Sensitivity analysis of traffic equilibria

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August 9, 2002

Abstract

The contribution of the paper is a complete analysis of the sensitivity of elastic demand traffic (Wardrop) equilibria. The existence of a directional derivative of the equilibrium solution (link flow, least travel cost, demand) in any direction is given a characterization, and the same is done for its gradient. The gradient, if it exists, is further interpreted as a limiting case of the gradient of the logit-based SUE solution, as the dispersion parameter tends to infinity. In the absence of the gradient, we show how to compute a subgradient. All of these computations (directional derivative, (sub)gradient) are performed by solving similar traffic equilibrium problems with affine link cost and demand functions, and they can be performed by the same tool as (or one similar to) the one used for the original traffic equilibrium model; this fact is of clear advantage when applying sensitivity analysis within a bilevel (or, mathematical program with equilibrium constraints, MPEC) application, such as for congestion pricing, OD estimation or network design. A small example illustrates the possible non-existence of a gradient and the computation of a subgradient.

Introduction

Performing a sensitivity analysis of traffic equilibria means evaluating the directions of change that occur in the flows and travel costs as parameters in the cost and demand functions change. A sensitivity analysis is particularly useful in control and pricing applications since, if we can anticipate the effects of a change in, say, the traffic infrastructure, on the behaviour of the travellers, then we can utilize this knowledge to optimize these changes according to some goal fulfillment, like a reduction in flows, a higher revenue from congestion tolls, etc. The subject for now is not the applications of sensitivity analyses per se, but instead the foundations of them. In particular, we provide for the first time a characterization of when such an analysis can be performed, including when the gradient of the equilibrium link flows, least travel costs, and demands with respect to a vector of parameters does exist. From this analysis, we can then develop new computational algorithms that take into consideration that the gradient does not always exist, and it can also lead to more efficient implementations of already existing algorithms. To this end, the chapter provides computational formulas for the directional derivative, the gradient, and a subgradient in the latter's absence.

All previous analyses have drawbacks or limitations which this paper tries to mitigate. Some analyses are based on the notion that the gradient does exist, and heuristically based formulas are provided for calculating it; the effect is that sometimes the formula provides a value which cannot be interpreted as a gradient, either because it does not exist or because the formula gives the wrong value, or the formula can break down and does therefore not provide a value even in the case that it does exist (see the discussion in [BeI97, Section 5.4]). This type of analysis, represented by [ToF88, CSF00], further has the limitation—in our opinion—that the computational formulas are based on complicated matrix calculations that are far removed from the original problem's form. We show that directional derivatives and (sub)gradients are naturally associated with the solution of traffic equilibrium problems which are similar to the original one, and the sensitivity information sought can therefore be efficiently computed by using the same, or only slightly modified, traffic equilibrium software.

The other analyses are similar to ours in the choice of underlying theory, but are still limited for other reasons. The papers [QiM89, Yen95, Out97, PaR02b], which together with the above two references comprise the whole body of literature on the subject of the theoretical development of sensitivity analysis of traffic equilibria, provide *sufficient* conditions for the existence of directional derivatives. In all cases,

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the conditions given are stronger than necessary. Some of these papers deal only with the link–route representation of traffic flows, thus failing to show that also link–node based models can provide sensitivity information, of importance when the number of routes is very large. Further, and most importantly, the analysis of this paper not only presents a characterization of the existence of the directional derivative, and formulas for calculating it, but also a characterization of the existence of the gradient, as well as a formula for the calculation of a subgradient in the absence of the gradient, under weak conditions that are almost always satisfied when the directional derivative exists.

We also indicate how the analysis changes if the model is appended with additional constraints. The fact that the sensitivity analysis is performed by solving a network flow problem, in contrast to doing a matrix analysis, is of great importance in this context: the network flow problem is simply appended with additional constraints to accommodate the new information, and it seems much more troublesome to extend a matrix formula to accomplish the same task.

The paper illustrates, by means of an example, that the equilibrium solution is not differentiable everywhere, and provides the directional derivative in one direction as well as one subgradient, in terms of both the link flows and the OD travel costs.

The analysis is made both for the link–route and link–node flow representation, although the former occupies the most space; the two analyses are so similar that only one needs to be performed; the (minor) differences between the analyses for the two representations are reported.

The models are studied in the form of variational inequalities and nonlinear (mixed) complementarity problems, and the analysis tool which is utilized throughout the paper is that of variational analysis, that is, the extension of differential analysis and convex analysis to situations where neither differentiability nor convexity might be present, which is indeed the one we face.

The rest of the paper is organized as follows: In the next section, we present the parameterized problem in the framework of Wardrop equilibrium models, and provide formulations for the link–route and link–node representations of traffic flows. Parameters may be present both in the travel cost and demand function, although analyses of special cases will be considered. Section 2 gives an overview of the subject of sensitivity analysis, in particular that of previous work done for traffic equilibrium models. Section 3 provides a characterization of the existence of directional derivatives of the equilibrium link flow, demand and OD travel costs. Some special cases such as the cases of fixed, unperturbed or invertible demand functions, will be studied especially. The characterization of differentiability of the equilibrium solution is taken up in Section 4. In this section, we also show that the gradient, whenever it exists, can be obtained numerically, at least in principle, by performing the sensitivity analysis of the logit-based stochastic user equilibrium (SUE) model as the value of the dispersion parameter tends to infinity. Section 5 provides an illustration of a case where the equilibrium link flow is not differentiable, although the most popular gradient calculus formula does produce a "gradient" vector. We then show in Section 6 that in the absence of a gradient and under an additional regularity assumption, a computation similar to that of the directional derivative of the equilibrium solution in each coordinate direction supplies a subgradient. We also provide one subgradient for the numerical example. Section 7 finally illustrates how the analysis can be extended to the case of additional, side, constraints on traffic flows, and discusses prospects for future research in the area.

1 The Wardrop conditions

Let $\mathcal{G} = (\mathcal{N}, \mathcal{L})$ be a transportation network, where $\mathcal{N}$ and $\mathcal{L}$ are the sets of nodes and directed links, respectively. For certain ordered pairs of nodes, $(p, q) \in \mathcal{C}$, where node p is an origin, node q is a destination, and $\mathcal{C}$ is a subset of $\mathcal{N} \times \mathcal{N}$, there is a transport demand, which may be given by a function of the travel cost. We assume that the network is strongly connected, that is, that at least one route joins each origin–destination (OD) pair.

Wardrop's user equilibrium principle states that for every OD pair $(p, q) \in \mathcal{C}$, the travel costs of the routes utilized are equal and minimal for each individual user. We denote by $\mathcal{R}_{pq}$ the set of simple (loop-free) routes for OD pair (p, q), by h_r the flow on route $r \in \mathcal{R}_{pq}$, and by c_r the travel cost on the route as experienced by an individual user.

We introduce the parameter to be present in the sensitivity analysis: it is denoted ρ, and is assumed to be of dimension d. This parameter could be present in one or both of the travel cost and demand functions. We assume that the travel cost function has the form $c(\rho, \cdot) : \Re_+^{|\mathcal{R}|} \mapsto \Re^{|\mathcal{R}|}$ given a value of ρ, where $|\mathcal{R}|$ denotes the total number of routes in the network. Further, the demand function is given by

$g(\rho,\cdot) : \Re^{|\mathcal{C}|} \mapsto \Re_+^{|\mathcal{C}|}$. (We introduce the notation $\Re_+ := \{ x \in \Re \mid x \geq 0 \}$ and $\Re_{++} := \{ x \in \Re \mid x > 0 \}$.)

In an application to OD estimation, d is in the order of $|\mathcal{C}|$, while $d \approx |\mathcal{L}|$ holds in equilibrium network design, pricing and control models.

We also introduce the matrix $\Gamma \in \Re^{|\mathcal{R}| \times |\mathcal{C}|}$, which is the route–OD pair incidence matrix (i.e., the element γ_{rk} is 1 if route r joins OD pair $k = (p,q) \in \mathcal{C}$, and 0 otherwise). Then, demand-feasibility is described by the conditions that $h \in \Re_+^{|\mathcal{R}|}$ and

$$\Gamma^{\mathrm{T}} h = g(\rho, \pi) \tag{1}$$

holds, while the Wardrop equilibrium conditions for the route flows are that

$$\begin{aligned} h_r > 0 &\implies c_r(\rho,h) = \pi_{pq}, \qquad r \in \mathcal{R}_{pq}, \qquad (p,q) \in \mathcal{C}, &\text{(2a)}\\ h_r = 0 &\implies c_r(\rho,h) \geq \pi_{pq}, \qquad r \in \mathcal{R}_{pq}, \qquad (p,q) \in \mathcal{C}, &\text{(2b)}\end{aligned}$$

holds, where the value of $\pi_{pq} := \pi_{pq}(\rho,h)$ is the minimal (i.e., equilibrium) route cost in OD pair (p,q). By the non-negativity of the route flows, the system (1)–(2) can more compactly be written as the mixed complementarity problem (MCP)

$$\begin{aligned} 0^{|\mathcal{R}|} \leq h \perp (c(\rho,h) - \Gamma\pi) &\geq 0^{|\mathcal{R}|}, &\text{(3a)}\\ \Gamma^{\mathrm{T}} h &= g(\rho,\pi), &\text{(3b)}\end{aligned}$$

where $a \perp b$, for two arbitrary vectors $a, b \in \Re^n$, means that $a^{\mathrm{T}} b = 0$. (By nonnegativity, this implies that $a_j \cdot b_j = 0$ for all j.)

As we shall be interested in the sensitivity of link flows, we will assume that the route cost is additive. For each link $l \in \mathcal{L}$, the travel cost has the form $t_l(\rho, v)$, where $v \in \Re^{|\mathcal{L}|}$ is the vector of link flows. The route and link travel costs and flows are related through a route–link incidence matrix, $\Lambda \in \{0,1\}^{|\mathcal{L}| \times |\mathcal{R}|}$, whose element λ_{lr} equals one if route $r \in \mathcal{R}$ utilizes link $l \in \mathcal{L}$, and zero otherwise. Route r has an additive route cost $c_r(\rho,h)$ if it is the sum of the costs of using all the links defining it. In other words, $c_r(\rho,h) = \sum_{l \in \mathcal{L}} \lambda_{lr} t_l(\rho,v)$. In short, then, $c(\rho,h) = \Lambda^{\mathrm{T}} t(\rho,v)$. Also, implicit in this relationship is the assumption that the pair (h,v) is consistent, in the sense that v equals the sum of the route flows: $v = \Lambda h$. We shall use the representation in terms of v, as it is an entity for which we can introduce conditions ensuring that uniqueness holds at equilibrium.

A more familiar representation of the parameterized Wardrop conditions (3) is that of a variational inequality problem (VIP),

$$-f(\rho,x) \in N_C(x), \tag{4}$$

where $x \in \Re^n$, $C \subseteq \Re^n$ is a closed and convex set, $f(\rho,\cdot) : C \mapsto \Re^n$ is smooth, and where

$$N_C(x) = \begin{cases} \{ z \in \Re^n \mid z^{\mathrm{T}}(x-y) \leq 0, \ \forall y \in C \}, & x \in C, \\ \emptyset, & x \notin C, \end{cases}$$

denotes the normal cone to C at x. Letting

$$x := \begin{pmatrix} h \\ \pi \\ v \end{pmatrix} \in \Re^{|\mathcal{R}|} \times \Re^{|\mathcal{C}|} \times \Re^{|\mathcal{L}|}, \quad f(\rho,x) := \begin{pmatrix} \Lambda^{\mathrm{T}} t(\rho,v) - \Gamma\pi \\ \Gamma^{\mathrm{T}} h - g(\rho,\pi) \\ v - \Lambda h \end{pmatrix}, \quad \text{and} \quad C := \Re_+^{|\mathcal{R}|} \times \Re^{|\mathcal{C}|} \times \Re^{|\mathcal{L}|}, \tag{5}$$

we obtain an equivalent VIP formulation from (3), where f is parameterized by ρ. The equivalence between a nonlinear complementarity problem (NCP) [that is, (3a)] and a VIP over the non-negative orthant [that is, $-[c(\rho,h) - \Gamma\pi] \in N_{\Re_+^{|\mathcal{R}|}}(h)$] was established in [Kar69, Kar72]. That (3b) is equivalent to the statement that $-[\Gamma^{\mathrm{T}} h - g(\rho,\pi)] \in N_{\Re^{|\mathcal{C}|}}(\pi)$ follows trivially, since $N_{\Re^{|\mathcal{C}|}}$ is identically zero. Similarly, the equation $v = \Lambda h$ comes out as the last row of (5): $-[v - \Lambda h] \in N_{\Re^{|\mathcal{L}|}}(v)$. Solutions exist to the problem (4), (5) whenever $g(\rho,\cdot)$ is upper bounded by some nonnegative vector.

We note that the familiar form of VIP,

$$x \in C; \quad f(\rho,x)^{\mathrm{T}}(y-x) \geq 0, \qquad y \in C,$$

is equivalent to (4) which we however prefer as it is more compact, and also lends itself better to the immediate application of the variational analysis theory that we will employ in this paper.

We may also formulate the Wardrop conditions in terms of link flows only. We introduce the link–node incidence matrix, $E \in \{-1,0,1\}^{|\mathcal{N}|\times|\mathcal{L}|}$, whose element e_{il} equals -1 if node i is the origin node of link l, 1 if node i is the destination node of link l, and 0 otherwise. The link–node version of Wardrop's equilibrium conditions states that at an equilibrium link flow v, being the aggregate of commodity (OD pair) volumes $w_k \in \Re^{|\mathcal{L}|}$, $k := (p,q) \in \mathcal{C}$, there exist vectors $\nu_k \in \Re^{|\mathcal{N}|}$ of node prices such that

$$0^{|\mathcal{L}|} \leq w_k \perp \left(t(\rho,v) - E^{\mathrm{T}}\nu_k\right) \geq 0^{|\mathcal{L}|}, \qquad k \in C;$$

for a link $(i,j) \in \mathcal{L}$, this means that $0 \leq w_{ijk} \perp (t_{ij}(\rho,v) - [\nu_{jk} - \nu_{ik}]) \geq 0$, $k \in \mathcal{C}$. The set of feasible volumes is the set of vectors $w_k \geq 0^{|\mathcal{L}|}$ for which $Ew_k = i_k g_k(\rho,\pi)$ holds.[1] We write this formulation in terms of the VIP (4) by letting

$$x := \begin{pmatrix} (w_k)_{k\in\mathcal{C}} \\ (\nu_k)_{k\in\mathcal{C}} \\ v \end{pmatrix} \in \Re^{|\mathcal{C}|\cdot|\mathcal{L}|} \times \Re^{|\mathcal{C}|\cdot|\mathcal{N}|} \times \Re^{|\mathcal{L}|}, \quad f(\rho,x) := \begin{pmatrix} (t(\rho,v) - E^{\mathrm{T}}\nu_k)_{k\in\mathcal{C}} \\ (Ew_k - i_k g_k(\rho,\pi))_{k\in\mathcal{C}} \\ v - \sum_{k\in\mathcal{C}} w_k \end{pmatrix}, \tag{6a}$$

$$C := \Re_+^{|\mathcal{C}|\cdot|\mathcal{L}|} \times \Re^{|\mathcal{C}|\cdot|\mathcal{N}|} \times \Re^{|\mathcal{L}|}. \tag{6b}$$

This problem has solution whenever, in addition to what has already been stated, the link cost $t(\rho,\cdot)$ is cycle-wise nonnegative.

Although the formulations introduced here are somewhat abstract, we will later show how more familiar formulations, such as the optimization models of Beckmann et al. [BMW56] for traffic assignment come out as special cases. The sensitivity analysis concentrates on the two general models (5) and (6), however, because the sensitivity analysis framework that we will use depends on the VIP having this form, where the feasible set C is a nonempty polyhedron, and where the parameter is present only in the smooth mapping f.

2 An overview of sensitivity analysis for traffic equilibria

Recall that our model is of the form

$$-f(\rho,x) \in N_C(x), \tag{7}$$

where $\rho \in \Re^d$ is the parameter, $x \in \Re^n$ is the solution, $f : \Re^d \times \Re^n \mapsto \Re^n$ is a smooth function, and $C \subseteq \Re^n$ is a nonempty polyhedral set. Our attention is focused on the generalized differentiation of the solution mapping

$$S : \rho \mapsto S(\rho) := \{\, x \mid -f(\rho,x) \in N_C(x) \,\} \tag{8}$$

at a pair (ρ^*, x^*) with $x^* \in S(\rho^*)$, that is, the set of solutions to the variational inequality (7) at $\rho = \rho^*$. The study of the continuity and differentiability of the mapping S with respect to variations in ρ that one encounters in the literature on traffic equilibria, have roughly been of three different kinds. We shall first briefly review them before we turn to our analysis of the model.

2.1 Braess' paradox-type analyses

One type of analysis of traffic equilibria sensitivity is qualitative; often, such analyses have been performed in conjunction with studies of traffic flow paradoxes. It all started with Braess' [Bra68] famous illustrative example of a network in which the travellers realize a higher cost when a link is improved, and the practical case reported by Knödel [Knö69]. Following these examples, Fisk [Fis79] showed that, analogously, an increase in one OD pair's demand may result in a decrease in another OD pair's travel costs on some routes. The continuity, and local Lipschitz continuity, of the travel costs with respect to changes in the demands, were studied in [Hal78] and in [DaN84b, DaN84c] respectively. (Incidentally, similar but stronger results, in fact characterizations, will be brought out automatically from the analysis to follow,

[1] The vector $i_k \in \{-1,0,1\}^{|\mathcal{N}|}$ is an indicator vector which is zero in all positions but two where, by the sign convention introduced earlier, the element with value 1 (-1) corresponds to the sink (source) node. The vector i_k also relates the OD node price vectors $\nu_k \in \Re^{|\mathcal{N}|}$ and the OD least cost value $\pi_k \in \Re$ through the relation $\pi_k = i_k^{\mathrm{T}}\nu_k$.

under weaker assumptions than in these references.) In line with Braess' paradox, work was done studying the direction of change in the travel costs to changes in the data, showing, in particular, that when one OD pair's demand increases, the equilibrium travel cost increases in that OD pair ([Hal78, Fan80, DaN84b, DaN84c]), as well as results on average changes ([DaN84b, DaN84c]).

Related to these sensitivity results are the studies on the prevalence of Braess' paradox for networks with special topologies. Steinberg and Zangwill [StZ83] studied the effect of the addition of a route, and in [DaN84a] the effect of changes in the demand, on the travel costs; the prevalence of Braess' paradox was ultimately found to depend on the ratio of the determinants of two very large matrices. See also [HaA01] for more recent developments on the subject.

2.2 The heuristic calculation of a "gradient"

The mapping S defined in (8) is differentiable only for some parameter values ρ^*, and especially so when the set C is defined in part by inequality constraints. Further, the calculation of the gradient, when it exists, is nontrivial. Here, we provide a discussion of the heuristics utilized to date in the calculation of an approximation to the gradient.

A vector taking the role of the gradient, whether it exists or not, is necessary to obtain when applying gradient-based algorithms for bilevel programs, or mathematical programs with equilibrium constraints (MPEC), cf. [LPR96, OKZ98]. These are models in which the vector x is optimized with respect to an (upper-level) objective of the parameter ρ:

$$\begin{aligned} &\underset{\rho}{\text{minimize}}\ \phi(\rho, x), \\ &\text{subject to } \rho \in P, \\ &\qquad\qquad -f(\rho, x) \in N_C(x), \end{aligned}$$

where $\phi : \Re^d \times \Re^n \mapsto \Re$ is a smooth function, and $P \subseteq \Re^d$ is a nonempty and closed, typically also convex, set.

Heuristic constructions of "gradients" are grouped in two categories. In the first we place linear equations-based methods; the second refers to methods based on direct approximations of the mapping S.

The first category is primarily represented by the work of Tobin and Friesz [ToF88], and its extension in [CSF00]. Its basis is the classic Implicit Function Theorem ([Cla83, Section 7.1], [Ber95, Proposition A.25]): If a system of the form $\omega(\rho, x) = 0^n$, with $\omega : \Re^d \times \Re^n \mapsto \Re^n$ being continuous, is such that at (ρ^*, x^*) with $\omega(\rho^*, x^*) = 0^n$, ω has a continuous and nonsingular gradient matrix $\nabla_\rho \omega(\rho^*, x^*)$ in an open neighbourhood of (ρ^*, x^*), then there is a function $\psi : U_\rho \mapsto U_x$ from an open neighbourhood of ρ^* to an open neighbourhood of x^* which is continuous, and for which it holds that $x^* = \psi(\rho^*)$ and $\omega(\rho, \psi(\rho)) = 0^n$ on U_ρ; further, if ω is p times continuously differentiable, then so is ψ, and $\nabla\psi(\rho) = -\nabla_\rho \omega(\rho, \psi(\rho))[\nabla_x \omega(\rho, \psi(\rho))]^{-1}$ on U_ρ.

In order to utilize this result in the present context, Tobin and Friesz make two simplifying assumptions:

(a) The above system contains no inequality constraints. One must therefore assume that *every* route is used, or, alternatively, reduce the problem to one where only the routes being of minimum cost are included, and assume that all of them are used. (The positivity condition is spelled out explicitly in [CSF00].) As we will show in Section 5, there are cases where there does *not* exist a set of equilibrium route flows in which all shortest routes are used. In such a case, the result from the application of the above gradient formula does not necessarily contain the information sought. (In general, one cannot even interpret the resulting vector as a *subgradient*; see Section 6 for an analysis of subgradients.)

(b) In order for the Jacobian matrix $\nabla_\rho \omega(\rho^*, \psi(\rho^*))$ to be invertible, Tobin and Friesz suggest choosing one of the route flow equilibrium solutions that are extremal in the equilibrium set, that is, a feasible basis in the polyhedron $H^*(\rho^*)$. But a closer look at this matrix reveals that the existence of its inverse relies on the invertibility of the (smaller) matrix $\nabla_h c(\rho^*, h^*)$; this matrix will however *not* be invertible in general, especially not for deterministic models where the travel cost is additive, as the link–route incidence matrix Λ will not have full row rank when the number of routes is larger than the number of links. (See also the discussion made in [BeI97, Section 5.4].) (A case where this technique is ensured to work however is the (non-additive) logit-based stochastic user equilibrium model of Fisk [Fis80]. Further, as we shall show, the gradient of the logit solution provides useful results for the (limiting) deterministic model precisely when the latter's solution is differentiable.)

To summarize, this gradient formula may provide a result when the implicit function theorem is not applicable, and may not provide a result even when the equilibrium link flow solution is differentiable. However, the technique has been applied in a wide spectrum of areas in transportation research, such as in network design ([KiS90]), transit network optimization ([MiS95]), traffic control ([YaY95, Chi99, WYL01]), OD estimation ([Den94, Yan95]), car ownership studies ([TaL00]), bicriterion traffic equilibrium ([Leu98]), and congestion pricing ([YaL96]). Some of the experiments conducted seem to have been successful, which implies that (a) the cases where the equilibrium link flow is not differentiable is small (it is indeed a set with Lebesgue measure zero, although optimal solutions to MPEC problem tend to be nondifferentiable), or, in the experiments conducted to date, the algorithms implemented have not been able to encounter (near-)optimal solutions; (b) the problems solved so far have been very small, and the number of routes sufficiently small, such that the result's applicability has not yet been challenged by the topological dependency described earlier. The only numerical comparison reported between the matrix-based heuristic of [ToF88] and a variational analysis based approach (in this case the report [DrL92]; see below) has been performed in [Den94] for OD estimation models, with the conclusion that the latter was more easy to use and provided more reliable results.

In the solution of OD estimation/adjustment problems, approximations of the mapping S defined in (8) have also been used. From the relation $\Lambda h = v$ we have that

$$v_l = \sum_{(p,q)\in\mathcal{C}} \sum_{r\in\mathcal{R}_{pq}} \lambda_{lr} h_r = \sum_{(p,q)\in\mathcal{C}} \rho_{pq} \sum_{r\in\mathcal{R}_{pq}} \lambda_{lr}\gamma_r, \quad l \in \mathcal{L},$$

where ρ_{pq} is the OD demand parameter $[g(\rho) \equiv \rho]$, and $\gamma_r := \frac{h_r}{\rho_{pq}}$ is interpreted as the route flow probability. (Unless $H^*(\rho^*)$—the set of equilibrium route flows—is a singleton, this value is not uniquely defined, and it is further clearly dependent on the value of ρ.)

Spiess [Spi90] makes the approximation that γ_r does not vary locally around the current value of ρ. In that case, the "partial derivative" of the equilibrium value of v_l with respect to the value of ρ_{pq} is $\sum_{r\in\mathcal{R}_{pq}} \lambda_{lr}\gamma_r$. Based on this approximate value of $\nabla_\rho v$ (which may or may not exist), an approximate "gradient" of the upper-level function in the MPEC problem can be obtained.

Drissi-Kaïtouni and Lundgren [DrL92] replace Spiess' linear approximation by a quadratic one. The "Jacobian" of the link cost vector with respect to the demand vector is calculated as follows. For each OD pair $(p,q) \in \mathcal{C}$, the directional derivative of v at v^* in the unit direction of e_{pq} is approximately obtained by solving the problem to

$$\underset{v'}{\text{minimize}}\ \frac{1}{2}(v')^{\mathrm{T}}\nabla t(v^*)v', \tag{9a}$$

$$\text{subject to } \Gamma^{\mathrm{T}} h' = e_{pq}, \tag{9b}$$

$$v' = \Lambda h'. \tag{9c}$$

The traffic equilibrium problem is solved with the DSD algorithm of [LaP92], which provides the equilibrium link flow v^* and a consistent route flow, the data for which is a subset $\hat{\mathcal{R}}$ of $\mathcal{R}$ that is explicitly stored and utilized also in the solution of (9). As we shall show, this problem provides an approximation of the correct value of the directional derivative which is correct (for the route subset generated) when the equilibrium link flow is differentiable (cf. Section 4).

The OD estimation algorithm of Codina and Barceló [CoB00] is different in that it is based on the generation of approximate *subgradients* of v, and the use of a subgradient-based descent algorithm. Since it does not fit into the sensitivity analysis framework of this paper, we shall not mention its workings in more detail here, but remark that the idea of generating approximate subgradients is an interesting line of research also for more general bilevel optimization problems in transport. It is an especially intriguing technique, since subgradients exist even at values of ρ^* where the gradient does not. (See further Section 6 for an analysis of the calculation of subgradients.)

2.3 Sensitivity analysis by directional derivatives

The third approach to sensitivity analysis is based on studying the direction of change of the solution x from *directional* changes of the parameter ρ, that is, the (vector-valued) directional derivative of x at ρ^* with respect to a direction ρ'. We shall use the notation $DS(\rho^* \mid x^*)(\rho')$ in our application.

Sensitivity analysis in the form of directional derivatives is, like the gradient, based on a kind of implicit function theorem, and in fact generalizes it. The directional derivative exists under much milder conditions than the gradient; when the gradient exists, its value can be obtained component-wise through calculating the directional derivative along all of the coordinate directions of ρ from ρ^*.[2]

For the sake of the discussion, we introduce the vector-valued function $\omega : O \mapsto \Re^n$, where $O \subseteq \Re^d$ is open. We also introduce one particular notion of a derivative, the *B(ouligand)*-derivative, below.

Definition 1 (B-derivative, [Rob85]). *The function ω is B-differentiable at $\rho^* \in O$ if there is a positively homogeneous function $D\omega(\rho^*) : \Re^d \mapsto \Re^n$, the B-derivative, such that*

$$\omega(\rho) = \omega(\rho^*) + D\omega(\rho^*)(\rho - \rho^*) + o(\|\rho - \rho^*\|),$$

where $o(\cdot)$ is such that $o(t)/t$ converges to zero as $t \to 0$. □

We note that, if the function $D\omega(\rho^*)$ exists, then it is unique (e.g., [Rob91]), and a B-differentiable function is directionally differentiable. When ω is *locally Lipschitz at ρ^** (that is, there exists a positive constant L such that

$$\|\omega(\rho^1) - \omega(\rho^2)\| \leq L\|\rho^1 - \rho^2\|$$

holds for all pairs (ρ^1, ρ^2) in a neighbourhood of ρ^*), then not only does the B-derivative exist at ρ^*, but it is then also equivalent to several other forms of derivatives, as analyzed by Shapiro [Sha90a]. (It is also equivalent to the semi-derivative of [RoW98, DoR02] (cf. [RoW98, Theorem 7.21 and p. 295]) which was utilized in the sensitivity analysis of elastic demand traffic equilibria in [PaR02b], even in the absence of Lipschitz continuity.) We note also that the differentiability of ω at ρ^* entails precisely that $D\omega(\rho^*)$ is linear. Further properties of the B-derivative are given in [Pan90a, Pan90b, RoW98]. We need, in particular, later to introduce regularity conditions on the traffic equilibrium problem so that the solution mapping S defined in (8) is single-valued and locally Lipschitz continuous.

We return now to the problem (7). The B-derivative of x at ρ^* in the direction of ρ' will be shown to be the solution to a kind of linearization of (7). To this end, we define first the critical cone ([Rob85])

$$K := T_C(x^*) \cap f(\rho^*, x^*)^{\perp}. \tag{10}$$

The set K defines the set of variations around x^* that retain first-order feasibility and optimality. The set $T_C(x^*)$ is the tangent cone to C at x^*. When C is described by linear constraints, we have

$$C = \{\, x \in \Re^n \,|\, Ax \geq b;\ Bx = d \,\} \quad \Longrightarrow \quad T_C(x^*) = \left\{\, z \in \Re^n \,|\, \bar{A}z \geq 0;\ Bz = 0 \,\right\},$$

where $\bar{A}$ consists of the rows A_i of A corresponding to the binding inequality constraints at x^*, that is, the indices i with $A_i x^* = b_i$. Further, for any vector $z \in \Re^n$, $z^{\perp} := \{\, y \in \Re^n \mid z^{\mathrm{T}} y = 0 \,\}$ is the orthogonal subspace associated with the vector z.

Sensitivity analysis centers around the solution to the following problem, which is a variational inequality defined by a first-order approximation of the original cost function over the set K.

$$DS(\rho^* \mid x^*)(\rho') := \{\, x' \in \Re^n \,|\, r(\rho', x') + N_K(x') \ni 0^n \,\},$$

where

$$r(\rho', x') := \nabla_\rho f(\rho^*, x^*)\rho' + \nabla_x f(\rho^*, x^*)x'. \tag{11a}$$

From now on, we will assume that the function f is differentiable in a neighbourhood of (ρ^*, x^*) with $x^* \in S(\rho^*)$, so that (11a) is defined.

The central question is under which conditions $DS(\rho^* \mid x^*)(\rho')$ exists and equals the B-derivative of the solution. We begin by introducing the strong regularity condition (SRC) of Robinson [Rob80].

Definition 2 (strong regularity, [Rob80, Rob85]). *The problem (7) is strongly regular at ρ^* if the solution mapping S defined in (8) is single-valued and locally Lipschitz continuous in a neighbourhood of ρ^*. In the present setting where C is polyhedral, this is equivalent to the following: the affine variational inequality*

$$z \in \nabla_x f(\rho^*, x^*)y + N_K(y)$$

has a unique solution $y := y(z)$ for every $z \in \Re^n$. □

[2] The difference is most directly explained by the fact that the directional derivative, $D\omega(\rho^*)(\rho')$, say, of a function $\omega : \Re^d \mapsto \Re^n$ is associated with a mapping which is positively homogeneous—that is, $D\omega(\rho^*)(\tau\rho') = \tau D\omega(\rho^*)(\rho')$ holds for all $\tau \geq 0$ and $\rho' \in \Re^d$—, and piecewise linear, while the gradient is associated with a mapping which is linear, namely $\rho' \mapsto \nabla\omega(\rho^*)^{\mathrm{T}}\rho'$.

The following result provides a characterization of the existence of the B-derivative of S, in terms of the B-derivative itself. (For more general feasible sets, an excellent account of characterizations of strong regularity is found in [DoR98].)

THEOREM 3 (characterization of B-differentiability, [DoR02]). *Assume that the parameterization is such that* $\operatorname{rank} \nabla_\rho f(\rho^*, x^*) = n$. *Suppose that S is convex-valued around ρ^*, in the sense that $S(\rho)$ is a convex set for all ρ in some neighbourhood of ρ^*. (This is, in particular, satisfied when $f(\rho, \cdot)$ is monotone on C in this neighbourhood.) Then the following properties are equivalent:*

(a) *S is single-valued and Lipschitz continuous on some neighbourhood of ρ^*, hence strongly regular at ρ^*;*

(b) *$DS(\rho^*)$ is single-valued.*

Moreover, then S is B-differentiable at ρ^*, and $DS(\rho^*)$ is not only Lipschitz continuous and positively homogeneous but also piecewise linear. □

We remark that the first result is valid without the convex-valuedness, as it is a straightforward application of the definition of strong regularity (note that the matrix $\nabla_\rho f(\rho^*, x^*)$ has full rank). See also [DoR98, Corollary 2.3]. The full rank condition can always be fulfilled, by adding dummy parameters to ρ if necessary.

We also remark already at this stage that we will utilize Theorem 3 in such a way that we select the entities among the elements of x for which the conditions in (a) and (b) hold simultaneously, that is, that for those entities, both the equilibrium solution *and* the perturbation is unique. This means that the vector x for which we will apply the theorem will never contain the commodity variables h or w_k.

Kyparisis [Kyp90b, Lemma 2.1] established that if strong regularity holds at ρ^*, then the function $y \mapsto \nabla_x f(\rho^*, x^*) y$ is nonsingular on the subspace

$$K \cap (-K) = \left\{ z \in \Re^n \,|\, \bar{A}x^* = 0;\ Bz = 0 \right\} \cap f(\rho^*, x^*)^\perp;$$

if the set K defined in (10) is a subspace, that is, if $K = K \cap (-K)$ holds, then the converse is true also. He also showed (in [Kyp88, Lemma 2.1]) that the condition that

$$\nabla_x f(\rho^*, x^*) \text{ is positive definite on } K - K \tag{12}$$

implies SRC at ρ^*. (The set $K - K$ is the subspace consisting of all vectors of the form $\mu - \omega$ with $\mu, \omega \in K$.) The condition (12) has been used by several researchers in reaching sensitivity analysis results; see, e.g., [QiM89, Pan90b, PaR02b].

Differentiability, a stronger property than directional differentiability, can be established to hold under an additional condition on the properties of the mapping DS at ρ^*:

THEOREM 4 (characterization of differentiability, [Kyp90b]). *Suppose that SRC holds at x^*. Then, the mapping S is differentiable at ρ^* if, and only if,*

$$DS(\rho^* \mid x^*)(\rho') \in -K, \qquad \rho' \in \Re^d. \tag{13}$$

If further K is a subspace, that is, if $K = K \cap (-K)$, then the gradient can be represented as

$$\nabla_\rho x(\rho^*) = -Z \left[Z^{\mathrm{T}} \nabla_x f(\rho^*, x^*) Z \right]^{-1} Z^{\mathrm{T}} \nabla_\rho f(\rho^*, x^*), \tag{14}$$

for any $n \times \ell$ matrix Z such that $Z^{\mathrm{T}} Z$ is nonsingular and $z \in K \cap (-K)$ if and only if $z = Zy$ for some $y \in \Re^\ell$, where ℓ is the dimension of $K \cap (-K)$. □

[Independently, Pang [Pan90b] established this equivalence result with SRC replaced by the stronger condition (12).] Note that $DS(\rho^* \mid x^*)(\rho') \in K$ always holds when the former exists. This result is an extension of the differentiability result provided by the implicit function theorem, as it relies on neither strict complementarity, nor linear independence of the binding constraints. The latter part of the result shows that under particular circumstances, it is itself a kind of implicit function theorem; note also that (14) is similar to the formula stated in [ToF88].

Since the analysis of the generalized Jacobian of S, that is, the calculation of subgradients, is more complex, we wait until Section 6 to explain it.

2.4 An outline of previous sensitivity analyses of traffic equilibria

Sensitivity results of the form given here have been applied to traffic equilibrium problems only to a limited extent, and then to establish the existence of directional derivatives only. (Surprisingly, what appears to be the most interesting result for computational purposes, namely the result of Theorem 4, has not seen the light of day in traffic applications until now.) The results, which are given in [QiM89, Yen95, Out97, PaR02b] have also been published mostly in journals outside of the transportation science domain. A short summary of them are given below. More details, and a comparison with our results, will be given later.

Qiu and Magnanti [QiM89, Theorem 4.1.1] studied an elastic demand model using the inverse $d \mapsto g^{-1}(\rho, d)$ of the demand function, and established that the mapping S is strongly regular at ρ^*, if (a) in a neighbourhood of (ρ^*, v^*, d^*) [for $(v^*, d^*) \in S(\rho^*)$ where $d^* \in \Re^{|\mathcal{C}|}$ is the equilibrium demand], $(\rho, v, d) \mapsto [t(\rho, v), -g^{-1}(\rho, d)]$ is continuous and further Lipschitz continuous with respect to ρ at (v^*, d^*), and differentiable with respect to (v, d) at (v^*, d^*); (b) its Jacobian at (v^*, d^*) is positive definite on the subspace $K - K$, that is, the condition (12). Although they stated the solution mapping S in the link flow space, they concluded that since the equilibrium route flows are not unique, Robinson's theory of strong regularity could not be applied directly, and they selected a (uniquely determined) representative equilibrium route flow solution by means of solving a strictly convex quadratic projection problem; a process similar to that made in [ToF88], and which is also used in [Yen95].

Tobin and Friesz [ToF88] noted that the choice of any particular route flow (or, indeed, any commodity link flow), was immaterial to the result of the sensitivity analysis in the link flow space. Patriksson and Rockafellar [PaR02b] established the fundamental property that lies behind this fact: the tangent cone in the space of v is the sum of the tangent cones in the commodity link flow spaces, whence the choices made in the latter has no effect on the appearance of the former, aggregated, set. We will use this fact also in this paper. Our approach is simpler than all of the above, in that we simply choose the solution vector x in $S(\rho)$ such that x satisfies the conditions of Theorem 3; this is also a type of projection. Patriksson and Rockafellar also established the existence of directional derivatives of the demand and link flow vectors, under conditions similar to those in [QiM89], however for both the link–route and link–node representations.

Outrata [Out97, Proposition 1.2] established strong regularity for a general class of variational problems, under conditions which here would translate to strong monotonicity of the mapping $(v, d) \mapsto [t(\rho, v), -g^{-1}(\rho, d)]$ on the feasible set, and a matrix condition like the one in [QiM89] but for a larger subspace. He also has a special application to the cost-perturbed fixed demand traffic equilibrium model, for which he devises a subgradient formula. A similar strong regularity result is also reached independently by Yen [Yen95, Theorem 4.1], where however also the inelastic demand is parameterized.

As remarked in [PaR02b], the B-differentiability of S implies the semismoothness of S, which will enable the use of bundle-type descent approaches in applications to bilevel optimization. (See [PaR02a] for detailed discussions on this topic, [Mif77] for a definition of semismoothness, and the conclusion section.)

We are now ready to establish the existence of, and formulas for calculating, the directional derivative and gradient of the equilibrium link flow solution and the corresponding equilibrium route costs.

3 Directional differentiability of traffic equilibria

3.1 The sensitivity problem

The sensitivity problem is first developed for the link–route representation.

Let ρ^* be given, and let $S(\rho^*)$ be given by the set

$$\left\{ v^* \in \Re^{|\mathcal{L}|} \;\middle|\; \exists \begin{pmatrix} h^* \\ \pi^* \\ v^* \end{pmatrix} \text{ which solves (7), (5)} \right\}.$$

For an arbitrary choice of ρ', we develop $DS(\rho^* \mid v^*)(\rho')$, as follows. Let h^* be an arbitrary equilibrium route flow, consistent with v^*, and let π^* be the vector of least route costs given (ρ^*, v^*). The cone K

defined in (10) is the following. First,

$$T_C(x^*) = \left\{ \begin{pmatrix} h' \\ \pi' \\ v' \end{pmatrix} \in \Re^{|\mathcal{R}|} \times \Re^{|\mathcal{C}|} \times \Re^{|\mathcal{L}|} \,\middle|\, \begin{array}{l} h'_r \geq 0 \text{ if } h^*_r = 0 \\ [r \in \mathcal{R}_{pq},\ (p,q) \in \mathcal{C}] \end{array} \right\},$$

while

$$\begin{aligned} f(\rho^*, x^*)^\perp &= \left\{ \begin{pmatrix} h' \\ \pi' \\ v' \end{pmatrix} \in \Re^{|\mathcal{R}|} \times \Re^{|\mathcal{C}|} \times \Re^{|\mathcal{L}|} \,\middle|\, [\Lambda^{\mathrm{T}} t(\rho^*, v^*) - \Gamma \pi^*]^{\mathrm{T}} h' = 0 \right\} \\ &= \left\{ \begin{pmatrix} h' \\ \pi' \\ v' \end{pmatrix} \in \Re^{|\mathcal{R}|} \times \Re^{|\mathcal{C}|} \times \Re^{|\mathcal{L}|} \,\middle|\, \sum_{r \in \mathcal{R}:\, c_r(\rho^*, h^*) > \pi^*_{pq}} \left[c_r(\rho^*, h^*) - \pi^*_{pq}\right] h'_r = 0 \right\}. \end{aligned}$$

Hence, the set of directions that retain feasibility and optimality at h^* is

$$K := T_C(x^*) \cap f(\rho^*, x^*)^\perp = \left\{ \begin{pmatrix} h' \\ \pi' \\ v' \end{pmatrix} \in \Re^{|\mathcal{R}|} \times \Re^{|\mathcal{C}|} \times \Re^{|\mathcal{L}|} \,\middle|\, \begin{array}{l} h'_r \text{ free if } h^*_r > 0 \\ h'_r \geq 0 \text{ if } h^*_r = 0 \text{ and } c_r(\rho^*, h^*) = \pi^*_{pq} \\ h'_r = 0 \text{ if } h^*_r = 0 \text{ and } c_r(\rho^*, h^*) > \pi^*_{pq} \\ [r \in \mathcal{R}_{pq},\ (p,q) \in \mathcal{C}] \end{array} \right\}. \tag{15}$$

The cost mapping of $DS(\rho^* \mid x^*)(\rho')$ is

$$\begin{aligned} r(\rho', x') &= \begin{pmatrix} \Lambda^{\mathrm{T}} \nabla_\rho t(\rho^*, v^*) \\ -\nabla_\rho g(\rho^*, \pi^*) \\ 0 \end{pmatrix} \rho' + \begin{pmatrix} 0 \\ \Gamma^{\mathrm{T}} \\ -\Lambda \end{pmatrix} h' + \begin{pmatrix} -\Gamma \\ -\nabla_\pi g(\rho^*, \pi^*) \\ 0 \end{pmatrix} \pi' + \begin{pmatrix} \Lambda^{\mathrm{T}} \nabla_v t(\rho^*, v^*) \\ 0 \\ I \end{pmatrix} v' \\ &= \begin{pmatrix} \Lambda^{\mathrm{T}} [\nabla_\rho t(\rho^*, v^*)^{\mathrm{T}} \rho' + \nabla_v t(\rho^*, v^*)^{\mathrm{T}} v'] - \Gamma \pi' \\ \Gamma^{\mathrm{T}} h' - [\nabla_\rho g(\rho^*, \pi^*)^{\mathrm{T}} \rho' + \nabla_\pi g(\rho^*, \pi^*)^{\mathrm{T}} \pi'] \\ v' - \Lambda h' \end{pmatrix}, \end{aligned}$$

reaching the sensitivity problem

$$-\begin{pmatrix} \Lambda^{\mathrm{T}} [\nabla_\rho t(\rho^*, v^*)^{\mathrm{T}} \rho' + \nabla_v t(\rho^*, v^*)^{\mathrm{T}} v'] - \Gamma \pi' \\ \Gamma^{\mathrm{T}} h' - [\nabla_\rho g(\rho^*, \pi^*)^{\mathrm{T}} \rho' + \nabla_\pi g(\rho^*, \pi^*)^{\mathrm{T}} \pi'] \\ v' - \Lambda h' \end{pmatrix} \in N_K(h', \pi', v'), \tag{16}$$

where K is given by (15).

Comparing the above with the original model (5), we see that the sensitivity problem has affine link travel costs, $v' \mapsto \nabla_\rho t(\rho^*, v^*)^{\mathrm{T}} \rho' + \nabla_v t(\rho^*, v^*)^{\mathrm{T}} v'$, an affine demand function, $\pi' \mapsto \nabla_\rho g(\rho^*, \pi^*)^{\mathrm{T}} \rho' + \nabla_\pi g(\rho^*, \pi^*)^{\mathrm{T}} \pi'$, and that the non-negativity restrictions on the route flows are here replaced by the sign restrictions in (15); the problem is a special affine traffic equilibrium problem.

We develop a few special cases, before turning to the node–link representation.

First, we take a look at the fixed demand case. The equilibrium model then is equivalent to

$$-t(\rho, v) \in N_{\widehat{F}(\rho)}(v), \tag{17a}$$

where

$$\widehat{F}(\rho) := \left\{ v \in \Re^{|\mathcal{L}|} \,\middle|\, \exists h \in H(\rho) \text{ with } v = \Lambda h \right\}, \tag{17b}$$

and

$$H(\rho) := \left\{ h \in \Re^{|\mathcal{R}|}_+ \,\middle|\, \Gamma^{\mathrm{T}} h = g(\rho) \right\}. \tag{17c}$$

Noting that the set K is independent of the appearance of the demand function, let

$$H'_W = \left\{ h' \in \Re^{|\mathcal{R}|} \,\middle|\, \exists \begin{pmatrix} \pi' \\ v' \end{pmatrix} \in \Re^{|\mathcal{C}|} \times \Re^{|\mathcal{L}|} \text{ with } \begin{pmatrix} h' \\ \pi' \\ v' \end{pmatrix} \in K \right\}, \tag{18a}$$

(18b)

$$H'(\rho') = H'_W \cap \left\{ h' \in \Re^{|\mathcal{R}|} \,\middle|\, \Gamma^{\mathrm{T}} h' = \nabla g(\rho^*) \rho' \right\}, \tag{18c}$$

and

$$\widehat{F}'(\rho') = \left\{ v' \in \Re^{|\mathcal{L}|} \,\middle|\, \exists h' \in H'(\rho') \text{ with } v' = \Lambda h' \right\}. \tag{18d}$$

By the cone decomposition results in [PaR02b], the set $\widehat{F}'(\rho')$ is independent of the choice of h^* in the set $H^*(\rho^*)$ of equilibrium route flows. The statement that $-r(\rho', x') \in N_K(x')$ holds is therefore equivalent to the VIP of finding $v' \in \Re^{|\mathcal{L}|}$ such that

$$-[\nabla_\rho t(\rho^*, v^*)^{\mathrm{T}} \rho' + \nabla_v t(\rho^*, v^*)^{\mathrm{T}} v'] \in N_{\widehat{F}'(\rho')}(v'). \tag{19}$$

This problem then is $DS(\rho^* \mid v^*)(\rho')$. The cost changes π' are precisely the Lagrange multipliers for the demand constraints $\Gamma^{\mathrm{T}} h' = \nabla g(\rho^*)\rho'$.

To illustrate the connection to the original fixed demand traffic equilibrium model, we assume for now that $g(\rho) = \bar{g} + \rho$, where $\bar{g} \in \Re^{|\mathcal{C}|}_{++}$, in which case $\nabla g(\rho^*)\rho' = \rho'$ holds, and further that the link travel cost function $t(\rho^*, \cdot)$ is separable. Then, the above variational inequality is the first-order optimality conditions for the problem to

$$\begin{aligned}
\underset{v'}{\text{minimize}} \; & \sum_{l \in \mathcal{L}} \int_0^{v_l'} \frac{\partial t_l(\rho^*, v_l^*)}{\partial v_l} s \, ds + [\nabla_\rho t(\rho^*, v^*)\rho']^{\mathrm{T}} v' \\
& = \sum_{l \in \mathcal{L}} \left(\frac{1}{2} \frac{\partial t_l(\rho^*, v_l^*)}{\partial v_l} (v_l')^2 + \tau_l v_l' \right), && \text{(20a)} \\
\text{subject to } & \Gamma^{\mathrm{T}} h' = \rho', && \text{(20b)} \\
& h' \in H_W', && \text{(20c)} \\
& v' = \Lambda h', && \text{(20d)}
\end{aligned}$$

where τ_l is element l of the vector $\nabla_\rho t(\rho^*, v^*)\rho'$. Compared with the original fixed demand model, we notice that it is similar; some of the routes in (20) are restricted to be zero, while others are not sign restricted. Further, the original cost is replaced by an affine one, so that the objective function in (20) is quadratic.

In the case that the demand further is unperturbed ($g(\rho) \equiv \bar{g} \in \Re^{|\mathcal{C}|}_{++}$), $\nabla g(\rho^*) = 0^{|\mathcal{C}|}$ holds, so the right-hand side of (20b) is zero, whence this particular sensitivity problem is defined over a flow circulation subspace. Also, it follows that the set $\widehat{F}'(\rho')$ in (18d) then is independent of ρ', and is given by

$$\widehat{F}' := \left\{ v' \in \Re^{|\mathcal{L}|} \,\middle|\, \exists h' \in H_W' \text{ with } v' = \Lambda h';\; \Gamma^{\mathrm{T}} h' = 0^{|\mathcal{C}|} \right\},$$

so the sensitivity problem is

$$-[\nabla_\rho t(\rho^*, v^*)^{\mathrm{T}} \rho' + \nabla_v t(\rho^*, v^*)^{\mathrm{T}} v'] \in N_{\widehat{F}'}(v'). \tag{21}$$

Next, we address the special case of the model (5) wherein the demand function $\pi \mapsto g(\rho, \pi)$ has an inverse, $d \mapsto \xi(\rho, d)$, on $\Re^{|\mathcal{C}|}$. Then, we can write the disaggregated model equivalently as

$$-\begin{pmatrix} c(\rho, h) \\ -\xi(\rho, d) \end{pmatrix} \in N_{H_d}(h, d),$$

where H_d is given by

$$H_d := \left\{ \begin{pmatrix} h \\ d \end{pmatrix} \in \Re^{|\mathcal{R}|}_+ \times \Re^{|\mathcal{C}|} \,\middle|\, \Gamma^{\mathrm{T}} h = d \right\}.$$

We provide the sensitivity problem for this model as well. Looked upon in the aggregated space of link flows and demands, the sensitivity problem is to find $(v', d') \in \widehat{F}_d'(\rho')$ such that

$$-\begin{pmatrix} \nabla_\rho t(\rho^*, v^*)^{\mathrm{T}} \rho' + \nabla_v t(\rho^*, v^*)^{\mathrm{T}} v' \\ -\nabla_\rho \xi(\rho^*, d^*)^{\mathrm{T}} \rho' - \nabla_d \xi(\rho^*, d^*)^{\mathrm{T}} d' \end{pmatrix} \in N_{\widehat{F}_d'}, \tag{22}$$

where

$$\widehat{F}_d' := \left\{ \begin{pmatrix} v' \\ d' \end{pmatrix} \mid \exists h' \in H_W' \text{ with } \Lambda h' = v';\; \Gamma^{\mathrm{T}} h' = d' \right\}.$$

The sensitivity problem (22) is equivalent to the aggregated form (16) of the sensitivity problem for the general elastic demand model.

From Theorem 3 it follows that the sensitivity problem (16) defines the B-derivative—therefore also the directional derivative—of the link flow solution, in the direction defined by any vector ρ' if, and only if, the solution v' is unique. Then also the shortest route cost changes, π', will be unique and therefore have the interpretation as the B-derivative of π in the direction of ρ'.

The sensitivity problem for the link–node formulation is developed similarly, and is, for an arbitrary choice of commodity link flows w_k^*, $k \in \mathcal{C}$ and matching OD travel costs and node prices (π_k^*, ν_k^*), $k \in \mathcal{C}$, the following:

$$-\begin{pmatrix} ([\nabla_\rho t(\rho^*, v^*)^{\mathrm{T}} \rho' + \nabla_v t(\rho^*, v^*)^{\mathrm{T}} v'] - E^{\mathrm{T}} \nu_k')_{k \in \mathcal{C}} \\ (E w_k' - i_k [\nabla_\rho g_k(\rho^*, \pi^*)^{\mathrm{T}} \rho' + \nabla_\pi g_k(\rho^*, \pi^*)^{\mathrm{T}} \pi'])_{k \in \mathcal{C}} \\ v' - \sum_{k \in \mathcal{C}} w_k' \end{pmatrix} \in N_{K_w} \begin{pmatrix} (w_k')_{k \in \mathcal{C}} \\ (\nu_k')_{k \in \mathcal{C}} \\ v' \end{pmatrix}, \tag{23a}$$

where K_w is given by

$$K_w = \left\{ \begin{pmatrix} (w_k')_{k \in \mathcal{C}} \\ (\nu_k')_{k \in \mathcal{C}} \\ v' \end{pmatrix} \,\middle|\, \begin{array}{l} w_{ijk}' \text{ free if } w_{ijk}^* > 0 \\ w_{ijk}' \geq 0 \text{ if } w_{ijk}^* = 0 \text{ and } t_{ij}(\rho^*, v^*) = \nu_{jk}^* - \nu_{ik}^* \\ w_{ijk}' = 0 \text{ if } w_{ijk}^* = 0 \text{ and } t_{ij}(\rho^*, v^*) > \nu_{jk}^* - \nu_{ik}^* \\ [(i,j) \in \mathcal{L}, k \in \mathcal{C}] \end{array} \right\}. \tag{23b}$$

This sensitivity problem has the same link costs and demand function as the one for the link–route representation, and the flow conservation constraints are almost identical to the original model's, except for the sign restrictions on the commodity link flow variables: the flow change allowed for a given link (i,j) in an OD pair k depends on whether it lies on a shortest route for the OD pair or not, and whether there is already a commodity flow on it. The sensitivity problems (16) and (23) are equivalent, in as much as the two equilibrium models (4), (5) and (4), (6) are equivalent. Given the equivalence between the two flow representations in the traffic equilibrium model and its perturbation, we do not need to reiterate the sensitivity results, once we have established them for one of the representations. We have chosen to work with the link–route formulation.

3.2 Directional differentiability of traffic equilibria

Throughout this section, we assume that the functions $t : \Re^d \times \Re^{|\mathcal{L}|} \mapsto \Re^{|\mathcal{L}|}$ and $g : \Re^d \times \Re^{|\mathcal{C}|} \mapsto \Re^{|\mathcal{C}|}$ are smooth (in C^1) on sufficiently large neighbourhoods of the sets involved in the calculations, in particular of (ρ^*, π^*, v^*). We could reduce this assumption to differentiability properties which are milder and which in particular are valid only in a neighbourhood of (ρ^*, π^*, v^*), but as these results are to be used in situations where, for example, the value ρ^* may change due to a bilevel optimization, we have opted to leave this generality aside.

THEOREM 5 (characterizations of directional differentiability, elastic demand case). *The following two statements are equivalent, and they imply the third.*

(a) *The pair (v^*, π^*) of equilibrium link flows and OD pair travel costs solving the problem (5) is single-valued (that is, unique) and locally Lipschitz continuous in a neighbourhood of ρ^*.*

(b) *Either of the following two equivalent statements* (i)–(ii) *is true.*

(i) *The matrices $\nabla_\rho t(\rho^*, v^*)$ and $\nabla_\rho g(\rho^*, \pi^*)$ have full rank. Further, the solution (v', π') to the model* (16) *is unique.*

(ii) *The linear traffic equilibrium problem*

$$-\begin{pmatrix} \Lambda^{\mathrm{T}} [z_v + \nabla_v t(\rho^*, v^*)^{\mathrm{T}} y_v'] - \Gamma y_\pi' \\ \Gamma^{\mathrm{T}} y_h' - z_\pi - \nabla_\pi g(\rho^*, \pi^*)^{\mathrm{T}} y_\pi' \\ y_v' - \Lambda y_h' \end{pmatrix} \in N_K(y_h', y_\pi', y_v')$$

has a unique solution $y' = (y_v', y_\pi') := y'(z)$ for every $z = (z_v, z_\pi) \in \Re^{|\mathcal{L}|} \times \Re^{|\mathcal{C}|}$ and $\rho' \in \Re^d$.

(c) *The pair (v^*, π^*) of equilibrium link flows and OD pair travel costs is directionally differentiable, in fact B-differentiable, at ρ^*, in any direction ρ', and the directional derivative is given by the unique solution pair (v', π') to the model* (16)*. Further, the directional derivative function $DS(\rho^* \mid (v^*, \pi^*))$ is Lipschitz continuous and piecewise linear.*

PROOF. The result in (a) is precisely strong regularity, as defined in Definition 2. As applied to the model (5), strong regularity is equivalent to the statement (b)(ii). The equivalence between (a) and (b)(i) follows from Theorem 3, and the same result establishes the implication (c). ∎

THEOREM 6 (characterizations of directional differentiability, fixed demand case). *Suppose that the demand function g is independent of π. In the statement* (a) *and* (c) *of Theorem* 5, *replace the model* (5) *by* (17)*; in the statement* (b)(i), *remove the condition on the matrix $\nabla_\rho g(\rho^*, \pi^*)$ and replace* (16) *by* (19)*; finally, in the statement* (b)(ii), *replace the affine variational inequality by the following:*

$$-[z_v + \nabla_v t(\rho^*, v^*)^{\mathrm{T}} y] \in N_{\widehat{F}'(\rho')}(y), \qquad z_v \in \Re^{|\mathcal{L}|}.$$

Then, the conclusions of Theorem 5 *are valid for the fixed demand model* (17).

PROOF. The result follows by tracing the proof of Theorem 5. ∎

We next provide sufficient conditions in terms of the original data for directional differentiability to follow. We will utilize the fact that the property (12) implies strong regularity, translating it to the problem at hand and its special cases. The first result concerns the general model (5), and the directional differentiability of the equilibrium link flow, travel cost, and demand.

Let

$$K_0 := \left\{ \begin{pmatrix} h' \\ \pi' \\ v' \end{pmatrix} \in \Re^{|\mathcal{R}|} \times \Re^{|\mathcal{C}|} \times \Re^{|\mathcal{L}|} \;\middle|\; \begin{array}{l} h'_r \text{ free if } h^*_r > 0 \\ h'_r = 0 \text{ if } h^*_r = 0 \text{ and } c_r(\rho^*, h^*) > \pi^*_{pq} \\ [r \in \mathcal{R}] \end{array} \right\},$$

which is the set $(K - K)$, and

$$H'_{W_0} = \left\{ h' \in \Re^{|\mathcal{R}|} \;\middle|\; \exists \begin{pmatrix} \pi' \\ v' \end{pmatrix} \in \Re^{|\mathcal{C}|} \times \Re^{|\mathcal{L}|} \text{ with } \begin{pmatrix} h' \\ \pi' \\ v' \end{pmatrix} \in K_0 \right\}.$$

COROLLARY 7 (sufficient conditions for directional differentiability, elastic demand case). *The following property implies the statement* (b)(i), *and therefore also the statement* (c), *in Theorem* 5, *guaranteeing the directional differentiability of the equilibrium link flow, OD travel cost, and equilibrium demand: the matrix*

$$\begin{pmatrix} \nabla_v t(\rho^*, v^*) & 0 \\ 0 & -\nabla_\pi g(\rho^*, \pi^*) \end{pmatrix} \tag{24}$$

is positive definite on the subspace

$$\widehat{F}^d_0 := \left\{ \begin{pmatrix} v' \\ d' \end{pmatrix} \in \Re^{|\mathcal{L}|} \times \Re^{|\mathcal{C}|} \;\middle|\; \exists h' \in H'_{W_0} \text{ with } v' = \Lambda h';\ \Gamma^{\mathrm{T}} h' = d' \right\}.$$

PROOF. First, we study the matrix $\nabla_x f(\rho^*, x^*)$ appearing in (12). In the model (5), in the space of (h, π, v), this matrix is

$$\begin{pmatrix} \Lambda^{\mathrm{T}} \nabla_v t(\rho^*, v^*) & -\Gamma^{\mathrm{T}} & 0 \\ 0 & -\nabla_\pi g(\rho^*, \pi^*) & \Gamma \\ I & 0 & -\Lambda^{\mathrm{T}} \end{pmatrix}.$$

We are interested in the result in the space of (v, π), since uniqueness only resides in this space. The transformation between the space of (h, π, v) to the space of (v, π) is provided by the matrix

$$\begin{pmatrix} \Lambda & 0 & 0 \\ 0 & I & 0 \\ 0 & 0 & 0 \end{pmatrix};$$

the matrix of interest therefore is the matrix (24).

As was remarked above, in the space of (h, π, v), the set $(K - K)$ equals K_0. The remaining components in the definition of the subspace $\widehat{F}^d_0$ define both the aggregation to the link flow space, and the restriction to the subspace of demand-feasible perturbations. This completes the proof. □

We next supply the corresponding results for the fixed demand case, for both perturbed and unperturbed demands. In the unperturbed case, the sensitivity problem is an affine variational inequality over the set of feasible circulations of flows where some route flows are restricted in sign. The positive definiteness condition can in this case be reduced somewhat, since the demand change is zero.

COROLLARY 8 (sufficient conditions for directional differentiability, fixed demand case). (a) *Suppose that the demand function g is independent of π. Then, the following property implies the directional differentiability of the equilibrium link flow and OD travel cost: the matrix $\nabla_v t(\rho^*, v^*)$ is positive definite on the subspace*

$$\widehat{F}_0 := \left\{ v' \in \Re^{|\mathcal{L}|} \,\middle|\, \exists h' \in H'_{W_0} \text{ with } v' = \Lambda h' \right\}.$$

(b) *Suppose further that the demand function is unperturbed, that is, $g(\rho) \equiv \bar{g} \in \Re^{|\mathcal{C}|}_{++}$. Then, the following property implies the directional differentiability of the equilibrium link flow and OD travel cost: the matrix $\nabla_v t(\rho^*, v^*)$ is positive definite on the (smaller) subspace*

$$\widehat{F}_{00} := \left\{ v' \in \Re^{|\mathcal{L}|} \,\middle|\, \exists h' \in H'_{W_0} \text{ with } v' = \Lambda h';\ \Gamma^{\mathrm{T}} h' = 0^{|\mathcal{C}|} \right\}.$$

PROOF. In the absence of the elastic demand term in the cost, the variable π' disappears, and the matrix of interest clearly is $\nabla_v t(\rho^*, v^*)$.

(a) In the case of perturbed demands, the set over which we solve the sensitivity problem is $\widehat{F}'(\rho')$. As ρ' varies in $\Re^d$, h' cannot a priori be restricted to a subspace smaller than $\Re^{|\mathcal{R}|}$. The smallest subspace that contains the range of $\widehat{F}'(\rho')$ as ρ' varies in $\Re^d$ therefore is the set F_0.

(b) In the case of unperturbed demands, the sensitivity problem reduces to (21). The range of link flow perturbations is therefore contained in the subspace defined by $\widehat{F}_{00}$. □

In the case of fixed and unperturbed demands, the condition (b)(ii) in the above theorem is a statement about the uniqueness of the solutions to the affine VIP

$$-[z_v + \nabla_v t(\rho^*, v^*)^{\mathrm{T}} y] \in N_{\widehat{F}'}(y), \qquad z_v \in \Re^{|\mathcal{L}|},$$

which is independent of ρ', and is more simple to verify.

REMARK 9 (is the case of standard TAP one where directional differentiability is guaranteed to hold?). The answer turns out not to be so simple. Consider the separable cost model. Normally, when modelling the traffic network, dummy links with zero costs are needed to model certain parts of the network, like the presence of centroid nodes for the OD pairs and certain turning movements, so not all links will in fact have strictly increasing costs; some of the dummy links may therefore not have unique equilibrium values. Nevertheless, consider a case where the real network links have BPR cost functions, where some of those are parameterized:

$$v_l \mapsto t_l(\rho, v_l) = \alpha_l + \rho_1 + 0.15 \cdot \left(\frac{v_l/\rho_2}{c_l} \right)^4, \quad \alpha_l > 0,\, c_l > 0.$$

Here, the value of $\rho_1 \in \Re$ could play the role of a link toll, while $\rho_2 > 0$ is a network design parameter. These links will have a unique flow.

Consider now the perturbed problem, which in our setting is (21). This problem is further one where the cost function is the gradient of a convex function. The characterization of directional differentiability is that the solution to the perturbed problem is unique. We will utilize the possibility to choose what "solution" means. Let S denote the mapping which assigns the optimal value of the link flows for which the travel costs are strictly increasing. Given the optimal solution v_l^*, the perturbed link cost is the sum of a constant and the term

$$0.6/(c_l^4 \rho_2) \cdot (v_l^*/\rho_2)^3 \cdot v_l'.$$

Clearly, this affine cost function is strictly increasing whenever $v_l^* > 0$, whence we will have a unique value of v_l' provided that link a has a positive flow.

A link that has a strictly increasing travel cost without parameters will give rise to a strictly increasing (respectively, increasing) perturbed link cost if its flow is positive (respectively, zero), and dummy links will have links with zero cost also in the perturbed problem. All these links will therefore have convex or strictly convex terms in the objective of the perturbed problem.

In general, then, if we project our problem for the given values of the parameters, such that S lies in the space of congested links for which the flow is positive, directional differentiability follows for those links. This is a positive result, because presumably they are the links for which we are indeed interested in the effects of perturbations in the data. □

To summarize the above development, under conditions that imply the uniqueness of the equilibrium link flows and demands, the sensitivity problem provides unique link flow and travel cost perturbations that have interpretations as directional derivatives.

4 Differentiability of traffic equilibria

4.1 Main results

As was stated in Theorem 4, once we have established directional differentiability, differentiability is equivalent to the condition (13), which we therefore need to analyze in detail. Complementarity has a crucial role here; we will show that the classic strict complementarity condition—that all the shortest routes are actually used—is a sufficient, but an unnecessarily strong condition to obtain differentiability.

Consider the set K defined in (15). Keeping in mind that this set depends on the choice of $h^* \in H^*(\rho^*)$, we have that

$$K \cap (-K) = \left\{ \begin{pmatrix} h' \\ \pi' \\ v' \end{pmatrix} \in \Re^{|\mathcal{R}|} \times \Re^{|\mathcal{C}|} \times \Re^{|\mathcal{L}|} \;\middle|\; \begin{array}{l} h'_r \text{ free if } h^*_r > 0 \\ h'_r = 0 \text{ if } h^*_r = 0 \\ {[r \in \mathcal{R}_{pq},\ (p,q) \in \mathcal{C}]} \end{array} \right\}.$$

As we consider the aggregated version in the space of v', we note as earlier that the set is independent of the choice of equilibrium route flow. The aggregated set in the space of v' in fact is the set of vectors $v' \in \Re^{|\mathcal{L}|}$ for which there exists an $h' \in \Re^{|\mathcal{R}|}$ with $v' = \Lambda h'$, and

$$\begin{array}{lll} h'_r \text{ free if } h^*_r > 0 \text{ for } \textit{some } h^* \in H^*(\rho^*), & r \in \mathcal{R}_{pq}, & (p,q) \in \mathcal{C}, \\ h'_r = 0 \text{ if } h^*_r = 0 \text{ for } \textit{every } h^* \in H^*(\rho^*), & r \in \mathcal{R}_{pq}, & (p,q) \in \mathcal{C}. \end{array}$$

Hence, each route r belongs to precisely one of these two sets; a methodology for determining this partition of $\mathcal{R}$ is given in Section 4.2.

The difference between this set and the set K is that in the set K, a variable h'_r which is associated with a shortest route that is forced to be zero on $H^*(\rho^*)$ because the consistency with v^* requires it, is allowed to become positive, whereas in the set $K \cap (-K)$, it is forced to be zero. As this condition must hold for every choice of perturbation ρ', according to Theorem 4, we can state the condition corresponding to (13) as follows:

Theorem 10 (characterization of differentiability of traffic equilibria). *For the case of elastic and fixed demands, respectively, let the assumptions of Theorem 5, statement* (a) *or* (b)*, be satisfied, or the corresponding assumptions in Theorem 6. Then, the following two statements are equivalent.*

(a) *The pair (v^*, π^*) of equilibrium link flows and OD pair travel costs is differentiable at ρ^*.*

Further, $DS(\rho^* \mid v^*)(\rho') = \nabla_\rho v(\rho^*)^{\mathrm{T}} \rho'$, and the corresponding formula holds for the derivative of π^* also. In particular, $\nabla_\rho v(\rho^*)$ is composed by the d elements $DS(\rho^* \mid v^*)(e_i)$, $i = 1, \ldots, d$, where e_i is the i^{th} unit d-vector.

(b) *Let $\rho' \in \Re^d$ be arbitrary. Let $r \in \mathcal{R}$ be a route for which $h^*_r = 0$ holds on the set $H^*(\rho^*)$. On the set of route flow changes h' consistent with the vector v' uniquely solving the sensitivity problem* (16) *[the case of elastic demands], respectively* (19) *[the case of fixed demands], $h'_r = 0$ holds.*

Proof. Follows by appealing to Theorem 4, and the above remarks. □

The presence of differentiability hinges on whether changes in the value of the parameter vector ρ changes the set of equilibrium routes. As "$h \geq 0^{|\mathcal{R}|}$" are the only inequality constraints present in any of the models discussed in this paper so far, it is not surprising that the conditions for differentiability are equivalent among them. In extensions to traffic equilibrium models where inequality side constraints on the flows are present, the situation will of course change.

An interesting application of the differentiability result presented above is that of the differentiation of the projection of a vector $\rho^* \in \Re^{|\mathcal{L}|}$ onto the fixed and unperturbed demand flow polyhedron. This case corresponds to the minimization of the function $\frac{1}{2}\|v - \rho^*\|$ over $\widehat{F}$, which one places in the framework of the traffic model by setting $t(\rho^*, v) := v - \rho^*$. The sensitivity problem has a special form—in particular, $r(\rho', v') = v' - \rho'$ holds—; it is therefore also a projection problem, of the vector ρ' onto the intersection of the tangent cone and the subspace perpendicular to the vector $v^* - \rho^*$. (Strong regularity obviously holds for the projection problem, so directional derivatives of Euclidean projections always exist on polyhedral sets.) The differentiability of this projection mapping at a limit point is at the heart of the convergence analysis of the descent algorithm of Patriksson and Rockafellar [PaR02a] for an MPEC model in traffic management, and its characterization has also been the subject of several theoretical studies (see, e.g., [Har77, Sha90b, Sha94, BCS98, BoS00]), mostly for more general sets and spaces. The convergence theorem of [PaR02a] utilizes the sufficient condition of strict complementarity discussed below.

The classic condition for the differentiability of the solution mapping S at a reference value ρ^* is that the solution x^* is (a) strictly complementary (or, non-degenerate), meaning that the Lagrange multiplier for a constraint is positive if and only if the constraint is binding, (b) that the binding constraint gradients (normals) are linearly independent (that is, the multiplier values are unique), and (c) that a second-order sufficiency condition is satisfied, which is a positive definiteness condition on a Jacobian matrix on a particular subspace. This is typically what is needed for problems posed over non-polyhedral constraints (cf. the surveys [Kyp90a, DoR98]). As Theorem 4 shows, for polyhedral constraints that do not include parameters, these conditions can be relaxed substantially.

In particular, as a corollary to Theorem 10, we can establish that strict complementarity is a sufficient—but not necessary—condition for the differentiability of the solution to the traffic equilibrium problem: Under the assumptions of that theorem, suppose that there exists a strictly complementary solution to the problem (5), that is, that for some $h^* \in H^*(\rho^*)$, it holds that for all $r \in \mathcal{R}$, $h_r^* > 0$ if and only if $c_r(\rho^*, h^*) = \pi_{pq}^*$. This condition implies that the set K equals $-K$, which means that the condition (13) is automatically satisfied. Theorem 4 then yields the result that the pair (v^*, π^*) of equilibrium link flows and OD pair travel costs is differentiable at ρ^*.

The calculus formula for the gradient adopted in [ToF88], which we discussed earlier in Section 2.2, is precisely the one that is contained in the second half of Theorem 4, and which is valid whenever $K = -K$ (and the matrix Z having the properties stated exists!). The gradient calculus of Tobin and Friesz [ToF88] relies on strict complementarity, although this condition is not a necessary one for differentiability.

4.2 Sensitivity analysis of stochastic user equilibria

The logit-based stochastic user equilibrium (SUE) model of Fisk [Fis80] is interesting in our context because it is one in which all the routes are used—by definition, because of the presence of the logit function. Therefore, strict complementarity is satisfied, and the SUE link *and* route flow solutions are differentiable whenever they are uniquely determined, which they are if, for example, $t(\rho^*, \cdot)$ is monotone on $\widehat{F}(\rho^*)$. (We limit ourselves in this section to the fixed demand model.) Moreover, if the function $t(\rho^*, \cdot)$ is strictly monotone on $\widehat{F}(\rho^*)$, we know that as the dispersion parameter tends to zero, the SUE solution tends to the unique equilibrium link flow solution solving (17) and the sequence of route flow solutions tends to a special equilibrium route flow solution, namely one which is strictly complementary in $H^*(\rho^*)$ if there is one (see Proposition 11 below). It is therefore natural to ask whether a sensitivity analysis of the SUE model can aid in the sensitivity analysis of the deterministic model (17). As it turns out, the answer is in the affirmative precisely when the deterministic link flow solution is differentiable.

Given the dispersion parameter $\theta > 0$, and assuming for simplicity for now that $t_l(\rho^*, v) \equiv t_l(\rho^*, v_l)$, $l \in \mathcal{L}$, all are differentiable and strictly increasing functions of v_l for every choice of ρ, the stochastic user equilibrium model of Fisk [Fis80] extends the deterministic optimization model as follows:

$$\underset{(v,h)}{\text{minimize}} \sum_{l \in \mathcal{L}} \int_0^{v_l} t_l(\rho^*, s)\, ds + \frac{1}{\theta} \sum_{r \in \mathcal{R}} h_r \log h_r, \tag{25a}$$

$$\text{subject to } \Gamma^{\mathrm{T}} h = g(\rho^*), \tag{25b}$$

$$h \geq 0^{|\mathcal{R}|}, \tag{25c}$$

$$v = \Lambda h. \tag{25d}$$

Thanks to the Cartesian product structure of the feasible set, there exists a strictly positive route flow solution, whence the unique optimal route flow also is strictly positive. Due to this property, the sensitivity analysis of this problem is somewhat easier than that of the deterministic model (17), as the route flow solution is strictly complementary; the optimal route flow is hence guaranteed to be differentiable in ρ under the same conditions as for the directional differentiability of the deterministic solution. We provide the sensitivity analysis for this problem, after which we relate it in detail to that of the model (17). (We note in passing that the sensitivity analyses in [Dav94, YiM01] are quite unrelated to ours.)

For $\theta > 0$, we denote the optimal route flow solution to (25) by $h^\theta(\rho^*)$. From now on, we assume for illustration purposes that $g(\rho) = \bar{g} + \rho$, with $g(\rho^*) \in \Re^{|\mathcal{C}|}_{++}$. Noting that $h^\theta(\rho^*) > 0$, the critical cone $K = T_C(x^*) \cap f(\rho^*, x^*)^\perp = \Re^{|\mathcal{R}|} \times \Re^{|\mathcal{C}|} \times \Re^{|\mathcal{L}|}$, so that not only is K a subspace, it is the entire space. Further,

$$r(\rho', x') = \begin{pmatrix} \Lambda^{\mathrm{T}}[\nabla_\rho t(\rho^*, v^*)^{\mathrm{T}} \rho' + \nabla_v t(\rho^*, v^*)^{\mathrm{T}} v'] + \dfrac{1}{\theta} \mathrm{diag}\,(1/h_r^\theta(\rho^*)) h' - \Gamma \pi' \\ \Gamma^{\mathrm{T}} h' - \rho' \\ v' - \Lambda h' \end{pmatrix},$$

where $\mathrm{diag}\,(1/h_r^\theta(\rho^*))$ denotes the diagonal matrix with diagonal entries $1/h_r^\theta(\rho^*)$, $r \in \mathcal{R}$.

By the assumptions on the link cost function $t(\rho^*, \cdot)$, the sensitivity problem is therefore equivalent to the problem to

$$\underset{(v',h')}{\text{minimize}} \sum_{l \in \mathcal{L}} \left(\frac{1}{2} \frac{\partial t_l(\rho^*, v_l^*)}{\partial v_l} (v_l')^2 + \tau_l v_l' \right) + \frac{1}{2\theta} \sum_{r \in \mathcal{R}} \log h_r^\theta(\rho^*) (h_r')^2, \tag{26a}$$

$$\text{subject to } \Gamma^{\mathrm{T}} h' = \rho', \tag{26b}$$

$$v' = \Lambda h', \tag{26c}$$

where τ is defined as in (20).

Note that the Jacobian of the cost mapping in (26) with respect to h' is

$$\Lambda^{\mathrm{T}} \nabla_v t(\rho^*, v^*) + \frac{1}{\theta} \mathrm{diag}\,(1/h_r^\theta(\rho^*));$$

the matrix $\mathrm{diag}\,(1/h_r^\theta(\rho^*))$ is positive definite on $\Re^{|\mathcal{R}|}$, whence we satisfy the condition (12) and therefore also the conditions for the differentiability Theorem 4 to be applicable.

Before we turn to the relations between the sensitivity analysis of the SUE and the deterministic solution, we cite an important result in this context on the relations between the solution $h^\theta(\rho^*)$, $\theta > 0$, to the SUE model and the set of equilibrium route flows in the deterministic model (17) as the value of θ tends to infinity.

The *most probable* equilibrium route flow solution (see, e.g., [RMH89, Jan93]) is the unique equilibrium route flow in the set $H^*(\rho^*)$, denoted $h^+(\rho^*)$, which solves the problem to

$$\underset{h}{\text{minimize}} \sum_{r \in \mathcal{R}} h_r \log h_r, \tag{27a}$$

$$\text{subject to } h \in H^*(\rho^*). \tag{27b}$$

Proposition 11 (the limit of the SUE solution, [LLPR01]). *Under the condition that each link cost $t_l(\rho^*, \cdot)$ is positive and strictly monotonically increasing,*

$$\lim_{\theta \to \infty} h^\theta(\rho^*) = h^+(\rho^*)$$

holds. □

This result implies that if, and only if, there exists a strictly complementary solution in the set $H^*(\rho^*)$, then so is $h^+(\rho^*)$. As strict complementarity is sufficient for the differentiability of the deterministic equilibrium link flow solution, a study of the limit of the sequence of solutions to the SUE model as $\theta \to \infty$ could therefore provide a proof that the deterministic solution is differentiable. The result is, in fact, even better, in that strict complementarity is not a necessary property for the analysis to carry over from the non-deterministic case.

The question then is whether we can use the fact that the SUE solution is differentiable to produce gradients for the deterministic model by studying the SUE model for large values of θ. We therefore study the sensitivity problem (26) as θ tends to infinity, and its relation to the sensitivity problem (20).

The two problems clearly are related; although the problem (26) lacks the sign constraints on h' of (20), as θ tends to infinity the additional term in the objective (26) seems to work as an interior penalty for h' becoming negative. Indeed, that is the case.

Consider first a route r for which $h_r^+ > 0$ holds. Then, in the limit as $\theta \to \infty$, the constant term $\log h_r^\theta(\rho^*)/(2\theta)$ tends to zero, so the second term in the objective of (26) disappears. This case is in line with the problem (20), where for such a route, h_r' is a variable with no sign restrictions.

Next, let's consider a route r for which $h_r^+ = 0$. [We note that such a route exists if and only if there does not exist a strictly complementary route flow solution in $H^*(\rho^*)$.] Notice that the logit formula gives that

$$h_r^\theta(\rho^*) = g_{pq}(\rho^*)\frac{\exp\left(-\theta c_r(\rho^*, h^\theta(\rho^*))\right)}{\sum_{\ell\in\mathcal{R}_{pq}} \exp\left(-\theta c_\ell(\rho^*, h^\theta(\rho^*))\right)}, \qquad r \in \mathcal{R}_{pq}, \qquad (p,q) \in \mathcal{C}.$$

We analyze the term $(2\theta)/\log h_r^\theta(\rho^*)$, the inverse of the term investigated, as a function of θ. The derivative formula for one-variable quotient functions then gives that the limit of this function as $\theta \to \infty$ equals that of the function

$$2c_r(\rho^*, h^\theta(\rho^*))h_r^\theta(\rho^*) \sum_{\ell\in\mathcal{R}_{pq}} \exp\left(-\theta c_\ell(\rho^*, h^\theta(\rho^*))\right) - 2h_r^\theta(\rho^*) \sum_{\ell\in\mathcal{R}_{pq}} c_\ell(\rho^*, h^\theta(\rho^*)) \exp\left(-\theta c_\ell(\rho^*, h^\theta(\rho^*))\right),$$

the limit of which is zero. Hence, the coefficient $\log h_r^\theta(\rho^*)/(2\theta)$ of h_r' tends to infinity with θ, and it is clear that for these variables, the additional objective term of (26) acts as a penalty for having $h_r' \neq 0$. In summary, in the limit, the problem (26) tends to the following problem as θ tends to infinity:

$$\underset{(v',h')}{\text{minimize}} \sum_{a\in\mathcal{L}} \left(\frac{1}{2}\frac{\partial t_l(\rho^*, v_l^*)}{\partial v_l}(v_l')^2 + \tau_l v_l'\right), \tag{28a}$$

$$\text{subject to } \Gamma^{\mathrm{T}} h' = \rho', \tag{28b}$$

$$h_r' = 0, \qquad r \in \mathcal{R} \text{ with } h_r^+ = 0, \tag{28c}$$

$$v' = \Lambda h'. \tag{28d}$$

This is a restriction of the problem (20), since in that problem, $h_r' \geq 0$ is allowed for routes that have a zero flow but are minimum-cost routes. Consider then the result of Theorem 10. According to its statement, differentiability holds precisely when the solution to (20) is such that $h_r' = 0$ for routes $r \in \mathcal{R}$ with $h_r^+ = 0$! Therefore, while the limit sensitivity problem (28) is not equivalent—in the sense of its feasible set—to the deterministic one, (20), their optimal solutions are identical precisely when the deterministic solution is differentiable. This result is summarized below.

Theorem 12 (sensitivity analysis from the SUE solution). *Assume that each link cost $t_l(\rho^*, \cdot)$ is positive and strictly monotonically increasing. Then, the following two statements are equivalent.*

(a) *The deterministic equilibrium link flow v^* is differentiable at ρ^*, with the gradient $\nabla v^*(\rho^*)$.*

(b) *The optimal solutions v' to the sensitivity problems (28) and (20) coincide.*

Further, then

$$\lim_{\theta\to\infty} \Lambda \nabla h^\theta(\rho^*) = \lim_{\theta\to\infty} \nabla v^\theta(\rho^*) = \nabla v^*(\rho^*),$$

where $\nabla h^\theta(\rho^*)$ [$\nabla v^\theta(\rho^*)$] is the gradient of the SUE route [link] flow solution at ρ^*. The same equivalence applies to the equilibrium shortest route costs π^*.

Proof. The result follows from Theorem 10 and the above remarks. □

Although the above development was made under the assumption that the traffic equilibrium model is equivalent to a convex optimization problem, it can be reproduced for a general variational inequality model. The SUE model (25) then is replaced by its variational inequality foundation, and the link cost mapping $t(\rho^*, \cdot)$ is assumed to be strictly monotone on the set of feasible flows. Under this condition, the conclusion of Proposition 11 is still valid, as it is a result on the limiting effect of a strictly monotone regularization; the below proposition establishes that strictly monotone regularizations provide the result sought. As the logit formula remains valid, the rest of the argument goes through with no alterations, and the conclusion of Theorem 12 follows for the general model.

Proposition 13 (on strictly monotone regularizations of monotone variational inequality problems). *Consider the variational problem $-f(x^*) \in N_X(x^*)$, where $X \subset \Re^n$ is nonempty, convex and compact, and $f : X \mapsto \Re^n$ is monotone on X. Let X^* denote the (convex and compact) set of solutions to this problem. Suppose that $r : X \mapsto \Re^n$ is strictly monotone on X, and consider the trajectory $\{x_\varepsilon\}$, where x_ε is the unique solution to the regularized problem $-[f + \varepsilon r](x_\varepsilon) \in N_X(x_\varepsilon)$. Then, as $\varepsilon \mapsto 0$, the sequence $\{x_\varepsilon\}$ converges to a limit, x_r^*, which is the unique point in X^* satisfying $-r(x_r^*) \in N_{X^*}(x_r^*)$.*

Proof. Let $\hat{x}$ be an arbitrary limit point of the sequence $\{x_\varepsilon\}$; at least one such point exists by the boundedness of X. By the continuity of f and r, it follows that $\hat{x} \in X^*$.

Let $x^* \in X^*$ be arbitrary. This solution can equivalently be characterized as follows:

$$f(x^*)^{\mathrm{T}}(x - x^*) \geq 0, \qquad x \in X,$$

while the solution x_ε to the regularized problem, for $\varepsilon > 0$, is equivalently characterized as follows:

$$[f(x_\varepsilon) + \varepsilon r(x_\varepsilon)]^{\mathrm{T}}(x - x_\varepsilon) \geq 0, \qquad x \in X.$$

Summing these two inequalities, with $x := x_\varepsilon$ and $x := x^*$, respectively, we obtain that

$$r(x_\varepsilon)^{\mathrm{T}}(x^* - x_\varepsilon) \geq \frac{1}{\varepsilon}[f(x^*) - f(x_\varepsilon)]^{\mathrm{T}}(x^* - x_\varepsilon) \geq 0,$$

where the last inequality follows by the monotonicity of f.

By the continuity of r, in the limit of the subsequence of $\{x_\varepsilon\}$ converging to $\hat{x}$, this yields that

$$r(\hat{x})^{\mathrm{T}}(x^* - \hat{x}) \geq 0,$$

and since $x^* \in X^*$ was arbitrary we thus have that

$$r(\hat{x})^{\mathrm{T}}(x^* - \hat{x}) \geq 0, \qquad x^* \in X^*.$$

As r is strictly monotone and $\hat{x} \in X^*$, $\hat{x}$ is the unique solution to this problem, which implies that the sequence $\{x_\varepsilon\}$ converges. This completes the proof. □

More general demand functions can of course be considered in the above development for the SUE model, with little changes in the analysis.

We return now to the heuristic "gradient" calculation made in the OD matrix adjustment method of [DrL92] in Section 2.2. The formula (9) for the $(p,q)^{\text{th}}$ element of the gradient, that is, the $(p,q)^{\text{th}}$ coordinate-wise directional derivative, can be compared to the problem (28). In the OD estimation model, there is no parameter in the travel costs. Therefore, the two objective functions coincide in this case. Further, the problem (9) includes (in principle) only the set of routes that are active at v^* (the set $\hat{\mathcal{R}}$), while the problem (28) omits routes that are forced to be zero at v^*. Under the assumption that every route that is active at *some* route flow solution in $H^*(\rho^*)$ (that is, all routes $r \in \mathcal{R}$ for which $h_r^+ > 0$ holds) is stored in the set $\hat{\mathcal{R}}$, the difference between their optimal solutions disappears precisely when Theorem 12 applies, that is, when the fixed demand traffic equilibrium link flow is differentiable; under this particular circumstance, the heuristic calculation in [DrL92] is exact.

5 An illustrative example

The following numerical example is on the fixed demand model, where the perturbation vector ρ is present in the demand vector. It illustrates a case in which the equilibrium link flow solution is not differentiable.

Consider the network in Figure 1.

For this network, we have the data in Table 1.

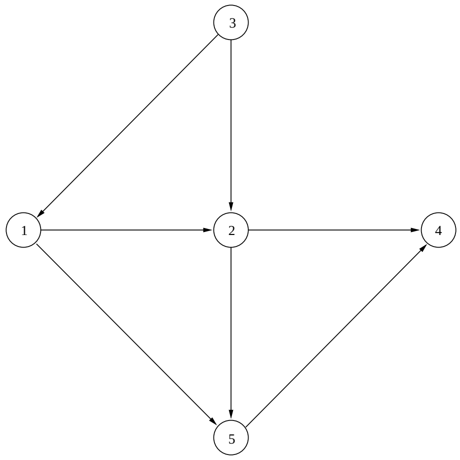

Figure 1: A traffic network.

Link	$t_{ij}(v_{ij})$	*OD pair*	$g_{pq}(\rho)$
1: $(1,2)$	$10v_{12}$	1: (1,4)	$1+\rho_1$
2: $(1,5)$	$\frac{1}{2}v_{15}$	2: (3,5)	$1+\rho_2$
3: $(2,4)$	$3+10v_{24}$		
4: $(2,5)$	$1+10v_{25}$		
5: $(3,1)$	v_{31}		
6: $(3,2)$	$2+v_{32}$		
7: $(5,4)$	v_{54}		

Table 1: Network data.

At $\rho^* := (\rho_1^*, \rho_2^*)^{\mathrm{T}} = (0,0)^{\mathrm{T}}$, the solution to (17) is

$$v^* = \begin{pmatrix} 0 \\ 2 \\ 0 \\ 0 \\ 1 \\ 0 \\ 1 \end{pmatrix}, \qquad t(v^*) = \begin{pmatrix} 10 \\ 1 \\ 3 \\ 1 \\ 1 \\ 2 \\ 1 \end{pmatrix}, \qquad \pi^* = \begin{pmatrix} 2 \\ 2 \end{pmatrix}.$$

The following routes are identified:

$$\{(1,2),(2,4)\}, \quad \{(1,2),(2,5),(5,4)\}, \quad \{(1,5),(5,4)\},$$

for OD pair $(1,4)$, with the associated route flow variables h_{11}, h_{12}, and h_{13}, and

$$\{(3,1),(1,5)\}, \quad \{(3,1),(1,2),(2,5)\}, \quad \{(3,2),(2,5)\},$$

for OD pair $(3,5)$, with corresponding route flow variables h_{21}, h_{22}, and h_{23}. The equilibrium route flow solution is unique in this case, with

$$h_{11}^*(\rho^*) = 0, \quad h_{12}^*(\rho^*) = 0, \quad h_{13}^*(\rho^*) = 1,$$

and

$$h_{21}^*(\rho^*) = 1, \quad h_{22}^*(\rho^*) = 0, \quad h_{23}^*(\rho^*) = 0,$$

respectively. This solution therefore also solves the problem (27). This solution is not strictly complementary, as we can see from a calculation of the route costs:

$$c_{11}(\rho^*, h^*) = 13, \quad c_{12}(\rho^*, h^*) = 2, \quad c_{13}(\rho^*, h^*) = 2,$$

and

$$c_{21}(\rho^*, h^*) = 2, \quad c_{22}(\rho^*, h^*) = 2, \quad c_{23}(\rho^*, h^*) = 3,$$

respectively. We see that in each OD pair, there is one route of least cost, but which is forced to have a zero flow (the second route in each pair). The link flow is clearly directionally differentiable in any direction ρ', as the Jacobian matrix $\nabla t(v^*)$ is positive definite on $\Re^{|\mathcal{L}|}$.

Assume now that $(\rho'_1, \rho'_2) = (1, 1)$. In the sensitivity problem, we have the following data: the link cost mapping is

$$v' \mapsto \nabla t(v^*) v' = \begin{pmatrix} 10v'_{12} \\ \frac{1}{2}v'_{15} \\ 10v'_{24} \\ 10v'_{25} \\ v'_{31} \\ v'_{32} \\ v'_{54} \end{pmatrix}.$$

The sensitivity problem is to

$$\begin{aligned} &\underset{(v',h')}{\text{minimize}}\ 5(v'_{12})^2 + \frac{1}{4}(v'_{15})^2 + 5(v'_{24})^2 + 5(v'_{25})^2 + \frac{1}{2}(v'_{31})^2 + \frac{1}{2}(v'_{32})^2 + \frac{1}{2}(v'_{54})^2, \\ &\text{subject to } \Gamma^{\mathrm{T}} h' = \rho', \\ &\qquad\qquad h'_{11} = 0;\ h'_{12} \geq 0;\ h'_{13} \text{ free}, \\ &\qquad\qquad h'_{21} \text{ free};\ h'_{22} \geq 0;\ h'_{23} = 0, \\ &\qquad\qquad v' = \Lambda h'. \end{aligned}$$

The unique solution to this problem is the directional derivative

$$v' = \begin{pmatrix} 0.0488 \\ 1.9512 \\ 0 \\ 0.0488 \\ 1 \\ 0 \\ 1 \end{pmatrix}, \qquad \pi' = \begin{pmatrix} 1.976 \\ 1.976 \end{pmatrix},$$

and a consistent, feasible route flow change is

$$h' = \begin{pmatrix} 0 \\ 0.0488 \\ 0.9512 \\ 1 \\ 0 \\ 0 \end{pmatrix}.$$

As stated already, the differentiability of the link flow solution is equivalent to the statement that every route $r \in \mathcal{R}$ for which $h^*_r = 0$ holds on the set $H^*(\rho^*)$ also satisfies $h'_r = 0$ in every solution to the sensitivity problem. Here, however, $h'_{12} = 0.0488 > 0$; hence, the present case is one where differentiability does not hold. (Had we applied sensitivity analysis for SUE in this context, we would have forced $h'_{12} = 0$ to hold, and obtained an erroneous result.) We also remark that the calculus formula in [ToF88] does produce a result for this instance, but its conclusion is incorrect as it cannot be given the interpretation of a gradient. The question whether it is a subgradient is a matter which merits further studies; one means to calculate a subgradient is given next.

6 Subgradients of traffic equilibria

If we would like to consider finding an optimal value of the parameter ρ by solving the bilevel programming model mentioned in Section 2.2, then in the absence of a gradient, devising a descent algorithm is, potentially, quite a lot more complicated. In nonsmooth analysis and optimization (see, e.g., [RoW98] and [HiL93], respectively), *subgradients* (or, generalized gradients), have been shown to be very useful, as they can be used in place of a gradient in specially constructed algorithms, for example in bundle methods.

A subgradient of S at ρ^* is defined as follows: it is any member of the generalized Jacobian, $\partial S(\rho^*)$, of S at ρ^*, with

$$\partial S(\rho^*) := \operatorname{conv} \left\{ \lim_{\ell \to \infty} \nabla S(\rho^\ell) \middle| \{\rho^\ell\} \to \rho^* \text{ and } \rho^\ell \in \delta_S \right\},$$

where δ_S is the set on which S is differentiable. Hence, the set of subgradients is the convex hull of the set of all limits of gradients of S at points converging to ρ^*. (This set is always nonempty, as soon as S is locally Lipschitz at ρ^*, cf. [Cla83].)

For many nonsmooth problems, generating a descent direction is much more complicated than to generate just one subgradient, as an arbitrary subgradient is not guaranteed to provide a descent direction. Bundle algorithms work by generating a collection of subgradients at nearby points and generating a search direction from their convex hull. We refer to the book [OKZ98] for a general discussion of such algorithms in the context of bilevel programming.

In this section, we will focus on the basic question of when and how a subgradient can be calculated, and how its calculation is related to the directional derivative and gradient calculus. Throughout this section, we work with the perturbed elastic demand model (5) in link–route space, assuming that the condition of Theorem 5, statement (a) or (b), holds, so that v^* is directionally differentiable.

In the case of a *real-valued* function S (rather than the vector-valued function S that we are considering in this paper), the generalized Jacobian (or, subdifferential) is characterized by, and generated by, the set of directional derivatives of S; cf. [RoW98, Chapter 8]. In our case, however, subgradients are more complicated to calculate in general, and additional assumptions will have to be made in order for the directional derivatives to generate the generalized Jacobian. We will briefly sketch one possibility to generate a subgradient of S, being aware that there may also be others. (If S is differentiable at ρ^*, then our subgradient formula will reduce to that of the gradient, like any such formula should.)

We now turn to the question of when, and how, a subgradient can be calculated, in the absence of a gradient. Let ρ^* be given, and likewise (h^*, π^*, v^*), where h^* is arbitrary in $H^*(\rho^*)$. At ρ^* and this equilibrium solution, two regularity conditions are next introduced under which a calculus formula to be given later will provide one subgradient. The first, and weakest, condition states that there is a subset of the routes with zero flow at equilibrium, the flows in which will remain at zero after *some* infinitesimal perturbation in ρ, and such that the resulting flow is strictly complementary.

We introduce the index sets

$$\begin{aligned}
\mathcal{J}(\rho^*, h^*, \pi^*) &:= \left\{ r \in \mathcal{R} \,\middle|\, c_r(\rho^*, h^*) > \pi^*_{pq} \right\}, \\
\mathcal{O}(\rho^*, h^*, \pi^*) &:= \left\{ r \in \mathcal{R} \,\middle|\, h^*_r > 0 \right\}, \\
\mathcal{M}(\rho^*, h^*, \pi^*) &:= \left\{ r \in \mathcal{R} \,\middle|\, c_r(\rho^*, h^*) = \pi^*_{pq} \text{ and } h^*_r = 0 \right\},
\end{aligned}$$

of, respectively, the non-equilibrium routes, the routes with positive flow, and the equilibrium routes with zero flow, at h^*. Recall that strict complementarity amounts to the condition that $\mathcal{M}(\rho^*, h^*, \pi^*) = \emptyset$, in which case differentiability follows (see the discussion following Theorem 10). The below condition is derived from [OuZ95].

Definition 14 (regularity properties of the equilibrium solution, I). *There exists a set*

$$\mathcal{J}_0(\rho^*, h^*, \pi^*) \subset \mathcal{J}(\rho^*, h^*, \pi^*) \cup \mathcal{M}(\rho^*, h^*, \pi^*), \tag{29}$$

for which the following holds: there exists a vector $\bar{\rho}' \in \Re^d$ such that for all sufficiently small $\tau > 0$, there is an equilibrium flow $h^*(\rho^* + \tau\bar{\rho}')$ with

$$\mathcal{J}_0(\rho^*, h^*, \pi^*) = \mathcal{J}(\rho^* + \tau\bar{\rho}', h^*(\rho^* + \tau\bar{\rho}'), \pi^*(\rho^* + \tau\bar{\rho}')) \tag{30}$$

and

$$\mathcal{M}(\rho^* + \tau\bar{\rho}', h^*(\rho^* + \tau\bar{\rho}'), \pi^*(\rho^* + \tau\bar{\rho}')) = \emptyset. \tag{31}$$

In other words, there exists a perturbation $\bar{\rho}'$ and a subset of the routes with zero flow at equilibrium at ρ^* with the properties that after perturbation, (i) their flow remains at zero, (ii) they become non-equilibrium routes, and (iii) the equilibrium flow becomes strictly complementary. □

This condition does not rely on performing any sensitivity analysis. However, there is no method inherent in it to find the vector $\bar{\rho}' \in \Re^d$, or a means to investigate its "approximate" fulfillment for use in practice. Moreover, as can be seen in the proof of Theorem 17 below, it may not extend very far in terms of applicability to more general traffic equilibrium models, in particular to those including additional flow constraints like capacities, as it relies on a linear independence assumption on the active inequality constraints. [Linear independence is fulfilled for the elastic demand model (5).] The second condition that we introduce is stronger, but is also more practical.

We introduce the vector ρ', and let (h', π', v') be the result of solving the sensitivity problem (16), where h' is arbitrary in the solution. We further let

$$\mathcal{M}_1(h') := \{ r \in \mathcal{M}(\rho^*, h^*, \pi^*) \mid c_r'(\rho^*, h^*, h') > \pi_{pq}' \},$$
$$\mathcal{M}_2(h') := \{ r \in \mathcal{M}(\rho^*, h^*, \pi^*) \mid h_r' > 0 \},$$

where the vector $c'(\rho^*, h^*, h')$ is defined by $\Lambda^{\mathrm{T}}(\nabla_\rho t(\rho^*, v^*)^{\mathrm{T}} \rho' + \nabla_v t(\rho^*, v^*)^{\mathrm{T}} v')$, that is, the route cost changes in the solution of (16). We recall that the characterization of differentiability of v at ρ^* given in Theorem 10 amounts to the condition that $\mathcal{M}_2(h') = \emptyset$ for all h' solving (16), clearly a less strong assumption than strict complementarity, as we have already concluded.

The condition stated below says that the solution to *some* sensitivity problem should behave nicely, in the sense that there exists a strictly complementary solution to it; this condition is derived from Outrata [Out97, Theorem 2.3].

Definition 15 (regularity properties of the equilibrium solution, II). *There exists a vector, $\bar{\rho}' \in \Re^d$, for which some solution $\bar{h}'$ to the sensitivity problem (16) satisfies*

$$\mathcal{M}_1(\bar{h}') \cup \mathcal{M}_2(\bar{h}') = \mathcal{M}(\rho^*, h^*, \pi^*) \qquad \text{and} \qquad \mathcal{M}_1(\bar{h}') \cap \mathcal{M}_2(\bar{h}') = \emptyset.$$

In other words, the sets $\mathcal{M}_1(\bar{h}')$ and $\mathcal{M}_2(\bar{h}')$ partition $\mathcal{M}(\rho^*, h^*, \pi^*)$, and so $\bar{h}'$ is strictly complementary. □

Proposition 16 (Definition 15 implies Definition 14). *Suppose that there is a vector $\bar{\rho}' \in \Re^d$ such that the property in Definition 15 holds. Then, for the same value of $\bar{\rho}'$, and with*

$$\mathcal{J}_0(\rho^*, h^*, \pi^*) := \mathcal{J}(\rho^*, h^*, \pi^*) \cup \mathcal{M}_1(\bar{h}'), \tag{32}$$

the property in Definition 14 holds.

Proof. With Definition 15 in force, it follows that for the same $\bar{\rho}'$, for every sufficiently small value of $\tau > 0$, (31) is satisfied. Let $\mathcal{J}_0(\rho^*, h^*, \pi^*)$ be given by (32); this is the set of routes that were either more expensive at ρ^* or becomes expensive at $\rho^* + \tau\bar{\rho}'$ for small enough $\tau > 0$. With this choice, we satisfy (29) and (30). The result follows. □

In the case of strict complementarity at h^*, both of the above definitions are in force, as in that case, $\mathcal{M}(\rho^*, h^*, \pi^*) = \emptyset$. It may however be that neither of the two conditions hold when we satisfy the mildest possible condition for differentiability, as given in Theorem 10.

The condition in Definition 15 is based on the use of sensitivity analysis to find a proper value of $\bar{\rho}'$. There are two advantages of this condition over the one given in Definition 14. First, as can be seen in the proof of Theorem 17 below, its validity does not rely on a linear independence assumption, which is important for the application of sensitivity analysis to some extensions of the original model (see the conclusion section); second, and most important, it is possible to use it in practice, as the set $\mathcal{J}_0(\rho^*, h^*, \pi^*)$ can naturally be approximated. Before turning to an example of how this can be done, we provide the calculus formula for a subgradient. The formula has the same appearance in both cases, except for a difference in the definition of the subset of the routes in $\mathcal{M}(\rho^*, h^*, \pi^*)$ which are forced to remain at zero.

Let $\mathcal{I}(\rho^*, h^*, \pi^*)$ be a route index set, which is equal to either $\mathcal{J}_0(\rho^*, h^*, \pi^*)$ or $\mathcal{J}(\rho^*, h^*, \pi^*) \cup \mathcal{M}_1(\bar{h}')$, depending on whether we work under Definition 14 or 15.

Let

$$\bar{K} := \left\{ \begin{pmatrix} h' \\ \pi' \\ v' \end{pmatrix} \in \Re^{|\mathcal{R}|+|\mathcal{C}|+|\mathcal{L}|} \;\middle|\; \begin{array}{l} h_r' = 0 \text{ if } r \in \mathcal{I}(\rho^*, h^*, \pi^*) \\ [r \in \mathcal{R}] \end{array} \right\},$$

For a given $\rho' \in \Re^d$, consider the problem

$$-r(h', \pi', v') \in N_{\bar{K}}(h', \pi', v'), \tag{33}$$

where the mapping r is the same as in the sensitivity problem (16).

We note that the variational inequality problem (33) is equivalent to a linear system uniquely solvable in v', which is also quite similar to the directional derivative problem (16), and hence then also to the definition of the gradient, when it exists; the difference is that the nonnegativity restrictions on some routes are removed, and replaced by the restriction that h'_r be zero for $r \in \mathcal{I}(\rho^*, h^*, \pi^*)$. Interestingly, both the linear system (33) and the sensitivity problem (16) are really network flow problems, which should make it possible to devise, for example, a bundle algorithm that is feasible also for large-scale problems.

Before establishing that the formula (33) provides the result sought, we discuss its possible application in practice, based on Definition 15 and the link–route formulation. Clearly, it is the set $\mathcal{I}(\rho^*, h^*, \pi^*)$ that requires our attention. Assume that the model (5) has been solved by the use of the DSD algorithm ([LaP92]), that is, an algorithm which explicitly keeps the set $\mathcal{O}(\rho^*, h^*, \pi^*)$, and possibly also a subset of $\mathcal{M}(\rho^*, h^*, \pi^*)$. If this subset, $\hat{\mathcal{R}}$, of $\mathcal{R}$, is rich enough, then the solution to the problem (33) is possible to find with the route data available. In particular, if $\mathcal{M}(\rho^*, h^*, \pi^*) \subset \hat{\mathcal{R}}$, then once we have identified the vector $\bar{\rho}'$, the subset $\mathcal{M}_1(\bar{h}')$ is identified and can be removed from $\hat{\mathcal{R}}$. We note that differentiability follows precisely when $\mathcal{M}_1(\bar{h}') = \mathcal{M}(\rho^*, h^*, \pi^*)$, whence the whole set of unused routes can be stricken. This suggests the following heuristic:

when solving the problem (33), keep only the route set in $\mathcal{O}(\rho^*, h^*, \pi^*)$.

This heuristic is exact whenever the equilibrium link flow is differentiable, and is equivalent to the assumption that $\mathcal{M}_2(\bar{h}')$ is empty. Outrata [Out97] concludes from computational experience with a bundle algorithm for bilevel programming that he had no difficulties when using this heuristic. The conclusion was however drawn from solving small-scale problems.

We are now ready to establish that the formula (33) provides a subgradient, under the conditions of either Definition 14 or 15. The proof is mainly an exercise in identification and will not be given in full detail, in order to save space.

THEOREM 17 (a subgradient formula). *Let the assumptions of Theorem* 5, *statement* (a) *or* (b), *be satisfied. Let further the conditions of Definition* 14 *or* 15 *be satisfied. Define the single-valued and linear operator* Π *which, for each* ρ', *gives a (unique) solution in* v' *to the problem* (33). *Then,* $\Pi \in \partial S(\rho^*)$.

Consequently, the collection of d *solutions* v' *to the problem* (33) *for* $\rho' = e_i$, $i = 1, 2, \dots, d$, *is a subgradient of* S *at* ρ^*. *The corresponding solution in* π' *is a subgradient of* π^* *at* ρ^*.

PROOF. (Definition 14) To put our model into the form of the problem in [OuZ95, p. 116], we note that it is a special case of the problem (7) in which

$$C := \{ y \in \Re^n |\ \exists z \in \Re^m \text{ with } Ay + Bz \le b \}.$$

An identification of our set C in (5) is made from

$$y = \begin{pmatrix} \pi \\ v \end{pmatrix}; \quad z = h; \quad A = 0; \quad B = -I; \quad \text{and} \quad b = 0.$$

Their condition (LI)' is fulfilled by our model, as the only inequality constraints are the conditions that $h \ge 0^{|\mathcal{R}|}$, so any active such constraints are linearly independent. As is also remarked on page 116 in that paper, the conditions (A1)–(A3) imposed in their Proposition 3.4 are there to ensure the local Lipschitz continuity of the mapping S, which we instead ensure by our assumptions of Theorem 5. The rest of Proposition 3.4 of [OuZ95] is a restatement of our result in (a), where we identify the set Q with our $\mathcal{J}$, their M with $\mathcal{J} \cup \mathcal{M}$, and where we may remove the projection argument of that theorem, as we have earlier concluded that the choice of route flow solution is immaterial to the sensitivity analysis.

(Definition 15) The problem studied by Outrata [Out97] is the special case of the problem (7) in which

$$C := \{ y \in \Re^n |\ \exists z \ge 0^m \text{ with } Ay - Bz = d \}.$$

We put our problem (5) into this framework by identifying

$$y = \begin{pmatrix} \pi \\ v \end{pmatrix}; \quad z = h; \quad A = \begin{pmatrix} 0 & 0 \\ 0 & I \end{pmatrix}; \quad B = \begin{pmatrix} 0 \\ \Lambda \end{pmatrix}; \quad \text{and} \quad d = \begin{pmatrix} 0 \\ 0 \end{pmatrix}.$$

Theorem 2.3 of [Out97] is established under the assumption that two conditions [(A1) and (A2) in that paper] are fulfilled. These conditions are stronger than our conditions of Theorem 5, statement (a) or (b), but they are only used in [Out97] to establish the local Lipschitz continuity and directional differentiability of S, and we have already established that our conditions of Theorem 5 then are sufficient. The rest of the statement of the theorem is identical to that of Theorem 2.3 of [Out97], with the identifications made above, whence the result follows. $\square$

The formula (33) reduces to the one for the gradient, cf., for example, (28), whenever $\mathcal{I}(\rho^*, h^*, \pi^*) = \{ r \in \mathcal{R} \mid h_r^+ = 0 \}$. With $\mathcal{I}(\rho^*, h^*, \pi^*)$ given by $\mathcal{J}_0(\rho^*, h^*, \pi^*)$, this equality is satisfied for every choice of vector $\bar{\rho}' \in \Re^d$ precisely when the equilibrium link flow solution is differentiable. Hence, (33) is the formula to use, as it automatically provides a gradient if it exists, and a subgradient if it does not.

It is unknown whether a subgradient can be generated from an explicit calculus formula under milder assumptions than those stated in the above definitions. Subgradient formulas for more general feasible sets are found, for example, in [OuZ95] and [OKZ98].

With reference to the numerical example in Section 5, we remark that the route flow change h' given there is not the only one; an alternative which also aggregates to v' is

$$h' = \begin{pmatrix} 0 \\ 0 \\ 1 \\ 0.9512 \\ 0.0488 \\ 0 \end{pmatrix}.$$

We note that in this solution, $h'_{22} > 0$ holds, while $h'_{12} > 0$ holds in the first alternative solution. Taking any positive convex combination of these two alternative route flow changes, for example with equals weights of $\frac{1}{2}$ giving the perturbation $(0, 0.0244, 0.9756, 0.9756, 0.0244, 0)^{\mathrm{T}}$, we reach a route flow change, $\bar{h}'$, in which both the degenerate routes mentioned receive a positive flow. In other words, in such a solution, $\mathcal{M}_1(\bar{h}') = \mathcal{M}(\rho^*, h^*, \pi^*)$ holds; therefore, this is a case where indeed we satisfy the conditions of the above theorem, based on Definition 15.

With $\mathcal{I}(\rho^*, h^*, \pi^*)$ consisting of the two routes defining the variables h_{11} and h_{23}, solving the problem (33) for ρ' being the two coordinate directions, respectively, yields:

$$\rho' = \begin{pmatrix} 1 \\ 0 \end{pmatrix}: \qquad v' = \begin{pmatrix} 0.0244 \\ 0.9756 \\ 0 \\ 0.0244 \\ 0 \\ 0 \\ 1 \end{pmatrix}; \qquad \pi' = \begin{pmatrix} 1.4878 \\ 0.4878 \end{pmatrix}$$

and

$$\rho' = \begin{pmatrix} 0 \\ 1 \end{pmatrix}: \qquad v' = \begin{pmatrix} 0.0244 \\ 0.9756 \\ 0 \\ 0.0244 \\ 1 \\ 0 \\ 0 \end{pmatrix}; \qquad \pi' = \begin{pmatrix} 0.4878 \\ 1.4878 \end{pmatrix}.$$

The reader is asked to compare these solutions, which yield the partial subgradients

$$\begin{pmatrix} 0.0244 & 0.9756 & 0 & 0.0244 & 0 & 0 & 1 \\ 0.0244 & 0.9756 & 0 & 0.0244 & 1 & 0 & 0 \end{pmatrix} \quad \text{and} \quad \begin{pmatrix} 1.4878 & 0.4878 \\ 0.4878 & 1.4878 \end{pmatrix}$$

of the equilibrium solution with respect to v and π, respectively, to the result of the sensitivity analysis in Section 5; the directional derivative for $\rho' = (1, 1)^{\mathrm{T}}$ is in fact the sum of the respective subgradient components. The route flow changes received from our subgradient computation were $h' =$

$(0, 0.2622, 0.7378, 0.2378, -0.2378, 0)^{\mathrm{T}}$, for the case of $\rho' = (1,0)^{\mathrm{T}}$, and $h' = (0, -0.2378, 0.2378, 0.7378, -0.2622, 0)^{\mathrm{T}}$, for the case of $\rho' = (0,1)^{\mathrm{T}}$, respectively, which sum up to the convex combined perturbation above.

We finally note that in the link–node representation, the conditions in Definitions 14 and 15 have their counterparts in conditions on the degenerate links in a commodity which lie on a shortest route and yet have no flow. The corresponding subgradient formula has the same appearance as the directional derivative formula in (23), except that for a given subset of the degenerate links, flow is forced to remain at zero. Whether it is an advantage to work with this formula rather than (33) depends largely on the size of the problem under study.

7 Conclusions, extensions and further research

This paper offers characterizations of when directional derivatives and gradients of the link flow and OD travel costs exist, in the context of the elastic (and also fixed) demand traffic equilibrium model. In the case of directional derivatives of link flows, the results established here are the strongest possible, and they improve upon the results previously stated. In the case of gradients, the paper provides the first generally valid results which at the same time also are the strongest possible. Moreover, we have remarked that the most popular gradient formula may produce erroneous results when used in at least two circumstances, as it does not provide the correct gradient value when the network topology makes the formula break down (as was observed by Bell and Iida [BeI97, Section 5.4]), and when the first part of the differentiability Theorem 4 applies but not the second; according to the numerical example, it can also supply a value when the gradient does not exist, and also possibly fail to yield a subgradient.

Apart from these technical results, we remark that the statements of the calculus formulas show that a sensitivity analysis can be performed by solving one (in the case of a directional derivative) or d (in the case of a gradient or a subgradient) network flow problem(s), similar to the original network model; the main difference is in the definition of the network itself, which imposes further restrictions on the sign of the commodity flow variables. The structure of the problems being so similar, we anticipate that in the case of the link–route formulation, for example, efficient projection-type column generation algorithms based on route flows, such as DSD ([LaP92]), could be adjusted to not only solve the original model, but also provide the sensitivity analysis sought. Whether it is possible to incorporate an efficient sensitivity analysis package within transportation planning software is an interesting subject for further study.

The advantage of using the general framework of variational analysis in deriving sensitivity analysis results, rather than performing specialized matrix-based studies of the network equilibrium model, should be apparent from the our analysis, but it becomes even more pronounced when we wish to extend the analysis to more general traffic models. While a specialized analysis could easily break down, the general technique used here would incorporate model extensions quite readily. To illustrate this fact, let us consider an extension to the model (17) in which we further impose upper bounds on the link flows. In other words, to the constraints defining the set $\widehat{F}(\rho^*)$ we further add capacity constraints of the form

$$v \in G := \left\{ v \in \Re^{|\mathcal{L}|} \,\middle|\, v_l \le u_l,\ l \in \mathcal{L} \right\},$$

where $u_l \in [0, \infty]$, $l \in \mathcal{L}$. (Applications and properties of the capacitated model are found in [Hea80, LaP95, LaP99].) What happens in the sensitivity analysis when adding such constraints? According to the properties of tangent cones, we have that $T_{\widehat{F}(\rho^*)\cap G}(v^*) = T_{\widehat{F}(\rho^*)}(v^*) \cap T_G(v^*)$, where the tangent cone $T_{\widehat{F}(\rho^*)}(v^*)$ was already analyzed as part of the description of the critical cone in the simpler model, and where

$$T_G(v^*) = \left\{ v' \in \Re^{|\mathcal{L}|} \,\middle|\, v'_l \le 0,\ l \in \mathcal{L} \text{ with } v^*_l = u_l \right\}.$$

So, incorporating such an extension only has the effect of adding constraints to the sensitivity problem. Needless to say, it will be more difficult to solve a sensitivity model in which both individual disaggregated (that is, commodity) flow (h', w'_k) and aggregated link flow (v') changes are sign constrained, since the Cartesian product structure no longer is present, but that is to be anticipated since the capacitated model itself lacks this favourable product structure. What this example brings to light, however, is that the change in the analysis is much smaller than one perhaps might think. It is known that the multipliers for the capacity constraints are not unique in general (cf. [LaP99]), but whether binding constraints are linearly independent or not has already earlier in this paper been deemed immaterial, with the strong sensitivity analysis theory that we are using. Apart from the relatively small and easily derived change in the sensitivity problem itself, what is left to check is the conditions for the existence of directional derivatives and gradients. According to Theorem 5, uniqueness of the solution to the sensitivity problem is enough for directional derivatives to exist, and as the current model is more constrained, so is the critical cone, whence the conditions for the original model are sufficient also for this model. The existence of a gradient is slightly more complicated, but not much: the corresponding change in the set $K \cap (-K)$ is a further condition of the form "$v'_l = 0$ if $v^*_l = u_l$," meaning that differentiability, according to the results of Theorem 10, follows if, in addition to the conditions stated in (b) in that theorem, a link $l \in \mathcal{L}$ that was used to full capacity in the original model will remain at capacity after all possible, infinitesimally small, perturbations. In the case of subgradients, we resort to the use of the condition in Definition 15, since linear independence among the active inequality constraints may fail to hold.

If the capacity u is a smooth function of ρ—which could model traffic signal control optimization, for example—the extension of the sensitivity analysis becomes no more complicated. Like the case of demand fulfillment, in which the right-hand side depends on ρ, we incorporate the constraint $v \leq u(\rho)$ within the function f, as follows. We introduce a multiplier vector $\beta \in \Re^{|\mathcal{L}|}_+$, and then obtain a model of the form (7), with

$$x = \begin{pmatrix} h \\ \pi \\ v \\ \beta \end{pmatrix}; \qquad f(x) = \begin{pmatrix} \Lambda^{\mathrm{T}} t(\rho, v) - \Gamma\pi \\ \Gamma^{\mathrm{T}} h - g(\rho, \pi) \\ v - \Lambda h \\ u(\rho) - v \end{pmatrix}; \qquad C = \Re^{|\mathcal{R}|}_+ \times \Re^{|\mathcal{C}|} \times \Re^{|\mathcal{L}|} \times \Re^{|\mathcal{L}|}_+.$$

The added model component describes the complementarity condition

$$0^{|\mathcal{L}|} \leq \beta \perp (u(\rho) - v) \geq 0^{|\mathcal{L}|},$$

which, in the case of a delay-based model, states that there is no queue where the equilibrium flow is not at capacity (cf. [LaP99]). Directional differentiability follows as above, although the formulas will have an added cost term from the derivative of u; the (sufficient) positive definiteness conditions for directional differentiability in the above two models will differ slightly, as was the case for unperturbed/perturbed demand as analyzed in Corollary 8. The question of the differentiability of the equilibrium link flow becomes more complex, because of the explicit presence of the Lagrange multipliers; this is because the differentiability Theorem 4 is in fact not independent of the representation of the feasible set. However, subgradient formulas based on Definition 15 should be readily constructed, at least heuristically.

Another, and in fact much simpler extension, is to combined traffic models, where the demand side is disaggregated further into different classes of traffic, perhaps with additional side constraints on the total demand between traffic zones. This is a case of the addition of linear equalities to the original elastic demand model, and the analysis of this type of model is straightforward.

To which traffic models the framework used in this paper may be applied in sensitivity analyses in the future is still open, but at least the above examples show that it is relatively straightforward to apply sensitivity analysis to the most basic models, and even go beyond them.

On the issue of existence of directional derivatives, the analysis in Remark 9 shows that even in the case of the simplest and most classic traffic assignment model, directional derivatives of the link flows may not exist for the entire network. Although this may seem to limit the use of the analysis, the example does show that the sensitivity analysis is valid for any link with positive flow. However, recent research (which must be reported in detail elsewhere) shows that even in this case, directional derivatives at least exist in terms of all the travel costs entities, t, c, and π (and in the case of π therefore improves upon the result stated in Corollary 7); in an application to MPEC where the travel cost is the entity which we wish to influence rather than the flow itself, an analysis shows that the properties of the classic TAP model are sufficient.

Finally, we mention that the subject of utilizing subgradients in algorithms for bilevel programming models in this area is an interesting subject for future research. It has been shown (see, e.g., [MGN87, DeV97]) that a constraint qualification (CQ), similar to the two regularity conditions that we have introduced, will be satisfied at any point almost surely, so that a subgradient, for use in bundle methods, can be calculated by means of a linear system. Further, even if the direction found fails to be a subgradient at certain points because a CQ is not satisfied there, we can always reach a point which is stationary for the MPEC, although "stationarity" will be understood in a weaker sense if we fail too frequently.

Acknowledgement The presentation of the paper benefitted from several remarks from three anonymous reviewers.

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