Aggregate Calibration of Microscopic Traffic Simulation Models

by

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Abstract

The problem of calibration of microscopic simulation models with aggregate data has received significant attention in recent years. But day-to-day variability in inputs such as travel demand has not been considered. In this thesis, a general formulation has been proposed for the problem in the presence of multiple days of data. The formulation considers the day-to-day variability in all the inputs to the simulation model. It has then been formulated using Generalized least squares (GLS) approach. The solution methodology for this problem has been proposed and the feasibility of this methodology has been shown with the help of two case studies. One of them is with an experimental network and the other is with network from Southampton, UK. The results indicate that estimation of day-to-day OD flows is feasible. They also reinforce the importance of having good apriori information on the OD flows and locating the sensors so as to obtain maximum information.

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Chapter 1

Introduction

With the ever increasing travel needs of people, it is not surprising in the least to say that traffic congestion is among the foremost problems being faced by cities in developed as well as developing countries. As per the 2003 Urban Mobility Study report published by Texas Transportation Institute [29], the largest university-affiliated transportation research agency in the US, traffic congestion in 2001 resulted in the loss of 3.5 billion hours of productivity valued at $69.5 billion. A similar study by the UK government estimates that 1.6 billion hours were lost by drivers and passengers in 1996 due to congestion. The situation is not very different in the developing countries, where the growth rate of fleet size is 10-30 per cent per year as against below 5 per cent in developed countries [16].

While congestion cannot be eliminated completely, measures can be adopted to alleviate the traffic conditions. Transportation agencies generally use three types of strategies to manage congestion:

- construction
- managing travel demand
- improving operations

Construction Traditionally, construction of more roads has been the strategy adopted to deal with congestion. In the present circumstances, it has several drawbacks having to face a variety of physical, economic, social and environmental constraints. Furthermore, it provides only temporary relief for congestion because it tends to encourage further development and therefore traffic growth. Most importantly, it is not possible to catch up with the growth rate in traffic. Increase in route miles of highways in the US by about 1.5 per cent as against 76 per cent increase in vehicle miles between 1980 and 1999 illustrates this clearly.

Managing travel demand This strategy aims at altering driver behavior so that vehicle trips during congested periods and at congested locations are reduced. Some of the programs which belong to this category are flexible work schedules that allow employees to travel off-peak, amenities to improve safety and efficiency of biking and walking, ridematching services for vanpools and carpools, community-based carsharing, employer-subsidized transit passes, guaranteed emergency rides home for transit users, incentives to decrease employer-paid parking and transit-oriented regional development.

Improving operations This method essentially tries to make use of the transportation system to the best extent possible through some strategies and thus tries to increase the efficiency and reliability of the system. Some of these strategies are: Advanced Traffic Management Systems (ATMS), Advanced Traveler Information Systems (ATIS), Incident Management Systems and Managed lanes (HOV lanes, truck-only facilities, congestion pricing, reversible and contra-flow roadways). These also involve altering the driver behavior.

1.1 Intelligent Transportation Systems

Intelligent Transportation Systems (ITS) is nothing but a composition of a number of technologies including information processing, communications, control and electronics applied to improve operations of the transportation systems. It was introduced as Intelligent Vehicle Highway Systems (IVHS) in late 80s with the multiple objectives of improving safety, reducing congestion, enhancing mobility, reducing environmental impact, saving energy and increasing economic productivity. The five functional areas that have been identified for implementation of advanced technologies are Advanced Traffic Management Systems, Advanced Traveler Information Systems, Advanced Vehicle Control Systems, Commercial Vehicle Operations and Advanced Public Transportation Systems [22].

1.2 Microscopic simulation models

Traffic management strategies using the aforementioned advanced technologies may be counter productive if not implemented correctly, as shown by some studies (Gartner et al. [21]). Additionally, often there would be many feasible alternatives that could be adopted to deal with congestion problem in a particular region. While coming up with the feasible alternatives is not very difficult, identifying the best alternative is a hard task. Therefore, evaluation of the alternatives is a critical component in the development of an efficient strategy. These evaluations can be performed with the help of either field tests or simulation models.

Field tests involve implementing all the identified alternatives and choosing the best among them based on certain measures of performance. Disadvantages of these tests are that they are time consuming and are not economical. Further, the test results are affected by uncontrollable parameters. In the case of ATIS, if some of the implemented alternatives do not improve the situation, it might affect the travelers' compliance with guidance provided in the future.

Simulation models , on the other hand, provide a very economical way of analyzing the alternatives. Obviously, credibility of the results obtained from such a model is dependent on its ability to replicate reality to the best extent possible. Some of the microscopic simulation models which have been developed are MITSIMLab [8], PARAMICS [30], FLEXSYT-II [34], etc. More detailed information on various microscopic simulation models can be obtained from the website [32]

1.3 Calibration of microscopic simulation models

All the microscopic simulation models require demand for the use of the road network, in the form of Origin - Destination (OD) flow matrix, as a necessary input. Each element in this matrix represents the number of trips from a specific origin to a specific destination. Another important set of inputs to the microscopic simulation models is the underlying behavior model parameters. However, many of these parameters are network dependent. Therefore, before applying the simulation model to a network, it should be calibrated and validated for that particular network. In addition to OD flows and model parameters, habitual travel times form another set of inputs to the simulation model.

Calibration is the process of determining the OD flow matrix and the behavior model parameters so that the simulator reflects the local traffic conditions being modeled. *Validation* is the process of determining the extent to which the calibrated model can accurately replicate traffic behavior.

1.3.1 OD flows

In practice, OD flows are not available and so need to be estimated. Cascetta [10], classifies the various methods of estimation of OD flows into three groups.

- direct sample estimation
- model estimation
- estimation from traffic flows

Direct sample estimation methods involve conducting surveys, such as home or destination interviews, roadside interviews, flagging techniques or combination of them and estimating the OD flow matrix with these survey results using sampling theory classical estimators. *Model estimation* methods, which are commonly used, estimate OD flow matrix by applying a system of models that give the number of journeys made as a function of several socio-economic variables. The third method of *estimating OD flow matrix from traffic flows* is a more recent one. This problem can be understood as the opposite of traffic assignment problem. This method has received a lot of attention owing to its cost effectiveness as compared to conducting surveys. Furthermore, these flows can be measured repeatedly so that evolution of the phenomenon can be followed.

Since this thesis deals with only the third method of estimation, it should be understood that henceforth the terms "OD estimation" and "Estimating OD flows from traffic flows" are used interchangeably.

1.3.2 Behavior model parameters

Behavior model parameters are the other set of inputs to a microscopic simulation model which need to be estimated. These parameters can be classified into two groups, namely, travel behavior and driving behavior parameters. Travel behavior relates to decisions taken by drivers at a higher level and is represented by a route choice model. Driving behavior models, on the other hand, represent the decisions taken by drivers at micro level as a reaction to other vehicles in the vicinity. Some of these models include lane-changing, car-following and intersection models. These models will be discussed briefly in chapter 4.

1.3.3 Habitual travel times

Habitual travel times represent the drivers' perceptions of travel times based on which they make the route choice decisions. They cannot be measured since they represent perceptions of the travelers. Usually, the network is assumed to be in equilibrium (i.e, the travel times which the drivers expect on the network are consistent with what they experience) in order to estimate these habitual travel times.

1.4 Calibration methodology

The typical methodology followed for calibration of microscopic simulation models is based on the framework shown in Figure 1-1 (which is reproduced from Ben-Akiva et al [7]). According to this framework, calibration involves two steps. In the first step, individual models (driving behavior and travel behavior models) that make up the simulation model are statistically estimated using disaggregate data such as trajectory data. In the second step, aggregate data (flows, speeds etc) is used to fine tune these parameters and estimate the OD flows. Using aggregate data to fine tune parameters helps in capturing the inter-dependencies among the parameters. But in most cases disaggregate data, being very expensive to collect, is not available. Therefore, calibration of the model parameters also has to be done using aggregate data only.

This problem of (i) estimating the OD flows and (ii) calibrating the model parameters using aggregate data is called *aggregate calibration* .

1.5 Thesis focus

In this thesis, a general formulation for calibration of microscopic simulation models in the presence of multiple days of aggregate data will be proposed. Further, various assumptions one could make to simplify the formulation will be presented. Finally, the application of this general formulation is demonstrated through some case studies with focus being more on OD estimation.

1.6 Thesis outline

This thesis is organized as follows. In chapter 2, a brief review of the different methods adopted for both components of aggregate calibration - OD estimation and parameter calibration - is presented. In chapter 3, aggregate calibration in the presence of multiple days of data is formulated as an optimization problem and various assumptions that could be made to be able to solve the problem are outlined. In chapter 4 MIT-

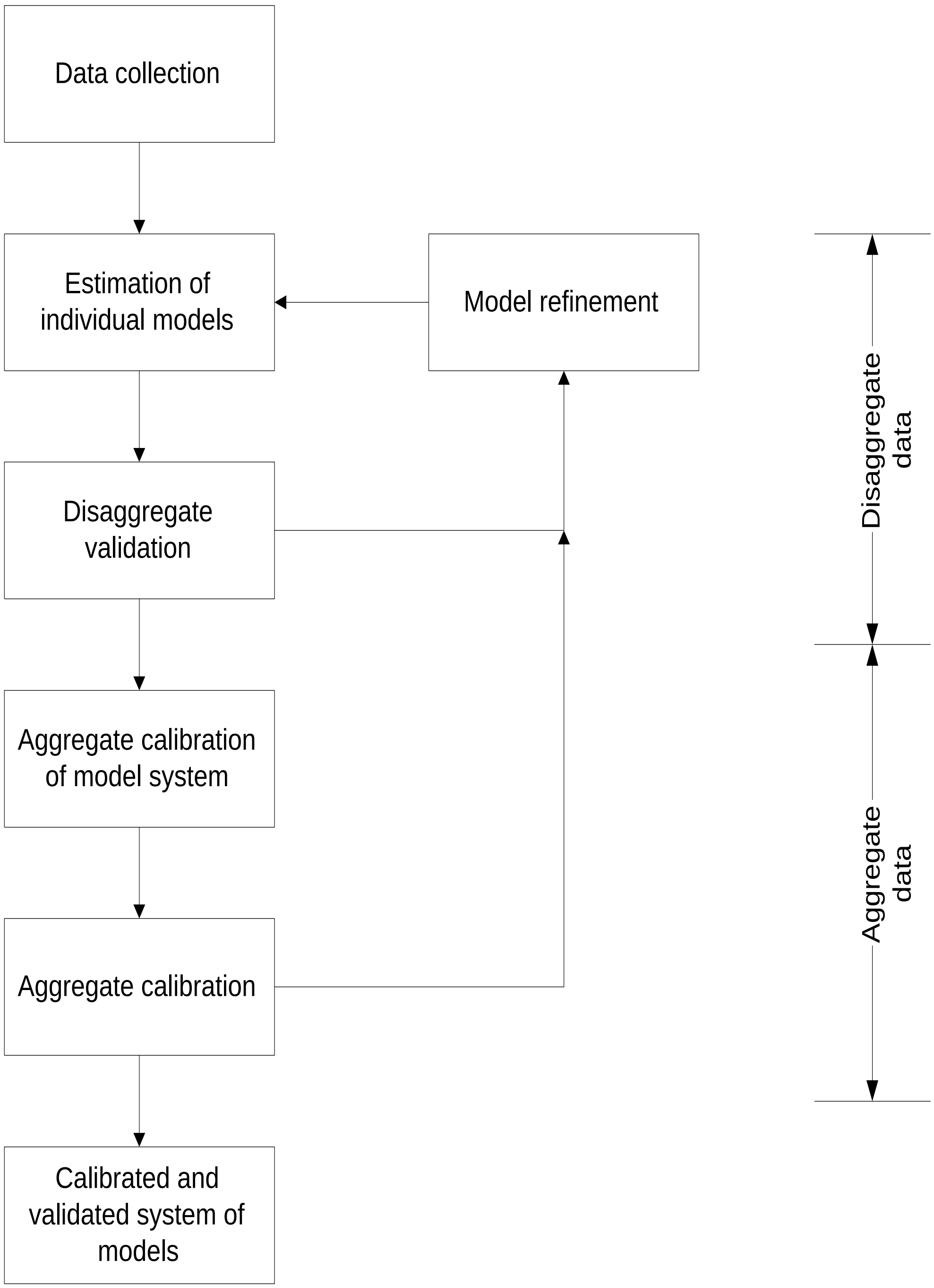

Figure 1-1: Calibration Framework

SIMLab, the microscopic simulation model which has been used in the following study is introduced. Case studies demonstrating the feasibility of the proposed calibration methodology are also discussed. Finally, conclusions drawn from the implementation of this methodolody and directions for future research are presented in chapter 5.

Chapter 2

Literature Review

The problem of aggregate calibration, which involves OD estimation and parameter calibration, has received a great deal of attention during the past few years. This chapter reviews literature pertaining to OD estimation, parameter calibration and obtaining user equilibrium travel times. Since the thesis focuses more on OD estimation, the other two are not discussed in detail.

2.1 OD estimation

In this section, various methods proposed for the estimation of OD flows from aggregate measurements (traffic counts) are reviewed. Most of the following review can be found in the book by Cascetta [11].

This problem of estimating OD flows by combining traffic counts with other available information is also referred to as origin-destination count based estimation (OD-CBE) problem. Typically information on OD flows contained in traffic counts is not sufficient enough to identify a unique set of OD flows. This is because of the relatively high number of OD pairs as compared to the number of links on which sensor measurements are available. Therefore additional information, giving apriori knowledge of the OD flows, is needed to estimate a unique set of OD flows. An overview of the inputs and outputs of the OD estimation problem can be seen in figure 2-1. In literature, apriori information on OD flows is also referred to as *direct measurements*

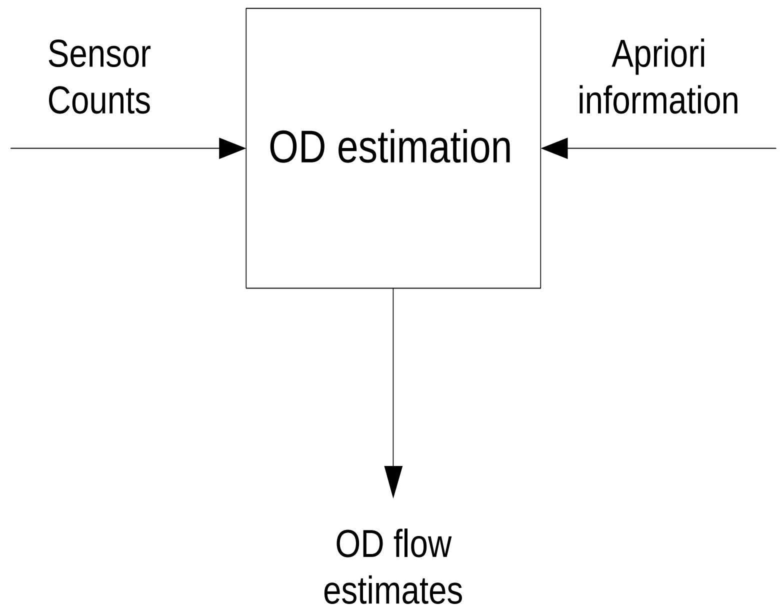

Figure 2-1: Overview of OD estimation inputs and outputs

while traffic counts are referred to as *indirect measurements* (since they represent a function of the true OD flows intended to be estimated).

OD matrices estimated can be either static or dynamic in nature, depending on the purpose of the study. A static OD matrix represents the average travel demand in a day, while a Dynamic OD matrix captures the temporal variation of travel demand within a day.

2.1.1 Static OD estimation

Methods which have been used for static OD estimation are entropy maximization or information minimization (Van Zuylen and L.G. Willumsen [37]), maximum likelihood estimation (Spiess [33]), generalized least squares (Cascetta [10]; McNeil et al. [28]; Bell [6]) and bayesian estimation (Maher [27]). Some of these are described briefly below.

Maximum likelihood estimators are obtained by maximizing the probability of observing the apriori information and the sensor measurements. Making the reasonable assumption that these two probabilities are independent, the maximum likelihood estimator can be expressed as:

$$\hat{x}_{ML} = arg \max_{x \in S}[lnL(x^H/x) + lnL(y/x)] \tag{2.1}$$

where:

x	is the travel demand vector to be estimated
x^H	is the apriori information on the travel demand, which could be obtained from sampling surveys or earlier planning studies
y	is the vector of observed traffic counts
$lnL(x^H/x)$	is the log-likelihood function of the apriori information on travel demand, i.e. the logarithm of the probability of observing the apriori travel demand x^H is x is the true travel demand
$lnL(y/x)$	is the log-likelihood function of the traffic counts, i.e. the logarithm of the probability of observing the traffic counts y if x is the true travel demand
S	is the feasibility set of the true travel demand, usually coincident with the non-negative orthant, i.e. $S = x : x \geq 0$

The log-likelihood functions in the equation (2.1) can be formulated after assumptions are made on the probability distributions of x^H and y, conditional on x.

Generalized Least Squares is another estimator based of classical statistics. This can be derived from the system of linear stochastic equations (2.2) and (2.3) mentioned below.

$$y = Ax + \epsilon \tag{2.2}$$

$$x^H = x + \eta \tag{2.3}$$

with the following additional assumptions

$$E(\epsilon) = 0, Var(\epsilon) = V$$

$$E(\eta) = 0, Var(\eta) = W$$

A is called *Assignment matrix* . This matrix is nothing but a mapping between the traffic counts and the OD flows. The *GLS* estimator of the travel demand, which is the best linear unbiased estimator, can be expressed as:

$$\hat{x}_{GLS} = arg \min_{x \in S} [(y - Ax)' V^{-1} (y - Ax) + (x^H - x)' W^{-1} (x^H - x)] \tag{2.4}$$

Bayesian estimation methods combine sampling information with prior or subjective information. In this particular problem of OD estimation, bayesian estimation involves updating the OD flows obtained apriori with the additional information from traffic counts. The estimator is obtained from the a posteriori distribution $h(x/y, x^H)$, of OD flows conditioned on the apriori information and traffic counts. According to Bayesian theory, this posterior probability is proportional to the product of the apriori probability distribution of OD flows $g(x/x^H)$ and the probability of observing the traffic counts conditional upon the unknown OD flows $L(y/x)$. Mathematically, this is expressed as:

$$h(x/y, x^H) \propto L(y/x) g(x/x^H) \tag{2.5}$$

Bayesian estimator of OD flows can be obtained by maximizing the a posteriori probability in equation (2.5) or its natural logarithm (since natural logarithm is a monotonous function).

$$\hat{x}_B = arg \max_{x \in S} [lng(x/x^H) + lnL(y/x)] \tag{2.6}$$

As in the case of Maximum Likelihood estimator, the specification of the Bayesian estimator depends on the assumptions made for the probability distributions $g(x/x^H)$ and $L(y/x)$.

Cascetta and Nguyen [13] examined Maximum Likelihood and Generalized Least Squares estimators and compared them to Bayesian estimator. They also discuss the computational issues for each of the approaches.

2.1.2 Dynamic OD estimation

The disadvantage of a static OD is that they only represent average traffic conditions in a day. They do not capture the temporal variation within a day and hence are not very useful for applications at operational level. Owing to this reason, several researchers have investigated the problem of dynamic OD estimation.

Various methods of dynamic OD estimation have been proposed, some of which (Cremer and Keller [17]; Bell [6]; Chang and Tao [15]) are are restricted to intersections, junctions or small segments of network corridors and hence not applicable to general networks. A brief review of these estimation methods and the contexts in which they are applicable can be found in Ashok [3]. On the other hand, *Generalized Least Squares* approach and *Kalman Filter* approach can be applied to general networks. Refer to Ashok [3] and Balakrishna [4] for more information on these two approaches.

Generalized least squares

Cascetta et al. [12] have extended the generalized least squares estimation approach to the dynamic case as well. Let the total period under consideration (H) be divided into T intervals, which can be assumed to be of equal length without loss of generality. Let n_l and n_{OD} be the number of sensors in the network and the number of OD pairs respectively. Let x_h be the column vector ($n_{OD} \times 1$) of travel demand of all the OD pairs during interval h; and x_h^H be the column vector of apriori OD flows for interval h. Similarly, let y_h the corresponding column vector ($n_l \times 1$) of traffic counts measured in interval h by all sensors.

The linear stochastic equations in the dynamic case are similar to equations (2.2) and (2.3):

$$y_h = \sum_{p=h-p'}^{h} A_p^h x_p + v_h \tag{2.7}$$

$$x_h^H = x_h + u_h \tag{2.8}$$

where p' is the maximum number of intervals required by a vehicle to complete its journey, A_p^h is the assignment matrix which relates the flows departing in interval p to counts observed in interval h. v_h and u_h are vectors of random errors. Let variance-covariance matrices of v_h and u_h be V_h and W_h respectively.

They proposed two estimation procedures - simultaneous estimation and sequential estimation. In the simultaneous estimation approach, OD flows for all the intervals are estimated in a single step using the traffic counts for all the intervals. The OD flow estimates are given by:

$$(\hat{x}_1, \hat{x}_2, \ldots, \hat{x}_T) = argmin \sum_{h=1}^{T} [(x_h - x_h^H)' W_h^{-1} (x_h - x_h^H)]$$

$$+ \sum_{h=1}^{T} [(y_h - \sum_{p=h-p'}^{h} A_p^h x_p)' V_h^{-1} (y_h - \sum_{p=h-p'}^{h} A_p^h x_p)] \tag{2.9}$$

with non-negativity constraints, $x_i \geq 0, \forall i = 1, 2, \ldots, T$.

On the other hand, in sequential estimation approach the OD flows for all the intervals are estimated one at a time. When estimating the OD flows for interval h, the OD flow estimates of past intervals are kept constant. Hence the counts of period h are linear functions of the unknown demand of the same period only. The OD flow estimates of an interval h are given by:

$$\hat{x}_h = argmin[(x_h - x_h^H)' W_h^{-1} (x_h - x_h^H)]$$

$$+[(y_h - \sum_{p=h-p'}^{h-1} A_p^h \hat{x}_p - A_h^h x_h)' V_h^{-1} (y_h - \sum_{p=h-p'}^{h-1} A_p^h \hat{x}_p - A_h^h x_h)] \tag{2.10}$$

Simultaneous estimation gives more consistent results, but it involves solving a very complex optimization problem. Hence, in practical situations where computational considerations are of prime importance, sequential estimation approach can be employed.

Kalman filtering

This approach casts OD estimation problem as a *state-space* model. A state-space model describes the behavior of a system using two linear stochastic equations -

measurement equation and transition equation. The measurement equation (2.11) relates the unknown state of the system to the observable data, and the transition equation (2.12) describes the evolution of system over time.

$$y_h = A_h x_h + v_h \tag{2.11}$$

$$x_{h+1} = \phi_h x_h + w_h \tag{2.12}$$

In the context of OD estimation, the set of equations (2.7) and (2.8) together form the measurement equations (2.15). Equation (2.12) represents the transition equation.

$$y_h - \sum_{p=h-p'}^{h-1} A_p^h \hat{x}_p = A_h^h x_h + v_h \tag{2.13}$$

$$x_h^H = x_h + u_h \tag{2.14}$$

Expressing both equations (2.13) and (2.14) using matrix algebra, we have

$$\begin{bmatrix} y_h - \sum_{p=h-p'}^{h-1} A_p^h \hat{x}_p \\ x_h^H \end{bmatrix} = \begin{bmatrix} A_h^h \\ \mathbf{I}_{n_{OD}} \end{bmatrix} x_h + \begin{bmatrix} v_h \\ u_h \end{bmatrix}$$

or

$$\mathbf{y}_h = \mathbf{A}_h x_h + \epsilon_h \tag{2.15}$$

The kalman filter algorithm, which is recursive in nature, is described here. Let $\hat{x}_{n|k}$ and $\Lambda_{n|k}$ denote the OD flow estimates and their variance covariance matrix of period n based on observations upto period k respectively. Let w_h be white noise with zero mean and variance Q_h. Similarly, let the variance of ϵ_h be C_h. Assuming that the initial system state is known ($\hat{x}_{0|0} = \mu_0$ and $\Lambda_{0|0} = \Lambda_0$), the steps in the algorithm are:

1. Generate the next estimate and its variance covariance matrix using the transi-

tion equation. Equations (2.16) and (2.17) are referred to as predictor equations.

$$\hat{x}_{h|h-1} = \phi_{h-1}\hat{x}_{h-1|h-1} \tag{2.16}$$

$$\Lambda_{h|h-1} = \phi_{h-1}\Lambda_{h-1|h-1}\phi'_{h-1} + Q_{h-1} \tag{2.17}$$

2. Compute the kalman gain matrix

$$K_h = \Lambda_{h|h-1}\mathbf{A}'_h(\mathbf{A}_h\Lambda_{h|h-1}\mathbf{A}'_h + C_h)^{-1} \tag{2.18}$$

3. Generate the filtered estimate and the corresponding variance covariance matrix using the measurement equation. Equations (2.19) and (2.20) are referred to as corrector equations.

$$\hat{x}_{h|h} = \hat{x}_{h|h-1} + K_h(y_h - \mathbf{A}_h\hat{x}_{h|h-1}) \tag{2.19}$$

$$\Lambda_{h|h} = \Lambda_{h|h-1} - K_h\mathbf{A}_h\Lambda_{h|h-1} \tag{2.20}$$

4. Increment h and go back to step 1.

Many variations of this basic kalman filter algorithm have also been proposed. This method finds special use in on-line applications where prediction of traffic conditions is needed.

2.2 Parameter calibration

The problem of parameter calibration involves identifying the correct set of parameters to be used in the underlying behavior models which reproduce the observed sensor measurements. This is very complex because of the absence of a clear analytical formulation for the objective function in terms of the variables to be estimated. Various methods for calibrating parameters that have been used are:

- manual changes (Daigle et al. [18])

- linear search (Balakrishna [4])
- simplex-based approach (Kim and Rilett [24])
- steepest descent (Kurian [25])
- box algorithm (Darda [19], Toledo et al. [36])
- genetic algorithms (Abdulhai et al. [1], Lee et al. [26])

2.3 Equilibrium travel times

Equilibrium implies that the habitual travel times based on which the drivers make their route choice decisions are consistent with what they experience on the network. These travel times are a property of the true behavioral models. Since the simulation model is used to approximate reality, the same can be used to obtain these equilibrium travel times. If $S()$ is used to denote the simulation model and TT to denote the equilibrium travel times, then TT is a solution to the following equation (2.21).

$$TT = S(TT) \tag{2.21}$$

This is nothing but a fixed point problem. Various iterative schemes have been proposed to solve this problem. Refer to Cascetta et al [14], Bottom [9] for a review.

The studies mentioned in the above sections concentrate on one of the problems only and not the calibration of all the input parameters jointly. Other studies like Darda et al [19] and Jha et al [23] have captured the interactions between the parameters by calibrating them jointly. Though aggregate calibration is the focus of this thesis, it has to be referred that validation of the calibrated simulation models is also an important task. In their paper, Toledo et al [36] have described various statistical measures that can be used to perform validation, but they do not take into account the correlations among the measurements. Barcelo et al [5] proposed a method for calibration and validation to account for these correlations between the sensor measurements. This method was implemented to calibrate the parameters of route choice model. But it is not easily scalable because it involves manually looking for good set of parameters. Additionally, some useful guidelines for developing simulation models have been presented in the paper.

2.4 Summary and Motivation

When data is available for many days, it is not surprising if the sensor data is not the same for all the days. While this variation could be partly because of pure noise, there are few other possible reasons for this. Observed data could vary from day-to-day because of changes in

- model parameters
- travel demand (OD flows)
- habitual travel times
- network conditions (which includes weather conditions)

But the earlier approaches assume that the variation in observed data is purely because of randomness and estimate a single OD matrix for all the days. So we might be losing wealth of information that is hidden in the data. Additionally, since the earlier approaches estimate an average OD matrix for the entire duration under study, they are suitable only for planning purposes and not for operational purposes or reliability studies (where information on distribution of OD flows over days is needed). Hence, the objective in this thesis is to incorporate the variation of the inputs from day-to-day in the calibration methodology.

Chapter 3

Problem formulation

In this chapter, an optimization based general formulation has been proposed for the problem of aggregate calibration in the presence of multiple days of data. The equivalent formulation under the generalized least squares approach has also been presented.

3.1 A general formulation

Before proceeding to the formulation, some of the important variables involved in this problem and the notation used to denote them are mentioned. These variables are:

- Observed aggregate measurements
- Simulated aggregate measurements
- Network conditions
- Travel demand (OD flows)
- Behavior model parameters
- Habitual travel times

Definition and notation of other variables would be mentioned as and when needed.

3.1.1 Notation

N	number of days for which data is available
$\mathcal{N}$	$1, 2, \ldots, N$
M_i^{obs}	observed measurements on day i
M_{iw}^{sim}	simulated measurements on day i and replication w. Simulation models are stochastic in nature. Hence the simulated measurements are random variables.
M_i^{sim}	mean simulated measurements on day i $M_i^{sim} = E[M_{iw}^{sim}]$
G_i	network conditions on day i
$G_{[i]}$	network conditions on days $1, 2, \ldots, i$ $G_{[i]} = \{G_1, G_2, \ldots, G_i\}$
OD_i	OD flows on day i
OD_i^0	apriori information on OD flows on day i
$OD_{[i]}$	OD flows on days $1, 2, \ldots, i$ $OD_{[i]} = \{OD_1, OD_2, \ldots, OD_i\}$
β_i	behavior model parameters for day i
β_i^0	apriori information on behavior model parameters for day i
$\beta_{[i]}$	behavior model parameters on days $1, 2, \ldots, i$ $\beta_{[i]} = \{\beta_1, \beta_2, \ldots, \beta_i\}$
TT_i^{hab}	habitual travel times for day i
$TT_{[i]}^{hab}$	habitual travel times for days $1, 2, \ldots, i$ $TT_{[i]}^{hab} = \{TT_1^{hab}, TT_2^{hab}, \ldots, TT_i^{hab}\}$
TT_{iw}^{exp}	experienced travel times for day i and replication w. Since simulation model is stochastic, the simulated experienced travel times are random variables.
TT_i^{exp}	mean experienced travel times for day i $TT_i^{exp} = E[TT_{iw}^{exp}]$
$TT_{[i]}^{exp}$	mean experienced travel times for days $1, 2, \ldots, i$ $TT_{[i]}^{exp} = \{TT_1^{exp}, TT_2^{exp}, \ldots, TT_i^{exp}\}$

S^M function which relates the inputs of a simulation model to the simulated measurements

S^{TT} function which relates the inputs of a simulation model to the simulated experienced travel times

3.1.2 Model equations

The equations which relate the measurements (both direct and indirect) of OD flows and model parameters to their true values form the basis of the optimization based methodology.

$$M_i^{obs} = M_i^{sim} + \epsilon_i, \quad \forall i \in \mathcal{N} \tag{3.1}$$

$$OD_i^0 = OD_i + \gamma_i, \quad \forall i \in \mathcal{N} \tag{3.2}$$

$$\beta_i^0 = \beta_i + \delta_i, \quad \forall i \in \mathcal{N} \tag{3.3}$$

Equation (3.1) represents indirect measurements while equations (3.2) and (3.3) represent the direct measurements of OD flows and model parameters. ϵ_i, γ_i and δ_i represent the errors made in these measurements for day i.

3.1.3 Objective function

Let $f_1(M_i^{obs}, M_i^{sim})$ represent the measure of deviation of the observed sensor measurements from the mean sensor measurements produced by the simulation model for day i. Similarly, let $f_2(OD_i, OD_i^0)$ and $f_3(\beta_i, \beta_i^0)$ represent the measures of deviations of the estimated OD flows from the apriori OD flows on day i and estimated model parameters from the apriori model parameters on day i respectively. The sum of all the three deviations for all days can serve as the objective function to be minimized:

$$\sum_{i=1}^{N} f_1(M_i^{obs}, M_i^{sim}) + f_2(OD_i, OD_i^0) + f_3(\beta_i, \beta_i^0)$$

Without the second and third terms, the objective function will typically have multiple minima. So, with the inclusion of these two terms also in the objective function, we aim to match the observed sensor measurements and at the same time we try not to deviate much from the apriori information we have on the OD flows and model parameters.

3.1.4 Constraints

This optimization problem would have two sets of constraints - expressions for simulation outputs and the feasibility conditions for the OD flows and model parameters to be estimated. Equation (3.4) defines the simulated measurements used in the objective function as a function of model parameters, OD flows, habitual travel times and network characteristics. w is random seed which is used to represent the stochastic nature of the simulator. Equation (3.6) describes how drivers update their habitual travel times day-to-day and is usually referred to as *learning model* in literature. The equation means that the habitual travel times on a day are a function of the habitual travel times and mean experienced travel times of all the previous days. Equation (3.5) defines the experienced travel times used in equation (3.6) as a function of the inputs to the simulation model and random seed.

$$M_{iw}^{sim} = S^M(\beta_i, OD_i, TT_i^{hab}, G_i, w) \tag{3.4}$$

$$TT_{iw}^{exp} = S^{TT}(\beta_i, OD_i, TT_i^{hab}, G_i, w) \tag{3.5}$$

$$TT_i^{hab} = g(TT_{[i-1]}^{hab}, TT_{[i-1]}^{exp}) \tag{3.6}$$

The other set of conditions are that the OD flows estimated should be non-negative and the estimated model parameters lie within a feasible region.

3.1.5 Complete formulation

The complete formulation would therefore be:

$$\min_{OD_i \geq 0, \beta_i \in S_i} \left[\sum_{i=1}^{N} f_1(M_i^{obs}, M_i^{sim}) + f_2(OD_i, OD_i^0) + f_3(\beta_i, \beta_i^0) \right] \tag{3.7}$$

$$s.t.\ M_i^{sim} = S^M(\beta_i, OD_i, TT_i^{hab}, G_i)$$

$$TT_i^{exp} = S^{TT}(\beta_i, OD_i, TT_i^{hab}, G_i)$$

$$TT_i^{hab} = g(TT_{[i-1]}^{hab}, TT_{[i-1]}^{exp})$$

Only OD flows and model parameters are considered to be the decision variables because the the habitual travel times are dependent on the inputs for the previous days and the network conditions on all the days under consideration are assumed to be known.

3.1.6 Possible assumptions

As noted earlier, the observed measurements will vary from day-to-day and the variability in these measurements could be because of stochasticity or changes in OD flows, model parameters, network conditions and habitual travel times. The optimization problem presented in section (3.1.5) is very difficult to solve. Hence, depending on the purpose of the study, assumptions need to be made on the sources of variability in observed measurements. Since there are four possible sources of variability (excluding randomness which is always supposed to exist), there will be $2^4 = 16$ possible assumptions one can make.

But it is not logical to assume that the habitual travel times *vary (do not vary)* when *none of the others vary (at least one of the others varies)* . It is also not logical

Cases	Model parameters	OD flows	Network conditions	Habitual travel times
1	DNV	DNV	DNV	DNV
2	DNV	V	DNV	V
3	DNV	DNV	V	V
4	DNV	V	V	V
5	V	DNV	V	V
6	V	V	V	V

Table 3.1: Possible assumptions on sources of variability in observed measurements

to assume that model parameters vary while the network conditions do not vary. Because of these conditions, the number of possible cases comes down to 6. These cases are mentioned in the table (3.1). In the table 'DNV' stands for *do not vary* and 'V' stands for *vary* .

Even for each of these cases, additional assumptions need to be made to be able to solve the problem. Cases 1 and 6 are the two alternative assumptions one can make and cases 2 to 5 are special restricted cases of these two cases. Formulations for cases 1 and 6 (referred to as stationary state and non-stationary state respectively) are presented.

3.1.7 Stationary state formulation

As per the assumptions, observed measurements vary from day-to-day purely because of randomness and none of the input parameters vary. Since habitual travel times are assumed not to vary, an additional assumption that the network is in equilibrium needs to be made to keep the problem solvable. As per the definition of equilibrium, the experienced travel times of drivers are consistent with the travel times they expect (i.e., habitual travel times). The final formulation is shown in equation (3.8). Note that the subscripts for β, OD, TT^{hab}, M^{sim} and G have been avoided indicating that they do not vary. But since observed measurements vary (because of randomness), subscripts for M^{obs} have been used. This particular formulation for aggregate calibration has been used by Darda [19].

$$\min_{OD\geq 0, \beta \in S} \left[\sum_{i=1}^{N} f_1(M_i^{obs}, M^{sim}) + f_2(OD, OD^0) + f_3(\beta, \beta^0) \right] \tag{3.8}$$

$$s.t.\ M^{sim} = S^M(\beta, OD, TT^{hab}, G)$$

$$TT^{exp} = S^{TT}(\beta, OD, TT^{hab}, G)$$

$$TT^{hab} = TT^{exp}$$

3.1.8 Non-stationary state formulation

The non-stationary state formulation, where we assume that all inputs vary, is nothing but the general formulation in section (3.1.5). It can reasonably be assumed that the network conditions are finite in number and that the model parameters on any two days are different if and only if the network conditions on both the days are different.

Let c_i represent the network conditions on day i. Also, let c_i belong to a finite set K. Since model parameters for a day have been assumed to be dependent only on the network conditions of that day, β_i can be replaced by β_{c_i}. In addition, it can also be assumed that the travelers update their habitual travel times based on their experiences on earlier days with similar network condition. The underlying premise is that the travelers are aware of the network conditions before they embark on their journey. With these set of assumptions, the formulation would be:

$$\min_{OD_i \geq 0, \beta_{c_i} \in S_{c_i}} \left[\sum_{i=1}^{N} f_1(M_i^{obs}, M_i^{sim}) + f_2(OD_i, OD_i^0) + f_3(\beta_{c_i}, \beta_{c_i}^0) \right] \tag{3.9}$$

$$s.t. \;\; M_i^{sim} = S^M(\beta_{c_i}, OD_i, TT_i^{hab}, G_i)$$

$$TT_i^{exp} = S^{TT}(\beta_{c_i}, OD_i, TT_i^{hab}, G_i)$$

$$TT_i^{hab} = g(TT_{i^*}^{hab}, TT_{i^*}^{exp})$$

where i^* stands for set of days defined as $i^* = \{j/(j < i), (c_i = c_j)\}$. $TT_{i^*}^{hab}$ and $TT_{i^*}^{exp}$ are the habitual travel times and experienced travel times respectively of all days which belong to the set i^*.

3.2 Generalized least squares formulation

Let y_{ih} represent the sensor measurements on day i and interval h. Let y_i be the measurements in all intervals on day i and y be the vector of all the measurments. Let T be the number of intervals and N be the number of days. Then,

$$y_i = (y_{i1}^{'}, y_{i2}^{'}, \ldots, y_{iH}^{'})'$$

$$y = (y_1^{'}, y_2^{'}, \ldots, y_N^{'})'$$

Similarly, let the OD flows to be estimated and their apriori information be arranged in two column vectors OD and OD^0 respectively. The model equations corresponding to those in section (3.1.2) would be (3.10) and (3.11). Note that apriori estimates of model parameters are typically not available and hence have not been incorporated in the model equations.

$$y^{obs} = y^{sim} + \epsilon \tag{3.10}$$

$$OD^0 = OD + \gamma \tag{3.11}$$

Let ϵ and γ have means of zero. Let variance covariance matrices of ϵ and γ be V and W respectively. Representing them in a single matrix, the variance covariance matrix would be

$$\Omega = \begin{bmatrix} V & 0 \\ 0 & W \end{bmatrix}$$

Here, ϵ and γ are assumed to be uncorrelated. Since the direct and indirect measurements are obtained from two different sources, this assumption is reasonable.

3.2.1 Objective function

As per Gauss-Markov theorem in Econometrics, *Generalized least squares* is the best linear unbiased estimator. The objective function to be minimized to obtain the GLS estimator of the unknown OD flows and model parameters is given by

$$\begin{bmatrix} y^{obs} - y^{sim} \\ OD^0 - OD \end{bmatrix}' \Omega^{-1} \begin{bmatrix} y^{obs} - y^{sim} \\ OD^0 - OD \end{bmatrix} \tag{3.12}$$

which upon simplification becomes

$$(y^{obs} - y^{sim})'V^{-1}(y^{obs} - y^{sim}) + (OD^0 - OD)'W^{-1}(OD^0 - OD) \tag{3.13}$$

The constraints would be the same with the notation of M_i^{sim} and M_i^{obs} for sensor measurements replaced by y_i^{sim} and y_i^{obs} respectively.

3.3 Solution approach

The GLS formulation presented is difficult to solve as it is. This is because there are two sets of variables to estimated - OD flows and model parameters - which are very different in their characteristics.

- OD flows are typically very large in number compared to model parameters.
- Objective function can be expressed analytically as a function of OD flows, but not model parameters.
- Computational cost is very high for estimating model parameters as against estimating OD flows because many efficient methods for OD estimation have been proposed over the years.

Hence, it would be efficient if these two sets of variables are separated and estimated iteratively as shown in figure (3-1).

The objective function to be minimized in these two sub-problems of OD estimation and parameter calibration is (3.13). Note that for the sub-problem of parameter calibration, OD flows are held constant. Therefore removing the constant term from the equation (3.13) will not affect the estimates. The alternative objective function for parameter calibration would therefore be:

$$(y^{obs} - y^{sim})' V^{-1} (y^{obs} - y^{sim})$$

3.4 Estimating variance-covariance matrices

The variance covariance matrices V and W are not available. They need to be estimated directly from the measurement errors ϵ and γ. Let ϵ_{ih} and γ_{ih} be the measurement errors on day i and interval h. Since both within-day and day-to-day dynamics are being considered, we do not have multiple observations for measurement

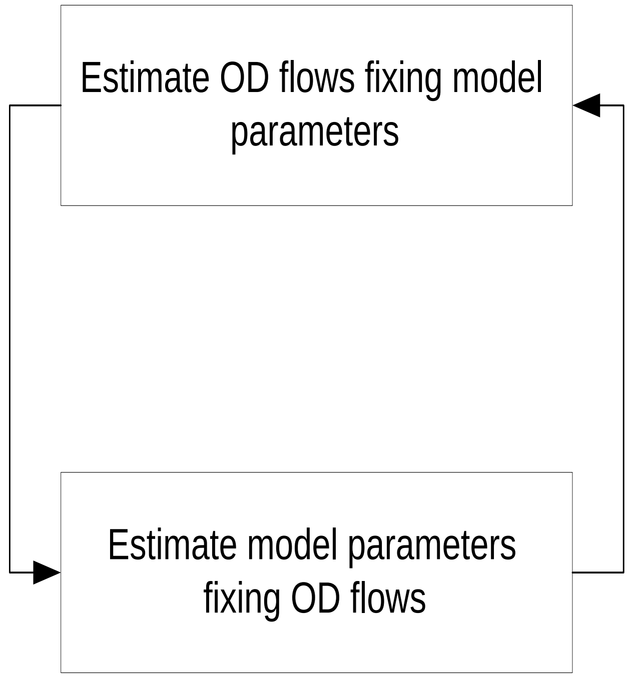

Figure 3-1: Iterative method of optimization

errors to compute the variances and covariances from their definitions. Therefore additional assumptions need to be made to estimate these matrices.

The variance covariance matrices can be expressed as a function of a set of parameters, which can then be estimated using the measurement errors. Alternatively, weak stationarity can be assumed. Any times series $x_1, x_2, \ldots, x_T$ is said to be weakly stationary if

$$E[x_t] = \mu, \;\; \forall t$$

$$E[(x_m - \mu)(x_n - \mu)] = E[(x_{t+m} - \mu)(x_{t+n} - \mu)], \;\; \forall t$$

Essentially, it means that all the variables have the same mean and the covariance between any two of them is dependent only on the time lag between them. Similarly, any two time series $x_1, x_2, \ldots, x_N$ and $y_1, y_2, \ldots, y_N$ are said to be jointly weak stationary if

$$E[x_t] = \mu,\ \ \forall t$$

$$E[y_t] = \nu,\ \ \forall t$$

$$E[(x_m - \mu)(y_n - \nu)] = E[(x_{t+m} - \mu)(y_{t+n} - \nu)],\ \ \forall t$$

Let δ_{ih} be the measurement error by a particular sensor on day i and interval h. Then the series formed by these errors would be

$$\delta_{11}, \delta_{12}, \ldots, \delta 1H \ \ \ldots\ldots\ldots \ \ \delta_{N1}, \delta_{N2}, \ldots, \delta NH$$

where N is the number of days and H is the number of intervals per day. Assuming that the error terms within a day form a weakly stationary series, we have

$$cov(\delta_{ih}, \delta_{i(t+h)}) = \frac{1}{N} \sum_{h'=1}^{H-t} \delta_{ih'} \delta_{i(t+h')} \tag{3.14}$$

Note that the variances of the error terms can be obtained by setting $t = 0$ in the above equation. With joint weak stationarity assumptions, the covariance between the measurement error by a particular sensor on two different days can be estimated using the following equation

$$cov(\delta_{ih}, \delta_{i'(t+h)}) = \frac{1}{N} \sum_{h'=1}^{H-t} \delta_{ih'} \delta_{i'(t+h')} \tag{3.15}$$

Covariance between measurement errors of two different sensors can be computed similarly. Though only the calculation of V has been presented in equations (3.14) and (3.15), W can be obtained similarly by replacing δ with the corresponding measurement error terms. Another method of estimating these variance covariance matrices could be assuming stationary processes such as AR(1). This is nothing but parameterizing the variance covariance matrices after assuming stationarity.

Chapter 4

Case studies

In this chapter, results from two case studies which have been performed to demonstrate the feasibility of the proposed methodology of aggregate calibration are presented. MITSIMLab (Microscopic Traffic Simulator Laboratory) has been chosen as the simulator to show the process of calibration. Before proceeding to the case studies, a brief overview of MITSIM has been presented.

4.1 Overview of MITSIM

MITSIM has been developed at MIT Intelligent Transportation Systems Lab by Yang [38] to model traffic flow at the microscopic level. Significant contributions to the development to MITSIM have also been made by Davol [20], Toledo [35]. It was developed primarily to be able to evaluate the impacts of Advanced Traveler Information Systems (ATIS) and Advanced Traffic Management Systems (ATMS). MITSIMLab is a synthesis of a number of different models and has the following characteristics:

- represents a wide range of traffic management system designs
- models the response of drivers to real-time traffic information and controls
- incorporates the dynamic interaction between the traffic management system and the drivers on the network

These are the main components of MITSIMLab:

- Traffic flow simulator (MITSIM)
- Traffic management simulator (TMS)
- Surveillance system
- Control and routing devices

The interaction between these components, which is shown in figure (4-1), is a critical element for a simulator. MITSIM is the traffic flow simulator and it models driver behavior and vehicular flow in the network at the microscopic level, while TMS is the traffic management simulator and it mimics the traffic control and routing functions chosen for evaluation. Traffic flow and route guidance affects the behavior of individual drivers, and hence, traffic flow characteristics as well. The changes in traffic flows are in turn measured by the surveillance system and consequently influence control and route guidance strategies. The simulator has a graphical user interface (GUI) also that is used for both debugging purposes and visual demonstration of traffic flow conditions through vehicle animation.

4.1.1 Components

Traffic flow simulator

MITSIM tries to replicate reality as well as possible. The traffic and network elements are represented in detail in order to capture the sensitivity of traffic flows to the control and route strategies. The main elements in MITSIM are

- *Network components:* The road network along with the traffic controls and surveillance devices are represented at the microscopic level. The road network consists of nodes, links, segments (segments are parts of links with uniform characteristics) and lanes.

- *Travel demand and Route choice:* The simulator requires as input time-dependent trip tables. These OD tables represent either expected conditions or are defined

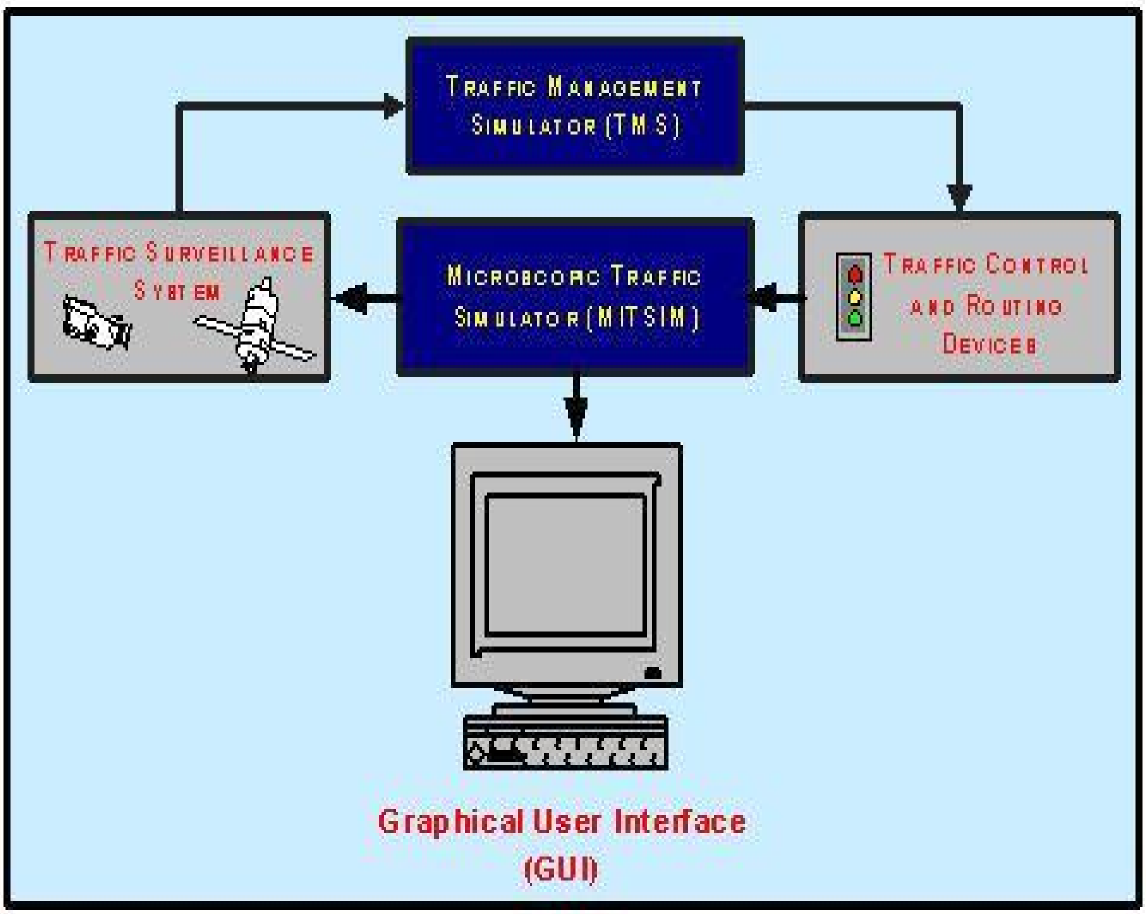

Figure 4-1: Components of MITSIM and their interactions

as part of a scenario for evaluation. A probabilistic route choice model is used to capture drivers' route choice decisions.

- *Driving behavior:* The OD flows are translated into individual vehicles wishing to enter the network at a specific time. Behavior parameters (such as desired speed, aggressiveness, etc.) and vehicle characteristics are assigned to each vehicle/driver combination. The movement of these vehicles is then simulated using car-following and lane-changing models. Car-following model captures the response of a driver to conditions ahead as a function of relative speed, headway and other traffic measures. The lane-changing model distinguishes between mandatory and discretionary lane changes. Merging, drivers' response to traffic signals, speed limits, incidents and toll booths are also captured.

Traffic management simulator

The traffic management simulator (TMS) mimics the traffic control system in the network. A wide range of traffic control and route guidance systems can be simulated, such as:

- Ramp control
- Freeway mainline control
- Lane control signs (LCS)
- Variable speed limit signs (VSLS)
- Portal signals at tunnel entrances (PS)
- Intersection control
- Variable message signs (VMS)
- In-vehicle route guidance

TMS has a generic structure that can represent different designs of such systems with logic at varying levels of sophistication (from pre-timed to responsive).

Surveillance system

The surveillance system measures the traffic conditions simulated by MITSIM and communicate them to the TMS. The following types of sensors can be simulated in MITSIMLab: Traffic sensors, Vehicle sensors, Point to point data sensors and Area wide sensors.

Control and routing devices

MITSIMLab supports a wide range of logics, including pre-timed signal controls, traffic adaptive controls, metering controls and control strategies in response to incidents. The vehicles respond to these signals or guidance according to some behavioral models.

4.1.2 Behavior models

In MITSIMLab vehicles move according to behavioral models, of which the most important ones are

- General acceleration
- Lane changing and gap acceptance
- Route choice models

General acceleration

A vehicle accelerates/decelerates in order to react vehicles ahead, perform a lane changing or merging maneuver or to respond to events. Depending on the degree of interaction with the vehicle ahead, the subject can be in free-flowing, car-following or emergency regime. The degree of interaction is determined by the time headway between the two vehicles. The acceleration in the free-flowing regime is a function of the vehicle's desired speed, while in the car-following and emergency regimes, the acceleration is a function of traffic conditions and relative position and speed of the two interacting vehicles.

In the free-flowing regime, the vehicle accelerates if its current speed is different from the driver's desired speed. The acceleration applied by a driver in this regime is assumed to have the following functional form:

$$\alpha_n^{ff}(t) = \lambda^{ff}\left[V_n^*(t-\tau_n) - V_n(t-\tau_n)\right] + \epsilon_n^{tt}(t) \tag{4.1}$$

where

$\alpha_n^{ff}(t)$	acceleration of driver n at time t
λ^{ff}	parameter
$V_n^*(t)$	desired speed of the driver at time t
$V_n(t)$	speed of subject vehicle at time t
τ_n	reaction time of driver n
$\epsilon_n^{tt}(t)$	error term

The car-following model is used for calculating a vehicle's acceleration or deceleration rate in various cases such as: (i) Car-following relationship with the leading vehicle (ii) Competition with other vehicles if two or more lanes merge into a single downstream lane and (iii) Yielding to another vehicle shifting into the same lane It can be expressed mathematically as:

$$\alpha_n^{cf}(t) = \alpha\frac{V_n(t-\tau_n)^\alpha}{[\Delta x(t-\tau_n)]^\beta}k^\delta[V_{n-1}(t-\tau_n) - V_n(t-\tau_n)]^\gamma + \epsilon_n^{cf}(t) \tag{4.2}$$

where

$\alpha_n^{cf}(t)$	acceleration of driver n at time t
$\Delta x(t)$	gap between vehicles at time t
k	density of traffic in the vicinity of the vehicle
$\alpha, \beta, \gamma, \delta$	parameters

In the emergency regime, the vehicle uses an appropriate deceleration rate to avoid collision. The deceleration rate depends on the state of the front and subject vehicles.

Lane changing and gap acceptance

The lane changing model is implemented in three steps: (i) checking if a change is necessary and defining the type of the change (ii) selecting the desired lane and (iii) executing the desired lane change if the available gaps are acceptable. Lane changing may be mandatory (MLC) or discretionary (DLC). Mandatory lane changing is performed when the current lane ceases to be an option, and thus the driver must move to another lane. Discretionary lane changing is performed when a driver is not satisfied with the driving conditions in the current lane.

The gap acceptance model captures drivers' assessment of gaps as acceptable or unacceptable. Drivers are assumed to consider only the adjacent gap. An adjacent gap is defined as the gap in between the lead and lag vehicles in the target lane. For merging into an adjacent lane, a gap is acceptable only if both lead and lag gaps are acceptable. Drivers are assumed to have minimum acceptable lead and lag gap lengths. These critical gaps vary not only among different individuals, but also for a given individual under different traffic conditions. The value of the critical gap is a function of traffic density, distance to the point by which the driver has to complete a mandatory lane change, etc.

Route choice

In MITSIMLab, drivers can make route choice decisions either pre-trip or en-route. Two probabilistic models, path-based and link-based, are available to capture the route choice decisions. The path-based model is path-size logit model (Ramming [31]). The link-based model calculates the probabilities of choosing an outgoing link at each intersection using the formula (4.3):

$$P(l/j,t) = \frac{exp[\beta(c_l(t) + C_k(t + c_l(t)))]}{\sum_{C_k(t+c_l(t)) \leq C_j(t)} exp[\beta(c_l(t) + C_k(t + c_l(t)))]} \tag{4.3}$$

where

$c_l(t)$	expected time to traverse link l for a vehicle that enters the link at time t
$C_k(t)$	expected shortest travel time from node k to the destination for a vehicle that arrives at k at time t
β	model parameter

The expected travel time to one's destination for each alternative downstream link at an intersection can be time dependent. If no information is available, habitual travel times are used.

Refer to Yang [38], Toledo [35] and Ahmed [2] for more information on these models as well as models.

4.2 Case study 1

4.2.1 Objective

The objective of this case study is to demonstrate the feasibility of the proposed methodology and at the same time investigate the importance of apriori information and the degree of information contained in sensor measurements. The network data has to be experimental in order to compare between these various factors which might affect the estimates obtained.

4.2.2 Generation of data

A 3×3 grid network, as shown in figure (4-2) has been chosen for the case study. Four OD pairs - $(0 \rightarrow 2)$, $(0 \rightarrow 8)$, $(6 \rightarrow 2)$ and $(6 \rightarrow 8)$ have been considered. A duration of one hour per day, discretized into four 15 minute intervals has been chosen as the period of study. Data (OD flows , habitual travel times and sensor counts) for 50 days was generated following the procedure outlined in figure (4-3). Default values have been assumed for the model parameters.

Equations (4.4), (4.5) and (4.6) describe how the OD flows have been generated. Here X_{ih} and X_{ih}^H represent the vector of true OD flows and historical OD flows on

Figure 4-2: Grid network

day i and interval h. Quadratic variation of historical OD flows from day-to-day has been assumed, as expressed by equation (4.4).

$$X_{ih}^{H} = X_{1h}^{H} + A_h(i-1) + B_h(i-1)^2 \quad \forall h = 1, 2, 3, 4 \tag{4.4}$$

$$(X_{i1} - X_{i1}^{H}) = \epsilon_1 \tag{4.5}$$

$$(X_{ih} - X_{ih}^{H}) = K(X_{i(h-1)} - X_{i(h-1)}^{H}) + \epsilon_2 \tag{4.6}$$

The values for X_{1h}^{H}, A_h and B_h have been chosen such that the historical OD flows increase monotonically by about 25 % from the first day to the last day. K is a constant. Non-occurrence of congestion in the network during all the days is also another consideration. For the first interval, deviation of true OD flows from historical OD flows is purely random. For the second, third and fourth intervals, the deviation of true OD flows from the historical OD flows is a function of the deviation in the previous interval and a random error term (autoregressive formulation). The values that have been used for the coefficients are

$$X_{11}^H = \begin{bmatrix} 800 \\ 2000 \\ 1800 \\ 950 \end{bmatrix} X_{12}^H = \begin{bmatrix} 830 \\ 2150 \\ 1830 \\ 975 \end{bmatrix} X_{13}^H = \begin{bmatrix} 840 \\ 2100 \\ 1850 \\ 950 \end{bmatrix} X_{14}^H = \begin{bmatrix} 820 \\ 2000 \\ 1900 \\ 940 \end{bmatrix}$$

$$A_1 = \begin{bmatrix} 11.4 \\ 18.0 \\ 15.7 \\ 11.0 \end{bmatrix} A_2 = \begin{bmatrix} 11.3 \\ 17.0 \\ 15.5 \\ 11.2 \end{bmatrix} A_3 = \begin{bmatrix} 11.3 \\ 17.0 \\ 15.5 \\ 11.1 \end{bmatrix} A_4 = \begin{bmatrix} 11.3 \\ 17.0 \\ 15.5 \\ 11.0 \end{bmatrix}$$

$$B_1 = \begin{bmatrix} -0.12 \\ -0.18 \\ -01.6 \\ -0.11 \end{bmatrix} B_2 = \begin{bmatrix} -0.12 \\ -0.18 \\ -0.16 \\ -0.1 \end{bmatrix} B_3 = \begin{bmatrix} -0.12 \\ -0.18 \\ -0.16 \\ -0.11 \end{bmatrix} B_4 = \begin{bmatrix} -0.13 \\ -0.19 \\ -0.17 \\ -0.12 \end{bmatrix}$$

Regarding habitual travel times, the first day is assumed to be in equilibrium. For the other days, a learning model as shown in equation (4.7) is used. As per this equation, drivers update their habitual travel times with the experienced travel times from the previous day. A value of 0.75 has been used for α. This is based on the intuition that the drivers give more weightage to their habitual travel times (which are based on experiences on a lot of days) than the experienced travel times from just one day. Though the simulator is stochastic, only one replication is used to get the experienced travel times of a day because it is assumed that the simulator represents the stochastic world. Same is the reason for using only one replication to get the sensor counts on a day.

$$TT_i^{hab} = \alpha \, TT_{i-1}^{hab} + (1 - \alpha) \, TT_{i-1}^{exp} \tag{4.7}$$

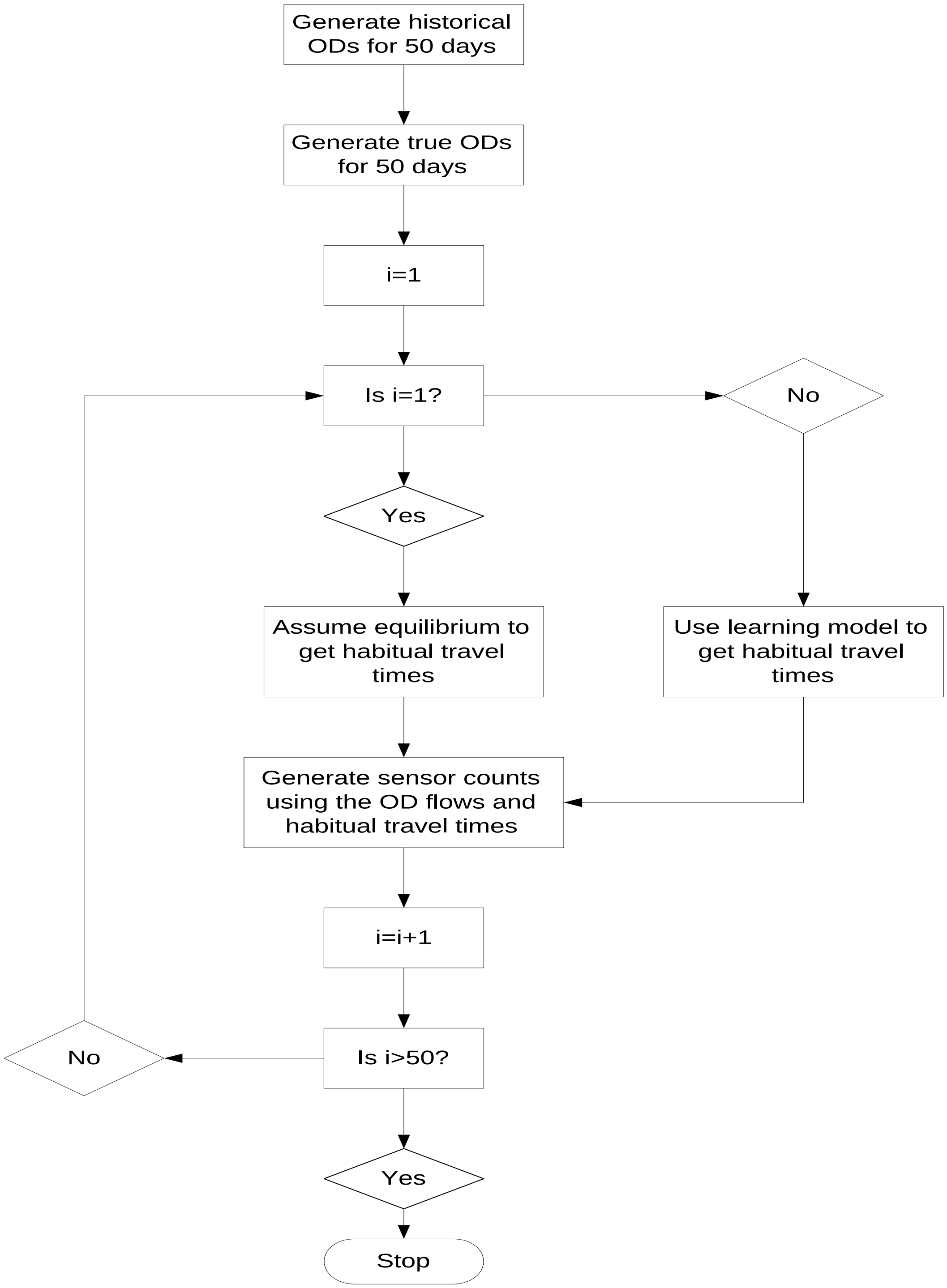

Figure 4-3: Flow chart for data generation

4.2.3 Experimental design

One of objectives, as mentioned earlier, is to investigate the importance of amount of information contained in the sensor counts and the apriori information on OD flows (seed OD). In addition, use of more replications for OD estimation and the variance of the true OD flows has also been considered in this case study. As per intuition, higher the variance of the true OD flows worse are the estimated OD flows. Assignment matrix, a critical component in OD estimation, is estimated from the simulator and hence is stochastic in nature. In most cases, using a single realization to calculate this matrix may yield bad results.

So, in all four factors have been considered. The factors and their levels have been mentioned in table (4.1). Three levels of seed OD flows - true seed (TR), seed with similar structure (SS) and seed with wrong structure (WS) - have been considered. With regard to information on sensor counts, two scenarios have been considered - one in which the sensors can count all the vehicles that move on the network (represented as F standing for full information) and the other in which the sensors miss some vehicles (represented as NF standing for not full information). The location of sensors corresponding to NF and F levels are indicated in figures (4-4) and (4-5) respectively. Notice that in figure (4-4), the sensors will not be able to count the vehicles which take the routes $0 \rightarrow 1 \rightarrow 4 \rightarrow 5 \rightarrow 8$, $6 \rightarrow 7 \rightarrow 4 \rightarrow 5 \rightarrow 2$ etc.

Two levels of variance of true OD flows - low (L) and high (H) - have been considered. The variance of ϵ_1 for these cases of L and H have been chosen to be around 5% and 15% of the historical OD flows respectively. On the other hand, variance of ϵ_2 has been chosen so that the true OD flows of the second, third and fourth intervals also have the same variance as that of the first interval (i.e., variance of ϵ_1). Note that ϵ_1 and ϵ_2 are column vectors. Their variances are assumed to be diagonal matrices. The other factor considered in the design is the number of replications used to calculate the assignment matrix. Two levels (1 replication and 5 replications) are used.

Considering all these levels will give $3 \times 2^3 = 24$ cases. But the estimation has

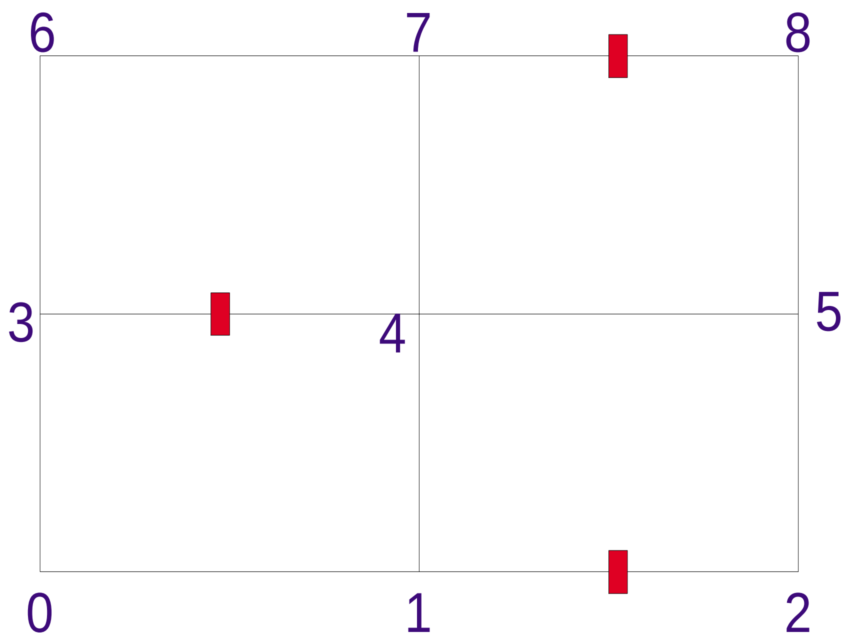

Figure 4-4: Sensor locations not capturing full information

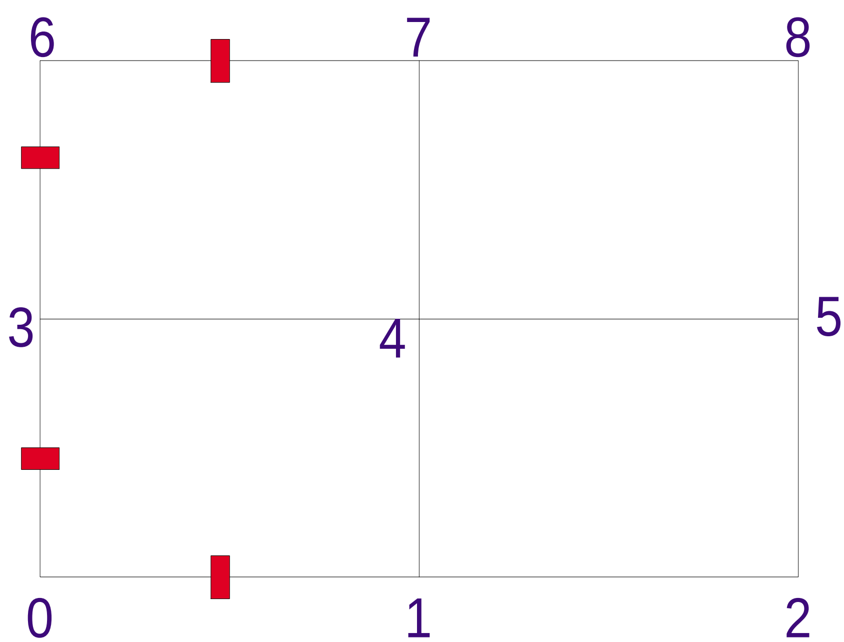

Figure 4-5: Sensor locations capturing full information

Factor	Level 1	Level 2	Level 3 (if it exists)
Seed OD	TR	SS	WS
Information in sensor counts	F	NF	
Variance of true OD flows	L	H	
No. of replications	1	5	

Table 4.1: Factors and their levels considered

not been performed for similar structure seed and wrong structure seed with one replication, bringing the number of cases down to 16.

4.2.4 Assumptions

The following assumptions have been made before the estimation process.

- Model parameters are known
- The OD historical process is known. That is, the matrices A_h and B_h in equation (4.4) are known. Hence the seed OD flows for all the 50 days can be generated with the seed OD flows for first day.
- The learning model along with the parameters is known.
- First day is in equilibrium.

4.2.5 Solution approach

GLS formulation is used to solve the problem. But the variance covariance matrices V and W which are needed are not available. So, instead FGLS (Feasible Generalized Least Squares) procedure is used. This procedure is as follows:

1. Find OLS (Ordinary Least Squares) estimates. This can be achieved assuming that V and W are identity matrices.
2. Using the latest estimates of OD flows and habitual link travel times (model parameters are assumed to be known), compute the residuals.

3. Use the residuals to obtain estimates of V and W. Stationary state assumptions mentioned in chapter 3, can be made use of.

4. With the variance covariance estimates $\hat{V}$ and $\hat{W}$, perform GLS estimation.

5. If convergence in estimates is not reached, go to step 2. Else stop.

The problem is too complex to solve even after we have estimates of V and W. The objective function involves all 50 days, making it a very difficult. Hence estimation procedure outlined in figure (4-6) has been adopted. In this procedure, the OD flows are estimated one day at a time.

Since the first day is assumed to be in equilibrium, equilibrium travel times are obtained with the seed OD. The assignment matrix is then estimated (using either 1 replication or 5 replications depending on the case under consideration) and the OD flows are estimated. Again equilibrium travel times are obtained and OD estimation is performed. This is continued until the OD flow estimates of the first day converge within certain tolerance. For the second day, since it is assumed that we know the learning model, the habitual travel times can be computed using the habitual travel times and the experienced travel times on the first day. With the seed OD for the second day, assignment matrix is obtained and the OD flows are estimated. These estimated OD flows are again used to obtain the assignment matrix. OD flows are again estimated. This is repeated until convergence. Note that once the habitual travel times for the second day are obtained, they are fixed. Similarly, the OD flows are estimated for all the 50 days.

4.2.6 Results

In this subsection, the results are presented. The graphical comparison of the OD flow estimates can be found in Appendix A. RMSE (Root Mean Square Error) and RMSPE (Root Mean Square Percentage Error) are the two statistics which have been used to measure the extent to which the OD flow estimates could match the true OD flows. RMSE and RMSPE are defined as follows:

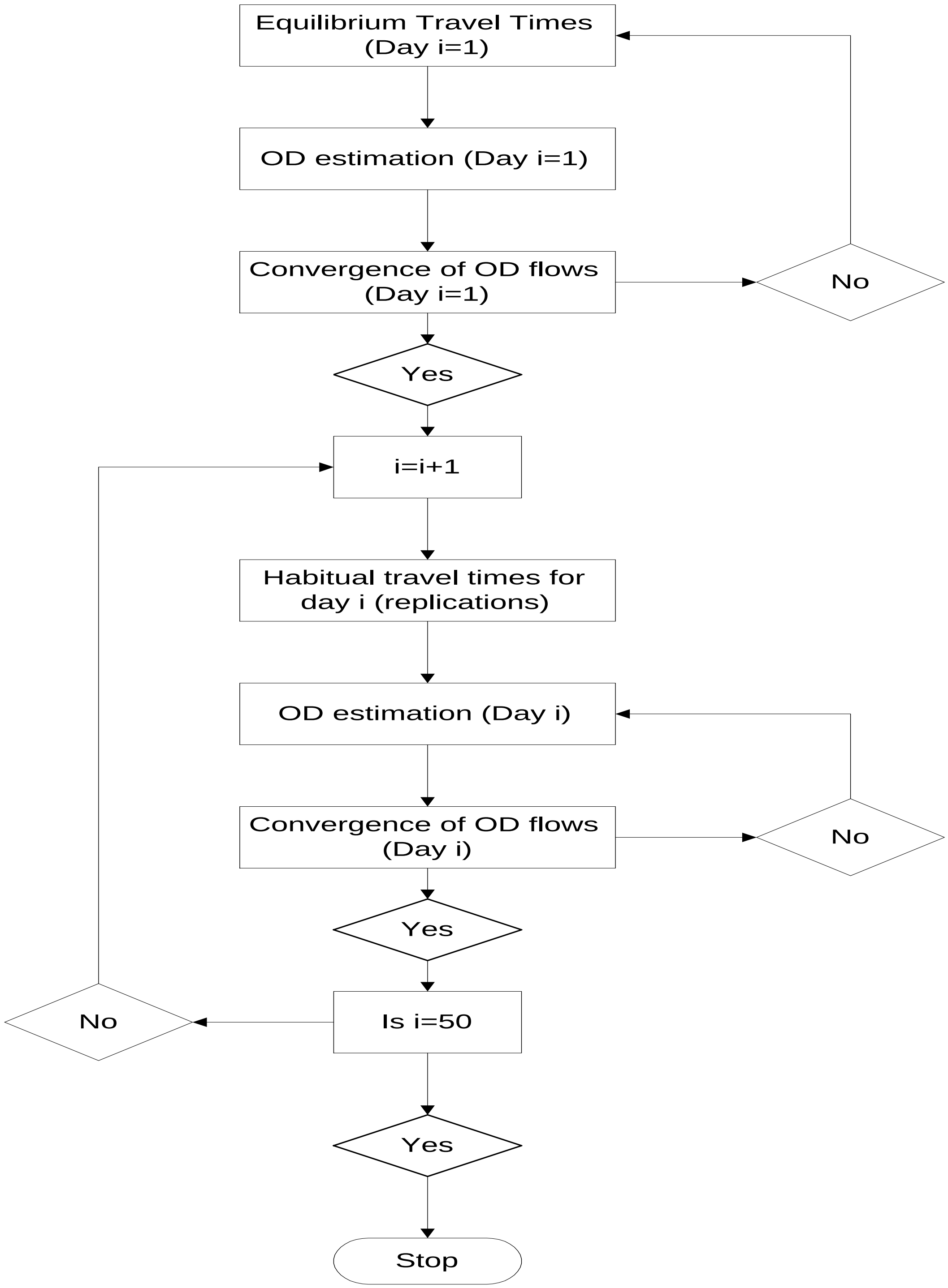

Figure 4-6: Sequential estimation of day-to-day OD flows

$$RMSE = \sqrt{\frac{\sum_{i=1}^{N}(y_i^{obs} - y_i^{est})^2}{N}}$$

$$RMSPE = \sqrt{\frac{\sum_{i=1}^{N}(1 - \frac{y_i^{est}}{y_i^{obs}})^2}{N}}$$

where N is the number of observations, y_i^{obs} is the i^{th} observed value and y_i^{est} is the i^{th} estimated value.

The following notation will be used to indicate the various cases.

TR-1	With true seed and one replication
TR-5	With true seed and five replications
SS-5	With similar structure seed and five replications
WS-5	With wrong structure seed and five replications
L-NF	Low variance of true OD flows and Not full information in sensor counts
L-F	Low variance of true OD flows and Full information in sensor counts
H-NF	High variance of true OD flows and Not full information in sensor counts
H-F	High variance of true OD flows and Full information in sensor counts

The results are presented in the following tables and also in bar graphs for easier interpretation. *Observability* is an important propoerty of some dynamic systems. According to this, the system reaches a stable state over time irrespective of the starting point. In order to verify the existence of a similar effect in this system (i.e., estimated OD flows for the last few days being approximately the same irrespective of the initial seed OD flows), statistics have been calculated for the last 10 days also and presented.

	L-NF	L-F	H-NF	H-F
TR-1	26.0	22.4	26.6	26.6
TR-5	26.4	22.9	26.9	27.0
SS-5	26.3	26.0	25.6	27.3
WS-5	29.4	26.9	29.8	34.4

Table 4.2: RMSE: Observed counts Vs Simulated counts

	L-NF	L-F	H-NF	H-F
TR-1	4.6	4.6	4.9	5.6
TR-5	4.7	4.8	5.0	5.7
SS-5	4.6	5.1	4.6	5.7
WS-5	5.0	5.3	5.2	7.8

Table 4.3: RMSPE: Observed counts Vs Simulated counts

	L-NF	L-F	H-NF	H-F
TR-1	30.4	17.7	88.8	80.6
TR-5	25.3	15.1	87.9	79.8
SS-5	115.1	65.4	131.7	94.9
WS-5	217.2	135.9	287.5	242.6

Table 4.4: RMSE: True ODs Vs Estimated ODs (All 50 days)

	L-NF	L-F	H-NF	H-F
TR-1	2.6	1.2	5.6	5.2
TR-5	2.1	1.0	5.5	5.2
SS-5	8.0	5.1	8.3	6.8
WS-5	14.7	8.0	15.6	11.4

Table 4.5: RMSPE: True ODs Vs Estimated ODs (All 50 days)

	L-NF	L-F	H-NF	H-F
TR-1	27.2	19.9	83.9	78.2
TR-5	25.6	16.5	82.9	76.9
SS-5	114.9	67.4	116.3	90.7
WS-5	218.4	127.3	274.4	236.4

Table 4.6: RMSE: True ODs Vs Estimated ODs (Last 10 days)

	L-NF	L-F	H-NF	H-F
TR-1	2.0	1.2	5.2	4.9
TR-5	1.9	0.9	5.0	4.8
SS-5	7.2	4.9	6.7	5.9
WS-5	13.2	6.8	13.4	10.3

Table 4.7: RMSPE: True ODs Vs Estimated ODs (Last 10 days)

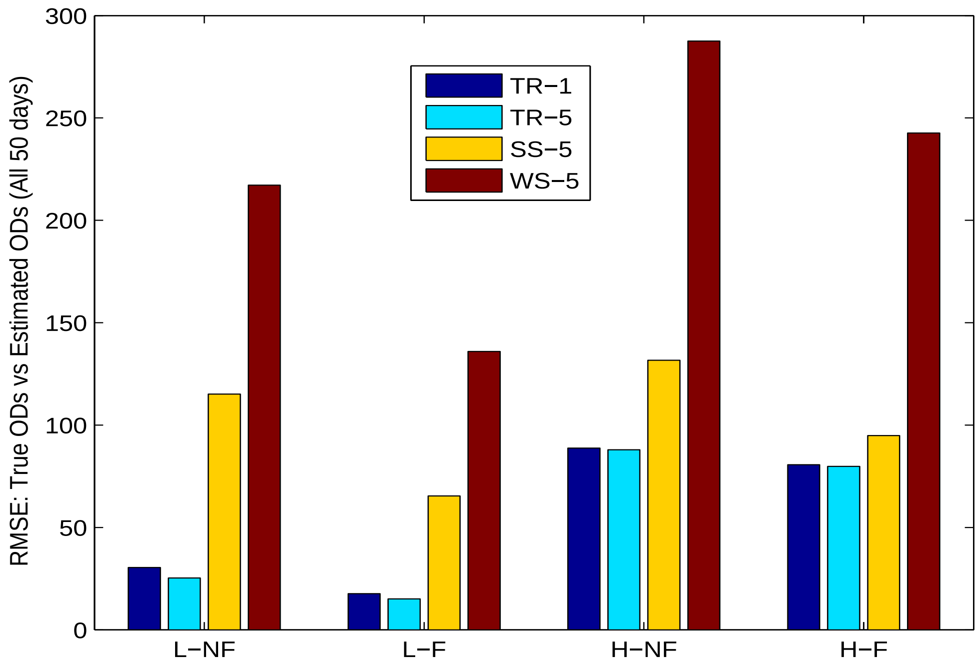

Figure 4-7: RMSE: True ODs vs Estimated ODs (All 50 days)

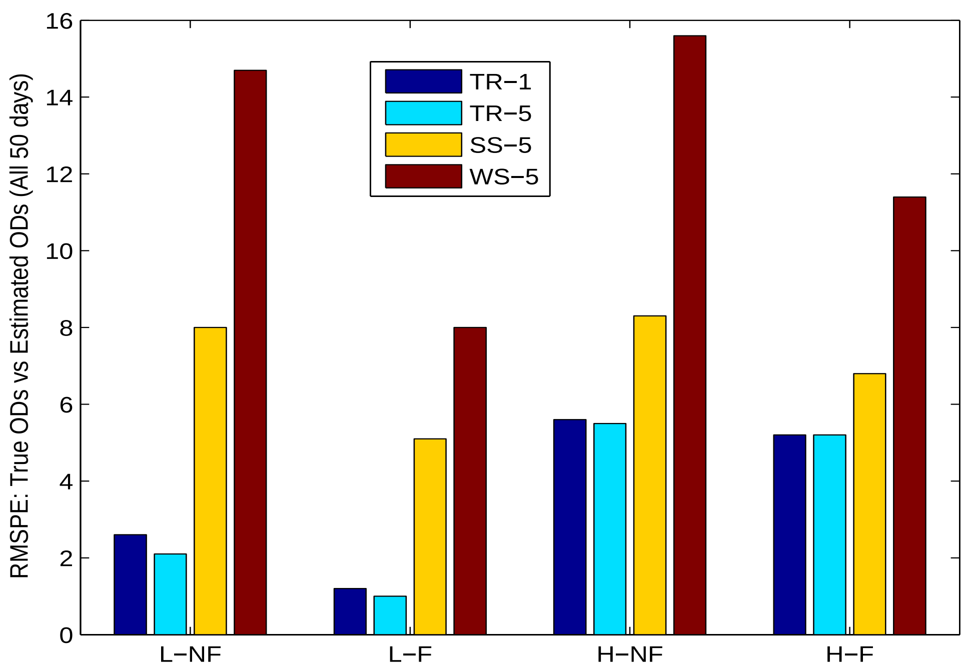

Figure 4-8: RMSPE: True ODs vs Estimated ODs (All 50 days)

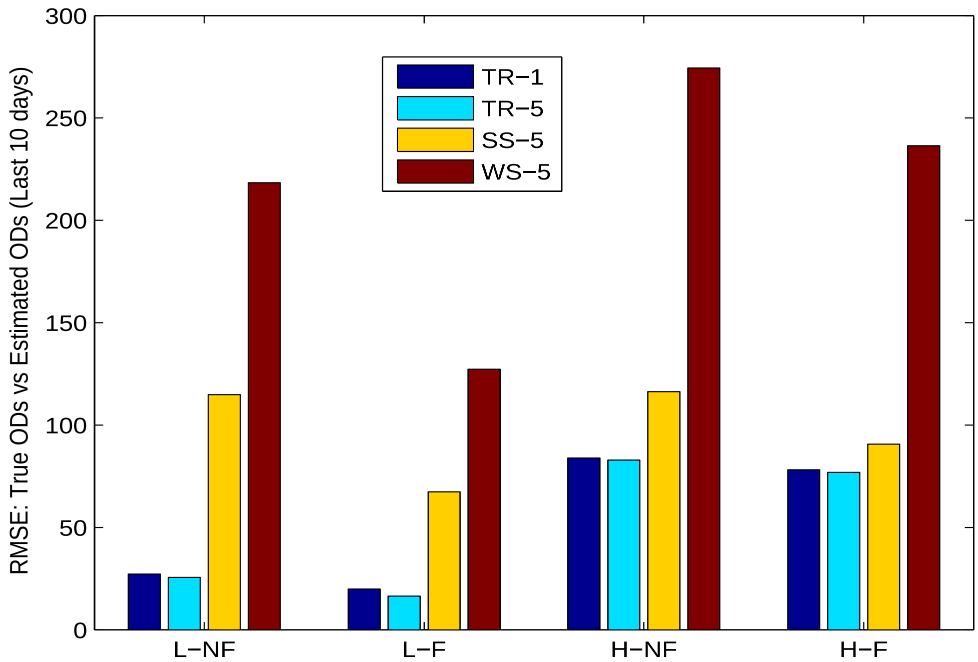

Figure 4-9: RMSE: True ODs vs Estimated ODs (Last 10 days)

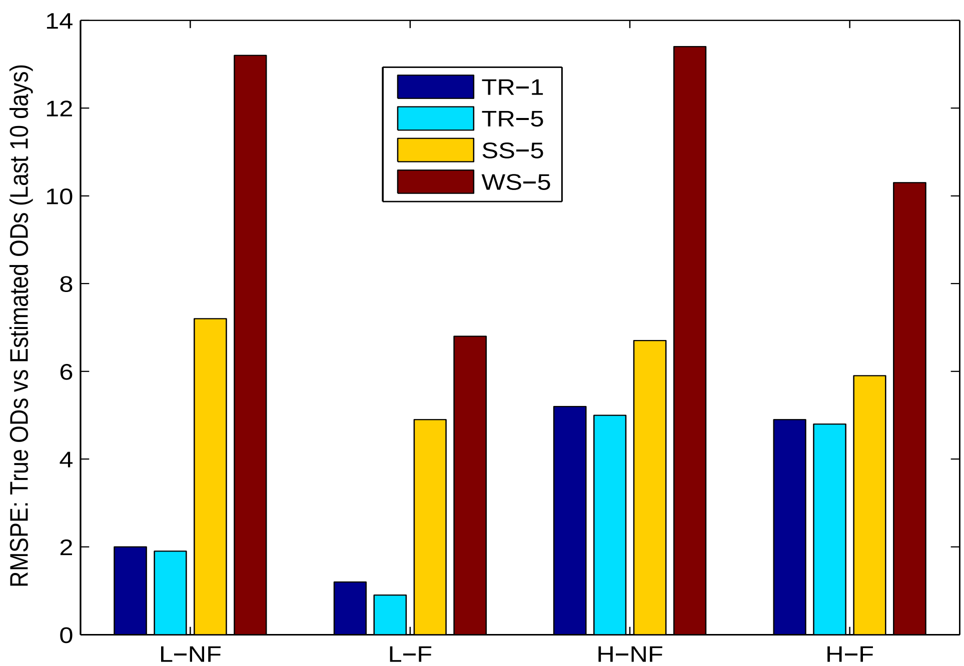

Figure 4-10: RMSPE: True ODs vs Estimated ODs (Last 50 days)

4.2.7 Conclusions

- From tables (4.2) and (4.3), the sensor counts seem to be matched well enough in all the cases. There is no substantial difference in the simulated counts. But the OD flows estimated are not the same. This reiterates the identification issue in OD estimation problems, i.e., existence of multiple solutions.

- The OD flow estimates seem to be close enough (less than 8%) to the true OD flows, as indicated by the RMSPE statistics in table (4.5) for the cases where true seed and seed with similar structure are used. This indicates that with good knowledge of the historical OD flows, this approach can be used to obtain good estimates of day-to-day OD flows.

- Between true seed with one replication and five replications, the estimates are not very different. Replications are useful to account for the stochasticity of the simulator. In this network, the OD flows are high in magnitude and each OD pair has only a few routes. So the assignment matrix will not be highly stochastic. This probably is the reason why replications did not seem to have much effect.

- The OD flow estimates with the true seed (RMSPE of around 1%-5%) are better than those obtained with similar structure seed (RMSPE of around 5%-8%). But both these estimates are better than the estimates obtained using wrong structure seed (RMSPE of around 8%-15%). This asserts the importance of seed in OD estimation.

- Comparing the estimates obtained using sensor counts containing full information and partial information, it is clear that accuracy of estimates depends on data collection methods as well. For example, the RMSPE of estimated OD flows with similar structure seed decreased from 8% to 5.1% in the low variance (of true OD flows) case and from 8.3% to 6.8% in the high variance (of true OD flows) case. This emphasizes the need for planned deployment of sensors on networks.

- Variance of true OD flows also affects the accuracy of the estimates. Higher the stochasticity of the true OD flows, greater is the difficulty in obtaining accurate estimates. This is corroborated by the results. For instance, in the case of estimation with true seed and partial information, the RMSPE increases from around 2% to 5.5%. In the other cases as well, the RMSPE statistics increase but by a lesser amount. This indicates that the affect of high variance of true OD flows diminishes with worsening quality of seed information, which is as per intuition.

- The statistics in tables (4.4) and (4.6), (4.5) and (4.7) indicate that the estimates do not get better over time. That is, there is not much to differentiate between the estimates of the last few days and estimates of all the days. Hence, observability is not a propoerty of this dynamic system.

4.3 Case study 2

4.3.1 Objective

The objective of this case study is to use data from real network to illustrate the proposed methodology and also compare the results with those obtained from earlier method of estimation.

4.3.2 Description of data

For this case study, a section of eastbound Motorway M27 near Southampton, United Kingdom has been selected. This network has two on-ramps and one off-ramp. Traffic counts are available from sensors at 8 locations. The network and the location of sensors is shown in figure (4-11).

Sensor data for the first five weeks in the Spring of 2001 was obtained from the UK Highway agency. Excluding the incident days (because of the absence of detailed information on the incidents in the accident log), days on which some of the sensors were malfunctioning (from to the sensor log), weekends and other holidays, 14 days of data was finally available. The morning peak, 6:00 AM to 8:45 AM, has been chosen as the period of study. The sensor data was aggregated into 15 minute intervals.

4.3.3 Assumptions

The variation of counts from the 8 sensors across days for all the 11 intervals (There are 11 15-minute intervals between 6:00 AM and 8:45 AM) is shown in figures (4-12) and (4-13). As can be seen, the variation of counts seems to random in nature. Hence the OD flows can be assumed to vary randomly from day-to-day. It is also assumed that there is no flow from node 2 to node 3. Consequently, only four OD pairs have been considered: $1 \rightarrow 3$, $1 \rightarrow 5$, $2 \rightarrow 5$ and $4 \rightarrow 5$.

Since there is no route choice in the network, no assumptions are needed regarding habitual travel times. The model parameters are not assumed to vary from day-to-day. This is reasonable since the weather conditions are not very different.

4.3.4 Solution approach

As mentioned earlier, in this case study, two aggregate calibration methodologies will be compared - assuming OD does not vary from day-to-day and OD varies from day-to-day. Note that habitual travel times are unimportant in this network as there is no route choice.

For the first approach, where OD is not assumed to vary, the objective function

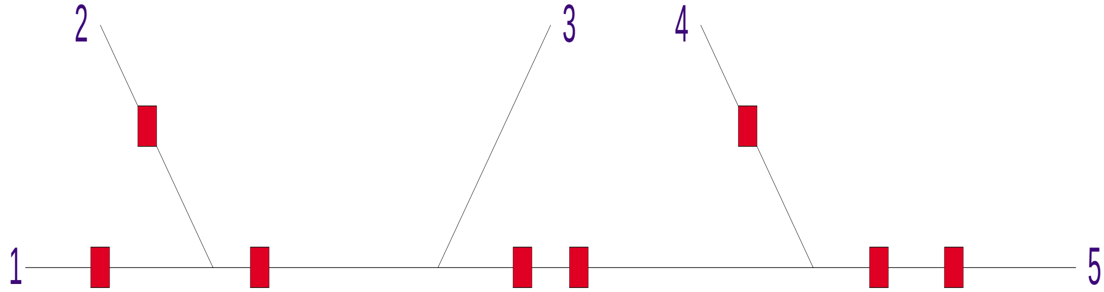

Figure 4-11: M27 network

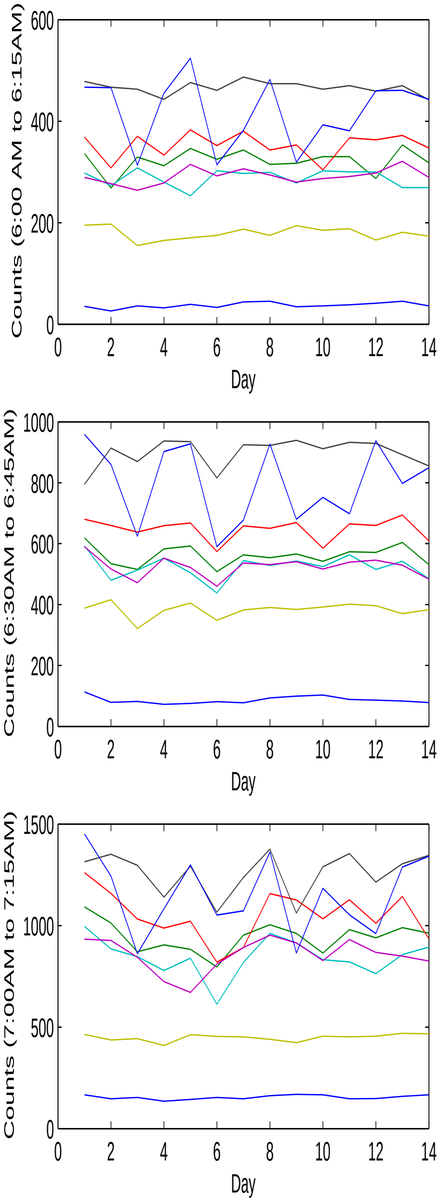

Figure 4-12: Day-to-day variation of counts from 6:15AM to 7:30AM at 15min intervals

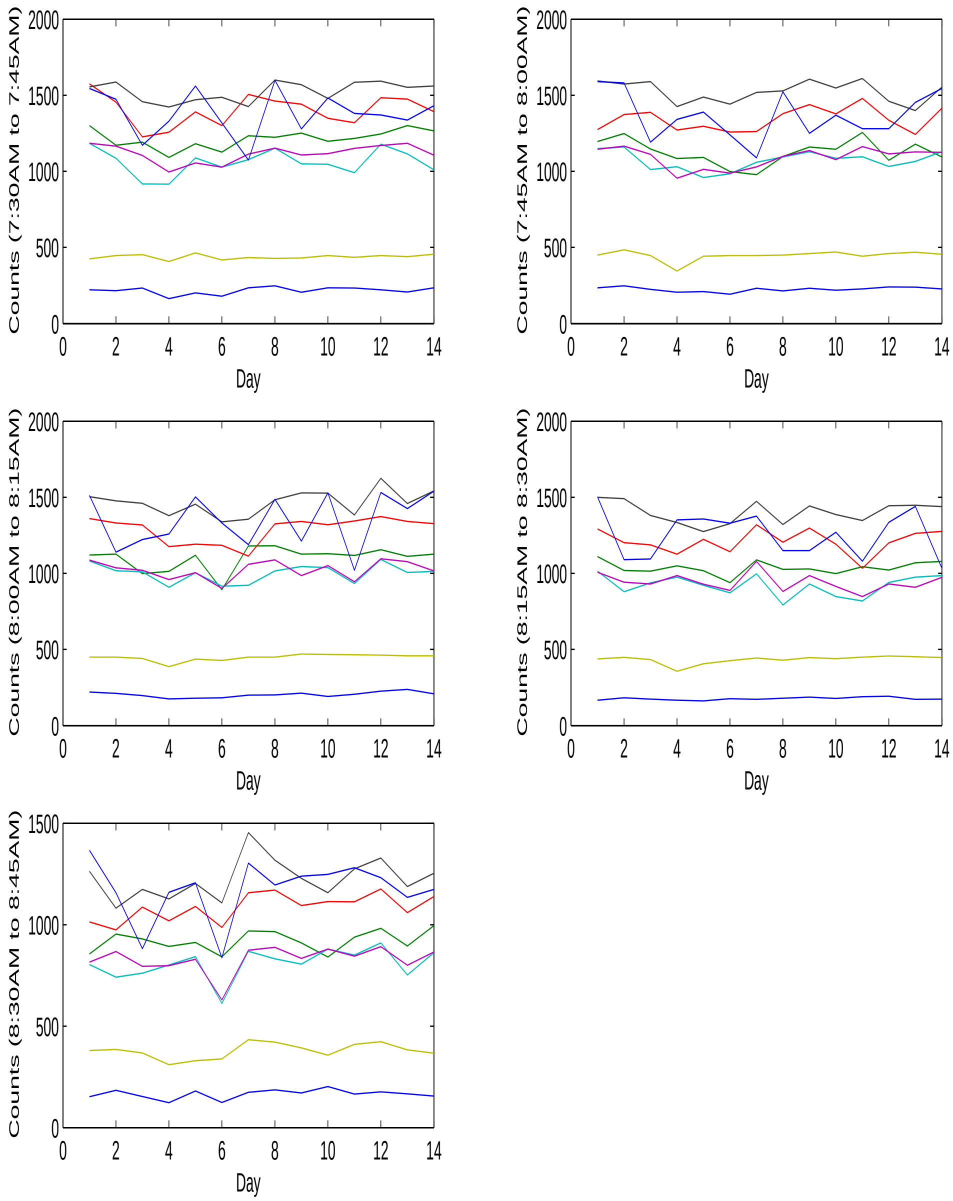

Figure 4-13: Day-to-day variation of counts from 7:45AM to 8:45AM at 15min intervals

Parameter	Estimate
Sensitivity parameter for acceleration in car-following	0.09
Sensitivity parameter for deceleration in car-following	-0.016
Mean of distribution of desired speed over speed limit	0.11%
Standard deviation of distribution of desired speed over speed limit	0.18%

Table 4.8: Estimated values of model parameters

includes all 14 days of data. FGLS procedure is adopted. OD flows and model parameters are estimated iteratively as shown in figure (3-1). Box algorithm (presented in Appendix C) has been used for estimation of model parameters. The following model parameters have been identified for calibration:

- Sensitivity parameters for acceleration and deceleration in car-following model. α in equation (4.2) is referred to as sensitivity parameter.

- Mean and standard deviation of drivers' desired speed over the speed limit in percentage

For the second approach, OD flows for each day have been estimated separately. Model parameters have not been estimated. Estimates from first approach have been used instead because the primary focus is on OD flows.

4.3.5 Results

Values of the estimated model parameters are listed in table (4.8). The results showing how the sensor counts are matched are in table (4.9) and figures (4-14) and (4-15).

The formulae used to compute $\bar{R}^2$ are mentioned in equations (4.8) and (4.9). Here N is the number of observations available and K is the number of parameters estimated. With the addition of more number of parameters, R^2 will only increase. Hence $\bar{R}^2$, which accounts for the number of parameters, is a better statistic to

	No day-to-day	Day-to-day
RMSE	82.4	62.2
RMSPE	10.4	9.7
$\bar{R}^2$	0.81	0.86

Table 4.9: Comparison of counts in both approaches

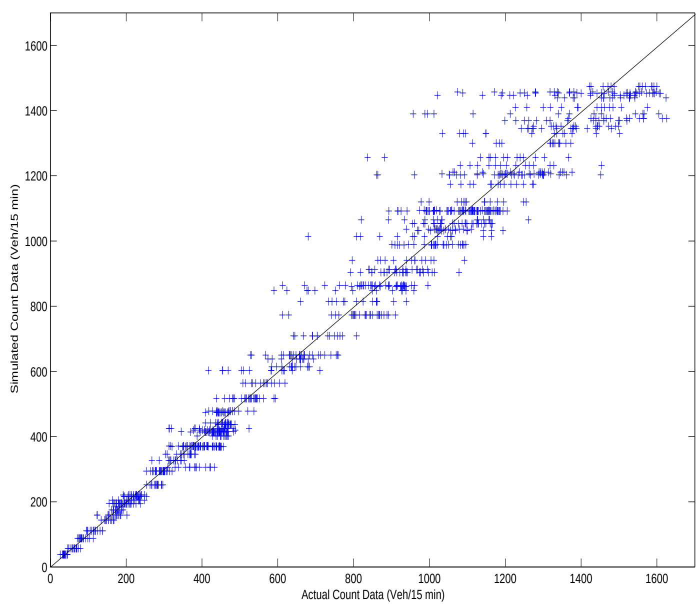

Figure 4-14: Count comparison when OD flows are not assumed to vary

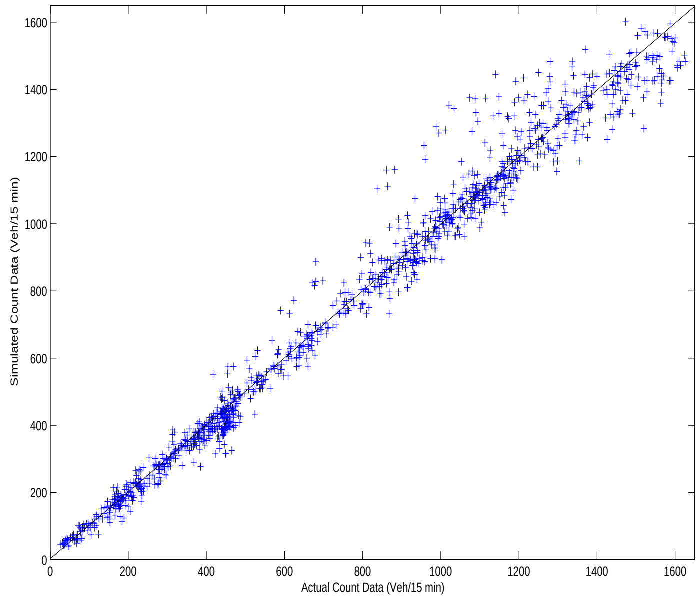

Figure 4-15: Count comparison when OD flows are assumed to vary

compare. y^{est}, y^{bas} and y^{obs} stand for simulated measurements with estimated model, simulated measurements with base model and observed measurements respectively. A base model is needed to compute R^2. For this purpose, a static OD matrix has been estimated for all the days. This OD matrix was used to simulate base model sensor measurements.

$$\bar{R}^2 = 1 - \frac{N-1}{N-K}(1-R^2) \tag{4.8}$$

$$R^2 = 1 - \frac{\sum_N (y_i^{est} - y_i^{obs})^2}{\sum_N (y_i^{bas} - y_i^{obs})^2} \tag{4.9}$$

Regarding OD flows, the estimates obtained from first approach would be referred to as *average OD* . With the second approach, OD flows have been obtained for all the 14 days. These figures have been relegated to Appendix B. Mean of the OD flows (for 14 days) would be referred to as *expected OD* . The aim of the first approach is to estimate OD flows which represent the average condition on all the days. But clearly, *expected OD flows* represent the average condition. RMSE and RMSPE between *average OD flows* and *expected OD flows* are 73.5 and 9.4 respectively.

Since OD flows have been estimated for each day, their coefficients of variation can be computed. Coefficient of variation of a random variable is the ratio of its standard deviation and its expected value. That is, $CV = \frac{\sigma}{\mu}$. Table (4.10) summarizes the results. Here the notation for OD flows is a-b-c, which stands for OD flows from node a to node b in interval c. The units are *vehicles per hour* .

4.3.6 Conclusions

From the results, it can be concluded that assuming day-to-day variation is useful. The sensor counts can be matched better, which can be observed from the difference in $\bar{R}^2$. Estimating day-to-day ODs introduces lot of parameters. Hence $\bar{R}^2$ can be used to compare the two methods after accounting for the significant increase in number of parameters. Also, the OD flows estimated assuming that they do not vary from day-to-day do not represent the mean traffic conditions. In this particular network, the difference from the mean conditions is about 9.4%, which is significant enough.

The variation of the OD flows have been computed. The coefficients of variation lie in the range 3% to 22%, which again are significant. Reliability studies can be performed because distribution of OD flows, which is the most important requirement, is known.

OD	Average OD	Expected OD	Standard Deviation	Coefficient of Variation
1-3-1	195	268	58.3	0.22
1-5-1	1183	1097	34.5	0.03
2-5-1	167	207	23.6	0.11
4-5-1	785	766	68.8	0.09
1-3-2	440	433	41.9	0.10
1-5-2	1273	1284	87.2	0.07
2-5-2	235	240	42.4	0.18
4-5-2	1010	998	68.6	0.07
1-3-3	499	539	33.5	0.06
1-5-3	1797	1752	87.4	0.05
2-5-3	356	385	46.3	0.12
4-5-3	1493	1484	113.5	0.08
1-3-4	642	682	58.5	0.09
1-5-4	2242	2218	162.6	0.07
2-5-4	449	471	96.3	0.20
4-5-4	1655	1628	135.2	0.08
1-3-5	849	923	117.4	0.13
1-5-5	2948	2883	222.6	0.08
2-5-5	577	624	117.0	0.19
4-5-5	1782	1758	232.4	0.13
1-3-6	1020	1219	115.2	0.09
1-5-6	3736	3552	210.9	0.06
2-5-6	870	944	124.3	0.13
4-5-6	1893	1710	218.7	0.13
1-3-7	1404	1361	99.3	0.07
1-5-7	3423	3461	142.9	0.04
2-5-7	828	827	95.0	0.11
4-5-7	1654	1647	124.5	0.08
1-3-8	1094	1117	118.6	0.11
1-5-8	3375	3359	158.0	0.05
2-5-8	885	876	75.5	0.09
4-5-8	1663	1646	111.1	0.07
1-3-9	1253	1210	134.6	0.11
1-5-9	3121	3162	165.8	0.05
2-5-9	782	767	111.3	0.14
4-5-9	1609	1616	178.7	0.11
1-3-10	1256	1193	69.5	0.06
1-5-10	2863	2924	157.4	0.05
2-5-10	697	658	91.7	0.14
4-5-10	1485	1564	115.4	0.07
1-3-11	1256	1098	77.3	0.07
1-5-11	2398	2531	158.9	0.06
2-5-11	645	598	131.2	0.22
4-5-11	1220	1366	182.7	0.13

Table 4.10: Summary of the OD flow estimates

Chapter 5

Conclusion

In this chapter, contributions of this thesis work have been summarized. Suggestions for future research have also been discussed.

5.1 Summary

Aggregate calibration of microscopic simulation models has received significant attention in the recent years following the need for better traffic management. The inputs to a simulation model are network, travel demand (OD flows), model parameters and habitual travel times. While network is known, the other need to be estimated. Earlier approaches do not consider the variation in OD flows, driving behavior and habitual travel times in aggregate calibration. They only try to estimate the mean conditions.

In this thesis, a very general formulation has been proposed considering the day-to-day variations and has been refined using the Generalized Least Squares approach. Two case studies have been performed to illustrate the proposed aggregate calibration methodology.

For the first case study, experimental data was used. Data was generated so that there was systematic variation in travel demand from day-to-day. The OD flows were then estimated for different cases. The results indicated the importance of having good apriori information on OD flows and efficient deployment of sensors to measure traffic data.

For the second case study, data from a motorway (M27) in Southampton, UK was used. Two approaches were used to estimate OD flows: assuming they vary from day-to-day and assuming they do not. The second approach was seen to be better in terms of matching the counts and also for further possible applications.

In summary, the contributions of this thesis are (i) a general formulation for the problem of aggregate calibration in the presence of day-to-day variation in various inputs (ii) two case studies (one with systematic travel demand variation and the other with random travel demand variation) indicating the feasibility of estimation using generalized least squares appraoch.

5.2 Scope of future research

The following are some of the further research issues:

- In the case studies, the learning model for updating habitual travel times is assumed to be known and the first day was assumed to be in equilibrium. Instead, the habitual travel times themselves can be seen as additional parameters to the simulation model along with the parameters in the learning model and can be estimated.

- In the first case study, true OD flows vary systematically from day-to-day. Using the estimated OD flows, statistical analysis can be performed to identify the trend in variation. Knowing the trend, OD flows can be predicted for any period in future (within certain range).

- In the case studies, day-to-day OD flows have been estimated. These can be used for reliability studies such as travel time reliability. Variation in travel times results not only from stochasticity in drivers' short term behavior (changing lanes etc) but also from variation in travel demand, driver behavior and habitual travel times. Knowing the variation of these inputs as well, the probability distribution of travel times can be obtained.

Appendix A

Case Study 1: OD estimates

The following graphs show how the OD estimates compare with the true OD flows. Here the estimates obtained for TR-1 and TR-5 cases have been shown as they cannot be seen at this small scale. In the graphs, x-axis is the day and y-axis is the OD flow. The label on y-axis gives an indication of which OD pair and which interval is being drawn.

The thick line in the graphs represents the true OD flows. The lines for OD estimates obtained using similar structure seed (SS-5) and wrong structure seed (WS-5) are represented by $+$ and $\diamond$ signs respectively.

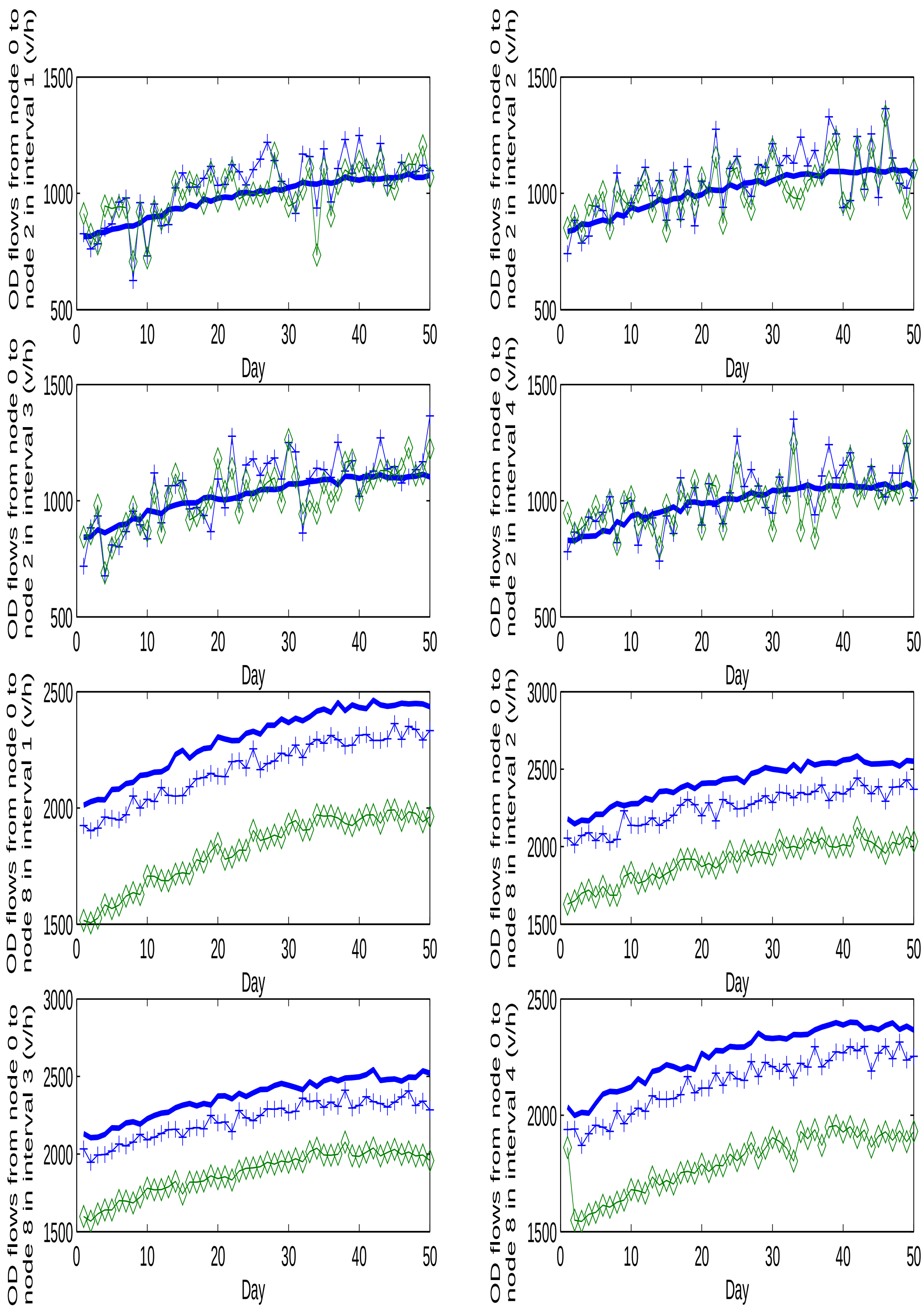

Figure A-1: OD estimates for L-NF case (a)

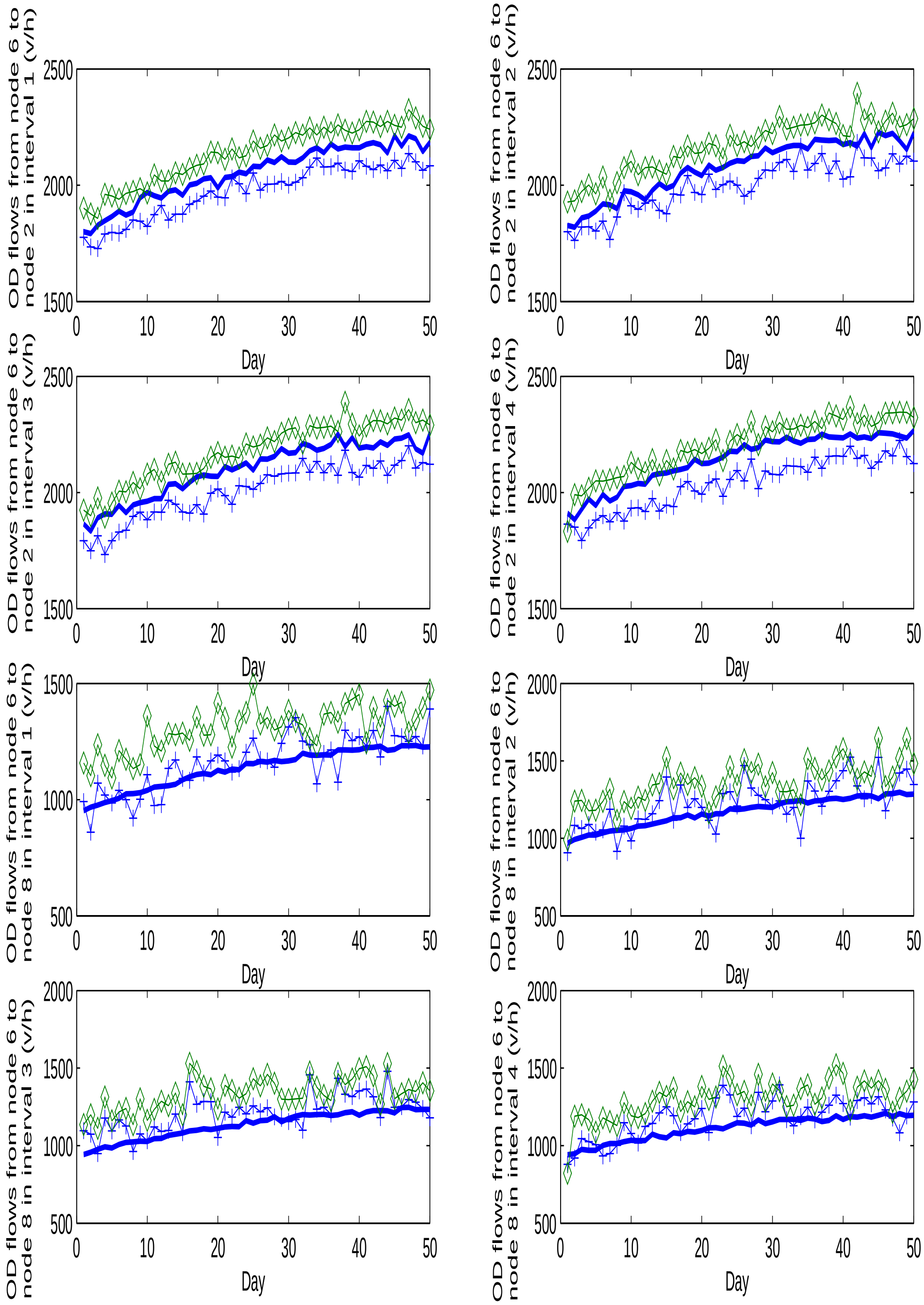

Figure A-2: OD estimates for L-NF case (b)

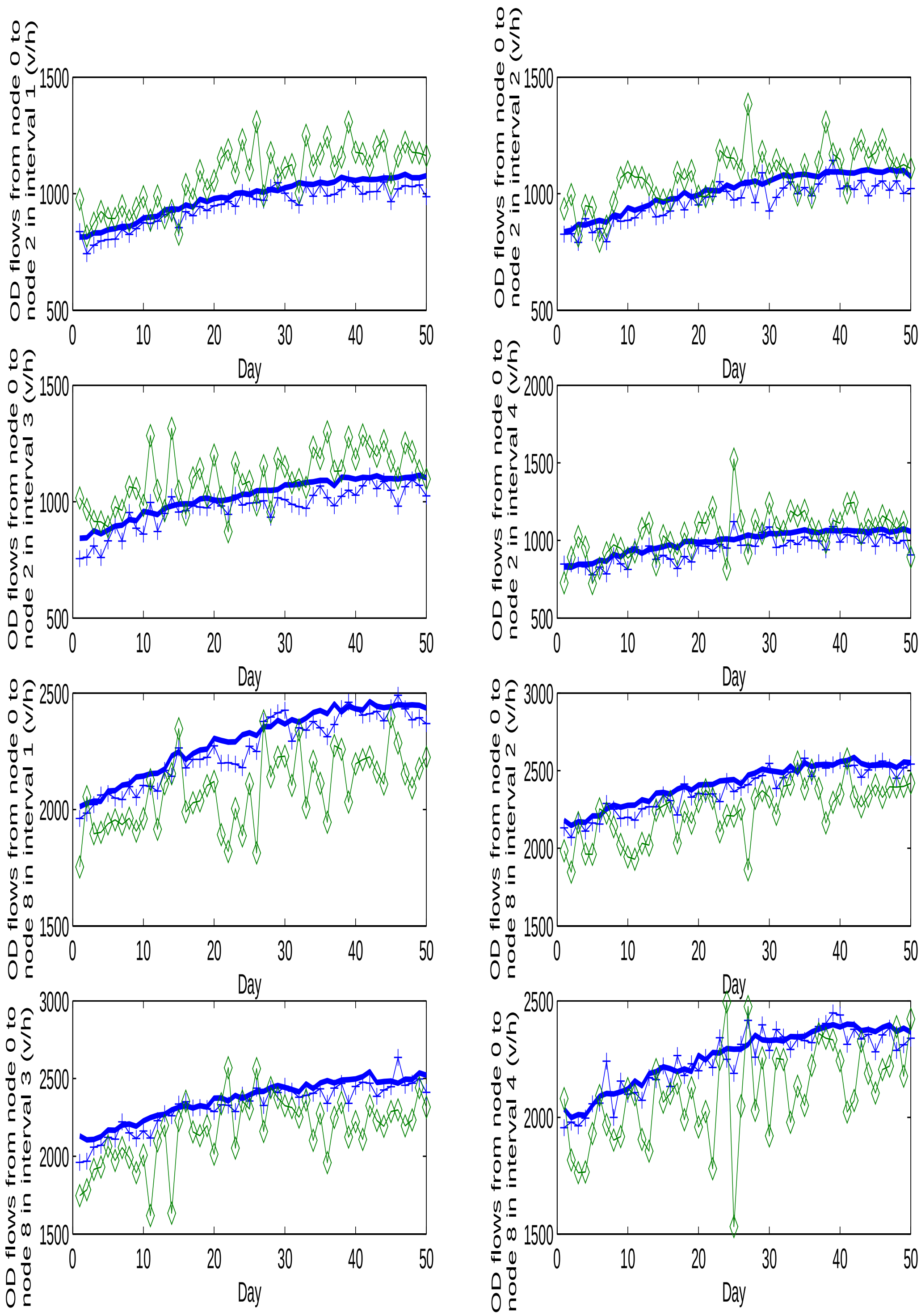

Figure A-3: OD estimates for L-F case (a)

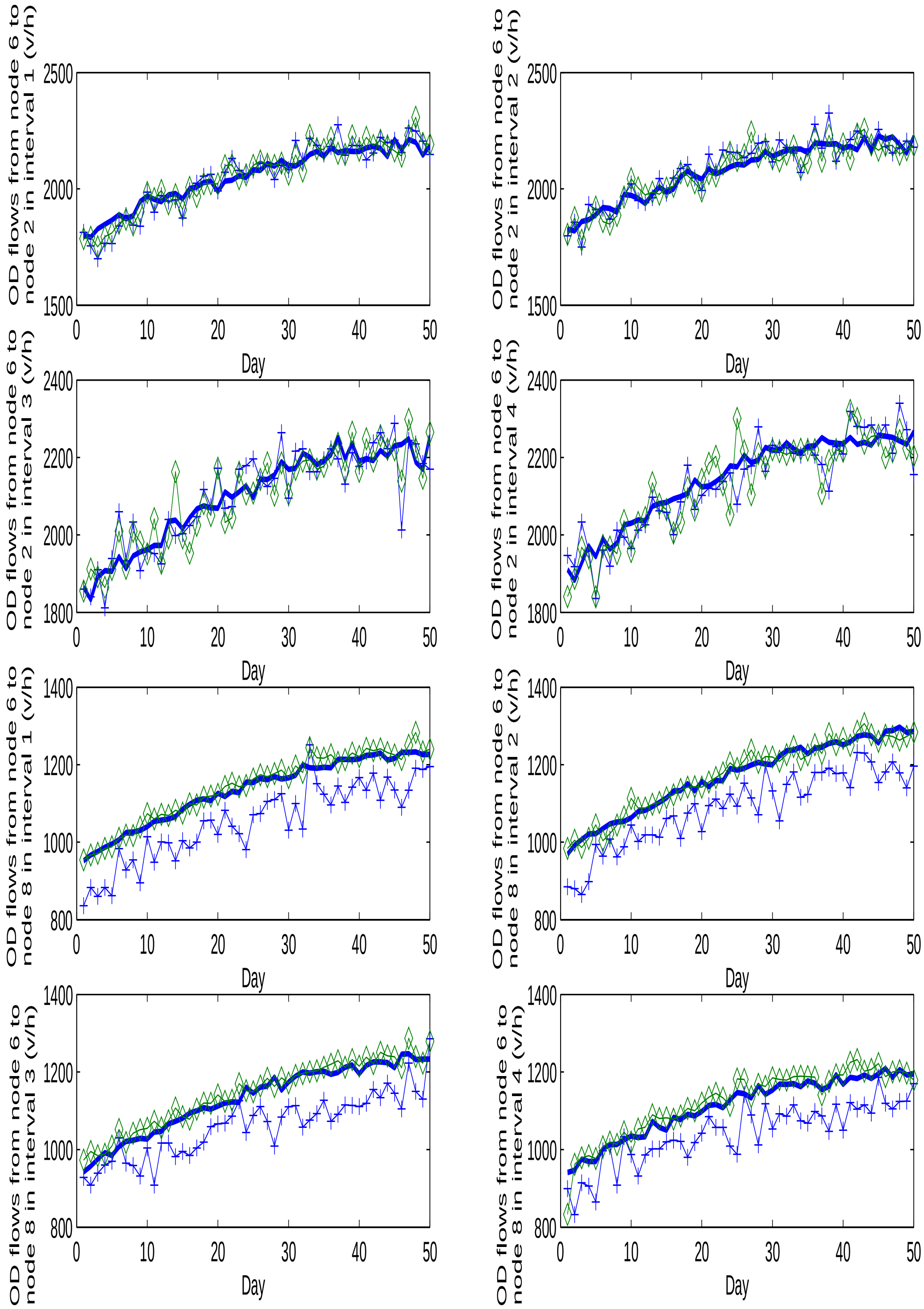

Figure A-4: OD estimates for L-F case (b)

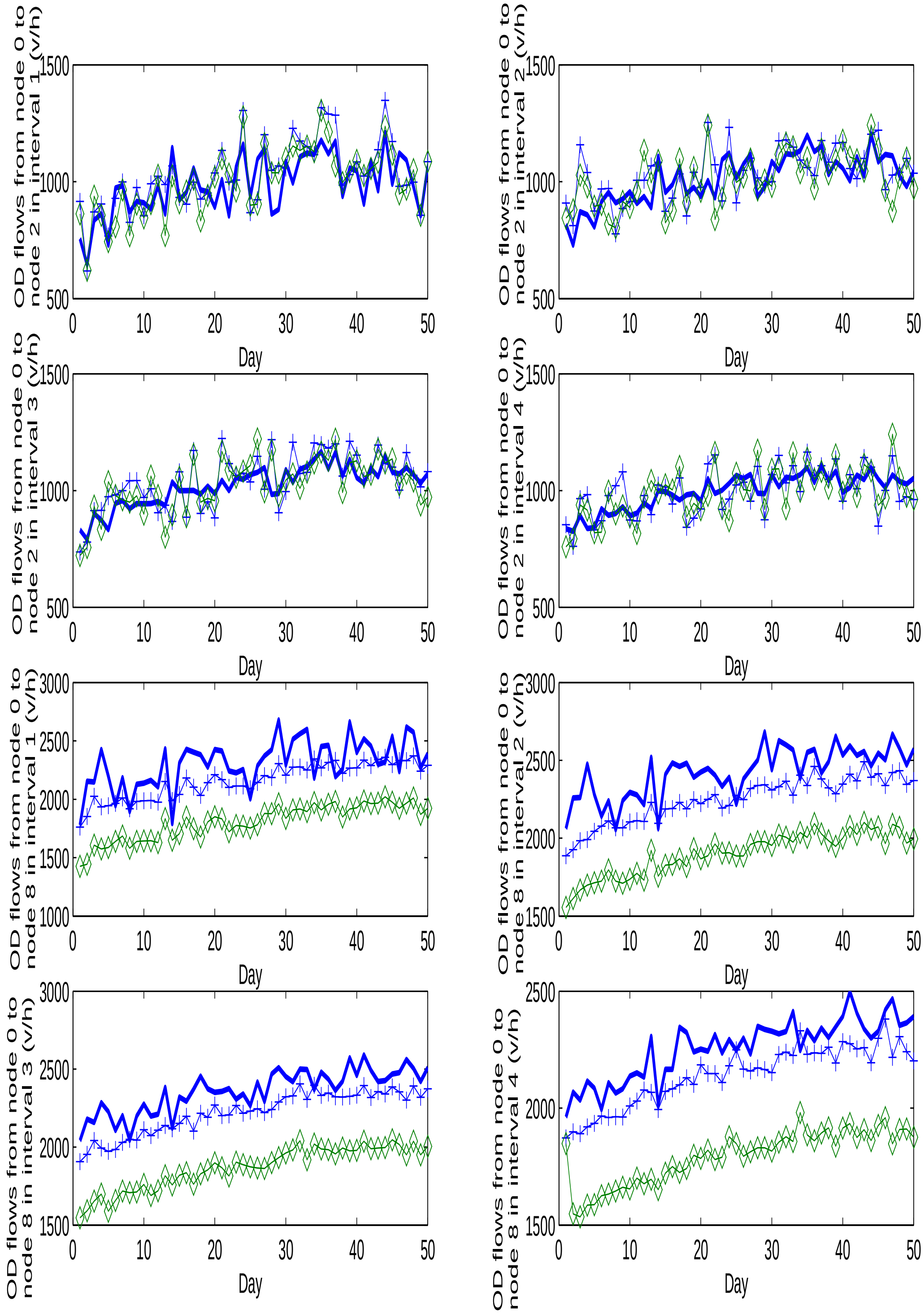

Figure A-5: OD estimates for H-NF case (a)

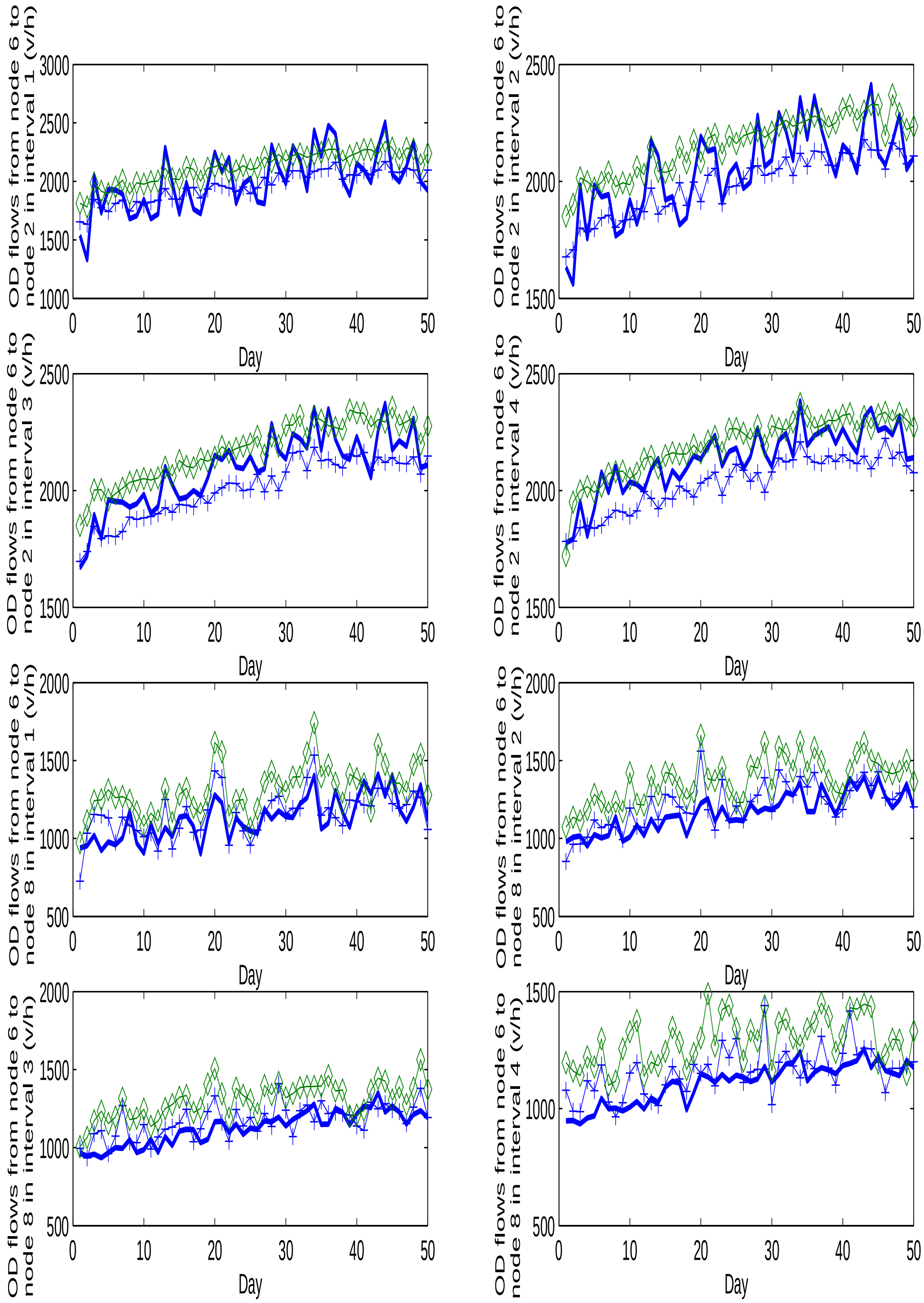

Figure A-6: OD estimates for H-NF case (b)

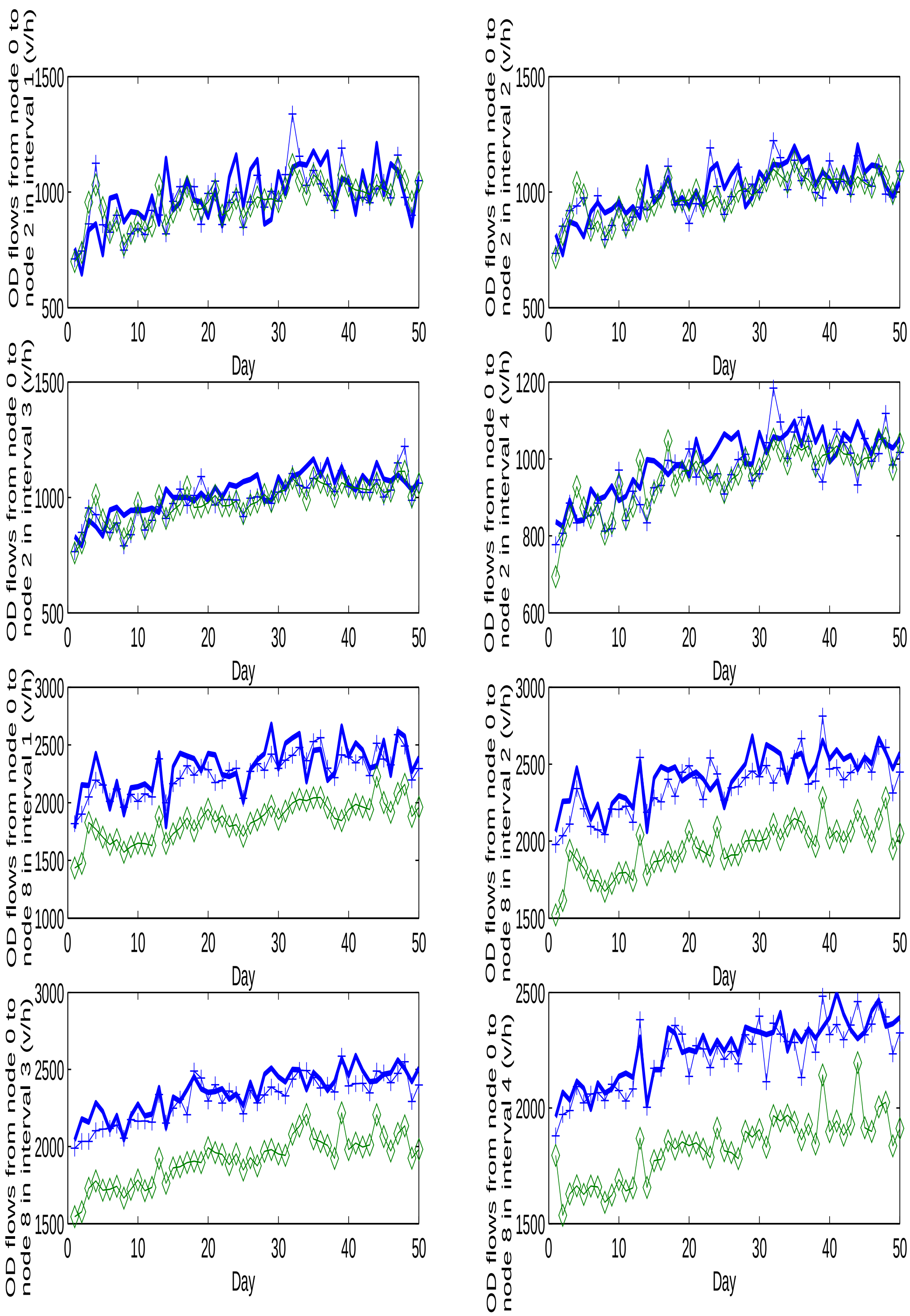

Figure A-7: OD estimates for H-F case (a)

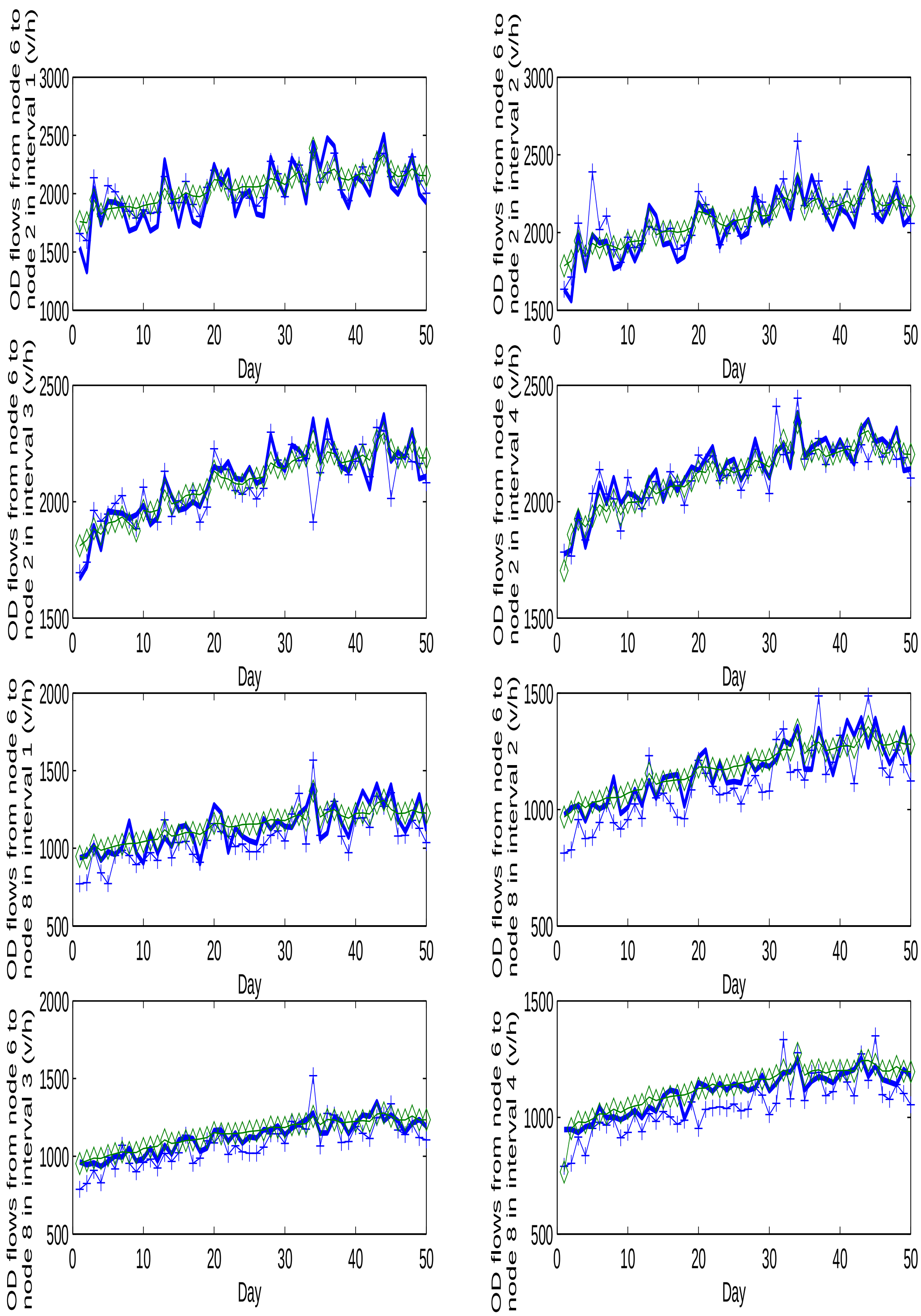

Figure A-8: OD estimates for H-F case (b)

Appendix B

Case Study 2: Variation in ODs

The following graphs show the variation of OD flows across days. The results are presented for each of the 11 intervals considered in the morning peak.

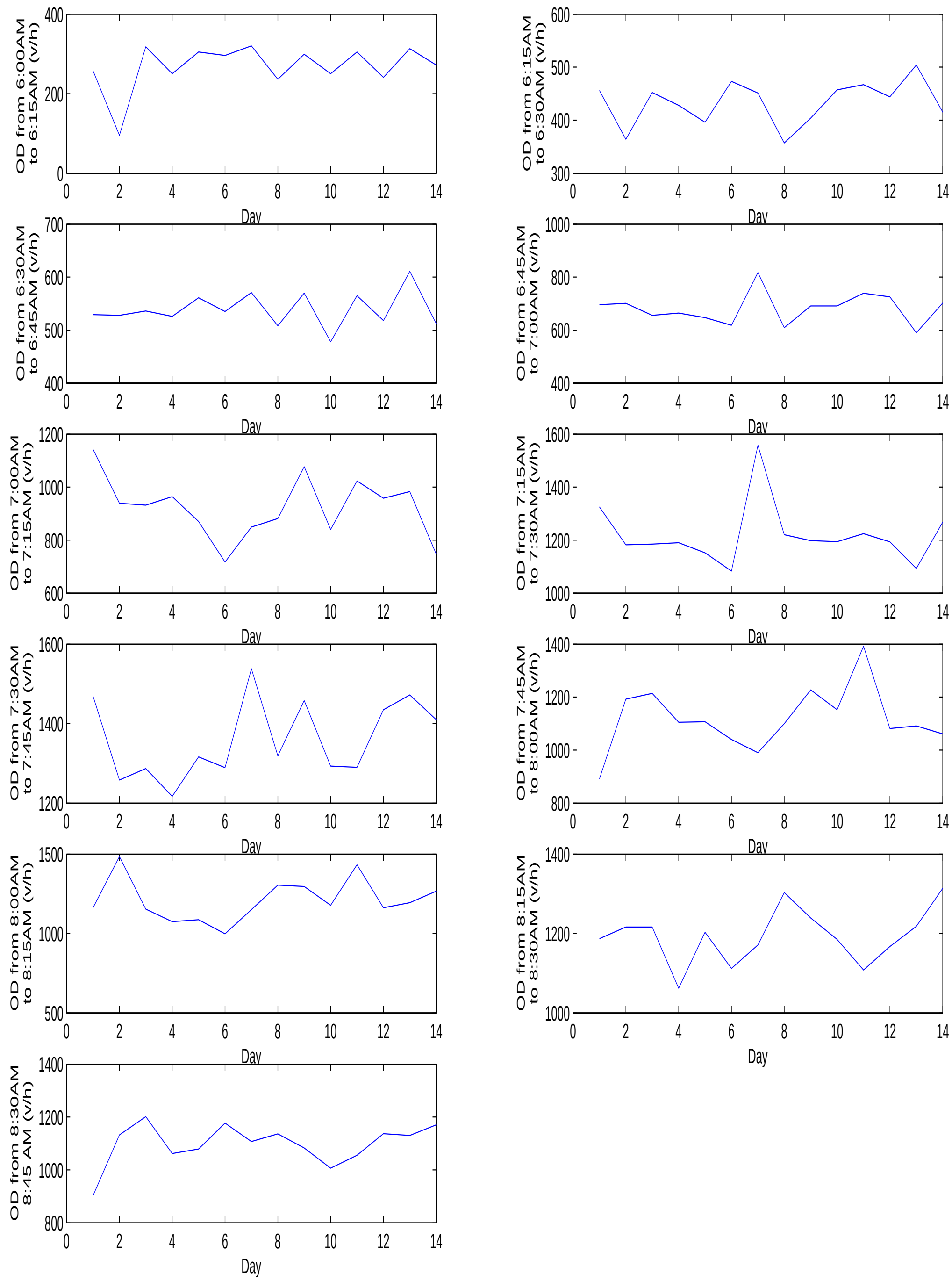

Figure B-1: Variation of OD flows from $1 \rightarrow 3$

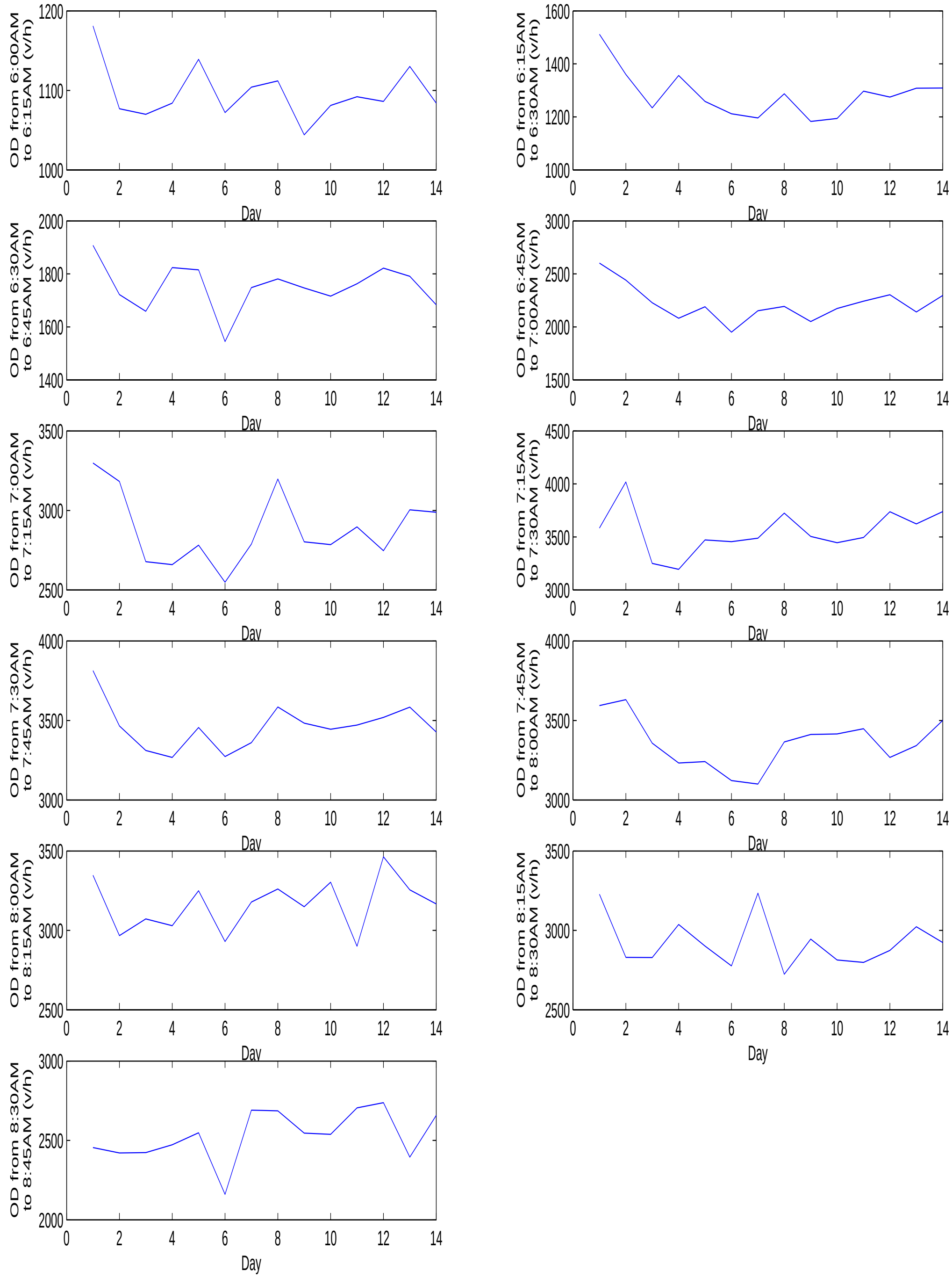

Figure B-2: Variation of OD flows from 1 → 5

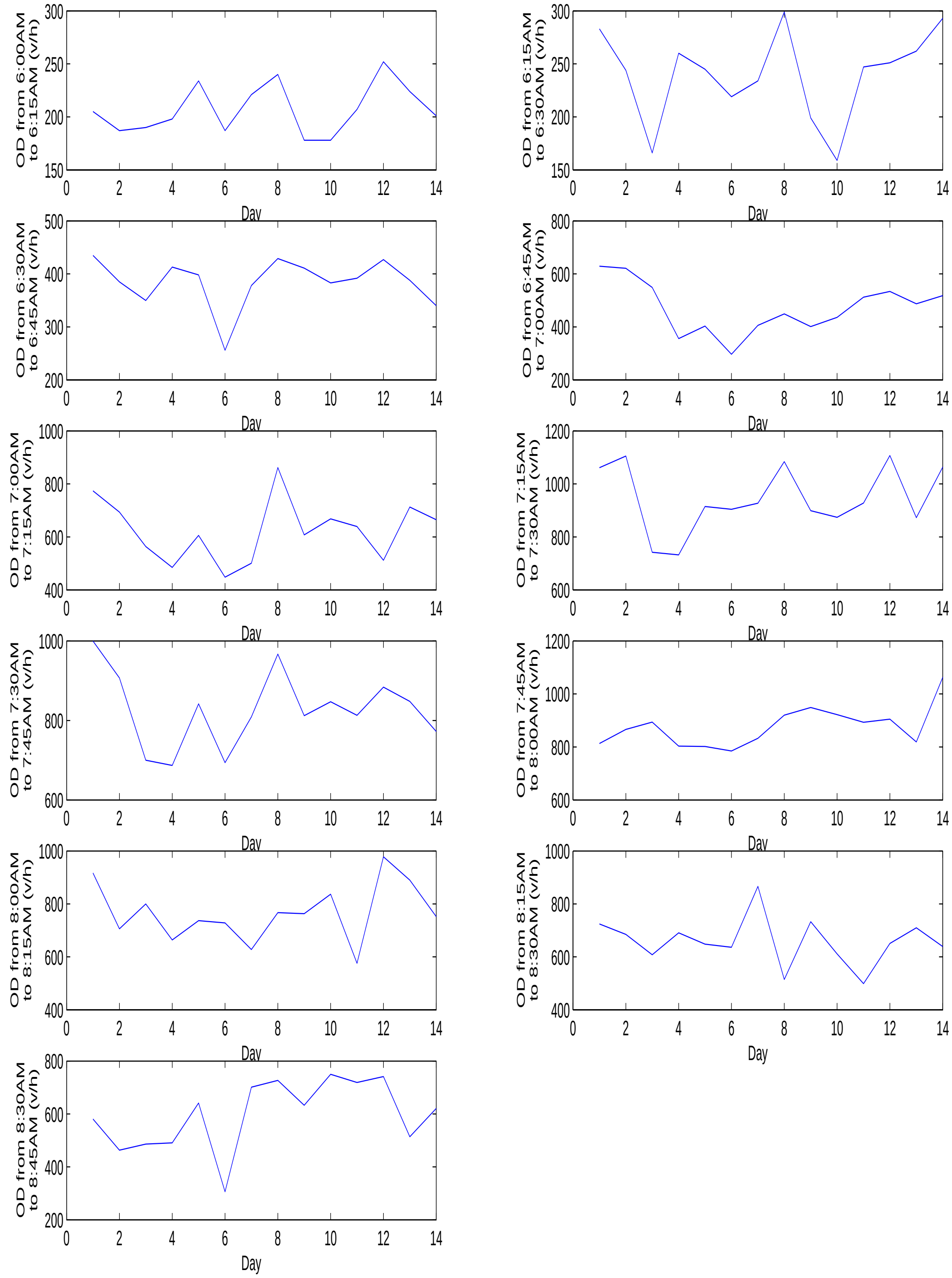

Figure B-3: Variation of OD flows from $2 \rightarrow 5$

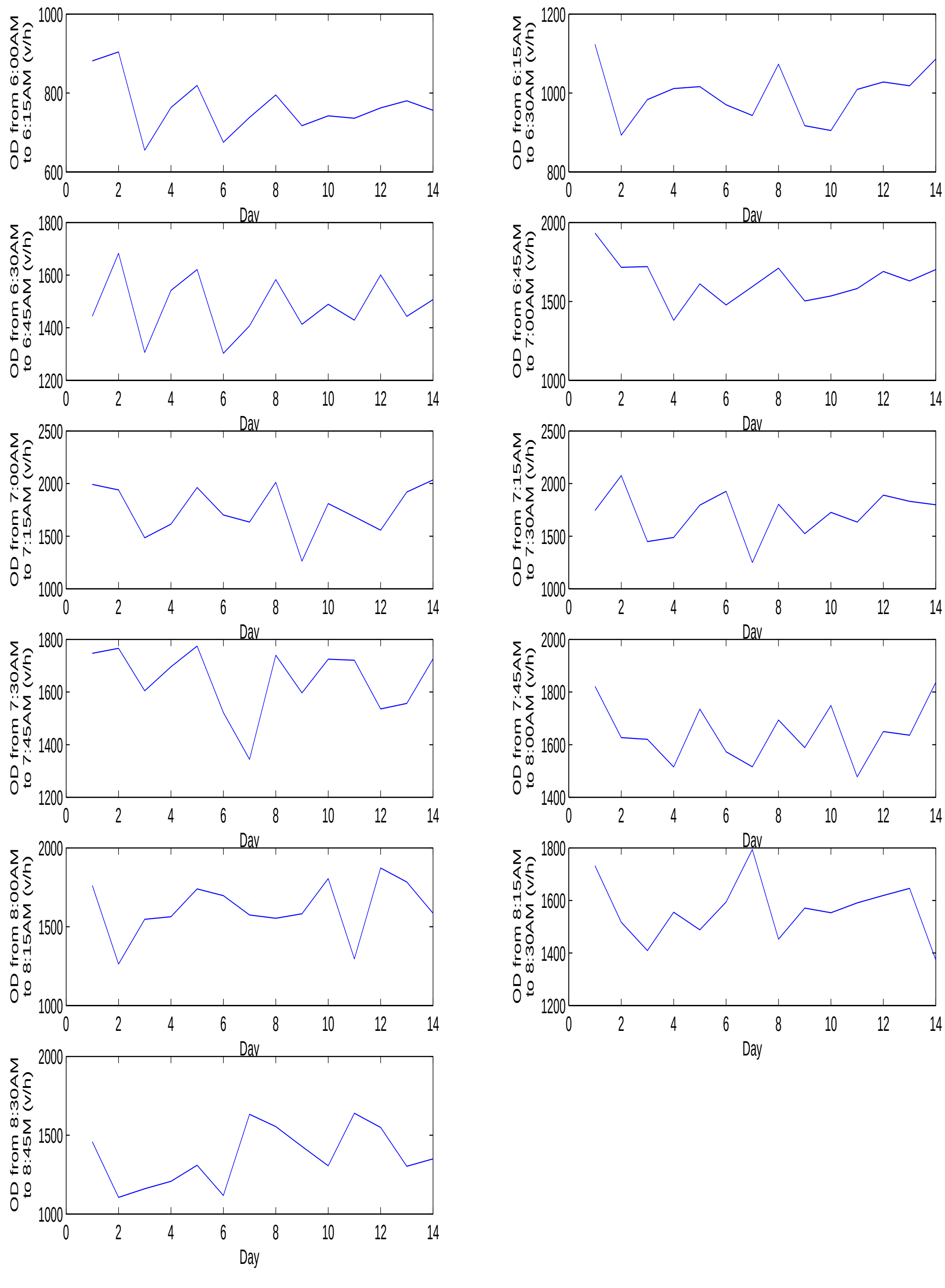

Figure B-4: Variation of OD flows from $4 \rightarrow 5$

Appendix C

Box algorithm

The algorithm finds the minimum of a multivariate, nonlinear function subject to nonlinear inequality constraints:

$$Minimize \;\; F(X_1, X_2, \ldots, X_N)$$

$$Subj\ to \;\; G_k \leq X_k \leq H_k, \quad k = 1, 2, \ldots, M$$

The implicit variables $X_{N+1}, \ldots, X_M$ are dependent functions of the explicit independent variables $X_1, X_2, \ldots, X_N$. The upper and lower constraints H_k and G_k are either constants or functions of the independent variables.

A *point* is defined as any combination of values $X_1, X_2, \ldots, X_N$ for which the objective function value can be computed. The algorithm enlists a *complex* set of K *points* to search for the minimum of the objective function, where K is an input parameter specified by the user. The basic algorithm is as follows:

1. An original complex of $K > N + 1$ points is generated consisting of a feasible point (specified by the user) and $K - 1$ additional points generated from random numbers and constraints for each of the independent variables.

$$X_{i,j} = G_i + r_{i,j}(H_i - G_i), \quad i = 1, 2, \ldots, N \;\; j = 1, 2, \ldots, K - 1$$

where $r_{i,j}$ are random numbers between 0 and 1

2. The selected points must satisfy both the explicit and implicit constraints. If at any time the explicit constraints are violated, the point is moved a small distance δ inside the violated limit. If an implicit constraint is violated, the point is moved one half of the distance to the centroid of the remaining points.

$$X_{i,j}^{new} = \frac{X_{i,j}^{old} + \bar{X}_{i,c}}{2}, \ \ i = 1, 2, \ldots, N$$

where the coordinates of the centroid of the remaining points are defined by

$$\bar{X}_{i,c} = \frac{1}{K-1}[\sum_{j=1}^{k} X_{i,j} + X_{i,j}^{old}], \ \ i = 1, 2, \ldots, N$$

This process is repeated as necessary until all the implicit constraints are satisfied.

3. The objective function is evaluated at each point. The point having the highest function value is replaced by a point according to the following equation. This is referred to as correction 1.

$$X_{i,j}^{new} = \alpha[\bar{X}_{i,c} - X_{i,j}^{old}] + \bar{X}_{i,c}, \ \ i = 1, 2, \ldots, N$$

A value of $\alpha = 1.3$ is usually recommended.

4. If a point repeats in giving the highest objective function value on consecutive trials, it is moved one half the distance to the centroid of the other points (correction 2).

5. The new point is checked against the constraints and is adjusted as before if the constraints are violated.

6. Convergence is assumed when the objective function values at each point are within some percentage for certain number of consecutive iterations.

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