Fast Calibration of Car Following models to Trajectory data using the Adjoint Method

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Abstract

Before a car-following model can be applied in practice, it must first be validated against real data in a process known as calibration. This paper discusses the formulation of calibration as an optimization problem, and compares different algorithms for its solution. The optimization consists of an arbitrary car following model, posed as either an ordinary or delay differential equation, being calibrated to an arbitrary source of trajectory data which may include lane changes and staggered observation times.

Typically, the calibration problem is solved using gradient free optimization. In this work, the gradient and Hessian of the optimization problem are derived using the adjoint method. The computational complexity of the adjoint method does not scale with the number of model parameters, which makes it far more efficient than evaluating the gradient numerically using finite differences. Numerical results are presented which show that quasi-newton algorithms using the adjoint method are significantly faster than a genetic algorithm, and also achieve slightly better accuracy of the calibrated model.
1 Introduction

1.1 The Case for Car Following and Trajectory Data

A complete traffic simulator consists of many different modules, including algorithms to determine the demand for different road sections, complex rules to govern lane changes, mergers, and diverges, a model to describe traffic flow and driving behaviors, and more. Out of all these modules, the description of traffic flow is the most fundamental. The decision of what model is used to describe traffic flow has impacts on the simulator’s strengths, weaknesses, and overall performance. In particular, one important distinction is whether to simulate at the macroscopic or microscopic level.

At the microscopic level, car following models are often used. Car following models describe how a vehicle behaves as a function of its surroundings; typically they are expressed as differential equations where any vehicle is coupled to the vehicle directly ahead (i.e. its lead vehicle). Many car following models are based on common sense rules of driving. Some simple examples are adopting a speed based on the distance between you and your leader, or accelerating based on the difference in speeds between you and your leader.

Whereas microscopic traffic models describe the motions of individual vehicles, their macroscopic counterparts treat traffic as a fluid. At the macroscopic level, there are no vehicles, only traffic densities. Congested road sections with high densities slowly trickle forward, while uncongested traffic at low densities flow freely. This connection to fluid dynamics was originally made by [1], and the influence of the resulting traffic flow theory can hardly be overstated. In the more than six decades since, numerous works have attempted to improve upon the so-called Lighthill-Whitham-Richards (LWR) model in order to better describe various complex elements of traffic flow. Among those, [2], [3], [4], [5], [6] are perhaps some of the most notable. Nonetheless, when it comes to macrosimulation, the LWR model, and its discrete numerical formulation [7], is still widely used today.

For all its merits, the LWR model is not without its limitations. A key relationship between flow and density known as the “fundamental diagram”, must be supplied. More importantly, it is assumed vehicles are homogeneous and exhibit static behavior. In real traffic, drivers behave differently; vehicles have varying performances; traffic demand fluctuates; controlled intersections and lane changes have complex effects. Traffic flow is incredibly dynamic and inhomogeneous. The shortcomings of the LWR model become apparent in practice [4, 8, 9]. In the fundamental diagram, instead of equilibrium curves, one finds a wide scattering of points. The time evolution of real traffic flow shows a much richer picture than what the LWR model predicts. Examining the evolution of a vehicle trajectory in the speed-spacing plane, e.g. [10] [11] or Fig. 2.1, one sees complex hysteresis loops which are inconsistent with current macroscopic theory. Given these limitations, one would hope for some car following model that could explain all these phenomena.

However, existing works are not prepared to offer guidelines as to which car following models are best. It is also not clear as to how much more accurate car following models are compared to macro-models (like LWR). Answering either of these pressing questions is difficult: the traffic microsimulation literature consists of literally hundreds of different models, many of which have never actually been thoroughly validated [12]. Works have attempted to address this long-standing problem of car following models [13, 14, 15, 16] but have had varying results as to which models are best.

Drawing conclusions on the efficacy of different car following models requires both a large vehicle trajectory (e.g. [17], [18], Fig. 1) dataset to facilitate comparison, as well as a reliable methodology for model calibration and validation. The aim of this work is to develop new methodology to improve the calibration of car following models. However, one should keep in mind that this only addresses one half of the challenge; equally important is the creation of new datasets and new approaches for collecting accurate and meaningful traffic data.

There is a need for an increased use of trajectory data to study traffic flow. This need goes far beyond the validation of existing car following models. As new technologies like autonomous vehicles, connected cities and on-demand mobility become fully realized, the LWR model assumption of homogeneous drivers exhibiting static behavior becomes increasingly unrealistic. The limitations of macrosimulation and the uncertainty of new technology are both good reasons to suspect a growing demand for microsimulation. At the same time, vehicle trajectory data (which is needed for microsimulation/car following) is easier to get than ever before because of new technologies like computer vision, lidar/radar, and GPS. Compared to the more commonly used loop detector data, trajectory data describes traffic flow at much higher temporal and spatial resolutions. These new sources of data, still largely unexploited, can help advance both micro- and macro- theory.
1.2 Calibration Using Trajectory Data

It is relatively simple to write down some mathematical equations and call them a traffic model. Far more difficult is applying this model in practice. In order to validate a model against real data, one must find the model parameters that best explain the data: this is known as calibration. Solving the calibration problem requires both a dataset describing the quantity of interest, as well as a mathematical model that explains the data. This paper deals with car-following models that are posed as differential equations, and may include elements such as delays, bounds on acceleration/speed, and multiple driving regimes. The car-following model is to be calibrated against trajectory data, time series data that describes the motion of individual vehicles.

Existing literature has covered various aspects of the calibration problem: the use of meta-models, sensitivity analysis, optimization algorithms, measures of performance (e.g. speed or spacing data), and goodness-of-fit function (i.e. loss function). [19, 20, 21] are good works focused primarily on methodology and [22, 23, 15, 16] are good works focused on both calibration and the benchmarking of various models.

In this paper calibration is posed as an optimization problem. For a wide class of models, being calibrated to trajectory data gathered from any source, the gradient and hessian of the optimization problem has been derived in an efficient way using the adjoint method. This enables the calibration problem to be solved by more efficient optimization routines which use gradient information. Several state of the art algorithms are benchmarked in order to determine both the accuracy of the fit they can achieve, as well as the computational effort required to apply the algorithm.

The paper is organized as follows. Section 2 introduces the different classes of car-following models considered in this work. Section 3 describes the optimization problem and discusses some issues arising in its solution. Section 4 applies the adjoint method to the optimization problem and compares it to finite differences. Section 5 compares different algorithms for solving the calibration problem.

2 Car-Following Models

We will consider any car-following model that can be expressed as either an ordinary or delay differential equation. This describes the majority of models in the literature, as well as the majority of models used in commercial microsimulation packages [24]. We deal with models of the following form

\[
\ddot{x}_n(t) = h(\dot{x}_{n-1}(t-\tau), x_{n-1}(t-\tau), \dot{x}_n(t-\tau), x_n(t-\tau), p)
\]  

(1)
where $x_n(t)$ is the position of vehicle $n$ at time $t$. $h$ is the car-following model, which depends on parameters $p$, the “following” vehicle $x_n$ and “lead” vehicle $x_{n-1}$. $\tau$ is a time-delay parameter which represents human reaction time.

Eq. (1) states that a driver’s behavior (how they choose to accelerate) is determined from the speed and position of their own car, the speed and position of the leading car, and parameters $p$. Given a lead vehicle trajectory $x_{n-1}(t)$, parameters $p$, and initial condition $x_n(t_n)$, the car following model (1) will produce the follower trajectory $x_n(t)$.

The presence of nonzero $\tau$ leads to a delay differential equation (DDE). Many car-following models (including most of those used in commercial software) treat reaction time explicitly by using a DDE.

Besides ODEs and DDEs, some car-following models are formulated as stochastic differential equations, cellular automata models, or queueing models. The consideration of such models is beyond the scope of this work.

2.1 Ordinary Differential Equations

Eq. (1) gives a general form for car-following models. The simplest type of model is a first-order ODE where the speed of the following vehicle $n$ is completely determined by the space headway ($x_{n-1} - x_n$). Then, each driver adopts a speed based on the distance between their car and the leading car.

This simple kind of model is important because of its connection to macroscopic theory and the LWR model. Specifically, if one assumes all vehicles are identical, and interprets the reciprocal of density as headway, then a functional relationship between traffic flow and density can be recast as a relationship between vehicle speed and headway [25]. Under these assumptions, the fundamental diagram can be thought of as describing a first-order car-following model. Consider Daganzo’s model as an example

$$\dot{x}_n(t) = \min\{v_f, \frac{x_{n-1} - x_n - s_{jam}}{\alpha}\}. \tag{2}$$

$v_f, \alpha$ and $s_{jam}$ are parameters describing a triangular fundamental diagram [22, 26, 27]. Namely $v_f$ is the speed of a vehicle during free flow, $s_{jam}$ is the distance between two completely stopped vehicles, and $\alpha$ is related to the shockwave speed. Actually, other models can also achieve correspondence with the fundamental diagram and hydrodynamic theory, and the Newell car-following model [28, 3] is one such example. In Newell’s model, the trajectory of a following vehicle is equivalent to the lead vehicle trajectory, translated over both space and time.

$$x_n(t) = x_{n-1}(t - \alpha) - s_{jam} \tag{3}$$

It is referred to as a trajectory translation model and is unique for not being a differential equation. In the special case where the Newell model is solved with a numerical time step equal to $\alpha$, the Daganzo and Newell models become equivalent [29], but in general the two models are different (see for example 2.1). Note also that the Daganzo model explicitly gives a maximum speed.

The reason these two models are related is because both preserve the LWR model’s shockwave behavior (shockwaves in the LWR model are thought to describe the propagation of traffic congestion). The advantages of the Newell or Daganzo models are that they contain a small number of parameters, and those parameters are easily interpretable under macroscopic theory.
Figure 2: Four different car following models are calibrated to a single empirical vehicle trajectory by minimizing the root mean square error between simulation and measurements. The trajectories are plotted in the speed - headway plane.

More complicated car-following models (compared to those of Newell and Daganzo) are criticized for two main reasons: first, for not having enough empirical support for their validity, and second, for having too many parameters. Despite these criticisms, more complicated models have behaviors that attract researchers. For example, the optimal velocity model (OVM) [30] exhibits a spontaneous phase transition between free flow and congested states, which may describe “phantom” traffic jams [31]. Another example is the intelligent driver model (IDM) [32], which can qualitatively reproduce a number of complex (empirical) traffic states. Besides newer models like OVM or IDM, there are also a plethora of older models to complicate the mix [12]. The default models in most modern traffic simulator packages (for example, VISSIM or AIMSUN) are still older car-following models [24], presumably because it is unclear if the newer car-following models offer any benefits.

Fig. 2.1 compares each of the four models just mentioned by calibrating them to a single vehicle trajectory from the reconstructed NGSim data [33]. The calibration minimized the root mean square error (RMSE) between the simulation and measurements. The vehicle (ID 1013) was recorded for only 55 seconds, but even in that time many hysteresis loops were recorded in the speed-headway plane. For the NGSim data, which was recorded on the freeway in congested conditions, trajectories that qualitatively resemble this one are the rule rather than the exception. The different models all give a different caricature of the oscillatory behavior observed. In particular, the Newell model (with a simulation time step of .1 s) seems to better capture the chaotic nature of the oscillations, whereas the more complicated (and computationally expensive to calibrate) IDM or OVM models result in a lower RMSE and better
It is useful to rewrite the second order differential equation Eq. (1) as a system of first order equations:

\[
\dot{x}_n(t) = \begin{pmatrix} \dot{x}_n(t) \\ \dot{v}_n(t) \end{pmatrix} = \begin{pmatrix} v_n(t) \\ h_n(x_{n-1}(t-\tau_n), x_n(t-\tau_n), p_n) \end{pmatrix} = h_n(x_n(t), x_n(t-\tau_n), x_{L(n)}(t-\tau_n), p_n) \tag{4}
\]

2.2 Delay-Differential Equations

Compared to ODEs, DDEs are more complicated to analyze and solve. Car-following models typically only consider the simplest case, where time delay (reaction time) is a constant. It seems the distinction between ODEs and DDEs has been given limited importance in the calibration literature, even though the addition of time delay as a parameter causes extra complications. As for the literature as a whole, the effect of nonzero time delay on car-following models is still not fully understood.

When studying the behavior of car-following models, one common approach is to consider a line of cars with identical model parameters on a closed loop. In this special setting, one can find an “equilibrium” solution where all vehicles have the same speed and same headway, with zero acceleration. The equilibrium solution is contrasted with an oscillatory/periodic solution, where the speed of a vehicle can oscillate in a manner reminiscent of stop-and-go or congested traffic. Since most analytic (i.e. not numerical) results come from studying the behavior around the equilibrium solution, the stability of the equilibrium solution is particularly important. Adjusting parameters in a model can be said to have a stabilizing (destabilizing) effect if the equilibrium solution will persist (degenerate) under a wider variety of conditions. Intuitively, one expects that drivers having slower reaction times will have a destabilizing effect, and this seems to be generally correct.

It has been shown for both the optimal velocity model (OVM) and intelligent driver model (IDM) that the inclusion of time delays has a destabilizing effect \[34, 35, 36\]. But time delay is not the only model parameter that can have such effects. For example, \[37\] showed that increasing (decreasing) the OVM’s “sensitivity parameter” has stabilizing (destabilizing) effects (the sensitivity parameter is proportional to how strongly the driver accelerates). Time delay can also have more subtle effects: \[34\] found the inclusion of time delays for OVM caused bistability between equilibrium and oscillatory solutions.

In \[28\] the OVM is considered with different reaction times \(0.3\) seconds. In this range, no qualitative changes to the model are observed. The authors state that changing the sensitivity parameter can account for the effects of reaction time. \[23, 34\] have done experiments on OVM with larger reaction times (\(\approx 1\) seconds) and found that while it is true that reaction time is not especially important at low values, once increased past some threshold it will start to cause unstable behavior leading to vehicle collisions. A similar behavior was found in \[19\] for the Gipps car-following model. These findings show the inclusion of reaction time will have a destabilizing effect, but large reaction times seem to have especially unstable effects, perhaps owing to some sort of phase transition.

In practice, one can observe that calibrated values for reaction time greatly vary across the literature, even for the same model. Consider that \[39, 15, 16\] all calibrate the Gipps model, but all find very different means and variances for drivers’ reaction times. One found the mean to be 0.57 s with a variance of 0.02 s. Another found the mean to be 1.73 s with variance 1.35 s.

Besides reaction time, another interesting extension to a model is the inclusion of “anticipation” effects. Examples of anticipation are a driver estimating the future speed/position of a leading vehicle, or a following vehicle reacting to multiple vehicles instead of just its leader. \[39\] showed that anticipation has a stabilizing effect for IDM, and \[40\] showed the same for OVM. Of course, due to nonlinearities, stabilizing and destabilizing effects will not simply cancel out.

3 Calibration

In this section, we first cover the notation used in the remainder of the work. Then we define calibration as an optimization problem and discuss some issues in its solution. The main methodological contributions are in the following sections.

3.1 Notation

It is useful to rewrite the second order differential equation Eq. (1) as a system of first order equations:

\[
\dot{x}_n(t) = \begin{pmatrix} \dot{x}_n(t) \\ \dot{v}_n(t) \end{pmatrix} = \begin{pmatrix} v_n(t) \\ h_n(x_{n-1}(t-\tau_n), x_n(t-\tau_n), p_n) \end{pmatrix} = h_n(x_n(t), x_n(t-\tau_n), x_{L(n)}(t-\tau_n), p_n) \tag{4}
\]
where \( x_n \) is now a vector consisting of the position and velocity of vehicle \( n \) at time \( t \). \( x_n^* \) and \( v_n \) are new dummy variables corresponding to the position and speed for vehicle \( n \). \( p_n \) denotes the parameters for vehicle \( n \). Additionally, the lead trajectory is denoted as \( x_{L(n)} \) instead of \( x_{n-1} \) to reflect the fact that the index corresponding to the lead vehicle may change (due to lane changing). The above equation is what we refer to when we say “car-following model” and its solutions are the “simulated trajectories”. Note that Eq. (4) is a more general form than what we initially presented in Eq. (1). We adopt the following notation:

- \( x_n(t) \): vector consisting of position and speed of vehicle \( n \), at time \( t \), calculated from the car-following model.
- \( L(n,t) \): the index of the vehicle \( n \)'s lead vehicle, so that \( x_{L(n)}(t) \) is the lead trajectory for vehicle \( n \) at time \( t \).
- \( \hat{x}_n(t) \): “true” measurements of vehicle \( n \), taken from data.
- \( t_n, T_n \): the first and last times that the leader of vehicle \( n \) is known.
- \( T_n \): the last time that measurements \( \hat{x}_n(t) \) for vehicle \( n \) are known.
- \( h_n(x_n(t), x_n(t - \tau_n), x_{L(n)}(t - \tau_n), p_n) \): generic car-following model such that \( \hat{x}_n = h_n \).
- \( p_n, p \): \( p_n \) is a vector consisting of model parameters describing vehicle \( n \). \( p = [p_1, p_2, \ldots, p_n] \).
- \( f(x_n(t), \hat{x}_n(t), t) \): loss function representing the goodness of fit of the car-following model for vehicle \( n \) at time \( t \).
- \( F \): objective function, defined as total loss

In what follows, we treat time as being a continuous variable. In practice, time will be discretized, and objective \( F \) and simulated trajectories \( x_n(t) \) are both computed numerically.

### 3.2 The Optimization Problem

The calibration is done for some arbitrarily sized platoon of \( n \) vehicles, indexed as \( 1, \ldots, n \). For each vehicle \( i \) to be calibrated, its lead trajectory is known between times \([t_i, T_{i-1}]\); the lead trajectory is not necessarily also calibrated, but it can be. The lead trajectories for \( i \) are known between \([t_i, T_i]\).

Given the lead vehicle trajectories not part of the platoon, initial conditions \( \hat{x}_i(t_i) \), \( i = 1, \ldots, n \), and parameters \( p \), the car following model [1] will produce simulated trajectories \( x_1(t), \ldots x_n(t) \). Calibration finds the parameters \( p \) that minimize the loss between simulation and measurements.

For an ODE, the optimization problem is

\[
\min_p F = \sum_{i=1}^{n} \int_{t_i}^{T_{i-1}} f(x_i, \hat{x}_i, t) dt
\]

s.t. \( \dot{x}_i(t) - h_i(x_i(t), x_{L(n)}(t), p_i) = 0 \), \( t \in [t_i, T_{i-1}] \), \( i = 1, \ldots, n \)

\( x_i(t_i) - \hat{x}_i(t_i) = 0 \) \( i = 1, \ldots, n \)

\( b_{low} \leq p \leq b_{high} \)

The objective function \( F \) is defined as the integral of the loss function \( f \) over time, summed over each simulated vehicle. We wish to minimize \( F \) with respect to the parameters of the car-following model, \( p \). The constraints are that the simulated trajectories \( x_i \) obey the car-following model \( h_i \) from time \( t_i \) to \( T_{i-1} \), with initial conditions \( x_i(t_i) = \hat{x}_i(t_i) \). There may also be some box constraints \( b_{low}, b_{high} \) that prevent parameters from reaching unrealistic values.

The DDE case is similarly defined:

\[
\min_p F = \sum_{i=1}^{n} \int_{t_i + \tau_i}^{T_{i-1} + \tau_i} f(x_i, \hat{x}_i, t) dt
\]

s.t. \( \dot{x}_i(t) - h_i(x_i(t), x_i(t - \tau_i), x_{L(n)}(t - \tau_i), p_i) = 0 \), \( t \in [t_i + \tau_i, T_{i-1} + \tau_i] \), \( i = 1, \ldots, n \)

\( x_i(t) - \hat{x}_i(t) = 0 \) \( t \in [t_i, t_i + \tau_i] \), \( i = 1, \ldots, n \)

\( b_{low} \leq p \leq b_{high} \)
where $T_{i-1}^* = \min\{T_{i-1} + \tau_i, T_i\}$, and the reaction time for vehicle $i$, $\tau_i$, is assumed to be a model parameter. $x_i(t) - \hat{x}_i(t) = 0$ defines the history function for $x_i$ (DDEs have history functions as their initial conditions). Note that trajectory $x_i(t)$ is simulated between different times depending on whether the model is an ODE or DDE.

Under these formulations, the leader for vehicle $i$ should be known at all times from $t_i$ to $T_{i-1}$, since the lead trajectory is needed in order to simulate any vehicle. In the case where there are gaps in time where the leader is not known, $[t_i, T_{i-1}]$ should define the longest time period with known leaders.

The rest of this section discusses extra details of the calibration problem. Section 3.3 deals with an issue caused by video data. Section 3.4 discuss the calibration of reaction times for DDEs. Section 3.5 discusses car following models that include extra constraints.

### 3.3 Video Data and Simulated Trajectories

Video data monitors a fixed section of road, so each vehicle in a platoon is tracked over the same spatial area, but has staggered observation times. Fig. 3 depicts this below (recall vehicle $n$ is observed during the time period $[t_n, T_n]$).

![Figure 3: Shows the observation times from video data for a platoon of vehicles where 1 follows 0 and 2 follows 1. The dashed region indicates times when a vehicle’s measurements are known, but its trajectory cannot be simulated because a lead trajectory is missing.](image)

Since car-following models require the lead vehicle trajectory as an input, the latest time vehicle $n$ can be simulated is $T_{n-1}$ for an ODE ($T_{n-1} + \tau_n$ for a DDE). The staggered observation times prevent vehicle $n$ being simulated between $[t_n, T_n]$ ($[T_{n-1}^*, T_n]$ for a DDE). Each vehicle only loses a small time interval of its simulated trajectory, but the effect compounds for a platoon of vehicles. In fig. 3 the entire platoon can only be simulated up to time $T_0$ without some strategy for dealing with this issue.

We want a way to simulate $x_i(t)$ when the lead trajectory $x_{i-1}(t)$ is unavailable. Here are three ideas:

1. Take the simulated trajectory to be the same as the measurements
2. Extrapolate the unobserved lead vehicle trajectory
3. Treat the unobserved lead vehicle trajectory as additional parameters to be optimized in Eq. (5), (6).

Approaches 2 and 3 have the advantage of allowing us to calibrate $x_i$ for the entire length $[t_i, T_i]$ of observations. Under approach 1, $x_i$ is only calibrated for $[t_i, T_{i-1}]$. The problem with approaches 2 and 3 is that there is no way to validate the imputed lead trajectory. Therefore we will consider approach 1.

But approach 1 also has a problem: setting $x_i(t) = \hat{x}_i(t)$ for $t = [T_{i-1}, T_i]$ will almost certainly cause a jump discontinuity at $t = T_{i-1}$ since

$$\lim_{t \to T_{i-1}^-} x_i(t) \neq \hat{x}_i(T_{i-1}).$$

Besides lacking a physical meaning, this jump discontinuity could cause problems for additional vehicles $x_{i+1}, \ldots$. The simplest fix, shown in fig. 4 is to simply remove the jump:

$$x_i(t) = \hat{x}_i(t) + (x_i(T_{i-1}) - \hat{x}_i(T_{i-1})) \text{ for } t \in [T_{i-1}, T_i]$$

(7)
Figure 4: Observed trajectory $\hat{x}_i(t)$ (red) and simulated trajectory $x_i(t)$ (black) are shown in space-time plots. Left shows the simulated trajectory is only known up to $T_{i-1}^-$. Middle shows the jump discontinuity that occurs at $T_{i-1}^-$. Right shows resulting simulated trajectory with the jump removed.

In the above we have treated the case of the model being an ODE. The times are slightly different for a DDE:

$$x_i(t) = \hat{x}_i(t) + (x_i(T_{i-1}^-) - \hat{x}_i(T_{i-1}^-)) \text{ for } t \in [T_{i-1}^-, T_i].$$  (8)

We do not consider (7) and (8) to be part of the car-following model. Rather, they are heuristics that are needed in order to define the calibration problem for a platoon using video trajectory data.

3.4 Reaction Time as a Parameter

Simulated trajectories are computed numerically with a specified time discretization. Since we want to compare the simulated trajectories with the actual measurements, it makes sense for the simulation to use the same time discretization as the data. For example, if the data is recorded every 0.1 seconds, the simulated trajectories should use a time step of 0.1 seconds. If the simulation used a different time step (e.g. 0.09), then the loss can only be calculated at a few points (e.g. 0.9, 1.8) unless we define some interpolation procedure.

For a DDE, the time discretization and reaction time need to be multiples of each other. If the simulation uses a time step of 0.1 seconds, then the reaction time will have to be an integer multiple of 0.1 (e.g. 0.1, 0.2). We can either:

1. Enforce that every vehicle’s reaction time is a integer multiple of 0.1
2. Allow reaction time to be a continuous variable and define the loss function through interpolation.

If we choose 1, it leads to a mixed integer nonlinear programming problem (MINLP). This is a much harder problem than the original nonlinear program. One approach used in [16] would be to split up all vehicles into small platoons (either pairs or triplets) and use a brute force search for reaction time. However, even when the platoons are small, using brute force vastly increases computation because the calibration has to be repeated for every possible combination of reaction times.

The other option is to use an approach similar to [23] where reaction time is a continuous variable and interpolation is used on the simulated trajectories. In general, any sort of interpolation could be used, but linear interpolation is the most common. In this approach, interpolation needs to be used on the lead trajectory and initial history function in order to define the model. Assuming the numerical time step is not equal to the delay, interpolation will need to be used on the simulated trajectory as well.

One issue with interpolation is how to compute the loss function. Specifically, assuming the simulation is defined on a different set of times than the measurements, should the simulation be interpolated onto the measurement’s times or vice versa? We suggest doing both. This avoids the possibility of error cancelation occurring during the interpolation and causing the loss function to be erroneously small. In this scenario it would be preferable to reweight the loss function as well since the loss will be computed over more points.
3.5 Constraints on the Car-Following Model

We have presented car-following models being in the form of Eq. (4). But often there are additional constraints to the car-following model, such as in Eq. (2) or the following example:

$$\dot{x}_n = \left( \min \{v_n, v_{\text{max}}\} \right) / \left( \max \{h^*, a_{\text{max}}, \min \{h^*, a_{\text{min}}\} \} \right) \quad (9)$$

In other words, we have now constrained our velocity $\dot{x}_n^*$ and acceleration $\dot{v}_n$ such that

$$\dot{x}_n^* \leq v_{\text{max}}, \quad a_{\text{min}} \leq \dot{v}_n \leq a_{\text{max}}$$

These sorts of constraints are very common in car-following models. Another common feature is a model having different regimes of driving behavior. For example, the Gipps model [41] has two regimes: one describing free flow conditions, and another “safety condition” that prevents collisions.

In general, these extra complexities might cause the simulated trajectory $x_n$ to no longer be smooth. Constraining the acceleration between $a_{\text{min}}$ and $a_{\text{max}}$ will keep the acceleration continuous but might cause the jerk to be discontinuous. The same can be said for constraining the velocity. In the next section, when we discuss the adjoint method, it will become apparent that $x_n$ being non-smooth means that the adjoint variables $\lambda_n$ will also be non-smooth. This is not a serious issue. First, since actual trajectories are smooth, a good model with realistic constraints should be very nearly smooth. Second, in practice we do not deal with the continuous time system and minor non-smoothness is not a big concern when integrating numerically.

4 Adjoint Method and Gradient/Hessian-Based Optimization

Eqs. (5) and (6) are nonlinear and non-convex optimization problems that must be solved numerically. Current approaches usually rely on gradient-free optimization, with genetic algorithm (GA) and Nelder-Mead simplex algorithm (NM) being the two most commonly applied algorithms [12, 42, 13, 14, 43, 23, 15, 16]. These methods have the disadvantage of being slow to converge, and require many objective function evaluations. The objective $F$ is relatively expensive to compute in this context because we first must solve a system of differential equations. As an alternative to directly solving the optimization problems (5) and (6), parameters can be estimated directly from data using statistics techniques [44, 26, 27, 45] but this approach is not guaranteed to find local minima. Also, many models have parameters that do not have clear physical interpretations, and therefore cannot be directly estimated.

There are a huge number of gradient/hessian-based optimization algorithms that can potentially solve the calibration problem much faster than gradient-free approaches. However, even though most optimization algorithms use gradient information, not many gradient-based algorithms have been examined in the calibration literature. To the author’s knowledge, the only gradient-based algorithms that have been considered are simultaneous perturbation stochastic approximation (SPSA) [46], Lindo’s Multistart [47] (a commercial solver’s global optimization routine), and sequential quadratic programming using filtering (SQP-filter) [48]. SPSA performed quite poorly in [19] [49], but the other gradient-based algorithms perform much better compared to gradient-free approaches. In [49] SQP-filter was found to give better solutions than NM or GA, as well as solve the problem up to 10 times faster; even better results were found when it was additionally combined with Lipschitzian algorithm DIRECT [50]. [19] did not consider computational speed, but found the Multistart algorithm had a much higher chance of finding the true global minimum compared to GA or NM.

Even if one only knows how to explicitly evaluate the objective function $F$, it is not necessary to use gradient-free optimization because the gradient $(dF/dp)^T$ can be calculated numerically ($T$ superscript indicates transpose). To do this, one varies the parameters $p$ one at a time, and recomputes the objective each time a parameter is varied. Then the gradient can be calculated using finite differences. We refer to this as the finite difference approach for computing the gradient. The problem with the finite difference approach is its complexity: $O(m)$, meaning computing the gradient takes about $m$ times as long as computing the objective [51]. For problems like (5), which are constrained by differential equations, the adjoint method offers a far more efficient way to compute the gradient. The adjoint method has complexity $O(1)$, and so it is the preferred method for computing the gradient when $m$ is large [51, 52]. The adjoint method extends in a straightforward way for computing the Hessian. Using finite differences would have complexity $O(m^2)$, whereas the adjoint method can be shown to have complexity $O(m)$ [53].

Implementing the adjoint method only needs to be considered when $m$ is large, which occurs either when the car-following model is complicated, or when a platoon of vehicles is calibrated (see section 5.2). If $m$ is small ($\lesssim 3$),
the finite difference approach will give similar performance. Note that many gradient-based optimization algorithms (such as the ones in Matlab and Scipy) will automatically compute the gradient using finite differences if explicit gradient functions are not given.

The rest of this section presents the adjoint method and then compares it against the simultaneous perturbation and finite difference methods for computing the gradient. The section after deals with a detailed case study where several common optimization algorithms are compared with each other.

4.1 Gradient for ODE Model

We start by applying the adjoint method to (6). In order to give an illustrative example, we first consider a platoon of a single vehicle \((n = 1)\) before dealing with the general case of an arbitrary number of vehicles. The adjoint method can be applied to the calibration problem (6) where the model includes time delay. It can also be extended to calculate the hessian in addition to the gradient. Both of these extensions follow the same techniques elaborated in this section, and are included in the appendix.

4.1.1 A single vehicle

First define the augmented objective function, denoted \(L\)

\[
L = \int_{t_n}^{T_n} dt \left[ f(x_n, \dot{x}_n, t) + \lambda^T(t) (\dot{x}_n(t) - h_n(x_n(t), x_{L(n)}(t), p_n)) \right]
\]

(10)

Here, \(\lambda(t)\) can be thought of as a Lagrange multiplier and will be referred to as the adjoint variable. \(T\) superscript indicates transpose. Note that \(L = F\) so that

\[
d\frac{dp}{dL} = \frac{d}{dp} L = \int_{t_n}^{T_n} dt \left[ \frac{\partial f}{\partial x_n} \frac{\partial x_n}{\partial p} + \lambda^T(t) \left( \frac{\partial \dot{x}_n}{\partial p} - \frac{\partial h_n}{\partial x_n} \frac{\partial x_n}{\partial p} - \frac{\partial h_n}{\partial p} \right) \right]
\]

(11)

where quantities are evaluated at time \(t\) if not explicitly stated. Note in this case there are no terms depending on the lead trajectory \(x_{L(n)}\) since the platoon consists only of \(x_n\) and the lead trajectory is regarded as fixed. Eq. (11) is not immediately useful to us because we have no way to calculate \(\frac{\partial x_n}{\partial p}\). The adjoint method allows us to avoid computing this unknown. Apply integration by parts:

\[
\int_{t_n}^{T_n} \lambda^T(t) \frac{\partial x_n}{\partial p} dt = \lambda^T(t) \frac{\partial x_n}{\partial p} \bigg|_{t_n}^{T_n} - \int_{t_n}^{T_n} \lambda^T(t) \frac{\partial x_n}{\partial p} dt
\]

(12)

The quantity \(\frac{\partial x_n(t_n)}{\partial p}\) is known because it simply depends on the initial conditions; based on (5) it is simply zero. We will choose \(\lambda(T_n-1) = 0\) to eliminate the \(\frac{\partial x_n(T_n-1)}{\partial p}\) term. Combining Eqs. (11) and (12):

\[
d\frac{dp}{dF} = \int_{t_n}^{T_n-1} dt \left[ \frac{\partial f}{\partial x_n} - \lambda^T(t) \frac{\partial h_n}{\partial x_n} \right] \frac{\partial x_n}{\partial p} - \lambda^T(t) \frac{\partial h_n}{\partial p}
\]

Then to avoid calculating \(\frac{\partial x_n}{\partial p}\) we will enforce:

\[
\frac{\partial f}{\partial x_n} - \lambda^T(t) - \lambda^T(t) \frac{\partial h_n}{\partial x_n} = 0, \quad t \in [T_n-1, t_n]
\]

(13)

Eq. (13) defines the “adjoint system”, a new differential equation in \(\lambda(t)\). Our choice \(\lambda(T_n-1) = 0\) becomes the corresponding initial condition. Then after solving for \(\lambda(t)\) we can calculate the desired gradient:

\[
d\frac{dp}{dF} = -\int_{t_n}^{T_n-1} \lambda^T(t) \frac{\partial h_n}{\partial p} dt
\]

(14)

4.1.2 N Car Platoon

Now we will apply the adjoint method to a platoon of arbitrary size, and sketch a general algorithm for computing the gradient. Define the augmented objective function and proceed as before. Again, we suppress \(t\) dependence for clarity.

\[
L = \sum_{i=1}^{n} \left( \int_{t_i}^{T_{i-1}} f(x_i, \dot{x}_i) + \lambda_i^T (\dot{x}_i - h_i(x_i, x_{L(i)}, p_i)) dt \right)
\]

(15)
\[
\frac{d}{dp} F = \frac{d}{dp} L = \sum_{i=1}^{n} \left( \int_{T_{i-1}}^{T_{i}} \frac{\partial f}{\partial x_i} \frac{\partial x_i}{\partial p} - \lambda_i^T(t) \frac{\partial \dot{x}_i}{\partial p} - \lambda_i^T(t) \frac{\partial h_i}{\partial x_i} \frac{\partial x_i}{\partial p} - \lambda_i^T(t) \frac{\partial h_i}{\partial p} \right) + \sum_{i=1}^{n} \int_{t_i}^{T_i} \mathbb{1}(G(i, t) \neq 0) \lambda_{G(i)}^T(t) \frac{\partial h_{G(i)}}{\partial x_i} \frac{\partial x_i}{\partial p} dt
\]

Here, \( \lambda_n \) corresponds to the adjoint variables for vehicle \( n \). Similar to how \( L(n, t) \) was defined, \( G(n, t) \) is defined as the index of vehicle \( n \)’s follower at time \( t \), so that \( x_{G(n)} \) is the following trajectory of vehicle \( n \). If vehicle \( n \) has no follower at time \( t \), or if the follower is not part of the platoon being calibrated, let \( G(n, t) \) return zero. \( \mathbb{1} \) is the indicator function. Apply integration by parts, choose \( \lambda_i(T_{i-1}) = 0 \), and gather terms with \( \partial x_i/\partial p \) to form the adjoint system:

\[
\frac{\partial f}{\partial x_i} - \lambda_i^T(t) \frac{\partial h_i}{\partial x_i} - \mathbb{1}(G(i, t) \neq 0) \lambda_{G(i)}^T(t) \frac{\partial h_{G(i)}}{\partial x_i} \frac{\partial x_i}{\partial p} = 0, \quad t \in [T_{i-1}, t_i], \quad \forall i
\]

Comparing this adjoint system to the one for a single vehicle (13), the difference here is that there is an extra contribution which occurs from the coupling between vehicles. This coupling term occurs only when a vehicle acts as a leader for another vehicle in the same platoon. After solving the adjoint system,

\[
\frac{d}{dp} F = \sum_{i=1}^{n} \left( \int_{T_{i-1}}^{T_i} \lambda_i^T(t) \frac{\partial h_i}{\partial p} dt - \int_{T_{i-1}}^{T_i} \mathbb{1}(G(i, t) \neq 0) \lambda_{G(i)}^T(t) \frac{\partial h_{G(i)}}{\partial x_i} \frac{\partial x_i}{\partial p} dt \right)
\]

Then we can sketch a general algorithm for computing \( \frac{d}{dp} F \):

1. Compute simulated trajectories \( \hat{x}_0(t), \ldots, \hat{x}_n(t) \), model parameters \( p_1, \ldots, p_n \).

2. Solve adjoint system Eq. (16) for \( \lambda_n(t), \lambda_{n-1}(t), \ldots, \lambda_1(t) \), with initial condition \( \lambda_i(T_{i-1}) = 0 \).

3. Compute gradient Eq. (18).

Note the differential equations for \( x_i(t) \) and its corresponding adjoint variable \( \lambda_i(t) \) are both defined over the same times, but \( x_i \) is solved forwards in time whereas \( \lambda_i \) is solved backwards in time. This means for the adjoint system, \( \lambda_n(t) \) is computed first, whereas one starts with \( x_1(t) \) for the vehicle trajectories. All the partial derivatives in Eqs. (16), (18) are computed exactly for a given loss function and car-following model. Solving for \( x_n(t), \lambda_n(t) \), and \( dF/dp \) is done numerically with an appropriate time discretization.

It should be noted that for any model having multiple regimes/constraints similar to Eq. (9), the adjoint calculation will need to be done for each regime. Further, the model will need to keep track of which regime the model is in at each timestep in order for the adjoint calculation to be performed.

### 4.1.3 Exact Gradient for Platoon with Video Data

In moving from Eqs. (17) to (18) we threw away the term

\[
\sum_{i=1}^{n} \int_{T_{i-1}}^{T_i} \mathbb{1}(G(i, t) \neq 0) \lambda_{G(i)}^T(t) \frac{\partial h_{G(i)}}{\partial x_i} \frac{\partial x_i}{\partial p} dt,
\]

resulting in an approximation. Note that the above term vanishes either if \( n = 1 \) (calibration of a leader/follower pair) or if \( T_{i-1} = T_i \) for \( \forall i \) (all vehicles are observed up to the same time). Thus, the adjoint method always gives an exact calculation except when calibrating a platoon of vehicles to video data. The issue is caused by the staggered observation times which are a unique property of video data.

For a platoon being calibrated to video data, an exact calculation can be made that preserves the favorable asymptotic computational complexity \( O(1) \) of the adjoint method. Define modified objective function \( F_1 \) and its modified augmented objective function \( L_1 \):

\[
F_1 = \sum_{i=1}^{n} \int_{t_i}^{T_i} f(x_i, \dot{x}_i) dt
\]
where we have augmented the objective with Eq. (7) in addition to the car-following model. Proceeding as usual, choose $\lambda_i(T_i) = 0$ as initial conditions for the adjoint variables. The adjoint system and gradient are
\[
\frac{\partial f}{\partial x_i} - \lambda_i^T - \mathbb{1}(t \leq T_i)\lambda_i^T \frac{\partial h_i}{\partial x_i} - \mathbb{1}(G(i, t) \neq 0)\lambda_i^T \frac{\partial h_{G(i)}}{\partial x_i} = 0, \quad t \in [T_i, t_i], \quad \forall i
\]
\[
\frac{dF_1}{dp} = \frac{dL_1}{dp} = \sum_{i=1}^{n} \left[ - \int_{t_i}^{T_i} \lambda_i^T \frac{\partial h_i}{\partial p} dt \right]
\]
Eqs. (22) and (23) then give an exact calculation for the gradient of the modified objective $F_1$. The strange thing about $F_1$ is that
\[
f(x_i, \hat{x}_i, t) = f(x_i, \hat{x}_i, T_i - t) \quad \text{for} \quad t \in [T_i - t_i, T_i]
\]
which is a consequence of Eq. (7). This means that $F_1$ gives a significant amount of extra weight to the point $x_i(T_i - t_i)$. This effect is not intended, and can be nullified by defining a modified loss function $f_1$ to use instead of $f$
\[
f_1(x_i, \hat{x}_i, t) = \begin{cases} 
  f(x_i, \hat{x}_i, t) & t \in [t_i, T_i] \\
  \frac{1}{T_i - T_{i-1}} f(x_i, \hat{x}_i, t) & t \in [T_i - t_i, T_i]
\end{cases}
\]
Then under this rescaling, the objective of the original optimization problem and the modified one are identical.

Note that here we operated under the assumption of using the strategy discussed in section 3.3 and defined by (3) to deal with the staggered observation times for video data. More generally, one can choose to deal with video data under some different strategies, and this would lead to a different modified adjoint system.

### 4.2 Implementation of Adjoint Method and Calibration Problem

To test the adjoint method and optimization algorithms, the calibration problem (3) was implemented in python for the optimal velocity model. The equations below show the functional form of the model as originally formulated in (13).
\[
\ddot{x}_n(t) = c_4(V(s) - \dot{x}_n(t)) \\
V(s) = c_1[\tanh(c_2s - c_3) - \tanh(-c_3)]
\]
c_1 through c_3 are the 5 parameters of the model. s is the space headway, defined as $x_{L(i)} - x_i - l_{L(i)}$, where $l_i$ is the length of vehicle i.

The optimal velocity model and its adjoint system were both discretized with a forward euler scheme. The data used was the reconstructed NGSim data (33), so a time step of .1 seconds was used to be consistent with this data. Because this is video data, the modified adjoint system and rescaled objective proposed in (4.1.3) were both used. The loss function $f$ used was square error, which was discretized with a riemann sum.
\[
f(x_i, \hat{x}_i, t) = (x_i(t) - \dot{x}_i(t))^2
\]
\[
F = \sum_{i=1}^{n} \sum_{t_i}^{T_{i-1}} f(x_i, \hat{x}_i, t)
\]
which is equivalent to minimizing the root mean square error (RMSE)
\[
\text{RMSE} = \sqrt{\frac{F}{\sum_{i=1}^{n} T_{i-1} - t_i}}
\]
Since only a car following model is being calibrated, any lane changes in the measurements will be the same lane changes in the simulation. This also means that the leader/follower relationships in the simulation are the same as they are in the data. This allows trajectories to be calibrated at the level of individual vehicles, since it does not make sense to directly compare the simulated and measured trajectories of a vehicle if the simulation and measurements have different lead vehicles.
4.3 Adjoint method compared to other methods for calculating the gradient

Many optimization algorithms will automatically use finite differences to compute the gradient if an explicit gradient function is not given. Simultaneous perturbation is another option when using an optimization algorithm like the one outlined in [10]. Then, assuming that one has chosen to use a gradient-based algorithm for calibration, it is of practical interest to investigate how the adjoint method compares to both of these methods. Specifically, how does the speed and accuracy of these three methods compare in practice?

4.3.1 Comparison of Speed

The theoretical computational complexities frequently cited in the relevant literature give the adjoint method $O(1)$ complexity, while forward differences has $O(m)$, where $m$ is the number of parameters. These complexities refer to how expensive the gradient is to compute compared to the objective. The simultaneous perturbation method has $O(k)$ complexity, where the final gradient is the average of $k$ estimates of the gradient.

To test these theoretical results in practice, the gradient of the calibration problem was calculated and the platoon size was varied. Since the OVM was used, the total number of parameters is 5 times the number of vehicles. We considered a platoon having between 1 and 15 vehicles. The results are shown in the figures below.

![Figure 5: Time for a single evaluation of the gradient for a progressively larger calibration problem. The objective varied from the loss from a single vehicle (5 parameters) to 15 vehicles (75 parameters).](image)

Figure 5: Time for a single evaluation of the gradient for a progressively larger calibration problem. The objective varied from the loss from a single vehicle (5 parameters) to 15 vehicles (75 parameters).

By examining the left panel, one can see the total CPU time, measured in seconds, needed to calculate the gradient of the calibration problem using the three different methods. The simultaneous perturbation was done with both 1 and 3 trials, denoted SPSA and SPSA-3. The right panel shows the time needed to calculate the gradient divided by the time needed to calculate the objective. To minimize the randomness in the CPU times, each data point was repeated 10 times and the results were averaged. Some variation is still present because some vehicles are observed for shorter times; these vehicles are inherently less expensive to calibrate because they have less observations. The same 15 vehicles were used in the experiment and always added in the same order. It should also be stated that for either a finite differencing scheme or for the adjoint method, one needs to first compute the objective before computing the gradient. Therefore, it should be implicitly understood that “time to calculate the gradient”, really refers to “time to calculate both the objective and gradient” for those two methods.

This shows that using a finite difference method quickly becomes intractable when the number of parameters increases. The time increases quadratically in the left panel because adding an additional vehicle requires not only additional parameters, but also additional effort in the simulation. In the right panel, when the time needed to calculate the gradient is divided by the time needed to calculate the objective, one observes the predicted $O(m)$ complexity. In that figure, we also see the $O(1)$ and $O(k)$ complexities for the adjoint method and simultaneous perturbation.
The table below clearly shows the cpu times for 5-15 parameters. Evidently, even when the number of parameters is small the adjoint method is still significantly faster. For a relatively model having only 5 parameters, using finite differences is about 50% slower. One can observe that this implementation of the adjoint method requires the equivalent of 4 objective function solves, whereas forward differences requires \( m + 1 \) (where there are \( m \) parameters).

Table 1: Table of speeds for adjoint method compared to finite differences for computing the gradient. Relative time refers to the equivalent number of objective function evaluations.

| Parameters | Obj. time (s) | Adjoint time (s) | Adjoint relative time | Finite time (s) | Finite relative time |
|------------|--------------|------------------|-----------------------|----------------|---------------------|
| 5          | .0062        | .0250            | 4.03                  | .0390          | 6.3                 |
| 10         | .0109        | .0438            | 4.02                  | .1250          | 11.5                |
| 15         | .0172        | .0686            | 3.99                  | .2811          | 16.3                |

### 4.3.2 Comparison of Accuracy

For the calibration problem, there is no way to calculate the gradient exactly because there is no closed form solution for the car following model. Since a forward Euler discretization was used to numerically integrate the model, the global truncation error is \( O(\Delta t) \), where \( \Delta t \) is .1 seconds in this case. The adjoint system used the same discretization and will have this same \( O(\Delta t) \) error.

For forward differences, the truncation error is also first order, i.e. \( O(\Delta p) \), where \( \Delta p \) is the step size used to perturb the parameters. The difference is that one can choose a \( \Delta p \ll \Delta t \). In particular, it is known that the optimum step size to use for forward differences is \( \approx \sqrt{\epsilon_m} \), where \( \epsilon_m \) is the machine epsilon. This leads to \( \Delta p = 10^{-8} \), and this is the step size that was used for the forward differences.

Although we have no “true solution” to compare our accuracy with, since the step size for forward differences is much smaller than the step size for the adjoint method, it is reasonable to assume that using forward differences gives a more accurate gradient than the adjoint method. When evaluating the accuracy of the adjoint method and simultaneous perturbation, we will treat the result from forward differences as the true solution.

To test the accuracy of the adjoint method, points were evenly sampled between an initial starting guess and the global minimum of the calibration problem for a single vehicle. At each of these points in the parameter space, the relative error was calculated

\[
\text{relative error} = \frac{||\nabla_{fd} F - \nabla F||_2}{||\nabla_{fd} F||_2}
\]

where \( \nabla_{fd} F \) is the gradient calculated with forward differences, \( \nabla F \) is the gradient calculated with the adjoint method or simultaneous perturbation, and \( ||\cdot||_2 \) denotes the 2 norm. The results of the experiment are shown below.

Figure 6: Compares the accuracy of the gradient for the adjoint method and simultaneous perturbation. The finite differences gradient is treated as the exact gradient.
For the adjoint method, the relative error is usually small, on the order of $10^{-6}$. When the parameters start to become close to a local minimum, the relative error starts to rapidly increase to the order of $10^{-4} - 10^{-3}$. When at the optimum, the relative error becomes as high as .3. The reason why the relative error increases is because as the parameters approach the minimum, the norm of the gradient decreases. The right panel shows the relationship between the log of the norm of the gradient calculated with finite differences, and the log of the relative error. One can see that they are inversely proportional to each other. This makes theoretical sense: we expect the residual $\nabla_{fd}F - \nabla F$ to always be on approximately the same order of magnitude since it depends mainly on the truncation error of the adjoint method, which does not change with the parameters. Then, it follows that the relative error is dominated by the $||\nabla_{fd}F||$ term in the denominator, which is what we observe.

The relative error for simultaneous perturbation follows the same shape as the adjoint method, but is always about 6 orders of magnitude larger. Of course, you would not use simultaneous perturbation as a substitute for the finite difference gradient, since it is used with its own optimization algorithm. Nonetheless, this shows that although the two methods (adjoint and simultaneous perturbation) both have a flat computational cost with the number of parameters, they have different uses. The reason why the the error for simultaneous perturbation is quite high in this context is because the gradient is scaled very poorly for the OVM model, meaning the parameters have very different sensitivities. This poor scaling is a common feature for car following models.

5 Benchmarking different Algorithms and the Adjoint method

The ideal optimization algorithm would be one that can not only solve the problem quickly, but also one that is able to avoid bad solutions corresponding to local extrema. Because existing literature has focused on gradient-free optimization algorithms, not much is known about using gradient/Hessian-based optimization to solve the calibration problem. The only works the authors know of in the car following calibration literature that consider gradient based optimization are [49] and [19]. Both those works found the gradient based algorithms to work best overall. This result is consistent with other engineering applications; for example [54] and [55] deal with aerodynamic shape optimization and material science respectively, and report that gradient-based optimization can offer significant speed increases.

To establish the benefits of gradient based optimization and the adjoint method, we consider 2 gradient-free and 5 gradient-based optimization algorithms. The different algorithms, their specific implementations, and abbreviations used throughout the rest of the paper, are detailed below.

- Genetic Algorithm (GA) - an initial population of trial solutions is randomly selected throughout the parameter space. In each iteration, the population is altered through stochastic processes referred to as “mutation” and “crossover”, and then updated in a selection step. An implementation following [56] is part of the scipy package in python.

- Nelder-Mead Simplex (NM) - a given initial guess is used to define a collection of points (a simplex). In each iteration, the corners of the simplex are updated according to deterministic rules. Implemented in scipy following [57]. NM works on unconstrained problems, so a large penalty term was added to the objective if the parameters went outside the bounds.

- Limited memory BFGS for bound constraints (BFGS) - at every iteration, gradient information from the previous iterates is used in the BFGS formula to form an approximation to the hessian. A quadratic approximation to the objective is formed, and the generalized cauchy point of this approximation is then found, which defines a set of active bound constraints. A minimization is then performed over the variables with inactive constraints, while the variables with active constraints are held fixed. The solution to this last minimization finally defines the search direction for the algorithm, and a line search is performed to determine the step length. The algorithm, referred to as l-bfgs-b, is due to [58] [59] and wrapped as part of the scipy package.

- Truncated Newton Conjugate (TNC) - at every iteration, instead of explicitly computing the Newton direction $-\nabla^2 F^{-1} \nabla F$, the conjugate gradient method is applied to the newton system $\nabla^2 Fd = -\nabla F$ (where $d$ is the search direction to be determined). Conjugate gradient is itself an iterative algorithm, and it is terminated early (truncated) to give an approximate solution to the newton system which is also guaranteed to define a direction of descent. A line search is then performed to define the step length. The conjugate gradient algorithm only needs hessian-vector products which can be computed efficiently using finite differences, so the full hessian never needs to be calculated. An implementation due to [60] is wrapped as part of scipy. That implementation uses a conjugate gradient preconditioner based on the BFGS update, and the search direction is projected to enforce the bound constraints.
• Simultaneous Perturbation Stochastic Approximation (SPSA) - At each iteration, the gradient is approximated using simultaneous perturbation. Then the algorithm moves in the direction of the negative gradient with a fixed step length, so no line search is performed. The size of the step length is gradually reduced in subsequent iterations. Implemented in python following [46].

• Gradient Descent (GD) - At every iteration, the negative gradient is computed and scaled according to the spectral step length (also known as the Barzilei Borwein method). The scaled gradient is then projected onto the bound constraints to define the search direction, and a non monotone backtracking linesearch is used to define the step length. Implemented according to [61] in python. The algorithm was tested with different line searches (backtracking, weak/strong wolfe, watchdog) [62] and the nonmonotone backtracking gave the best performance.

• Sequential quadratic programming (SQP) - At every iteration the hessian is computed and the search direction is defined by the newton direction projected onto the bound constraints. This algorithm explicitly computes the hessian instead of approximating it. Because the hessian may fail to be positive definite, the search direction is safeguarded so that if the newton direction fails to define a direction of descent, the algorithm instead searches in the direction of the negative gradient. A small regularization is also added to the hessian so that it can always be inverted. The algorithm is a simple python implementation of sequential quadratic programming based on [62]. We again found the nonmonotone backtracking linesearch to be most effective.

In summary, out of all the algorithms tested: NM and GA are gradient-free; SPSA and GA are stochastic; BFGS and TNC are quasi-newton; GD and SPSA do not use hessian information; SQP explicitly computes the hessian; GA is the only global algorithm.

For the TNC, BFGS, GD, and SQP algorithms, we considered two separate modifications for each algorithm. First, either the finite difference method or the adjoint method can be used to compute the gradient, and we denote this by either “Fin” or ”Adj” respectively. Second we considered starting from multiple initial guesses. Multiple initial guesses are specified, and after each calibration, if the RMSE was above a specified threshold, the next initial guess would be used. The same 3 initial guesses were used in the same order for all algorithms requiring an initial guess. So with a threshold of 0, 3 guesses are always used, and with an arbitrarily large threshold, only a single guess will be used. The thresholds of 0, 7.5 and ∞ were used, and denoted in reference to the algorithm. The initial guesses used are based off of the calibrated parameters found from [45].

5.1 Evaluating Algorithm Performance

As detailed in [12] we tested the calibration problem on the OVM car following model using squared error in distance as the loss function (equivalent to minimizing the RMSE). In this experiment, for each algorithm, every vehicle in the reconstructed NGSim dataset was calibrated using the true measurements of its lead trajectory. In total, there were 7 unique algorithms and 23 total algorithms tested when including the variants described above.

The calibration results are evaluated primarily based on three different measures: the average calibration time for a single vehicle, the % of the time the algorithm found the global minimum, and the average RMSE of a calibrated vehicle. Since there is no way to know the actual global minimum for the calibration problem, we regard the global minimum for a vehicle as being the best result out of all the algorithms, and we regard an algorithm as having found the global minimum if its RMSE is within 1/12 ft (1 inch) of this best result.

Based on these three metrics, all algorithms on the pareto front were identified and are shown in the table below. In figure 7, every algorithm is plotted in the RMSE - time and % found global optimum - time plane. The algorithms on the pareto front are circled in black.

Table 2: Algorithms on the Pareto front. All algorithms tested shown in appendix.

| Algorithm | % found global opt | Avg. RMSE (ft) | Avg. Time (s) | Avg. RMSE / % over global opt | Initial Guesses | # Obj. Evals | # Grad. Evals |
|-----------|--------------------|---------------|---------------|-----------------------------|----------------|-------------|-------------|
| Adj BFGS-0 | 94.0 | 6.46 | 7.42 | .10 / 2.0% | 3 | 307.1 | 307.1 |
| Adj BFGS-7.5 | 85.2 | 6.56 | 4.16 | .20/6.8% | 1.67 | 165.0 | 165.0 |
| GA | 95.0 | 6.47 | 33.5 | .10/2.2% | - | 5391 | 0 |
| Fin BFGS-0 | 94.3 | 6.46 | 11.4 | .10/2.2% | 3 | 311.5 | 311.5 |
| Fin BFGS-7.5 | 85.7 | 6.55 | 6.32 | .19/6.3% | 1.66 | 164.8 | 164.8 |
| Adj TNC-0 | 90.7 | 6.43 | 6.87 | .05/2.4% | 3 | 285.7 | 285.7 |
| Adj TNC-7.5 | 82.7 | 6.48 | 3.82 | .11/5.0% | 1.63 | 152.3 | 152.3 |
| Adj TNC-∞ | 77.3 | 6.62 | 2.26 | .25/7.7% | 1 | 94.1 | 94.1 |
Figure 7: All algorithms plotted by the three metrics time, RMSE, and % found the global optimum. Algorithms on the pareto front with respect to these three metrics circled in black.

The only three algorithms on the pareto front were the GA, TNC, and BFGS. GA gave the best % of finding the global optimum. TNC with the adjoint method and three guesses gave the best overall RMSE, and was the fastest algorithm overall when used with the adjoint method and a single guess. BFGS was slightly slower than TNC and has a slightly higher RMSE, but it has a higher chance of finding the global optimum.

The conclusion of what algorithms are on the pareto front depends strongly on how “finding the global optimum” is defined. Here, we treat an algorithm as having found the global optimum if it gives a result within an inch (1/12) of the best RMSE. Let us refer to this value of 1/12 as the “tolerance” for finding the global optimum. If a smaller tolerance is used, then GA will no longer be on the pareto front. If a larger tolerance is used, GA and BFGS will no longer be on the pareto front. For example, with a tolerance of 0, the pareto front consists of only the adj TNC and adj BFGS variants, and adj BFGS-0 gives the highest chance of finding the global optimum. With a tolerance of 1/2, the adj TNC variants are the only algorithms on the pareto front. The effects of changing the tolerance are shown in the table below. Adj TNC will always be on the pareto front regardless of the tolerance because it gives the best average RMSE for any given speed. No algorithms other than adj TNC, BFGS, and GA are ever on the pareto front.

Table 3: Algorithms on the Pareto front depend on how “finding the global optimum” is defined (without that metric, TNC with the adjoint method would be the only algorithm on the pareto front). Set notation indicates the strategies used for initial guesses.

| Tolerance for global opt (ft) | Algorithms on the pareto front               |
|------------------------------|---------------------------------------------|
| 0                            | Adj TNC-{0, 7.5, Inf}, Adj BFGS-{0, 7.5, Inf} |
| 1/24                         | Adj TNC-{0, 7.5, Inf}, Adj BFGS-{0, 7.5, Inf}, Fin BFGS-{0, 7.5} |
| 1/12                         | Adj TNC-{0, 7.5, Inf}, Adj BFGS-{0, 7.5}, Fin BFGS-{0, 7.5}, GA |
| 1/4                          | Adj TNC-{0, 7.5, Inf}, GA                    |
| 1/2                          | Adj TNC-{0, 7.5, Inf}                        |

The behavior shown in table 3 is explained by figure 8. That figure looks at the distribution of the amount over the global optimum (in RMSE) each algorithm achieves in a log plot. The metric “% found the global optimum” can be directly read off from these plots by looking at the value of each distribution at the log of the tolerance used. For example, a tolerance of 1/12 corresponds to -1.07, and the top right panel shows that at that point, the GA has the highest chance of finding the global optimum. The same panel shows that if the tolerance increases, adj TNC-0 will have the highest chance, and that adj BFGS-0 will have the highest chance if the tolerance decreases.

The figure also gives some insight as to the differences between the distribution in RMSE for the different algorithms. BFGS typically found the best solution out of all the algorithms tested, but it also has a heavier tail in
the sense that there were also some vehicles for which BFGS couldn’t find a good solution. On the other hand, TNC is more consistent because its distribution shows less of a heavy tail. The GA has a tail similar to BFGS, and it isn’t good at finding the best solution possible, but it performs well when only a moderate tolerance is needed.

The appendix includes a plot that shows the distributions of RMSE (instead of log RMSE), and the differences between the three algorithms are essentially indistinguishable at that resolution.

Figure 8: Shows the distribution of RMSE over the global optimum for GA, Adj TNC-0, Adj BFGS-0 in top two panels. Bottom two panels show the distributions over all algorithms on the pareto front (with tolerance of 1/12).

Overall, these differences between the three algorithms (GA, adj TNC-0, adj BFGS-0) are relatively minor, with all three giving essentially the same average RMSE (GA had a slightly worse RMSE than the other two). It’s not clear to the authors whether the subtle differences between them would cause any differences in practice. However, the BFGS and TNC algorithms both give a significant speed increase; the adjoint method with BFGS or TNC is about 5 times faster than the GA on average. Even when using finite differences instead of the adjoint method, BFGS is still about 3 times faster than the GA (finite differences with TNC did not work well). A much larger speed increase can be realized with only a small trade off in accuracy. Adj TNC-Inf had an average RMSE of 6.62 compared to 6.47 for the GA, but is 15 times faster. Adj TNC-7.5 had an average RMSE of 6.48 while being 9 times faster than the GA.

The comparison between the different strategies for initial guesses (0, 7.5, Inf) shows the trade off between speed and accuracy when starting a local search based algorithm multiple times. For car following models, it seems that even a suboptimal local minimum still gives a reasonable accuracy. The difference in accuracy made by starting a algorithm multiple times is smaller than the difference from using another algorithm, so regardless of the initial guess, the local search seems to converge to similar parameters. We also saw that a good local search algorithm (in this case, the quasi-newton algorithms) can give results equivalent to a global search algorithm (the GA) when a small number of initial guesses are used. Of course, each initial guess used greatly increases the time needed for the algorithm, so a hybrid strategy similar to the one proposed in [49] can be considered if a large number of initial
Comparing the results of using the adjoint method to finite differences, the differences between the two methods depends heavily on the algorithm used. For BFGS, using finite differences instead of the adjoint method gives essentially the same result, in the same number of objective/gradient evaluations, and the difference is speeds is consistent with the speed increase found in section 5. For TNC, the algorithm does not perform well when finite differences is used. This is most likely due to the small amount of noise induced by the adjoint method (see 4.3.2 acting as a source of regularization which prevents the newton system from becoming too ill-conditioned. The parameters of car following models often have very different sensitivities (for example, see [21]), and this can cause the hessian to be ill-conditioned. Overall we found that the adjoint method offers a speed up for gradient based algorithms, and that the small amount of numerical inaccuracy it gives is not large enough to cause any negative effects.

All the attention so far has been concentrated on the TNC, BFGS, and GA algorithms since those gave good results. None of the other algorithms performed well. NM is designed for unconstrained problems, so it is unsurprising that it did not perform as well as an algorithm designed specifically to deal with box constraints (recall that here the box bounds were enforced by adding a penalty term). GD suffered from the problem widely reported in the literature where it takes a very large number of iterations to fully converge. The majority of the time, the algorithm terminates due to exceeding the maximum number of evaluations allowed. For the SQP (recall in this case we explicitly computed the Hessian), we found that the newton direction often fails to define a direction of descent, and the algorithm simply searches in the direction of the gradient instead. Then, the algorithm spends a lot of computational time computing the Hessian but ends up not using it for anything, so explicitly computing the hessian seems to not work well for car following calibration; BFGS updating to estimate the Hessian, or a truncated newton method for estimating the newton direction should be used instead. SPSA performed worst out of all algorithms tested because of the vastly different sensitivities for car following models, as well as the rapidly changing magnitude of the gradient.

The analysis in this section has shown the value of gradient based algorithms and the adjoint method, since they can give the same overall performance while offering a significant speed increase. We found that for the calibration of a single vehicle, the truncated newton (TNC) algorithm with the adjoint method gives a slightly more accurate calibration than a genetic algorithm, while also being 5 times faster. TNC is 15 times faster than the genetic algorithm if \( \approx 2\% \) decrease in accuracy is acceptable (when only a single initial guess is used). Actually, as we will see in the next subsection, when the calibration problem becomes larger, the benefit of gradient based algorithms and the adjoint method becomes even larger.

### 5.2 Calibration of larger platoons

Instead of calibrating an arbitrarily sized platoon of vehicles, it would be simpler to break up the platoon into several leader/follower pairs (or in other words, a single follower is calibrated at a time). This is how most of the literature treats the car following calibration, and was the strategy used in the above section. Clearly this is suboptimal since each trajectory depends on it’s lead trajectory. But calibrating many vehicles together also means that the calibration problem becomes harder, so it’s not clear what platoon size would give the best results in practice. To the author’s knowledge, [16] is the only paper focused on car following calibration that has taken a platoon size of larger than 1 (2 followers were calibrated at a time in that paper).

In this section, we are interested in two questions regarding the calibration of some arbitrarily sized platoon of vehicles. First, for the different methods considered so far (gradient free, gradient based with finite differences, adjoint method) how does the time needed to solve the calibration problem scale with the number of parameters. Second, what is the benefit (in terms of RMSE) from considering a larger platoon of vehicles.

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number of parameters). The results are shown below.

![Log (base 10) of equivalent number of objective evaluations required to solve the calibration problem for an increasing number of parameters.](image)

Figure 9: Log (base 10) of equivalent number of objective evaluations required to solve the calibration problem for an increasing number of parameters. The number of parameters is the number of vehicles times 5. The brackets show the standard deviation for the data points. The work required to solve the calibration problem increases at a much faster rate when using gradient free optimization or finite differences compared to the adjoint method.

Table 4: Compares the number of equivalent objective evaluations for the calibration problem for an increasing number of parameters, relative to the Adj TNC-0 algorithm.

| # parameters | Adj TNC | Fin TNC | Fin TNC relative evals. | GA | GA relative evals. |
|--------------|---------|---------|-------------------------|----|-------------------|
| 5            | 1098    | 1790    | 1.63                    | 5256 | 4.79              |
| 10           | 1200    | 3300    | 2.75                    | 37715 | 31.4              |
| 15           | 1780    | 7139    | 4.01                    | 135485 | 76.1              |

Assuming that a gradient based algorithm converges in approximately the same number of gradient/objective evaluations for either using finite differences or the adjoint method, the equivalent number of objective evaluations can be easily converted between the two methods. Namely, if the adjoint method requires \( g(m) \) gradient + objective evaluations, for some arbitrary function \( g \), then finite differences will require \( \frac{m+1}{2} g(m) \). So using finite differences will always scale an order of \( m \) worse than the adjoint method. For the GA, it is clear that its cost is growing extremely fast with the number of parameters, and we only considered a platoon up to size 3 because of this reason. It was about 75 times as expensive as using TNC with the adjoint method for a problem size of only 15 parameters. We conclude that when the number of parameters becomes large, using the adjoint method with gradient based optimization can offer an arbitrarily large speed increase compared to either gradient free optimization or finite differences.

As for the effect of platoon size on the overall RMSE of the entire platoon, the results are shown in figure 10. Note overall RMSE is different than average RMSE because vehicles are weighted according to how many observations they have (see 4.2). It should be noted that these results were only for 100 randomly selected vehicles, and that the RMSE is expected to be higher here since the calibration is being done sequentially using the leader’s simulated trajectory instead of the leader’s measured trajectory. The left panel shows the overall RMSE versus platoon size. The right panel shows the relative improvement in RMSE, the percentage differences in overall RMSE compared to a platoon size of 1. The standard deviation of the relative improvement is also shown in that panel. The standard deviations are quite large: partially because there were only 10 platoons total considered in this experiment, but mainly because the improvement could be as large as 50%, or the overall RMSE could actually be slightly worse. Still, we saw that a platoon size of 3 or 4 both give about a 20% average improvement compared to a platoon size of 1.
Overall, these results suggest that considering a larger platoon size can improve calibration results, and further research on larger platoon sizes should be considered. We also see from figure 10 that the GA starts to perform better than TNC when the platoon size increases. This suggests that while the simple strategy of just using multiple guesses is adequate for the calibration of a single vehicle, a more sophisticated strategy is needed when multiple vehicles are being calibrated.

6 Conclusion

We considered an optimization based formulation of the calibration problem for car following models being calibrated to trajectory data. It was shown how to apply the adjoint method to derive the gradient or hessian for an arbitrary car following model formulated as either an ordinary or delay differential equation. Several algorithms for solving the calibration problem were compared, and it was found that the best overall algorithms were the genetic algorithm, l-bfgs-b, and truncated newton conjugate.

For the calibration of a single vehicle at a time, it was found that using the adjoint method and a quasi-newton method gives slightly better performance than a genetic algorithm, and is 5 times faster. As the number of parameters increases, the speed increase offered by the adjoint method and gradient based optimization can become arbitrarily large (for 15 parameters, a truncated newton algorithm using the adjoint method was 75 times faster than a genetic algorithm). Compared to using finite differences to calculate the gradient, the adjoint method will always scale better as the number of parameters becomes large, because the adjoint method has a flat cost and finite differences has a cost proportional to the number of parameters. Numerical experiments used the reconstructed NGsim data and the optimal velocity model.

There are two main directions for future research. In this paper we consider only the calibration of a car following model, while a full microsimulator has several other important modules, such as route choice or lane changing decision models. The question of how to apply the adjoint method to those other components can be considered in the future so that the methodology could be applied to a full microsimulation model. There are also more questions regarding the calibration of car following models. Future research can consider the effect of a larger platoon size on the calibration problem, so that multiple vehicles (which share leaders) are calibrated at a time. Another interesting question is using the new highly accurate vehicle trajectory data [63] to compare and validate different car following models. Since it was found during this study that lane changing vehicle trajectories are not described well by car following models, another question is how to incorporate lane changing dynamics into an arbitrary car following model, and the authors have recently proposed a method for doing so [64].
## Appendix A - Supplemental figures/tables for comparison of algorithms

Table 5: The full table showing all variants of the 7 algorithms considered.

| Algorithm    | % found global opt | Avg. RMSE (ft) | Avg. Time (s) | Avg. RMSE / % over global opt | Initial Guesses | # Obj. | # Grad. | # Hess. |
|--------------|--------------------|----------------|---------------|-------------------------------|-----------------|--------|--------|--------|
| Adj BFGS-0   | 94.0               | 6.46           | 7.42          | .10 / 2.0%                    | 3               | 307.1  | 307.1  | 0      |
| Adj BFGS-7.5 | 85.2               | 6.56           | 4.16          | .20/6.8%                      | 1.67            | 165.0  | 165.0  | 0      |
| Adj BFGS-∞   | 75.6               | 6.96           | 2.55          | .59 / 15.4%                   | 1               | 107.3  | 107.3  | 0      |
| GA           | 95.0               | 6.47           | 33.5          | .10/2.2%                      | -               | 5391   | 0      | 0      |
| NM           | 39.4               | 7.25           | 6.85          | .88/21.0%                     | 1               | 1037   | 0      | 0      |
| Fin BFGS-0   | 94.3               | 6.46           | 11.4          | .10/2.2%                      | 3               | 311.5  | 311.5  | 0      |
| Fin BFGS-7.5 | 85.7               | 6.55           | 6.32          | .19/6.3%                      | 1.66            | 164.8  | 164.8  | 0      |
| Fin BFGS-∞   | 77.0               | 6.88           | 3.91          | .52/13.8%                     | 1               | 107.3  | 107.3  | 0      |
| Adj GD-0     | 20.2               | 7.58           | 25.5          | 1.21/28.2%                    | 3               | 1374   | 542.5  | 0      |
| Adj GD-7.5   | 13.4               | 7.83           | 18.1          | 1.46/40.8%                    | 1.93            | 1094   | 436.6  | 0      |
| Adj GD-Inf   | 8.8                | 8.90           | 8.75          | 2.53/67.2%                    | 1               | 719.3  | 282.6  | 0      |
| Adj SQP-0    | 29.1               | 8.37           | 21.1          | 2.01/61.7%                    | 3               | 287.6  | 83.8   | 80.8   |
| Adj SQP-7.5  | 21.5               | 8.59           | 15.4          | 2.22/71.4%                    | 2.17            | 244.8  | 71.3   | 69.1   |
| Adj SQP-∞    | 10.0               | 11.1           | 5.87          | 4.70/140.7%                   | 1               | 141.6  | 39.4   | 38.4   |
| SPSA         | 4.2                | 53.2           | 38.5          | 46.8/786%                     | 1               | 6001   | 0      | 0      |
| Fin GD-∞     | 9.1                | 8.86           | 14.7          | 2.50/66.2%                    | 1               | 657.3  | 258.5  | 0      |
| Fin SQP-∞    | 2.6                | 9.61           | 15.8          | 3.25/81.8%                    | 1               | 179.4  | 67.2   | 66.2   |
| Adj TNC-0    | 90.7               | 6.43           | 6.87          | .05/2.4%                      | 3               | 285.7  | 285.7  | 0      |
| Adj TNC-7.5  | 82.7               | 6.48           | 3.82          | .11/5.0%                      | 1.63            | 152.3  | 152.3  | 0      |
| Adj TNC-∞    | 77.3               | 6.62           | 2.26          | .25/7.7%                      | 1               | 94.1   | 94.1   | 0      |
| Fin TNC-0    | 36.3               | 6.84           | 13.2          | .47/11.0%                     | 3               | 302.4  | 302.4  | 0      |
| Fin TNC-7.5  | 24.9               | 7.05           | 8.35          | .69/20.8%                     | 1.82            | 183.2  | 183.2  | 0      |
| Fin TNC-∞    | 18.0               | 7.63           | 4.49          | 1.27/33.2%                    | 1               | 100.8  | 100.8  | 0      |
Figure 11: Shows the distribution of RMSE for different algorithms tested. Left panels show overall RMSE, right panels show the RMSE for vehicles that experience lane changes (solid) and those that don’t (dashed). The RMSE for lane changing vehicles is much higher because car following models don’t describe lane changes well [64]. For example, for the genetic algorithm, the average RMSE for vehicles which do not experience lane changes is 4.75, whereas it is 8.17 for vehicles which do. The other algorithms have very similar numbers.

Appendix B - Extension of adjoint method for Hessian

When calculating the gradient, the benefit of the adjoint method is that you avoid calculating $\partial x_i / \partial p$ terms. When calculating the Hessian, the adjoint method will be used to avoid calculating $\partial^2 x_i / \partial p^2$ terms. We will still be left with the unknowns $\partial x_i / \partial p$, which need to be calculated using the “variational” approach, also known as the “forward sensitivity” approach [52, 51].

To obtain the variational system, differentiate the model Eq. (4) with respect to the parameters

$$\frac{d}{dp} \dot{x}_i = \frac{d}{dp} h_i(x_i, x_{L(i)}, p_i)$$

and then switch the order of differentiation on the left hand side to obtain the variational system

$$\frac{d}{dt} \frac{\partial x_i}{\partial p} = \frac{\partial h_i}{\partial x_i} \frac{\partial x_i}{\partial p} + \frac{\partial h_i}{\partial p_i} + \mathbb{1}(L(i, t) \in [1, n]) \frac{\partial h_i}{\partial x_{L(i)}} \frac{\partial x_{L(i)}}{\partial p}, \quad t \in [t_i, T_{i-1}] \quad \forall i.$$ (24)

Eq. (24) gives $\partial x_i(t) / \partial p$ starting from the initial conditions $\partial x_i(t_i) / \partial p$. Note that the variational system for $x_i$ is only defined up to time $T_{i-1}$ because $\partial x_i(t) / \partial p = \partial x_i(T_{i-1}) / \partial p$ for $t \in [T_{i-1}, T_i]$. Now starting from Eq. (10),
For a platoon being calibrated to video data, the last term cannot be calculated and one proceeds as in 4.1.3.

\[
\frac{d^2}{dp^2} F = \frac{d^2}{dp^2} L = \sum_{i=1}^{n} \left[ \int_{t_i}^{T} \frac{\partial^2 \hat{x}_i(t)}{\partial p^2} T \frac{\partial^2 f^T}{\partial x_i^2} \frac{\partial x_i}{\partial p} + \frac{\partial f}{\partial x_i} \frac{\partial^2 \hat{x}_i}{\partial p^2} + \lambda_i^T \frac{\partial^2 \hat{x}_i}{\partial p^2} \lambda_i \frac{\partial x_i}{\partial p} - \lambda_i^T \frac{\partial h_i}{\partial x_i} \frac{\partial^2 x_i}{\partial p^2} + \ldots \right.
\]

\[
- \frac{\partial x_i^T}{\partial p} \frac{\partial^2 h_i}{\partial p \partial x_i} \lambda_i - \lambda_i^T \frac{\partial^2 h_i}{\partial p^2} - \frac{\partial^2 h_i}{\partial x_i \partial p} \lambda_i \frac{\partial x_i}{\partial p} dt \] + \ldots
\]

\[
+ \sum_{i=1}^{n} \int_{t_i}^{T} (G(i,t) \neq 0) \left[ - \frac{\partial x_i^T}{\partial p} \frac{\partial^2 h_{G(i)}}{\partial p^2} \lambda_{G(i)} \frac{\partial x_i}{\partial p} - \frac{\partial x_i^T}{\partial p} \frac{\partial^2 h_{G(i)}}{\partial p \partial x_i} \lambda_{G(i)} - \frac{\partial x_i^T}{\partial p} \frac{\partial^2 h_{G(i)}}{\partial p \partial x_{G(i)}} \lambda_{G(i)} \frac{\partial x_i}{\partial p} dt \right]
\]

\[
\frac{d^2}{dp^2} F = \sum_{i=1}^{n} \left[ \int_{t_i}^{T} \frac{\partial^2 \hat{x}_i(t)}{\partial p^2} T \frac{\partial^2 f^T}{\partial x_i^2} \frac{\partial x_i}{\partial p} - \frac{\partial x_i^T}{\partial p} \frac{\partial^2 h_i}{\partial p \partial x_i} \lambda_i - \lambda_i^T \frac{\partial^2 h_i}{\partial p^2} + \ldots \right.
\]

\[
- \frac{\partial^2 h_i}{\partial x_i \partial p} \lambda_i \frac{\partial x_i}{\partial p} dt \] + \sum_{i=1}^{n} \int_{t_i}^{T} (G(i,t) \neq 0) \left[ - \frac{\partial x_i^T}{\partial p} \frac{\partial^2 h_{G(i)}}{\partial p^2} \lambda_{G(i)} \frac{\partial x_i}{\partial p} - \frac{\partial x_i^T}{\partial p} \frac{\partial^2 h_{G(i)}}{\partial p \partial x_i} \lambda_{G(i)} - \frac{\partial x_i^T}{\partial p} \frac{\partial^2 h_{G(i)}}{\partial p \partial x_{G(i)}} \lambda_{G(i)} \frac{\partial x_i}{\partial p} dt \right] + \ldots
\]

The adjoint variables are defined the same way whether the gradient or Hessian is being computed. Eq. (16) gives the adjoint system for the unmodified objective \( F \). After solving for all the adjoint variables, in addition to solving the variational system Eq. (24), one can calculate the Hessian:

\[
\frac{d^2}{dp^2} F = \sum_{i=1}^{n} \left[ \int_{t_i}^{T} \frac{\partial^2 \hat{x}_i(t)}{\partial p^2} T \frac{\partial^2 f^T}{\partial x_i^2} \frac{\partial x_i}{\partial p} - \frac{\partial x_i^T}{\partial p} \frac{\partial^2 h_i}{\partial p \partial x_i} \lambda_i - \lambda_i^T \frac{\partial^2 h_i}{\partial p^2} + \ldots \right.
\]

\[
- \frac{\partial^2 h_i}{\partial x_i \partial p} \lambda_i \frac{\partial x_i}{\partial p} \] + \sum_{i=1}^{n} \int_{t_i}^{T} (G(i,t) \neq 0) \left[ - \frac{\partial x_i^T}{\partial p} \frac{\partial^2 h_{G(i)}}{\partial p^2} \lambda_{G(i)} \frac{\partial x_i}{\partial p} - \frac{\partial x_i^T}{\partial p} \frac{\partial^2 h_{G(i)}}{\partial p \partial x_i} \lambda_{G(i)} - \frac{\partial x_i^T}{\partial p} \frac{\partial^2 h_{G(i)}}{\partial p \partial x_{G(i)}} \lambda_{G(i)} \frac{\partial x_i}{\partial p} dt \right] + \ldots
\]

(25)

For a platoon being calibrated to video data, the last term cannot be calculated and one proceeds as in 4.1.3.

**Exact Hessian for Platoon with Video Data**

Proceeding as in section 4.1.3, use the modified objective function \( F_1 \) and modified augmented objective function \( L_1 \). Under these modifications, the adjoint system is given by Eq. (22). No modifications to the variational system are needed. The Hessian is then

\[
\frac{d^2}{dp^2} F_1 = \sum_{i=1}^{n} \left[ \lambda_i^T (\frac{\partial^2 \hat{x}_i(t_i)}{\partial p^2} + \frac{\partial^2 f^T}{\partial x_i^2} \frac{\partial x_i}{\partial p} + \frac{\partial f}{\partial x_i} \frac{\partial^2 \hat{x}_i}{\partial p^2} + \lambda_i^T \frac{\partial^2 \hat{x}_i}{\partial p^2} \lambda_i \frac{\partial x_i}{\partial p} - \lambda_i^T \frac{\partial h_i}{\partial x_i} \frac{\partial^2 x_i}{\partial p^2} + \ldots \right.
\]

\[
- \lambda_i^T \frac{\partial^2 h_i}{\partial p^2} - \frac{\partial^2 h_i}{\partial x_i \partial p} \lambda_i \frac{\partial x_i}{\partial p} dt \] + \sum_{i=1}^{n} \int_{t_i}^{T} (G(i,t) \neq 0) \left[ - \frac{\partial x_i^T}{\partial p} \frac{\partial^2 h_{G(i)}}{\partial p^2} \lambda_{G(i)} \frac{\partial x_i}{\partial p} - \frac{\partial x_i^T}{\partial p} \frac{\partial^2 h_{G(i)}}{\partial p \partial x_i} \lambda_{G(i)} - \frac{\partial x_i^T}{\partial p} \frac{\partial^2 h_{G(i)}}{\partial p \partial x_{G(i)}} \lambda_{G(i)} \frac{\partial x_i}{\partial p} dt \right] + \ldots
\]

(26)

To obtain the exact Hessian calculation for a platoon of vehicles using video data, simply solve Eqs. (22) and (26) instead of (16) and (25). As before, this modification gives extra weight to the point \( x_i(T_{i-1}) \) so it makes sense to reweight the loss function as was done in the section 4.1.3.

**Appendix C - Gradient for DDE model**

We will now deal with calculating the gradient for Eq. (24). As before, if not explicitly stated, quantities can be assumed to be evaluated at time \( t \). Define the augmented objective function:

\[
L = \sum_{i=1}^{n} \left( \int_{t_i + \tau_i}^{T_i} f(x_i, \dot{x}_i) + \lambda_i^T (\dot{x}_i(t) - h_i(x_i(t), x_i(t - \tau_i), x_{L(i)}(t - \tau_i), p_i)) dt \right)
\]

(27)
and since \( F = L \)

\[
\frac{d}{dp} F = \sum_{i=1}^{n} \left[ \int_{t_i + \tau_i}^{T_{i-1}} \left( -\lambda_i^T(t) \frac{\partial h_i}{\partial x_i} - \lambda_i^T(t) \frac{\partial h_i}{\partial p} - \lambda_i^T(t) \frac{\partial h_i}{\partial h_i} \frac{\partial x_i(t - \tau_i)}{\partial p} \right) dt \right]
\]

\[
- \lambda_i^T(t) \frac{\partial h_i}{\partial x_i(t - \tau_i)} \frac{\partial x_i(t - \tau_i)}{\partial p} - \lambda_i^T(t) \frac{\partial h_i}{\partial p} dt \right] + \sum_{i=1}^{n} \sum_{j \in S(i)} \int_{t_i + \tau_i}^{T_{i-1}} 1(G(i, t - \tau_j) = j) \left[ + \ldots \right]
\]

\[
- \lambda_i^T(t) \frac{\partial h_i}{\partial x_i(t - \tau_j)} - \lambda_i^T(t) \frac{\partial h_i}{\partial p} \frac{\partial x_i(t - \tau_j)}{\partial p} dt \right]
\]

(28)

where \( S(i) \) is defined as the set of all followers for vehicle \( i \) and we have chosen \( \lambda_i^T(T_{i-1}^{*}) = 0 \). For a DDE, use a change of coordinates on terms containing \( \partial x_i(t - \tau)/\partial p \).

\[
- \int_{t_i + \tau_i}^{T_{i-1}} \lambda_i^T(t) \frac{\partial h_i}{\partial x_i(t - \tau_i)} dt = - \int_{t_i + \tau_i}^{T_{i-1} - \tau_i} \lambda_i^T(t + \tau_i) \frac{\partial h_i}{\partial x_i(t - \tau_i)} dt + \sum_{i=1}^{n} \sum_{j \in S(i)} \int_{t_i + \tau_j}^{T_i} 1(G(i, t) = j) \lambda_i^T(t + \tau_j) \frac{\partial h_i}{\partial x_i(t - \tau_j)} dt
\]

(29)

Where we make use of the fact that \( \partial x_i(t)/\partial p = 0 \) for \( t \in [t_i, t_i + \tau_i] \) since the initial history function doesn't depend on the parameters. Now substituting Eq. (29) into Eq. (28) and grouping terms, one obtains the adjoint system:

\[
\frac{\partial f}{\partial x_i} - \lambda_i^T(t) - \lambda_i^T(t) \frac{\partial h_i}{\partial x_i} - 1(t \leq T_{i-1}^{*} - \tau_i) \lambda_i^T(t + \tau_i) \frac{\partial h_i}{\partial x_i(t - \tau_i)} \ldots
\]

\[
- \sum_{j \in S(i)} 1(G(i, t) = j) \lambda_j^T(t + \tau_j) \frac{\partial h_j}{\partial x_i(t - \tau_j)} = 0, \quad t \in [T_{i-1}^{*}, t_i + \tau_i], \quad \forall i
\]

(30)

with initial conditions \( \lambda_i(T_{i-1}^{*}) = 0 \). For a DDE model, the adjoint system also becomes a DDE. After solving for the adjoint variables, one can compute the gradient:

\[
\frac{d}{dp} F = \sum_{i=1}^{n} \left[ \int_{t_i + \tau_i}^{T_{i-1}} \left( -\lambda_i^T(t) \frac{\partial h_i}{\partial x_i(t - \tau_i)} \frac{\partial x_i(t - \tau_i)}{\partial p} - \lambda_i^T(t) \frac{\partial h_i}{\partial p} dt \right) \right]
\]

\[
+ \sum_{i=1}^{n} \sum_{j \in S(i)} \int_{t_i + \tau_j}^{T_i} 1(G(i, t) = j) \lambda_j^T(t + \tau_j) \frac{\partial h_j}{\partial x_i(t - \tau_j)} \frac{\partial x_i(t - \tau_j)}{\partial p} dt
\]

(31)

The last term of (31) contains a \( \partial x_i(t)/\partial p \) term that cannot be directly evaluated. This problematic term always vanishes for the calibration of a single vehicle (because \( S(i) \) will always be empty) or for data in which all vehicles are observed up to the same time (because \( T_{i-1}^{*} = T_i \)). A modification similar to 4.1.3 can be done in order to fix this problem. This will lead to the modified adjoint system:

\[
\frac{\partial f}{\partial x_i} - \lambda_i^T(t) - 1(t \leq T_{i-1}^{*}) \lambda_i^T(t) \frac{\partial h_i}{\partial x_i} - 1(t \leq T_{i-1}^{*} - \tau_i) \lambda_i^T(t + \tau_i) \frac{\partial h_i(t + \tau_i)}{\partial x_i(t - \tau_i)} \ldots
\]

\[
- \sum_{j \in S(i)} 1(G(i, t) = j) \lambda_j^T(t + \tau_j) \frac{\partial h_j(t + \tau_j)}{\partial x_i(t - \tau_j)} = 0, \quad t \in [T_i, t_i + \tau_i], \quad \forall i
\]

(32)

This modified adjoint system will eliminate the problematic last term in (31). The loss function should be reweighted in this case.
References

[1] M. J. Lighthill and G. B. Whitham. On kinematic waves ii. a theory of traffic flow on long crowded roads. *Proceedings of the Royal Society of London A: Mathematical, Physical and Engineering Sciences, 229*(1178):317–345, 1955.

[2] Boris S. Kerner. Three-phase theory of city traffic: Moving synchronized flow patterns in under-saturated city traffic at signals. *Physica A: Statistical Mechanics and its Applications, 397*:76 – 110, 2014.

[3] Jorge A. Laval and Carlos F. Daganzo. Lane-changing in traffic streams. *Transportation Research Part B: Methodological, 40*(3):251 – 264, 2006.

[4] D. Helbing, A. Hennecke, V. Shvetsov, and M. Treiber. Micro- and macro-simulation of freeway traffic. Mathematical and Computer Modelling, 35(5):517 – 547, 2002.

[5] Kai Nagel and Michael Schreckenberg. A cellular automaton model for freeway traffic. *Journal de Physique I, 2*(12):2221–2229, 1992.

[6] G.C.K Wong and S.C Wong. A multi-class traffic flow model an extension of lwr model with heterogeneous drivers. *Transportation Research Part A: Policy and Practice, 36*(9):827 – 841, 2002.

[7] Carlos F. Daganzo. The cell transmission model: A dynamic representation of highway traffic consistent with the hydrodynamic theory. *Transportation Research Part B: Methodological, 28*(4):269 – 287, 1994.

[8] B. S. Kerner and H. Rehborn. Experimental properties of phase transitions in traffic flow. *Phys. Rev. Lett., 79*:4030–4033, Nov 1997.

[9] Jorge A. Laval and Ludovic Leclercq. Microscopic modeling of the relaxation phenomenon using a macroscopic lane-changing model. *Transportation Research Part B: Methodological, 42*(6):511 – 522, 2008.

[10] Benjamin Coifman and Lizhe Li. A critical evaluation of the next generation simulation (ngsim) vehicle trajectory dataset. *Transportation Research Part B: Methodological, 105*:362 – 377, 2017.

[11] Dirk Helbing and Benno Tilch. Generalized force model of traffic dynamics. *Phys. Rev. E, 58*:133–138, Jul 1998.

[12] Mark Brackstone and Mike McDonald. Car-following: a historical review. *Transportation Research Part F: Traffic Psychology and Behaviour, 2*(4):181 – 196, 1999.

[13] Elmar Brockfeld, Reinhart Khne, and Peter Wagner. Calibration and validation of microscopic traffic flow models. *Transportation Research Record: Journal of the Transportation Research Board, 1876*:62–70, 2004.

[14] Elmar Brockfeld, Reinhart Khne, Alexander Skabardonis, and Peter Wagner. Toward benchmarking of microscopic traffic flow models. *Transportation Research Record: Journal of the Transportation Research Board, 1852*:124–129, 2003.

[15] Vincenzo Punzo and Fulvio Simonelli. Analysis and comparison of microscopic traffic flow models with real traffic microscopic data. *Transportation Research Record: Journal of the Transportation Research Board, 1934*:53–63, 2005.

[16] Saskia Ossen, Serge Hoogendoorn, and Ben Gorte. Interdriver differences in car-following: A vehicle trajectory-based study. *Transportation Research Record: Journal of the Transportation Research Board, 1965*:121–129, 2006.

[17] U. S. Department of Transportation. Next generation simulation (ngsim) vehicle trajectories and supporting data. [https://data.transportation.gov/Automobiles/Next-Generation-Simulation-NGSIM-Vehicle-Trajectory/8ect-6jqj](https://data.transportation.gov/Automobiles/Next-Generation-Simulation-NGSIM-Vehicle-Trajectory/8ect-6jqj) 2006. Accessed: 2018-05-05.

[18] Robert Krajewski, Julian Bock, Laurent Kloeker, and Lutz Eckstein. The highd dataset: A drone dataset of naturalistic vehicle trajectories on german highways for validation of highly automated driving systems. In *2018 IEEE 21st International Conference on Intelligent Transportation Systems (ITSC), 2018*.

[19] Biagio Ciuffo, Vincenzo Punzo, and Marcello Montanino. The Calibration of Traffic Simulation Models: Report on the Assessment of Different Goodness of Fit measures and Optimization Algorithms. Technical Report EU Cost Action TU0903 MULTITUDE, European Commission Joint Research Centre, 2012.
[20] Vincenzo Punzo, Biagio Ciuffo, and Marcello Montanino. Can results of car-following model calibration based on trajectory data be trusted? *Transportation Research Record: Journal of the Transportation Research Board*, 2315:11–24, 2012.

[21] V. Punzo, M. Montanino, and B. Ciuffo. Do we really need to calibrate all the parameters? variance-based sensitivity analysis to simplify microscopic traffic flow models. *IEEE Transactions on Intelligent Transportation Systems*, 16(1):184–193, Feb 2015.

[22] Hwasoo Yeo, Alexander Skabardonis, John Halkias, James Colyar, and Vassili Alexiadis. Oversaturated freeway flow algorithm for use in next generation simulation. *Transportation Research Record: Journal of the Transportation Research Board*, 2088:68–79, 2008.

[23] Arne Kesting and Martin Treiber. Calibrating car-following models by using trajectory data: Methodological study. *Transportation Research Record: Journal of the Transportation Research Board*, 2088:148–156, 2008.

[24] P. Hidas. A functional evaluation of the aimsun, paramics and vissim microsimulation models. *Road and Transport Research*, 14:45–59, 12 2005.

[25] Carlos F. Daganzo. In traffic flow, cellular automata=kinematic waves. *Transportation Research Part B: Methodological*, 40(5):396 – 403, 2006.

[26] Hwasoo Yeo and Alexander Skabardonis. Parameter estimation for ngsim over-saturated freeway flow algorithm. In *Proceedings of the 10th AATT Conference*, 2008. cd-rom.

[27] Xiao-Yun Lu and Alexander. Skabardonis. Freeway shockwave analysis: Exploring ngsim trajectory data. In *Transportation Research Board 86th Annual Meeting*, 2007. cd-rom.

[28] G.F. Newell. A simplified car-following theory: a lower order model. *Transportation Research Part B: Methodological*, 36(3):195 – 205, 2002.

[29] Carlos F. Daganzo. In traffic flow, cellular automata=kinematic waves. *Transportation Research Part B: Methodological*, 40(5):396 – 403, 2006.

[30] M Bando, K Hasebe, A Nakayama, A Shibata, and Y Sugiyama. Dynamical model of traffic congestion and numerical simulation. *Physical review. E, Statistical physics, plasmas, fluids, and related interdisciplinary topics*, 51(2):10351042, February 1995.

[31] Yuko Sugiyama, Minoru Fukui, Macoto Kikuchi, Katsuya Hasebe, Akihiro Nakayama, Katsuhiro Nishinari, Shinichiro Tadaki, and Satoshi Yukawa. Traffic jams without bottlenecks: experimental evidence for the physical mechanism of the formation of a jam. *New Journal of Physics*, 10(3):033001, 2008.

[32] Martin Treiber, Ansgar Hennecke, and Dirk Helbing. Congested traffic states in empirical observations and microscopic simulations. *Physical Review E*, 62:1805–1824, 02 2000.

[33] Marcello Montanino and Vincenzo Punzo. Trajectory data reconstruction and simulation-based validation against macroscopic traffic patterns. *Transportation Research Part B: Methodological*, 80:82 – 106, 2015.

[34] L.C. Davis. Modifications of the optimal velocity traffic model to include delay due to driver reaction time. *Physica A: Statistical Mechanics and its Applications*, 319:557 – 567, 2003.

[35] Gábor Orosz and Gábor Stépán. Subcritical hopf bifurcations in a car-following model with reaction-time delay. *Proceedings of the Royal Society of London A: Mathematical, Physical and Engineering Sciences*, 462(2073):2643–2670, 2006.

[36] Martin Treiber, Arne Kesting, and Dirk Helbing. Delays, inaccuracies and anticipation in microscopic traffic models. *Physica A: Statistical Mechanics and its Applications*, 360(1):71 – 88, 2006.

[37] I. Gasser, G. Sirito, and B. Werner. Bifurcation analysis of a class of car following traffic models. *Physica D: Nonlinear Phenomena*, 197(3):222 – 241, 2004.

[38] L. C. Davis. Comment on “analysis of optimal velocity model with explicit delay”. *Phys. Rev. E*, 66:038101, Sep 2002.
[39] Biagio Ciuffo, Vincenzo Punzo, and Marcello Montanino. Thirty years of gipps’ car-following model. Transportation Research Record: Journal of the Transportation Research Board, 2315:89–99, 2012.

[40] H. X. Ge, S. Q. Dai, L. Y. Dong, and Y. Xue. Stabilization effect of traffic flow in an extended car-following model based on an intelligent transportation system application. Phys. Rev. E, 70:066134, Dec 2004.

[41] P.G. Gipps. A behavioural car-following model for computer simulation. Transportation Research Part B: Methodological, 15(2):105 – 111, 1981.

[42] Hesham Rakha and Brent Crowther. Comparison of greenshields, pipes, and van aerde car-following and traffic stream models. Transportation Research Record: Journal of the Transportation Research Board, 1802:248–262, 2002.

[43] Prakash Ranjitkar, Takashi Nakatsuji, and Motoki Asano. Performance evaluation of microscopic traffic flow models with test track data. Transportation Research Record: Journal of the Transportation Research Board, 1876:90–100, 2004.

[44] Aurielen Duret, Christine Buisson, and Nicolas Chiabaut. Estimating individual speed-spacing relationship and assessing ability of newell’s car-following model to reproduce trajectories. Transportation Research Record: Journal of the Transportation Research Board, 2088:188–197, 2008.

[45] Masako Bando, Katsuya Hasebe, Ken Nakanishi, Akihiro Nakayama, Akihiro Shibata, and Yuki Sugiyama. Phenomenological Study of Dynamical Model of Traffic Flow. Journal de Physique I, 5(11):1389–1399, 1995.

[46] J. C. Spall. Multivariate stochastic approximation using a simultaneous perturbation gradient approximation. IEEE Transactions on Automatic Control, 37(3):332–341, March 1992.

[47] Inc. LINDO Systems. Lindo api 12.0 user manual, 2018.

[48] R. Fletcher, N. Gould, S. Leyffer, P. Toint, and A. Wchter. Global convergence of a trust-region sqp-filter algorithm for general nonlinear programming. SIAM Journal on Optimization, 13(3):635–659, 2002.

[49] Li Li, Xiquan (Micheal) Chen, and Lei Zhang. A global optimization algorithm for trajectory data based car-following model calibration. Transportation Research Part C: Emerging Technologies, 68:311 – 332, 2016.

[50] D. R. Jones, C. D. Perttunen, and B. E. Stuckman. Lipschitzian optimization without the lipschitz constant. Journal of Optimization Theory and Applications, 79(1):157–181, Oct 1993.

[51] Jonathan Calver and Wayne Enright. Numerical methods for computing sensitivities for odes and ddes. Numerical Algorithms, 74(4):1101–1117, Apr 2017.

[52] Alternative optimization and adaptive parameters. SIAM Journal on Scientific Computing, 24(3):1076–1089, 2003.

[53] D. I. Papadimitriou and K. C. Giannakoglou. Direct, adjoint and mixed approaches for the computation of hessian in airfoil design problems. International Journal for Numerical Methods in Fluids, 56(10):1929–1943, 2007.

[54] David W. Zingg, Marian Nemec, and Thomas H. Pulliam. A comparative evaluation of gradient and adjoint-based methods applied to aerodynamic optimization. European Journal of Computational Mechanics, 17(1-2):103–126, 2008.

[55] B.M. Chaparro, S. Thuillier, L.F. Menezes, P.Y. Manach, and J.V. Fernandes. Material parameters identification: Gradient-based, genetic and hybrid optimization algorithms. Computational Materials Science, 44(2):339 – 346, 2008.

[56] Rainer Storn and Kenneth Price. Differential evolution: a simple and efficient heuristic for global optimization over continuous spaces. J. of Global Optimization, 11(4):341–359, December 1997.

[57] Fuchang Gao and Lixing Han. Implementing the nelder-mead simplex algorithm with adaptive parameters. Computational Optimization and Applications, 51(1):259–277, Jan 2012.

[58] Richard H. Byrd, Peihuang Lu, Jorge Nocedal, and Ciyou Zhu. A limited memory algorithm for bound constrained optimization. SIAM J. Sci. Comput., 16(5):1190–1208, September 1995.
[59] Cium Zhu, Richard H. Byrd, Peihuang Lu, and Jorge Nocedal. Algorithm 778: L-bfgs-b: Fortran subroutines for large-scale bound-constrained optimization. ACM Trans. Math. Softw., 23(4):550–560, December 1997.

[60] S. Nash. Newton-type minimization via the lanczos method. SIAM Journal on Numerical Analysis, 21(4):770–788, 1984.

[61] E. Birgin, J. Martnez, and M. Raydan. Nonmonotone spectral projected gradient methods on convex sets. SIAM Journal on Optimization, 10(4):1196–1211, 2000.

[62] Jorge Nocedal and Stephen J. Wright. Numerical Optimization. Springer, New York, NY, USA, 1999.

[63] Robert Krajewski, Julian Bock, Laurent Kloeker, and Lutz Eckstein. The highd dataset: A drone dataset of naturalistic vehicle trajectories on german highways for validation of highly automated driving systems. In 2018 IEEE 21st International Conference on Intelligent Transportation Systems (ITSC), 2018.

[64] Ronan Keane and H. Oliver Gao. A formulation of the relaxation phenomenon for lane changing dynamics in an arbitrary car following model. Manuscript in preparation, 2019.