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Calibration of fundamental diagram using trajectories of probe vehicles: Basic formulation and heuristic algorithm*

Toru Seo^{†‡} Takahiko Kusakabe[§] Yasuo Asakura[‡]
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Abstract

A fundamental diagram (FD), also known as flow-density relation, is one of the most important principles in traffic flow theory. It would be valuable if an FD could be calibrated by GPS-equipped probe vehicles; since they can continuously collect data from wide spatiotemporal area, compared to traditional fixed sensors. This paper proposes methods for calibrating an FD from trajectories of sampled vehicles. We formulate a method that identifies values of a free-flow speed and a critical density of a triangular FD, while it relies on exogenous assumptions on FD's functional form and a value of its jam density. Then, a heuristic algorithm for FD calibration in actual traffic environment is developed based on the proposed method. It was validated using traffic data generated by microscopic traffic simulator. The results suggested that the proposed methods can calibrate an FD precisely and robustly. It implies that FDs in road sections on which congestion happens frequently can be calibrated using probe vehicles, if probe vehicle data were collected for a long period. Therefore, the proposed methods would contribute to significant improvement of applicability of probe vehicle-based traffic management methods.

Keywords: traffic flow theory, fundamental diagram, GPS-equipped probe vehicle, trajectory

1 Introduction

Fundamental diagram (FD), also known as flow-density relation, is literally one of the most fundamental concepts in the traffic flow theory. An FD describes relation between flow and density¹ in *stationary traffic*. Stationary traffic is defined as traffic in which all the vehicles have the same constant speed and spacing (Daganzo, 1997). In theory, an FD itself contains useful information on traffic features, such as value of free-flow speed and flow capacity, and distinction between free-flow and congested states. Empirical studies also showed that clear relation can be found between flow and density in actual traffic at near-stationary states (Cassidy, 1998). In addition, macroscopic traffic flow dynamics can be modeled by combining an FD and other principles: the most known example is the Lighthill–Whitham–Richards (LWR) model (Lighthill and Whitham, 1955; Richards, 1956). Moreover, FDs can describe microscopic vehicle behavior to some extent (Newell, 2002). Therefore, FDs are applied to various academic and practical purposes in traffic and transportation engineering, such as macroscopic traffic simulation (e.g., Daganzo, 1994), traffic control (e.g., Papageorgiou et al., 2003), and traffic state estimation (e.g., Deng et al., 2013).

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¹Technically, relation between two variables among flow or headway, density or spacing, and speed or pace (Laval and Leclercq, 2013).

To calibrate parameters of an FD in actual traffic, one has to collect data from traffic, to assume its FD's functional form, and then to calibrate the FD's parameters by fitting the FD to the data. Those data are commonly collected using fixed sensors (e.g., cameras, detectors) from the era of Greenshields (1935); for example, see Chiabaut et al. (2009), Dervisoglu et al. (2009), Coifman (2014), and references therein. This is a straightforward way because usual fixed sensors can measure traffic count and occupancy, which are closely related to flow and density, respectively, at their location. The limitation of the fixed sensor-based calibration is obvious: it cannot calibrate FDs where sensors are not installed. Therefore, FDs on roads without sensors, such as most of arterial roads, are difficult to be known. Identification of bottlenecks' exact locations and characteristics is also difficult, even on freeways with some sensors.

Probe vehicles received high attention in these days.² The advantage of probe vehicles is their significantly wider data collection range (in spatiotemporal domain) compared with fixed sensors (Herrera et al., 2010). For example, one of the most typical and useful utilization of the advantage is traffic state estimation, which estimates flow, density, and speed of traffic using partial measurement data (c.f., Deng et al., 2013, and references within). However, existing studies on such application assume their FDs exogenously, in order to relate flow and density to speed measured by probe vehicles. This can be significant limitation for application of probe vehicles, since FD calibration is not a trivial task. Especially, FD calibration using probe vehicle data has been not well studied. Appendix in Herrera et al. (2010) mentioned a manual inference method for FD using probe vehicle data under special conditions. However, it lacks rigorous formulation and is not computable. Considering these days high availability of probe vehicle data, systematic and computational approaches for FD calibration would be desirable.³

The aim of this paper is to propose a method of calibrating FDs using probe vehicle data. In order to enable the calibration, we allow the method to rely minimum exogenous assumptions, such as FD's functional form and values of some of the FD's parameters (e.g., jam density which can be inferred from external knowledge). In addition, to show empirical validity of the proposed method, a computable method for FD calibration is developed and validated using microscopic traffic simulation data.

The rest of this paper is organized follows. Section 2 formulates a method of identifying FD parameters using sampled vehicle trajectories under idealized conditions. Section 3 describes a heuristic algorithm for actual traffic environment based on the proposed method. Section 4 validates the proposed heuristic algorithm using noisy traffic data generated by microscopic traffic simulation. Section 5 concludes this paper.

2 Formulation

This section describes a method of calibrating FD using sampled vehicle trajectories under simplified conditions.

Concept of the proposed method is as follows. The subjects of estimation are values of free-flow speed and critical density of a triangular FD. The jam density is assumed exogenously, as it can be easily inferred by external knowledge such as average vehicle body length. Suppose that two probe vehicles are driving the same road with homogeneous FD; and c-1 vehicles exist between the probe vehicles. If traffic in a time-space region between two probe vehicles is stationary (c.f., stationary traffic is defined as traffic in which all the vehicles have the same constant speed and spacing (Daganzo, 1997)), a traffic state (i.e., flow, density, and speed) in the region follows the FD by the definition. If the region is stationary and the distance traveled by the probe vehicles are the same, a traffic state of probe vehicles only in the region (i.e., probe-traffic-state) follows

²In this paper, unless otherwise specified, the term "probe vehicle" refers to be the Global Positioning System (GPS)-equipped probe vehicle, which continuously measure and report its position and time.

³If probe vehicles can measure spacing to their leading vehicles using advanced technologies (c.f., Huber et al., 1999; Seo et al., 2015a), FDs can be directly derived from such probe vehicle data in detail, for example, continuously (Kotani and Iwasaki, 1999), individually (Duret et al., 2008), stochastically (Jabari et al., 2014), and jointly with traffic state (Seo et al., 2015b). However, these technologies are not commonly available for large-scale data collection at this moment. Therefore, application of such advanced technologies is out of scope of this study.

a curve which is similar to the FD with 1/c scale (i.e., probe-FD). If the probe vehicles trajectories satisfies certain conditions (which are likely to be satisfied in many situations), the probe-FD can be identified. Finally, since the probe-FD is similar to the FD with 1/c scale and the value of the FD's jam density is already known, the free-flow speed and the critical density can be identified.

2.1 Assumptions and preconditions

Following two factors are assumed:

- (a) a functional form of an FD is triangular, and
- (b) value of jam density.

Note that parameters of a triangular FD are three: free-flow speed, critical density, and jam density. Therefore, parameters to be calibrated are free-flow speed and critical density.

Input data for the proposed method are:

• Multiple vehicles trajectories in a time-space region whose FD is to be calibrated.

These data are considered to be continuously collected by probe vehicles without error. Hereafter, the time–space region whose FD is to be calibrated is referred as *target region*.

The required conditions for calibrating FD's parameter are as follows:

- (i) The FD is constant with the assumed functional form and jam density in the target region.
- (ii) A first-in first-out (FIFO) principle and a conservation law are satisfied in the target region.
- (iii) Two vehicles' trajectories traveled through following three time-space regions in the target region:
 - a stationary region⁴ whose density is less than the critical density,
 - a stationary region whose density is greater than or equal to the critical density, and
 - a stationary region whose density is greater than the critical density and is not equal to those
 of the above regions.

The conditions (i) and (ii) are assumptions on traffic flow characteristics. They means the traffic is described by the LWR model. The condition (iii) is an assumption on appearance of probe vehicles. Practical meaning of these assumptions and conditions are discussed later (see section 2.3.2).

The output estimated by the proposed method are:

- values of free-flow speed and critical density, and
- number of vehicles exist between the two vehicles.

The objective of the proposed method is to obtain the former values.

2.2 Calibration method

The calibration method can be described by following general formula:

$$find u, k_c, \{c_{i,j}\}_{\forall i,j}, \tag{1a}$$

s.t.
$$q_i(\mathbf{a}) = Q(k_i(\mathbf{a}), u, k_c/c_{i,j}, \kappa/c_{i,j}),$$
 (1b)

$$\forall \mathbf{a} \in \mathbf{A}'(i, j, \mathbf{A}),\tag{1c}$$

$$\forall i, j \in \mathbf{P}(\mathbf{A}),\tag{1d}$$

where

⁴In this paper, the term "stationary region" is defined as a time-space region in which traffic is stationary.

A the target region which satisfies conditions (i) and (ii),

 $Q(k, u, k_c, \kappa)$ FD function which represents flow under density k, free-flow speed u, critical

density k_c , and jam density κ ,

P(A) set of all the probe vehicles in region A,

 $c_{i,j}$ total number of vehicles exist between probe vehicles i and j,

 $q_i(\mathbf{a}), k_i(\mathbf{a}), v_i(\mathbf{a})$ flow, density, and speed with respect to probe vehicle i only in region \mathbf{a} . Hereafter, they are referred to be *probe-traffic-state*, Their definition is provided

by eqs (4)–(6),

 $S_i(\mathbf{a})$ probe-traffic-state vector, namely, $(q_i(\mathbf{a}), k_i(\mathbf{a}))^{\top}$,

A'(i, j, A) set of time-space regions which satisfies following conditions:

- it is in region A,

- its edges are trajectories of probe vehicles i and j in region A,

its traffic is stationary

Eqs (1a) and (1b) mean that values of FD parameters are determined such that traffic state estimated from probe vehicle data follows the FD, considering conditions (i) and (ii). Eqs (1c) and (1d) mean that probe vehicle data which satisfy condition (iii) are utilized for calibration. Following *traffic state* is defined:

 $q(\mathbf{a}), k(\mathbf{a})$ flow and density with respect to all the vehicle in region \mathbf{a}

 $S(\mathbf{a})$ traffic state vector, namely, $(q(\mathbf{a}), k(\mathbf{a}))^{\top}$

The traffic state (considering all the vehicles) and probe-traffic-state (which is traffic state considering a probe vehicle only) are defined based on the Edie (1963)'s generalized definition as follows:

$$q(\mathbf{a}) = \frac{\sum_{n \in \mathbf{N}(\mathbf{a})} d_n(\mathbf{a})}{|\mathbf{a}|},\tag{2}$$

$$k(\mathbf{a}) = \frac{\sum_{n \in \mathbf{N}(\mathbf{a})} t_n(\mathbf{a})}{|\mathbf{a}|},\tag{3}$$

$$q_i(\mathbf{a}) = \frac{d_i(\mathbf{a})}{|\mathbf{a}|},\tag{4}$$

$$k_i(\mathbf{a}) = \frac{t_i(\mathbf{a})}{|\mathbf{a}|},\tag{5}$$

$$v_i(\mathbf{a}) = \frac{d_i(\mathbf{a})}{t_i(\mathbf{a})},\tag{6}$$

where

N(a) set of all the vehicle in region a,

 $d_n(\mathbf{a})$ distance traveled by vehicle n in region a,

 $t_n(\mathbf{a})$ time spent by vehicle n in region \mathbf{a} ,

 $|\mathbf{a}|$ area of region \mathbf{a} .

Following explains the logic of the FD calibration. For the sake of brevity, it explains a special case of the method where an element in $\mathbf{A}'(i,j,\mathbf{A})$ is defined as a time-space region between trajectories of probe vehicles i and j in space $[x,x+\Delta x)$, where Δx is arbitrary distance. Such element is denoted as $\mathbf{a}_{i,j}^{(x)}$. Under this specification, the calibration method can be illustrated as Figs. 1 and 2. Fig 1 is a time-space diagram showing free-flow traffic and congested traffic divided by a shockwave. Fig 2 is a flow-density plane corresponding to

Fig 1. In Fig 2, a dot indicates traffic state or probe-traffic-state; a solid line indicates transition of traffic states; and a dashed line indicates a FD. The blue areas (in Fig 1) and dots (in Fig 2) indicate stationary regions with free-flow traffic; the green ones indicate non-stationary regions with free-flow and congested traffic; and the red ones indicate stationary regions with congested traffic.

By the definition, traffic state $S(\mathbf{a}_{i,j}^{(x)})$ follows FD if region $\mathbf{a}_{i,j}^{(x)}$ is stationary. Probe-traffic-state $S_i(\mathbf{a}_{i,j}^{(x)})$ is equal to $S(\mathbf{a}_{i,j}^{(x)})/c_{i,j}$ if region $\mathbf{a}_{i,j}^{(x)}$ is stationary and distance traveled by each vehicles in $\mathbf{a}_{i,j}^{(x)}$ is equal to the others. It means that $S_i(\mathbf{a}_{i,j}^{(x)})$ follows a *probe-FD* which is a curve whose scale is $1/c_{i,j}$ of the true FD under the aforementioned conditions. The probe-FD can be also represented as $q = Q(k, u, k_c/c_{i,j}, \kappa/c_{i,j})$. In Fig 1, regions $\mathbf{a}_{i,j}^{(0,1,4,5)}$ are stationary; therefore, they are on the probe-FD which is represented as thick dashed lines in Fig 2. On the other hand, regions $\mathbf{a}_{i,j}^{(2,3)}$ are non-stationary; therefore, they are not on the probe-FD and discarded (not utilized by calibration) (eq (1c)).

Stationarity of region $\mathbf{a}_{i,j}^{(x)}$ can be inferred using trajectories of probe vehicles i and j. For example, $v_i(\mathbf{a}_{i,j}^{(x)}) = v_j(\mathbf{a}_{i,j}^{(x)})$ is a necessary condition for stationarity.

Finally, if the probe vehicles i and j have traveled other congested region $\mathbf{a}_{i,j}^{(o)}$ (the gray dot in Fig 2; it may locates at downstream outside of Fig 1), $\mathbf{A}'(i,j,\mathbf{A})$ consists of $\mathbf{a}_{i,j}^{(0)}, \mathbf{a}_{i,j}^{(1)}, \mathbf{a}_{i,j}^{(4)}, \mathbf{a}_{i,j}^{(5)}, \mathbf{a}_{i,j}^{(o)}$. Then, the FD can be uniquely determined by choosing values of u, k_c , and $c_{i,j}$ such that all the points in $\{S_i(\mathbf{a}_{i,j}^{(x)}) \mid \mathbf{a}_{i,j}^{(x)} \in \mathbf{A}'(i,j,\mathbf{A})\}$ are on the probe-FD $q = Q(k,u,k_c/c_{i,j},\kappa/c_{i,j})$ (eqs (1a) and (1b)).

2.3 Discussion

2.3.1 Summary of method

The proposed method can be summarized as follows.

Suppose that there is traffic described by the LWR model; two probe vehicles, namely, i and j, travel through a free-flow region and some congested regions in the traffic; and $c_{i,j}-1$ non-probe vehicles are traveling between the two probe vehicles (Fig 1). Let $q(\mathbf{a})$ be flow in time-space region \mathbf{a} ; $k(\mathbf{a})$ be density in time-space region $k(\mathbf{a})$; which determine flow under density $k(\mathbf{a})$; free-flow speed $k(\mathbf{a})$; critical density $k(\mathbf{a})$; and jam density $k(\mathbf{a})$.

Now the time-space region between the two probe vehicles is divided to multiple subregions (a in Fig 1) according to a specific rule. If traffic in a subregion is stationary, its traffic state $(S(\mathbf{a}) = (q(\mathbf{a}), k(\mathbf{a})))$ in Fig 2) will follow the true FD $(q(\mathbf{a}) = Q(k(\mathbf{a}), u, k_c, \kappa))$ by the definition. If traffic in a subregion is stationary and distance traveled in the subregion by each vehicle is equal to the others, its probe-traffic-state, $S_i(\mathbf{a}) = (q_i(\mathbf{a}), k_i(\mathbf{a}))$, which is flow and density of probe vehicles only, will be $1/c_{i,j}$ times the true traffic state in the subregion $(S_i(\mathbf{a}) = S(\mathbf{a})/c_{i,j})$. Such probe-traffic-states follow probe-FD of which scale is $1/c_{i,j}$ of the true FD. It can be represented as $q_i(\mathbf{a}) = Q(k_i(\mathbf{a}), u, k_c/c_{i,j}, \kappa/c_{i,j})$.

If probe vehicles traveled through regions that satisfy specific conditions, the probe-FD can be identified from the probe vehicle data only. For example, in Fig 2, a triangle with its vertex is at point (0,0), its edge is on line q=0, and its edges pass blue point, red point, and gray point can be determined uniquely. In other words, values of u, $k_{\rm c}/c_{i,j}$, and $\kappa/c_{i,j}$ can be determined from the probe vehicle data by assuming triangular shape for the FD. Finally, since the value of jam density κ is given, values of the rest of variables—namely, number of vehicles between probe vehicles $c_{i,j}$, free-flow speed u, and critical density $k_{\rm c}$ —can be determined.

2.3.2 Practical meaning of the assumptions and preconditions

The proposed method assumes a triangular FD with known jam density (assumptions (a) and (b)). This assumption can be regarded as useful and easy to be assumed. Triangular FD has several desirable characteristics in theory (Newell, 1993), is often employed by existing studies (c.f., Daganzo, 1997), and can

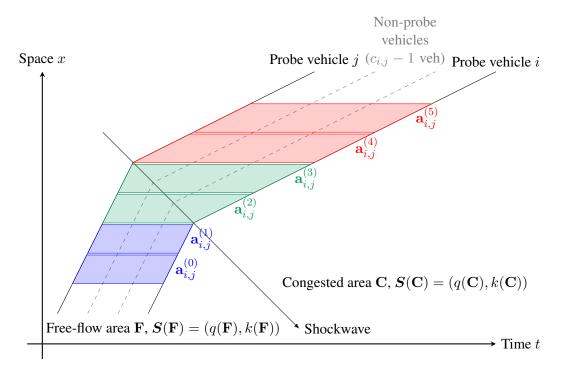


Figure 1: Vehicle trajectories on time-space diagram

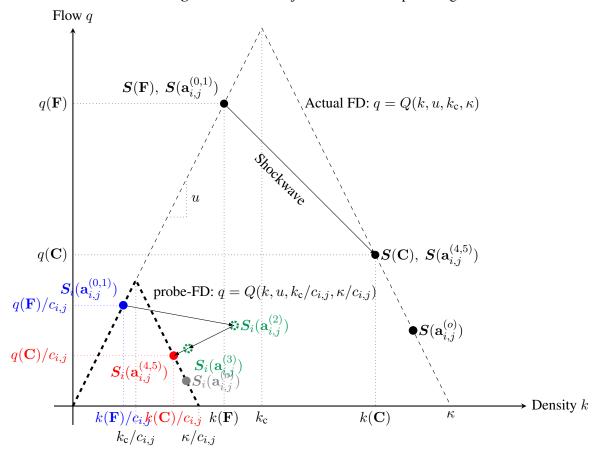


Figure 2: Traffic states transition on flow-density plane

be found in empirical data (Cassidy, 1998). As for the parameter assumption, we can expect that reasonable value can be assumed without strong dependency on time, space, nor flow characteristic; because value of jam density mainly depends on average length of vehicle bodies.

The method requires that the FD is constant in the target region (condition (i)). This assumption can be the method's limitation to some extent, especially on application to freeways; because the constant FD means there are no bottlenecks. Therefore, in freeway cases, the method has to be applied to near-homogeneous road section only. Note that bottlenecks at the boundaries of the section are acceptable for the method. For example, the method can be applied to a homogeneous section whose downstream end is an bottleneck. It should be noted that, although the FD of the bottleneck cannot be calibrated by the method in such situation, its capacity can be inferred; because flow during congested state in the section can be derived based on the calibrated FD and the probe vehicle data. On the other hand, the condition (i) will not be significant limitation of the method on application to arterial roads, where traffic is governed by signals rather than bottlenecks. In fact, the method would be useful in such arterial roads, since the condition (iii) is likely to be satisfied near signals (see below).

The method requires certain properties for presence of probe vehicles (condition (iii)). This condition is likely to be satisfied in the real-world. For example, it will be satisfied at upstream congestion of a merging section, queue at signal, stop-and-go wave, and congestion due to a moving bottleneck. Furthermore, it will be satisfied if amount of probe vehicle data is large enough (e.g., data collection time period) and it is randomly sampled, even if the penetration rate is low.

3 Heuristic algorithm for actual traffic

The method presented in section 2 can determine an FD theoretically, if all the preconditions (i)–(iii) were satisfied (and appropriate computation procedure was implemented). However, actual traffic may not follow the LWR model (e.g., finite acceleration, heterogeneity among vehicles and lanes, measurement error). It means that the preconditions may not be satisfied in actual traffic. In order to derive FD in such actual traffic, this section describes a heuristic (and computational) algorithm for actual traffic based on the method of section 2.

The concept of the proposed algorithm is as follows. Exact solution of the problem (1) may not exist since the preconditions are not exactly satisfied in actual traffic. Therefore, an algorithm determines FD parameters by solving a residual minimization problem which relaxes eq (1) is proposed. Because of the residual minimization problem may not be convex, the proposed algorithm is considered as heuristic.

3.1 Algorithm

The algorithm can be described as follows:

- **Step 1** Define region **A**.
- **Step 2** Select probe vehicle *i* from set P(A). Go to Step 5 if all of the probe vehicles are already selected.
- **Step 3** Execute the following procedure:
 - **Step 3.1** Select probe vehicle j from $\mathbf{P}(\mathbf{A})$ such that $i \neq j$. Go back to Step 2 if all of the combination (i,j) are already selected. Define empty set $\mathbf{A}'(i,j,\mathbf{A})$.
 - **Step 3.2** Define region $\mathbf{a}_{i,j}^{(x)}$. Go back to step 3.1 if all of the combination (i,j,x) are already selected.
 - **Step 3.3** Determine whether region $\mathbf{a}_{i,j}^{(x)}$ is stationary or not based on the trajectories of i and j. Go back to Step 3.2 if it is not stationary.

⁵Lane-drops and sags are the typical bottlenecks in this LWR context. Contrary, merging sections and signals are not bottlenecks in the context, as FDs around those sections are commonly considered as constant.

Step 3.4 Add probe-traffic-state $S_i(\mathbf{a}_{i,j}^{(x)})$ to set $\mathbf{A}'(i,j,\mathbf{A})$. **Step 3.5** Go back to Step 3.1.

Step 4 Go back to Step 2.

Step 5 Determine free-flow speed u, critical density k_c , vehicle numbers $\{c_{i,j}\}$ by using residual minimization with set $\mathbf{A}'(i,j,\mathbf{A})$.

Note that Steps 2, 3, and 4 correspond to eqs (1c) and (1d); and Step 5 corresponds to eqs (1a) and (1b). Among the procedure, Step 5 is considered as heuristic while the other steps are not.

In Step 3.3, a region is determined to be stationary if relative difference of speed of probe vehicles i and j is less than θ , namely,

$$\frac{|v_i(\mathbf{a}_{i,j}^{(x)}) - v_j(\mathbf{a}_{i,j}^{(x)})|}{v_i(\mathbf{a}_{i,j}^{(x)})} \le \theta, \tag{7}$$

where θ is a constant which should be given appropriately. If values of θ and Δx are too small, $\mathbf{a}_{i,j}^{(x)}$ will not be regarded as stationary due to small-scale noises in traffic. On the other hand, if they are too large, $\mathbf{a}_{i,j}^{(x)}$ will be regarded as stationary even if it includes a shockwave and therefore should not be stationary.

The residual minimization in Step 5 is described as follows:

$$\min_{\substack{u,k_{c},\{c_{i,j}\}_{\forall i,j} \\ \forall i,j \in \mathbf{P}(\mathbf{A})}} \sum_{\substack{\mathbf{a} \in \mathbf{A}'(i,j,\mathbf{A}) \\ \forall i,j \in \mathbf{P}(\mathbf{A})}} \operatorname{diff}\left(c_{i,j}S_{m}(\mathbf{a}), u, k_{c}, \kappa\right)^{2}, \tag{8}$$
s.t. $u \geq 0$,
$$0 \leq k_{c} \leq \kappa$$
,
$$\forall c_{i,j} \geq 0, i, j \in \mathbf{P}(\mathbf{A})$$
,

where diff represents distance between a point (q, k) and a curve $q = Q(k, u, k_c, \kappa)$. Note that diff $(c_{i,j}S_m(\mathbf{a}), u, k_c, \kappa)$ and $c_{i,j}$ diff $(S_m(\mathbf{a}), u, k_c/c_{i,j}, \kappa/c_{i,j})$ are equivalent to each other except $c_{i,j} = 0$ case. The optimization can be executed by quasi-Newton method with multiple initial points; because optimization problem (8) is not necessarily convex.

3.2 Discussion

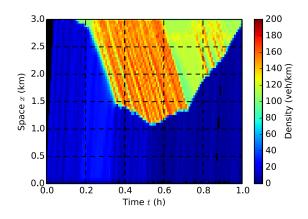
By using the proposed algorithm, values of the FD parameters can be calibrated. The result can be considered as an "average FD" where heterogeneity over time and space are averaged out. The heterogeneity among vehicles can be also averaged out if the data contains large number of probe vehicles.

The proposed algorithm can be robust against measurement error. The variables $d_i(\mathbf{a})$, $t_i(\mathbf{a})$, and $|\mathbf{a}|$ are derived from a vehicle trajectory over a distance of Δx . Therefore, measurement error will be negligible if Δx is sufficiently larger than GPS measurement error (typically around 10 meters).

The optimization problem (8) is not necessarily convex as mentioned. In addition, an obvious global optimal is $c_{i,j} = 0$ ($\forall i, j$), which is physically meaningless for FD calibration. However, it can be expected that local optima exist near the actual FD parameters. Therefore, FD parameters would be estimated properly by using a local optimization method (e.g., quasi-Newton method) with certain initial points. Validness of applying quasi-Newton method with various initial points to this problem (i.e., robustness of the proposed algorithm) is presented in section 4.

4 Validation

This section describes validation of the calibration algorithm of section 3 by applying it to synthetic traffic data generated by microscopic traffic simulation.



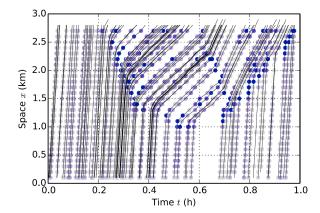


Figure 3: Density k in the simulation

Figure 4: An example of probe vehicle trajectories in the simulation

4.1 Simulation environment

Traffic data was generated by a microscopic traffic flow simulator Aimsun (TSS-Transport Simulation Systems, 2011), which is based on Gipps (1981)'s car-following model and Gipps (1986)'s lane-changing model. The car-following model's parameters are shown by Table 1. The road was configured to have two lanes corridor with a bottleneck at its downstream end. Probe vehicles were randomly sampled from the entire vehicles with 5% probability. As results, the synthetic traffic does not satisfy the precondition (i) and (ii) exactly and does not satisfy (iii) at all depending on a combination of probe vehicles—these are similar to actual traffic.

Fig 3 shows the traffic density generated by the simulation. According to the figure, several traffic features, such as queue extension, queue diminishing, and stop-and-go waves in the queue can be found. Fig 4 shows an example of probe vehicle trajectories. The curves represent trajectories of probe vehicles and the colored dots represent non-stationarity defined by the left hand side of eq (7), where thicker color shows larger non-stationarity.

Values of the parameter of the algorithm were set as follows: $\kappa = 200$ (veh.km), $\theta = 0.05$, and $\Delta x = 100$ (m). The initial values for the optimization problem (8) were given by certain i.i.d. uniform distributions such that $u \in [70, 100]$ (km/h), $k_c \in [10, 40]$ (veh/km), and $c_{i,j} \in [20, 100]$ (veh).

4.2 Calibration results

Fig 5 shows a calibration result where the red lines represent a calibrated FD and blue dots represent traffic states which are not necessarily stationary. The estimated FD parameter values are $\hat{u}=74.2$ (km/h) and $\hat{k}_{\rm c}=28.8$ (veh/km). The calibrated FD seems to describe the traffic well. Fig 6 compares estimated $\hat{c}_{i,j}$ and its truth. According to the figure, the results of $c_{i,j}$ estimation can be categorized into two: almost proper estimation and estimated as zero. The latter is caused by indefinite $c_{i,j}$, which is because of non-satisfaction of the precondition (iii), and the feature of the optimization problem discussed in section 3.2.

Table 1: Parameters of the car-following model

	mean	std.div.
Vehicle length (m)	4	0.5
Minimum spacing (m)	1	0.3
Desired speed (km/h)	80	10.0
Maximum acceleration rate for acceleration (m/s ²)		0.2
Standard acceleration rate for deceleration (m/s ²)		0.25
Maximum acceleration rate for deceleration (m/s ²)		0.5

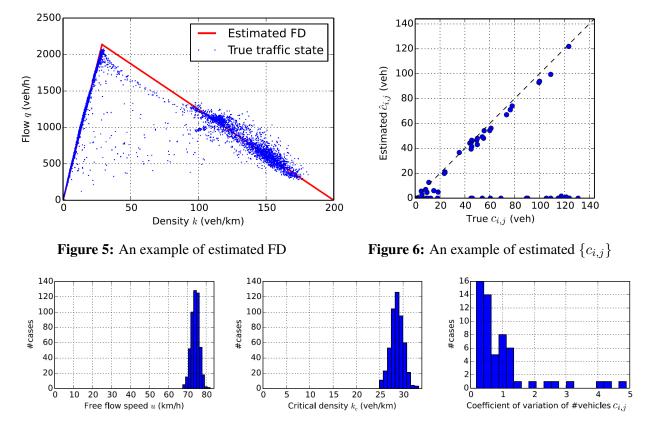


Figure 7: Distribution of free-flow **Figure 8:** Distribution of critical **Figure 9:** Distribution of cov. of speed \hat{u} density $\hat{k_c}$ $\hat{c}_{i,j}$

Robustness of the algorithm is validated by performing multiple calibration iterations for 500 times with different initial value to the non-convex optimization problem (8). Fig 7 and 8 shows distributions of estimated free-flow speed \hat{u} and critical density $\hat{k_c}$, respectively. According to the figure, the calibration is almost stable, although slight variation can be found. Fig 9 shows distribution of the coefficient of variation (cov.) of each $\hat{c}_{i,j}$. According to the figure, this result is not stable, since $\hat{c}_{i,j}$ can be zero as evidenced by Fig 6. Table 2 summarizes the calibration results. The results of \hat{u} and $\hat{k_c}$ were fairly stable. It means that although derivation of $\hat{c}_{i,j}$ was not necessarily stable due to the issue mentioned in section 3.2, the algorithm can estimate values of the FD parameters robustly. In addition, the mean of all the iterations fits well to the actual traffic; therefore, obtaining a final result by taking mean of multiple iterations would be precise.

In summary, the results suggested that the proposed algorithm can be precise and robust for traffic in which the preconditions are not exactly satisfied, although the optimization problem has some theoretical issues (e.g., non-convexity). The algorithm can be considered as precise and accurate as the calibration results are close to the actual phenomena, and can be considered as robust as the results did not strongly depend on initial points of the algorithm.

Table 2: Statistics of distributions of calibration results

	mean	std.div.	cov.
free-flow speed u (km/h)	74.2	2.1	0.028
critical density k_c (veh/km)	28.7	1.4	0.048
capacity $k_{\rm c}u$ (veh/h)	2126.1	106.7	0.050
cov. of $c_{i,j}$	0.997	_	_

5 Conclusion

This paper proposed methods of calibrating a fundamental diagram based on probe vehicle data. First, we formulated a method which identifies value of free-flow speed and critical density under idealized conditions, while it relies on exogenous assumptions about functional form of FDs and value of jam density. Then, a heuristic algorithm for calibrating FDs under actual traffic conditions is developed based on the method. The results of simulation-based validation suggested that the algorithm can calibrate an FD precisely and robustly. Therefore, it can be expected that the proposed method calibrate FDs in road sections on which congestion happens frequently, if probe vehicle data were collected for a long period. It means that applicability of probe vehicle-based traffic management methods can be significantly increased.

Several future works are considerable and being investigated by the authors. The first is to develop endogenous identification method for time–space regions with constant FDs. This is essentially important to improve the methods' applicability, since the current methods themselves do not identify a bottleneck. The second is to develop theoretically sophisticated algorithm (e.g., avoiding meaningless global optimal, developing convex optimization-based algorithm) for more rigorous calibration. The third is to validate the methods under more general conditions (e.g., using real world datasets). The forth is to adopt more precise identification method for stationary states (e.g., Yan et al., 2016) and to perform related sensitivity analyses.

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