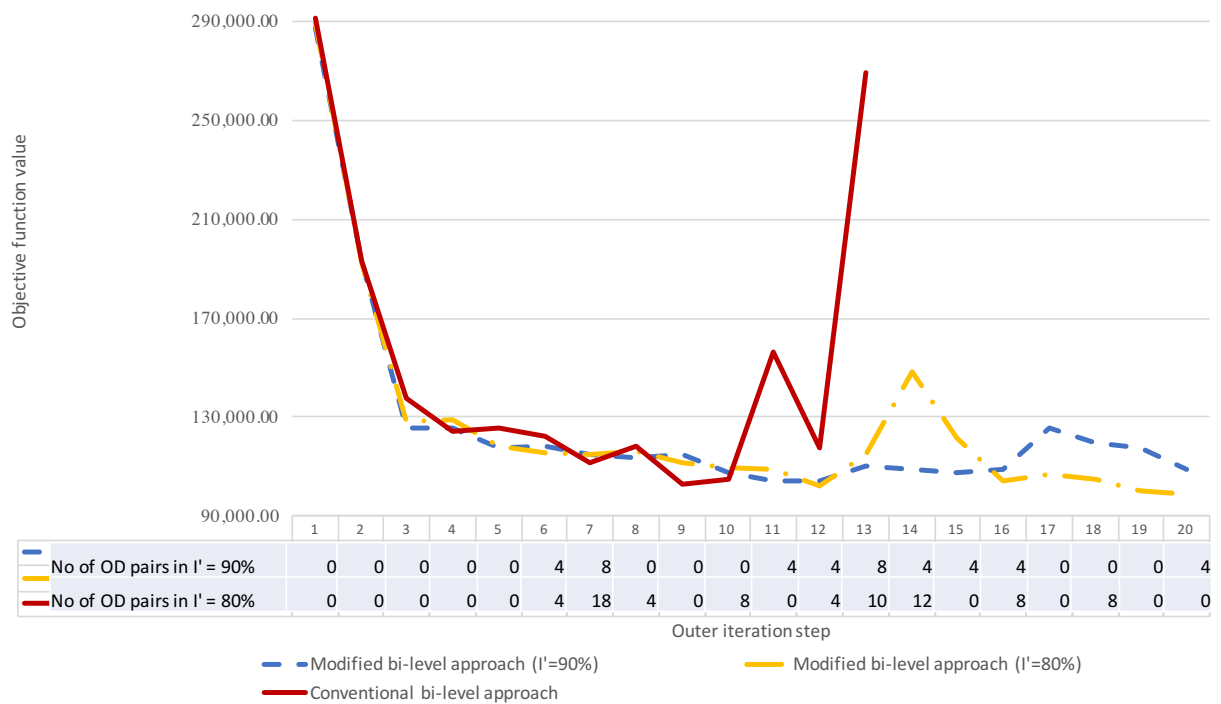
- 7 Three assessment scenarios have been defined for the performance assessment of the proposed solution ap-  
 8 proach. The main goal of this task is to evaluate the expected improvements due to exact implementation  
 9 of marginal effects of OD demand variations. Thus, dynamic OD estimation method that shares same per-  
 10 formance measure and solution framework, i.e. least square (LS) error measure defined in bi-level solution  
 11 framework is selected as a benchmark scenario. Further, two solution strategies in selecting the number of  
 12 OD pairs have been defined to assess the performance of the proposed OD estimation method. Subsets of OD  
 13 pairs involved in proposed modified solution approach are defined, such that in every iteration step we can  
 14 identify potential set of OD pairs that impacts the 90% and 80% of variation in traffic counts. For example,  
 15 the distance between observed and simulated traffic counts is computed, and arranged in decreasing order  
 16 of deviation magnitude in each iteration step. Then, OD pairs that dominate changes in the traffic detectors  
 17 with deviation higher then 90% are selected for their evaluation of the marginal effects in demand estimation  
 18 process, here denoted as  $I' = 90\%$ . In this evaluation task, three assessment scenarios are considered:

- 19 1. **Conventional bi-level approach:** LS solved by conventional bi-level solution approach without  
 20 explicit non-linear relationship formulation;  
 21 2. **Modified bi-level approach with  $I' = 90\%$**   
 22 3. **Modified bi-level approach with  $I' = 80\%$**

- 23 A point of interest now is finding out to which extent the estimation accuracy and computational  
 24 time are improved. To get a better grasp of the algorithms real world performance, results are presented in  
 25 the following section.

1 **RESULTS**

2 The performance of the objective function for all three scenarios are presented in Figure 3. For the purpose  
 3 of this study, convergence was defined as reaching an objective function value that is three times lower than  
 4 the initial value obtained (by any of the algorithms) within 20 iterations. The performance of the proposed  
 5 modified bi-level solution approach demonstrates satisfying results, since it is able to maintain the decrease  
 6 of the objective function value through iteration steps. Modified bi-level approach with both OD pair sub-  
 7 sets demonstrate convergence trend to a local minimum, in contrast to conventional bi-level optimization  
 8 framework. Note that conventional bi-level approach did not reach convergence, which seems to indicate  
 9 that search directions that algorithm produces are increasingly inefficient as the algorithm progress. For the  
 10 purpose of visualisation, we have shown results for the conventional bi-level approach up to iteration step  
 13 and stored the results for further analysis from this step.

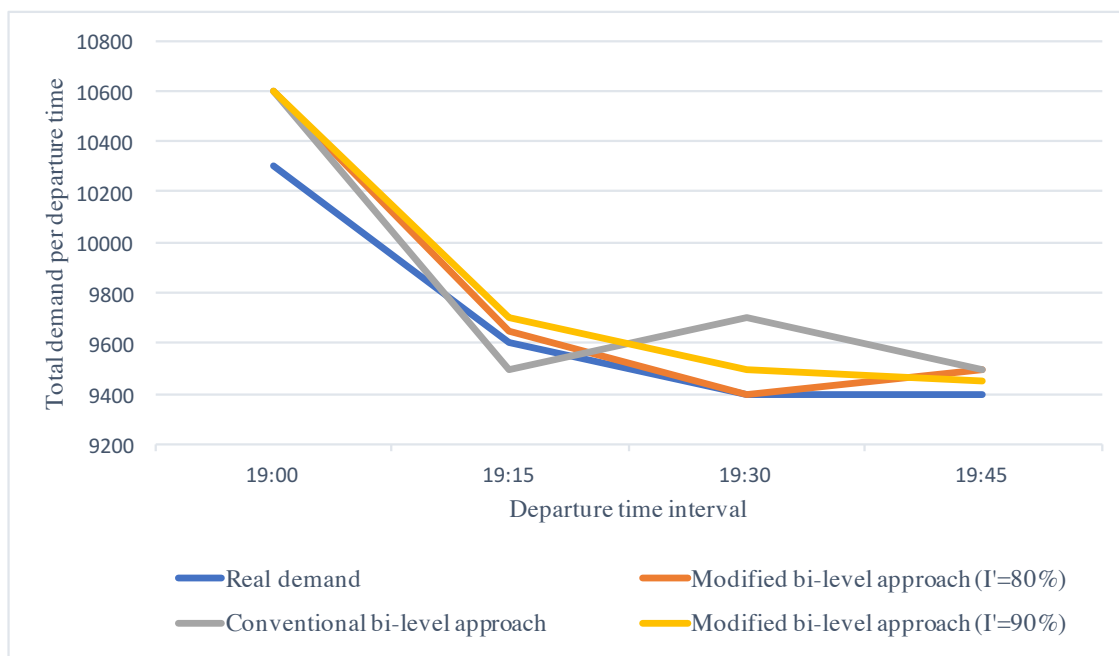


**FIGURE 3 Comparison of the objective function performance**

11 It can be observed from Figure 3 that the conventional bi-level approach runs into an unstable  
 12 convergence trend from the iteration step 9. This effect is a consequence of initial OD matrix that reflects  
 13 over fitted demand, very close to the congestion level. When demand obtained in iteration step 9 is assigned  
 14 in the network it will result in the network blockage due to spill-back propagation. Thus, assignment matrix  
 15 obtained out of this simulation step is not realistic and if used further by algorithm in iteration step 10 results  
 16 in sudden divergence of cost function and intractable solution. Results shown in Figure's 3 table reveal that  
 17 the proposed modified bi-level approach identified the cause of function deterioration in the iteration step  
 18 6, and by updating the elements of the assignment matrix in the recursive step guaranteed more stable  
 19 objective function convergence. Also, results show that extending the number of OD pairs involved in  
 20 updating the link flow proportions leads to objective function performance improvement (e.g., see modified  
 21 bi-level approach with  $I' = 80\%$  in Figure 3) although with slight higher objective function deterioration as  
 22

1 shown in iteration step 12 and 13. This effect can be explained by definition of the recursive step in modified  
 2 approach, where derivatives have been computed for the larger set of OD pairs and whose effect has a better  
 3 impact in finding more accurate demand solution. However, this effect can be further explored by extending  
 4 the list of OD pairs whose variance dominates deviations in the traffic flows.

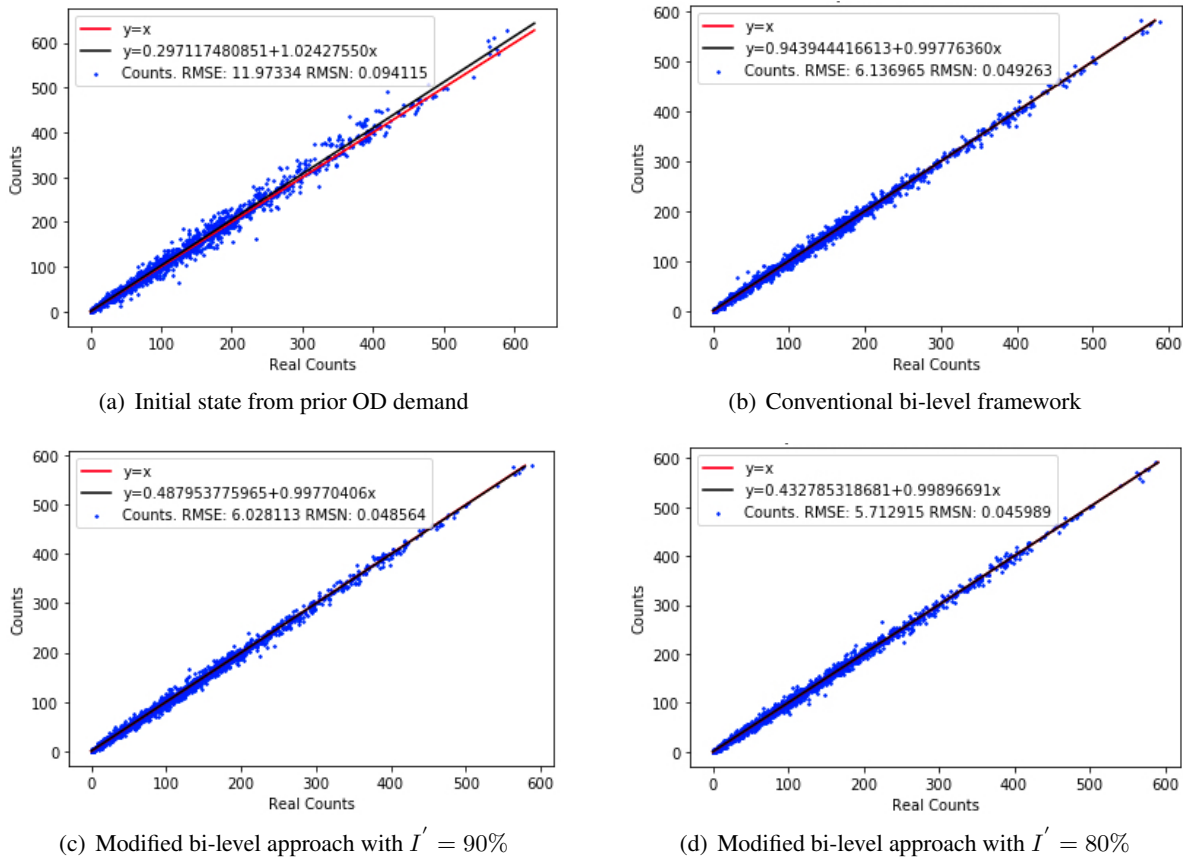
5 Figure 4 shows the estimated total OD demand per departure time interval for OD demand solu-  
 6 tion approaches. We have included the real OD demand in the figure as a point of reference. All three  
 7 tested solutions demonstrate a tendency to slightly overestimate demand as a consequence of incorrect data  
 8 interpretation from loop detectors when congestion level increase. However, performance of the proposed  
 9 modified bi-level approach demonstrates a capacity to recognize an overestimation trend and improves de-  
 10 mand estimation using the first order approximation given by Eq.(3) to update elements of the assignment  
 11 matrix in time intervals when congestion occurs in the network. In addition, results indicate unstable per-  
 12 formance of the conventional bi-level approach, where the misinterpreted impact of the congestion led to  
 13 under- and overestimation of total demand.



**FIGURE 4 Estimated OD demand per departure time interval**

14 Next, it is important to investigate how these estimated OD demands once assigned to the network  
 15 can produce traffic counts close to their real observations. Figure 5 provides a performance overview of ap-  
 16 proaches in terms of the relationship between simulated and observed traffic counts. It appears clearly from  
 17 Figure 5 that all the approaches show correlation increase and significant reductions in RMSE and RMSN  
 18 error. Results in Figure 5(d) indicate that proposed modified bi-level approach with higher sensitivity to de-  
 19 mand changes has the best performance with improvement of the RMSE value for 52.29% compared to the  
 20 initial value before OD demand estimation. It is interesting to observe from Figure 5(b) that a conventional  
 21 bi-level approach demonstrates slightly lower reduction of the RMSE value for 45.19%. However, note that  
 22 results presented here for the conventional bi-level approach are obtained from iteration step 13, since the  
 23 method did not show a tendency to converge until iteration step 20 as discussed above. In turn, performance  
 24 results of conventional bi-level approach should be considered with caution. A detailed examination of Fig-  
 25 ures 4, 5(d) and 5(c), shows that the more OD pairs are included in the evaluation of the marginal effects  
 26 of demand variation on the traffic flows the better the demand estimation results obtained, in terms of total

1 demand and traffic flows.



**FIGURE 5 Scatterplot of the observed and simulated traffic counts per solution approach**

2 Note that initial idea was to solve the computational complexity of the OD demand estimation  
 3 problem for real case applications while maintaining reliable estimation results in the congested networks.  
 4 Therefore, Table 1 shows the run time and number of simulation runs for each of the tested solutions.

**TABLE 1 CPU computation time and the number of the DTA simulations**

CPU time	No. of assignment simulations	Aimsun simulation time	Demand estimation time (Python)
Conventional bi-level method	13	26min	31min
Modified bi-level method $I' = 90\%$	64	2h 2 min	51min
Modified bi-level method $I' = 80\%$	96	3h 4min	1h 16min
Benchmark method (Shafiei (2017))	366	12h 12min	14h 32min

5 Table 1 shows that the conventional bi-level method requires the least number of simulation runs.  
 6 This can be explained as follows: the conventional algorithm requires one simulation run in each iteration,  
 7 compared to the other two solutions that require three simulation runs for each OD pair within one iteration

1 step to compute the numerical derivatives defined by Eq. (3). As a result, the gain in terms of run times  
2 obtained by the use of an assignment matrix without updates is large, but with a trade off on the lower  
3 quality of estimation results. Furthermore, this degradation in estimation accuracy is expected to increase  
4 for larger and more complex networks. We can observe significant CPU computation time reduction of  
5 the proposed modified bi-level solution approach compared to the benchmark method proposed by (10).  
6 This effect can be explained by definition of solution approaches. The proposed modified bi-level approach  
7 calculates derivatives for the subset of the OD pairs when deterioration of the objective function is observed  
8 in contrasted to the benchmark method that requires in the second iteration step evaluation of the derivatives  
9 for all the OD pairs. These times have been obtained by running Aimsun and Python on DELL Latitude  
10 E6430 with processor Intel Core i5-3320M, and 2.6GHz memory.

## 11 CONCLUSIONS

12 The common approach usually adopted in dynamic OD demand estimation and prediction consists of solv-  
13 ing an optimization problem in which the distance between observed and simulated traffic conditions is  
14 minimized by assuming the relationship between OD flows and traffic observations is independent of traffic  
15 conditions in the network. This approach has a severe shortcoming as it does not take into account the impact  
16 of demand flow variation on traffic observations in congested networks. Modelling of traffic observations  
17 dependency on variations in OD flows has been identified by many researchers as a key challenge in the  
18 estimation and prediction of high-quality OD matrices.

19 In this paper, we proposed a modified bi-level optimization framework to solve the high-dimensionality  
20 of non-linear OD estimation problem by computing the marginal effects of demand flow variation only for  
21 the most significant OD pairs with respect to traffic observations. This approach allows the modeller to  
22 control the trade-off between simplicity of the model and the level of realism. Several specific solution  
23 approaches that differ in the assumptions on the link-flow proportions derivation and solution algorithms  
24 were used in the performance evaluation study. From the results presented in this contribution, modified  
25 bi-level approach appears to outperform conventional bi-level solution with fixed linear relationship signif-  
26 icantly and achieves great improvement over the reference case. Results show that proposed approach is  
27 able to capture the effect of congestion in the network and to reproduce the observed traffic conditions with  
28 high level of accuracy. Furthermore, we show that deriving a non-linear relationship between OD demand  
29 and traffic counts for the subset of the OD pairs will lead to computational efficiency with a guaranteed  
30 improvement in result's accuracy.

31 An improvement of the algorithm presented in this paper can be seen in two directions: 1) ex-  
32 tension of the model as a multi-objective function with traffic condition data (i.e., speed, density, demand  
33 derived from floating car data) can be considered to overcome limitation of the method relying only on  
34 traffic count data; 2) explore alternative gradient solution approaches in solving the upper-level problem to  
35 avoid convergence in local minima, especially when initial OD matrix does not reflect congestion pattern in  
36 reality.

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