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SENSITIVITY ANALYSIS OF THE VARIABLE DEMAND PROBIT STOCHASTIC USER EQUILIBRIUM WITH MULTIPLE USER-CLASSES

Richard D. Connors¹, email: r.d.connors@its.leeds.ac.uk

Agachai Sumalee, email: a.sumalee@its.leeds.ac.uk

David P. Watling, email: d.p.watling@its.leeds.ac.uk

All: Institute for Transport Studies, University of Leeds, Leeds LS2 9JT, U.K.

Tel: 0113 3435325 Fax: 0113 3435334

Abstract

This paper presents a formulation of the multiple user class, variable demand, probit stochastic user equilibrium model. Sufficient conditions are stated for differentiability of the equilibrium flows of this model. This justifies the derivation of sensitivity expressions for the equilibrium flows, which are presented in a format that can be implemented in commercially available software. A numerical example verifies the sensitivity expressions, and that this formulation is applicable to large networks.

Keywords

Sensitivity Analysis, Probit Stochastic User Equilibrium

1. Introduction

In many network-based techniques for transport planning, design and estimation, there is a key role played by the implicit relationship between the data input to a traffic assignment model and the predictions of equilibrium network flows based on those data. For example, in equilibrium-based trip matrix estimation, the ‘data’ in question are the unknown trip matrix elements, which when assigned according to an equilibrium model are required to give predicted link flows that reproduce—to some given level, according to some distance metric—flows that have actually been observed on a subset of links (Yang et al. 1992). A second common application arises in the equilibrium-based network design problem, the ‘data’ reflecting some policy measure under the control of the planner (e.g. link capacities, road tolls, signal timings), where the objective is to optimize some measure of system/economic performance while anticipating the equilibrium response of travellers on the network (Magnanti/Wong 1984; Patriksson/Rockafellar 2002; Yang/Bell 1997). A third application is in the field of network reliability assessment, where the vulnerability of origin-destination/system performance to unreliable capacity or demand conditions can be imputed from the impact such input changes may have on the equilibrium state (Bell et al. 1999; Chen et al. 2002; Du/Nicholson 1997). A final application is in the area of error estimation, where the impact of sampling errors in the estimated input data (e.g. trip matrix elements, parameters of the link travel time functions) on errors in the forecast network evaluation measures can be deduced from the implicit equilibrium relationship (Bell/Iida 1997; Leurent 1998).

In such applications, it is commonly necessary to deal with the implicit equilibrium relationship as a sub-problem during the course of some overall, master solution algorithm, and it is therefore only natural to consider ways of either approximating this relationship and/or of computing its gradients or sub-gradients, should they exist. This is the role of *sensitivity analysis*, a technique with a substantial history both in non-linear programming generally and in the transportation network field specifically. As illustration of its significance, all of the references cited in the paragraph above were chosen not only to illustrate the application areas in which implicit equilibrium problems arise, but also because they all propose algorithms based on sensitivity analysis.

Aside from its importance for applied problems, the prominence of sensitivity analysis has been magnified in recent years from a technical perspective, due to the work of Patriksson & Rockafellar (2002; 2003), who brought into question the whole basis and validity of the seminal transportation paper by Tobin & Friesz (1988) upon which many of the subsequent applications were based. The technical problems and their ramifications continue to be debated, yet it is important to appreciate that these are problem-specific in the sense that they relate crucially to the choice of Wardrop deterministic user equilibrium as the network flow model. While these difficulties may be described in a number of different guises, on a simple level there are two main facets of this model that require careful handling. These are namely: i) non-uniqueness of the equilibrium path flows in general networks even for fixed input data; and ii) problems of ‘complementarity’ due to the active equilibrium path set (even if it were unique!)

¹ Corresponding Author

changing as the input data to the model are changed, the latter meaning that even directional derivatives of the equilibrium flows may not exist at certain points.

The nature of these difficulties has meant that it has been only natural to consider embedding alternative network flow models in the application problems mentioned above. Specifically, Davis (1994) and Ying & Miyagi (2001) describe the computation of sensitivity analysis for the logit Stochastic User Equilibrium (SUE) model, which may be observed to exist everywhere (and be efficiently computable) under mild conditions. The disadvantage of this approach is that one is then left with a question of plausibility of the adopted model, in the light of the well-known deficiencies of the logit model in being unable to represent correlated alternatives, of which the routes in a network are one of the most natural examples. The SUE approach is, however, sufficiently general to admit a range of alternative behavioural assumptions, through the form of joint distribution assumed for the stochastic path error terms. Examples of such models include the C-logit (Cascetta et al. 1996), nested logit (GentilePapola 2001), cross-nested logit (VovshaBekhor 1998), paired combinatorial logit (Gliebe et al. 1999; PrashkerBekhor 1999), mixed logit (Nielsen et al. 2002), and probit (DaganzoSheffi 1977). To this end, Clark & Watling (2002a) describe a computational procedure for sensitivity analysis of the probit SUE. In the probit case, given that the choice proportions are not expressible in closed form but are rather the result of a multidimensional integral, a key practical factor in this latter work is seen to be deducing the sensitivity analysis expressions in such a way that the relevant Jacobian matrices are computable by analytic means, without resort to the vagaries and errors of finite difference approximation.

Part of the analyst's role is to determine the appropriate balance between generality, accuracy and efficiency when choosing a modelling approach. In the light of the recent work on sensitivity analysis reported above, it is our contention that probit-SUE increasingly affords the best compromise for network modelling, particularly within the wider context of network design optimisation problems. Our aim in this paper is to justify this claim by presenting a formulation of the probit-SUE that admits individuals of different classes, and allows them to choose not to travel (elastic demand). We derive gradient information for this general formulation of the probit-SUE, showing that many of the analytical pitfalls detailed by Patriksson & Rockafellar are avoided, with the equilibrium flows varying smoothly with the design parameters. This may be contrasted with the DUE model, in which the systematically non-smooth variation of the equilibrium flows in the design parameters makes problems such as equilibrium-based network design extremely difficult. Even if one is careful to follow the techniques described by Patriksson and Rockafellar (2002, 2003), one must still face the prospect that even directional derivatives will not exist at some points in the design space. In any case, it is not difficult to make case that drivers do not know precisely, nor perceive identically, the travel costs they will experience on any journey, implying that some form of stochastic model would be more appropriate. Furthermore, in the whole family of equilibrium models mentioned above, the probit SUE has a claim to maximum generality in being able to approximate all such models by appropriate choice of the error distribution. These appealing features of the probit-SUE are achieved at a cost; computation and analysis of the probit-SUE flows are comparatively difficult and time consuming. Part of the purpose of this paper is to show that these obstacles are diminishing.

Specifically, in the present paper, our original contributions are to extend the work of Clark & Watling (2002a) in several key ways:

- The underlying probit SUE model is generalised from the single user class, fixed demand case to a case with multiple user classes and elastic demand.
- A formal proof is provided of the existence of the sensitivity analysis for this model.
- An improved computational procedure is described (even for the single user class, fixed demand case) for computing the base equilibrium solution and the choice probability Jacobian, which both improves the efficiency of the method and avoids the difficulties in interpreting Monte Carlo error (Monte Carlo techniques are not used).
- Explicit formulae are presented to allow the straightforward implementation of the method in widely available matrix-based mathematical languages, such as MATLAB.
- A practical application of the methods to a toll-pricing problem is reported for a realistic-sized network.

The structure of the paper is as follows. In Section 2 the necessary notation is introduced, and our particular formulation of elastic demand probit SUE presented. Differentiability of the equilibrium flows is established in Section 3, providing conditions to ensure existence of the sensitivity analysis. In Section 4 sensitivity expressions are derived for the equilibrium flows. Implementation and computational issues are described in section 5, and numerical experiments reported in Section 6, before presenting the conclusions in Section 7.

2. Definitions, Notation and Assumptions

We consider the road network represented by a directed graph consisting of Z nodes, with the set of connecting links labelled $a = 1, \dots, N$. The origin-to-destination (OD) movements on the network are labelled $r = 1, \dots, R$ and the user classes $m = 1, \dots, M$. The $[NM \times 1]$ vector of disaggregate link flows is ordered by class

$$\mathbf{x} = [\mathbf{x}^1, \dots, \mathbf{x}^M]^T = [x_1^1, \dots, x_N^1, x_1^2, \dots, x_N^M]^T; \quad (1)$$

x_a^m is the flow of class m on link a . While we have assumed here that all links are available to all user classes, it is a trivial change to disallow certain links to individual classes. Users on link a of class m experience a generalized cost $t_a^m(\mathbf{x})$ that may depend on the flows of any user class, anywhere on the network. We assume that

A1. The link cost functions are single valued and continuously differentiable.

This does not require the link cost functions to be monotonic, separable nor that the Jacobian, $\nabla_{\mathbf{x}} \mathbf{t}$, be symmetric.

The set of simple paths available to class m on the r -th OD movement is of size $K^{m,r}$; each class may have a different path-set. The total number of paths is $K = \sum_m \sum_r K^{m,r}$. An assignment of flows to all paths is denoted by the $[K \times 1]$ vector \mathbf{f} , whose elements are ordered by class and sub-ordered by OD movement:

$$\mathbf{f} = [f_1^{1,1}, \dots, f_{K^{1,1}}^{1,1}, f_1^{1,2}, \dots, f_k^{m,r}, \dots, f_{K^{M,R}}^{M,R}]^T, \quad (2)$$

with $f_k^{m,r} \geq 0 \forall m, r, k$. The $[MR \times 1]$ OD demand vector, $\hat{\mathbf{q}}$, is similarly ordered by class and OD movement, with entry $q^{m,r}$ representing the total potential travel demand by user-class m for the r -th OD movement.

The path flow assignment \mathbf{f} is *feasible* for demand $\hat{\mathbf{q}}$ if and only if, for each constituent class and OD movement, $\sum_{k \in K^{m,r}} f_k^{m,r} = q^{m,r} \forall m, r$. Ψ is the $[MR \times K]$ demand-path incidence matrix, such that

$$\hat{\mathbf{q}} = \Psi \cdot \mathbf{f}. \quad (3)$$

The set of feasible path flows is closed and convex.

The $[MN \times K]$ block-diagonal link path incidence matrix Δ , whose elements are Kronecker delta functions $\delta_{a,k}^{m,r}$, denotes the links comprising each path, for every class and OD pair. The vector of disaggregate link flows, (1), is therefore given by

$$\mathbf{x} = \begin{bmatrix} [\Delta^{1,1} \ \Delta^{1,2} \ \dots \ \Delta^{1,R}] & \mathbf{0} & \dots & \mathbf{0} \\ \mathbf{0} & [\Delta^{2,1} \ \Delta^{2,2} \ \dots \ \Delta^{2,R}] & \dots & \vdots \\ \vdots & \vdots & \ddots & \mathbf{0} \\ \mathbf{0} & \dots & \mathbf{0} & [\Delta^{M,1} \ \Delta^{M,2} \ \dots \ \Delta^{M,R}] \end{bmatrix} \cdot \begin{bmatrix} \mathbf{f}^{1,1} \\ \mathbf{f}^{1,2} \\ \vdots \\ \mathbf{f}^{1,R} \\ \mathbf{f}^{2,1} \\ \vdots \\ \mathbf{f}^{M,R} \end{bmatrix} = \Delta \cdot \mathbf{f} \quad (4)$$

where $\Delta^{m,r}$ is the $[N \times K^{m,r}]$ component link-path incidence matrix for class m on the r -th OD movement. The path costs are the summed constituent link costs: $\mathbf{c} = \Delta^T \cdot \mathbf{t}$ so that

$$c_k^{m,r}(\mathbf{x}) = \sum_a t_a^{m,r}(\mathbf{x}) \delta_{a,k}^{m,r}. \quad (5)$$

and hence the path cost vector, \mathbf{c} , has entries ordered as for \mathbf{f} .

2.1 The variable demand and choice models

Individuals are motivated to travel by the utility they gain from getting to their desired destination; they choose between travelling to their desired destination on one of the available routes, or not travelling (or going later or by a different mode that is outside of the road network). For each individual, the benefit of

travelling, as they perceive it, is weighed against the perceived cost of making their journey, specifically, the (perceived) minimum route cost. We assume that if the individual perceives no overall gain in utility from making their desired journey, they will choose not to travel.

For each OD pair, the option of “no travel” is represented in the network by a pseudo-link that provides drivers with another choice of OD route; this link thus comprises a pseudo-path. We note that although our terminology is similar, the method we describe should not be confused with the conventional way of implementing elastic demand DUE problems by the excess demand formulation (Gartner, 1980), which requires a separate demand function to be specified and inverted. In our case, the specification of the demand function is integral to the probit model as an additional choice alternative. Without loss of generality, we can assume that for each class and for each OD movement, the pseudo-path is $f_1^{m,r}$. With this formulation of variable demand, every driver is assigned to the network; those choosing not to travel are assigned to the pseudo-path connecting the relevant OD pair. We will assume that congestion on a “real” network does not depend on the number of potential travellers staying at home *i.e.* costs on the “real” links depend only on the flows on the “real” links, and not on the pseudo-link flows.

The motivation to travel is not the same for all users, even within a single class. For users of class m let the mean utility of travelling (across the population of class m) on the r -th OD movement be $V^{m,r}$. The initial motivation to make a particular OD movement does not depend on the state of the network; the cost of travel (due to the network flows) determines the *net gain* in utility and hence whether or not an individual decides to travel. Therefore $V^{m,r}$ is a constant.

Following discrete choice theory we assume that, for users of class m , the *perceived* utility of the r -th OD movement on route k is the random variable, dependent on \mathbf{x} :

$$U_k^{m,r}(\mathbf{x}) = v^{m,r} - c_k^{m,r}(\mathbf{x}) + \varepsilon_k^{m,r}, \quad (6)$$

where $v^{m,r}$ is the flow-independent (mean) utility of travelling, and $c_k^{m,r}(\mathbf{x})$ are the deterministic, flow-dependent path costs defined in (5) above. We assume that

A2. The stochastic terms $\varepsilon_k^{m,r}$ have a non-degenerate joint probability density function that is continuous, strictly positive, and independent of the deterministic path costs.

We assign the opportunity cost of not travelling (the utility gained by travelling) to the pseudo-link: $c_1^{m,r} = v^{m,r}$, so that the utility of not travelling has zero mean. The constant cost on the pseudo-path also represents the fact that there is no congestion effect on the “no travel” alternative (this assumption can be relaxed and the results to be derived still follow—indeed, the constant cost assumption is more problematic, as seen in section 3, but is chosen so as to be more consistent with conventional implementations of elastic demand problems). It will be convenient to define the vector of deterministic path utilities, $\mathbf{u}(\mathbf{x})$, with elements $u_k^{m,r}(\mathbf{x}) = v^{m,r} - c_k^{m,r}(\mathbf{x})$. This gives $U_k^{m,r}(\mathbf{x}) = u_k^{m,r}(\mathbf{x}) + \varepsilon_k^{m,r}$, and on the pseudo-paths, $u_1^{m,r}(\mathbf{x}) = 0$.

Drivers from class m , on OD movement r choosing the k -th path are those who perceive this to maximise their utility (given the current mean path costs for their class: \mathbf{c}^m). The corresponding choice probability is defined to be

$$P_k^{m,r}(\mathbf{u}^m) = \Pr(U_k^{m,r} \geq U_j^{m,r} \forall j | \mathbf{u}^m). \quad (7)$$

The $[K \times 1]$ vector of path choice probabilities is denoted \mathbf{P} . Note that since $\mathbf{P}(\mathbf{u}) = \mathbf{P}(\mathbf{v} - \mathbf{c})$, then $\nabla_{\mathbf{u}} \mathbf{P} = -\nabla_{\mathbf{c}} \mathbf{P}$ and so we can readily work in terms of either utility or cost derivatives. The choice model thus defined is single-valued and continuously differentiable (GentilePapola 2001) in the deterministic path utilities (equivalently in the path costs), and hence (using A1) in the path and link flows.

Daganzo (1982) shows that the choice probabilities are continuously differentiable, based on the slightly different assumption that the joint probability density function is regular everywhere rather than being strictly positive.

This variable demand model is a natural extension of the fixed demand case (with no pseudo-links) and is based on the same underlying principles of discrete choice theory used to model drivers’ route choice behaviour. A demand function is implicitly defined by the choice model; for the m -th class on the r -th OD movement this is

$$q_{travel}^{m,r}(\mathbf{x}) = D^{m,r}(\mathbf{x}) = q^{m,r} \cdot \left(1 - \Pr[U_1^{m,r} \leq U_k^{m,r}(\mathbf{x}) \forall k = 1, \dots, K^{m,r}]\right). \quad (8)$$

In this formulation of variable demand, the demand function is determined by an integrated demand and path-choice probability function, and a different demand function prototype cannot be freely chosen (in

contrast, for example, with the conventional manner of defining elastic demand DUE problems). While for a given joint probability distribution the demand function is of a fixed type, the variance-covariance matrix allows the cross elasticities to be defined, in particular for the no travel option.

2.2 The Stochastic User Equilibrium

The Stochastic User Equilibrium (SUE) is defined to be a feasible set of flows such that:

At SUE, no driver can improve his or her *perceived* travel cost by unilaterally changing route.

An SUE is a solution to the fixed-point problem (Sheffi 1985):

$$\mathbf{f} = \mathbf{q} \cdot \mathbf{P}(\mathbf{u}(\Delta\mathbf{f})), \quad (9)$$

for feasible path flows, path choice probabilities, and OD demands. Here $\mathbf{q} = \text{diag}(\Psi^T \hat{\mathbf{q}})$ is the matrix-expanded version of the potential demand vector, such that each constituent class-specific OD movement comprises

$$\begin{bmatrix} f_1^{m,r} \\ f_2^{m,r} \\ \vdots \\ f_{K^{m,r}}^{m,r} \end{bmatrix} = \begin{bmatrix} q^{m,r} & 0 & \cdots & 0 \\ 0 & q^{m,r} & & \\ \vdots & & \ddots & \\ 0 & 0 & & q^{m,r} \end{bmatrix} \cdot \begin{bmatrix} P_1^{m,r} \\ P_2^{m,r} \\ \vdots \\ P_{K^{m,r}}^{m,r} \end{bmatrix}. \quad (10)$$

A solution to (9) is denoted $\tilde{\mathbf{f}}$, with the corresponding link flow solution denoted $\tilde{\mathbf{x}} = \Delta\tilde{\mathbf{f}}$. By assumption (A1) and following Rosa (Rosa 2003), it is clear that, at equilibrium, there is a one-to-one mapping between a disaggregate path flow SUE and its corresponding disaggregate link flow representation, from path to link flows through $\tilde{\mathbf{x}} = \Delta\tilde{\mathbf{f}}$, and from link to path flows through via the sequence of relationships: disaggregate link flows \Rightarrow disaggregate link costs \Rightarrow disaggregate path costs \Rightarrow disaggregate path choice probabilities \Rightarrow disaggregate path flows, i.e. $\tilde{\mathbf{f}} = \mathbf{q} \cdot \mathbf{P}(\mathbf{u}(\tilde{\mathbf{x}}))$.

It remains to solve the fixed-point problem (9) in order to calculate the equilibrium flows for a given network. Fortunately, with this variable demand model, it is no more difficult than calculating the fixed demand SUE flows, methods for which have been extensively discussed elsewhere (Fisk 1980; MaherHughes 1997; Rosa 2003; Sheffi 1985; SheffiPowell 1981).

2.3 The Probit Model

The probit model is a particular instance of the formulation described above, in which for each user-class m and O-D movement r the joint distribution of the vector of path error terms $\boldsymbol{\varepsilon}^{m,r}$ —which has elements $\varepsilon_k^{m,r}$ for $k = 1, 2, \dots, K^{m,r}$ —follows a Multivariate Normal distribution with zero mean and covariance matrix $\boldsymbol{\Sigma}^{m,r}$. Many structures are possible for this covariance matrix; for example, a diagonal matrix with identical diagonal entries would allow us to approximate the i.i.d. assumption of the multinomial logit. Alternatively, as the magnitude of the terms in $\boldsymbol{\Sigma}^{m,r}$ becomes small, so it is well known that the SUE model increasingly approximates the DUE. As a further alternative, Yai *et al* (1997) propose a structure incorporating path-specific error terms. However, the most commonly adopted and arguably most natural assumption is to impute $\boldsymbol{\Sigma}^{m,r}$ from constituent *link* cost components, with the joint distribution of the link cost error components itself Multivariate Normal. Given that the Multivariate Normal assumption is preserved under linear transformation (from the link to path cost domain), such link error component models do indeed imply a probit path choice model, provided that the implied path cost error covariance matrix is well-conditioned (an important point to which we return in section ...). While the link error component assumption also permits *link* error correlations to be specified, a simplification is to neglect these correlations and assume independent Normal link cost error distributions for each link. In this latter, simplest case, if the link cost error distribution for link a as perceived by user-class m on O-D movement r is Normal with zero mean and variance σ_{amr}^2 , then the network structure gives the required components of $\boldsymbol{\Sigma}^{m,r}$ as:

$$\Sigma_{k,l}^{m,r} = \sum_{a=1}^N \delta_{a,k}^{m,r} \delta_{a,l}^{m,r} \sigma_{amr}^2 \quad (k = 1, 2, \dots, K^{m,r}; l = 1, 2, \dots, K^{m,r}). \quad (11)$$

Hence the joint distribution of error terms $\boldsymbol{\varepsilon}^{m,r}$ is known in order to apply (6), and which (it is supposed) satisfies assumption A2. Note that since the perceived utilities of the travel alternatives (6) are MVN distributed, the path choice probabilities, (7), and hence the demand function, (8), cannot be written in closed form.

2.4 Properties of the SUE flows

Existence of a solution to the SUE problem defined is guaranteed by Brouwer's theorem since, by A1 and A2, the fixed-point condition (9) is a continuous function of the flows, being a continuous composition of continuous mappings, and the feasible region is closed and convex. A sufficient condition for the uniqueness of this solution (Cantarella 1997) is that the link cost function, $\mathbf{t}(\mathbf{x})$, is monotone, non-decreasing.

2.5 Design Parameters

We wish to consider changes to the *design parameters*, $\mathbf{s} = [s_1, \dots, s_S]^T$, that define the network; namely, the OD demands and the parameters in the link cost functions. Davis (1994) remarked that

...“if the link use probabilities can be expressed as differentiable functions of the capacity increases and of the link volumes [the design parameters], which is the case for both logit and probit models, the NDP with SUE assignment becomes a differentiable optimization problem with a manageable number of differentiable constraints.”

This implies that the probit SUE flows are differentiable in the design parameters, though Davis provides no formal proof of this statement. In the next section, we determine sufficient conditions for the equilibrium flows to be differentiable in the design parameters, in the case of our variable demand multiple user class network model. Differentiability of the equilibrium flows is required to justify the concomitant derivation of sensitivity expressions for these flows as the design parameters are perturbed.

3. Differentiability of the Equilibrium Flows

Sufficient conditions for the differentiability of the equilibrium disaggregate link flows will be established using the implicit function theorem that states:

Consider $\mathbf{d}(\mathbf{x}; \mathbf{s}) = \mathbf{d}(x_1, \dots, x_N, s_1, \dots, s_S)$, a continuously differentiable, vector valued function mapping on an open set $E \subset \mathbb{R}^{N+S}$ into \mathbb{R}^N . Let $(\mathbf{x}_0, \mathbf{s}_0)$ be a point in E for which $\mathbf{d}(\mathbf{x}_0, \mathbf{s}_0) = \mathbf{0}$ and for which the $[N \times N]$ Jacobian determinant is non-zero

$$\left. \frac{\partial(d_1, \dots, d_N)}{\partial(x_1, \dots, x_N)} \right|_{[\mathbf{x}_0, \mathbf{s}_0]} \neq 0$$

Then there exists an S -dimensional neighbourhood W of \mathbf{s}_0 and a unique, continuously differentiable function $\mathbf{g} : W \rightarrow \mathbb{R}^N$ such that

$$\mathbf{g}(\mathbf{s}_0) = \mathbf{x}_0 \text{ and } \mathbf{d}(\mathbf{g}(\mathbf{t}); \mathbf{t}) = \mathbf{0} \text{ for all } \mathbf{t} \in W.$$

In the light of the SUE fixed-point condition, (9), consider the gap function for the link flows

$$\mathbf{d}(\mathbf{x}; \mathbf{s}) = \mathbf{x} - \Delta \cdot \mathbf{q}(\mathbf{s}) \cdot \mathbf{P}[\mathbf{u}(\mathbf{x}; \mathbf{s})]. \quad (11)$$

Clearly for design parameters, \mathbf{s} , the link flows $\tilde{\mathbf{x}}$ are a solution to the SUE if and only if $\mathbf{d}(\tilde{\mathbf{x}}; \mathbf{s}) = \mathbf{0}$. For every point, \mathbf{s}_0 , where the Jacobian is non-singular, $|\nabla_{\mathbf{x}} \mathbf{d}(\tilde{\mathbf{x}}(\mathbf{s}_0); \mathbf{s}_0)| \neq 0$, the implicit function theorem therefore states that the equilibrium flows are continuously differentiable as a function of the design parameters (in some neighbourhood of \mathbf{s}_0).

Note that, by assumptions (A1) and (A2), the gap function is differentiable with respect to the link flows, giving

$$\nabla_{\mathbf{x}} \mathbf{d} = \mathbf{I} - \Delta \cdot \mathbf{q}(\mathbf{s}) \cdot \nabla_{\mathbf{u}} \mathbf{P} \cdot \nabla_{\mathbf{x}} \mathbf{u}(\mathbf{x}; \mathbf{s}). \quad (12)$$

However, this does not mean that the equilibrium flows are a continuously differentiable function of the design parameters because there is no guarantee that the Jacobians in (13) are invertible. In fact, the constant cost pseudo-paths arising from our variable demand model contribute zero rows to $\nabla_{\mathbf{x}} \mathbf{u}$, which is therefore rank deficient and hence non-invertible.

To proceed, we consider a reduced formulation of the network flows, by removing the flows on the pseudo-paths and links. Using similar notation to that of Bellei *et al.* (2002), the $[K-MR \times K]$ matrix \mathbf{I}^- is constructed by removing from the $[K \times K]$ identity matrix the MR rows that correspond to the pseudo-paths $f_1^{m,r}$. Therefore the reduced vector of path flows, with the flow on alternatives corresponding to the pseudo-paths removed, is

$$\mathbf{f}^- = \mathbf{I}^- \mathbf{f}. \quad (13)$$

The $[K \times 1]$ vector $\mathbf{I}^- \mathbf{f}$ has correct entries for the “real” path flows, but all pseudo-path flows appear as zero. The $[MR \times 1]$ vector of removed path flows are

$$\mathbf{f}^1 = \mathbf{I}^1 \mathbf{f}, \quad (14)$$

where \mathbf{I}^1 is derived from the identity matrix with all rows deleted *except* those corresponding to the pseudo-paths.

For each class/OD movement only one of the constituent flows has been removed from \mathbf{f} to obtain \mathbf{f}^- . Flow conservation therefore allows us to retrieve the full path flow vector from the reduced path flow vector, \mathbf{f}^- .

$$\mathbf{f}^1 = \hat{\mathbf{q}} - \Psi \mathbf{I}^{-T} \mathbf{f}^- \quad (15)$$

Where Ψ is defined in (3). Consequently, the full path flow vector is

$$\mathbf{f} = \mathbf{I}^{-T} \mathbf{f}^- + \mathbf{I}^{1T} (\hat{\mathbf{q}} - \Psi \mathbf{I}^{-T} \mathbf{f}^-). \quad (16)$$

Let Δ^- be the link path incidence matrix with those rows and columns removed that correspond to the pseudo-links and pseudo-paths. The reduced link flow vector, with the flows on pseudo-links removed, is

$$\mathbf{x}^- = \Delta^- \mathbf{f}^- \quad (17)$$

The reduced path utility vector can be calculated from the set of link costs, \mathbf{t}^- , without the pseudo-links included

$$\mathbf{u}^- = \mathbf{I}^- \Psi^T \nu - \Delta^{-T} \cdot \mathbf{t}^-(\mathbf{x}^-; \mathbf{s}) \quad (18)$$

Note that the full vector of deterministic path utilities can be retrieved since pre-multiplying by \mathbf{I}^- inserts zeros at the positions of the removed paths and, by construction, the removed pseudo-paths have zero utility. Therefore

$$\mathbf{u} = \mathbf{I}^{-T} \mathbf{u}^-. \quad (19)$$

The fixed-point condition for the reduced path flows is obtained by pre-multiplying (9) by \mathbf{I}^-

$$\mathbf{f}^- = \mathbf{I}^- \cdot \mathbf{q} \cdot \mathbf{P}(\mathbf{I}^{-T} \mathbf{u}^-) \quad (20)$$

The argument of the choice model is the full path utility vector so the correct proportions of flow are assigned to all paths. The full demand matrix is used. This fixed-point condition is equivalent to (9) because the reduced flows uniquely determine the flows on each of the pseudo-paths. The reduced link flow fixed-point SUE condition is

$$\mathbf{x}^- = \Delta^- \mathbf{I}^- \cdot \mathbf{q}(\mathbf{s}) \cdot \mathbf{P}[\mathbf{I}^{-T} \{ \mathbf{I}^- \Psi^T \nu - \Delta^{-T} \mathbf{t}^-(\mathbf{x}^-; \mathbf{s}) \}] \quad (21)$$

We apply the implicit function theorem to the gap function

$$\mathbf{d}^-(\mathbf{x}^-; \mathbf{s}) = \mathbf{x}^- - \Delta^- \mathbf{I}^- \cdot \mathbf{q}(\mathbf{s}) \cdot \mathbf{P}[\mathbf{u}(\mathbf{x}^-; \mathbf{s})] \quad (22)$$

$\mathbf{d}^-(\cdot)$ is single-valued and C^1 because (by A1 and A2) the link cost functions and the choice model are C^1 . It remains to show that the Jacobian Determinant (with respect to \mathbf{x}^-) is non-zero

$$\nabla_{\mathbf{x}^-} \mathbf{d}^- = \mathbf{I}^- - \nabla_{\mathbf{x}^-} (\Delta^- \mathbf{I}^- \cdot \mathbf{q}(\mathbf{s}) \cdot \mathbf{P}[\mathbf{u}(\mathbf{x}^-; \mathbf{s})]). \quad (23)$$

Using (18) and (19) this gives

$$\nabla_{\mathbf{x}^-} \mathbf{d}^- = \mathbf{I}^- + (\Delta^- \mathbf{I}^-) \cdot \mathbf{q}(\mathbf{s}) \cdot (\nabla_{\mathbf{u}} \mathbf{P}) \cdot (\Delta^- \mathbf{I}^-)^T \cdot (\nabla_{\mathbf{x}^-} \mathbf{t}^-(\mathbf{x}^-; \mathbf{s})) \quad (24)$$

The choice probability Jacobian $\nabla_{\mathbf{u}} \mathbf{P}$ is positive semi-definite (Daganzo 1979). Assume that:

A3. The Jacobian $\nabla_{\mathbf{x}^-} \mathbf{t}^-(\mathbf{x}^-; \mathbf{s})$ is positive definite (and hence invertible).

Pre-multiplying (25) by this reduced link cost Jacobian gives

$$\nabla_{\mathbf{x}^-} \mathbf{t}^-(\mathbf{x}^-; \mathbf{s})^T \nabla_{\mathbf{x}^-} \mathbf{d}^- = \nabla_{\mathbf{x}^-} \mathbf{t}^-(\mathbf{x}^-; \mathbf{s})^T + \nabla_{\mathbf{x}^-} \mathbf{t}^-(\mathbf{x}^-; \mathbf{s})^T (\Delta^- \mathbf{I}^-) \cdot \mathbf{q} \cdot (\nabla_{\mathbf{u}} \mathbf{P}) \cdot (\Delta^- \mathbf{I}^-)^T \cdot (\nabla_{\mathbf{x}^-} \mathbf{t}^-(\mathbf{x}^-; \mathbf{s}))$$

The first term on the right hand side is positive definite by (A3). The second term is positive semi-definite since it is a quadratic form applied to a positive semi-definite matrix. This term is multiplied by the demand matrix that is positive definite since the demands are positive and the matrix diagonal. The entire

right hand side is therefore the sum of a positive semi-definite matrix and a positive definite matrix and is hence positive definite.

On the left hand side, $\nabla_{\mathbf{x}^-} \mathbf{t}^-(\mathbf{x}^-; \mathbf{s})^T \nabla_{\mathbf{x}^-} \mathbf{d}$ is therefore positive definite and hence invertible. In addition, $\nabla_{\mathbf{x}^-} \mathbf{t}^-(\mathbf{x}^-; \mathbf{s})^T$ is invertible (by A3). Finally then, $\nabla_{\mathbf{x}^-} \mathbf{d}$ is invertible, with

$$\left[\nabla_{\mathbf{x}^-} \mathbf{d} \right]^{-1} = \left[\nabla_{\mathbf{x}^-} \mathbf{t}^-(\mathbf{x}^-; \mathbf{s})^T \nabla_{\mathbf{x}^-} \mathbf{d} \right]^{-1} \nabla_{\mathbf{x}^-} \mathbf{t}^-(\mathbf{x}^-; \mathbf{s})^T. \quad (25)$$

Consider a setting of the design parameters $\mathbf{s} = \mathbf{s}_0$ and the corresponding SUE link flows, $\tilde{\mathbf{x}}_0^-$. Application of the implicit function theorem gives us that there is an open neighbourhood W of \mathbf{s}_0 , and a continuously differentiable function \mathbf{g} such that $\mathbf{g}(\mathbf{s}_0) = \tilde{\mathbf{x}}_0^-$ and $\mathbf{g}(\mathbf{s}) = \tilde{\mathbf{x}}^-$ for all $\mathbf{s} \in W$ i.e. $\mathbf{d}^-(\mathbf{g}[\mathbf{s}], \mathbf{s}) = \mathbf{0}$. This implies that the full vector of disaggregate SUE link flows is a continuously differentiable function of the design parameters, since all disaggregate link flows are uniquely specified by a continuously differentiable function of the reduced link flows

$$\mathbf{x} = \Delta \cdot \mathbf{q}(\mathbf{s}) \cdot \mathbf{P} \left[\mathbf{I}^{-T} \left\{ \mathbf{I}^{-T} \Psi^T \nu - \Delta^{-T} \mathbf{t}^-(\mathbf{x}^-; \mathbf{s}) \right\} \right]. \quad (26)$$

4. Link Based Sensitivity Analysis of the Equilibrium Flows

Standard optimisation algorithms need gradient information to find minima/maxima. For the SUE flows, computation of the relevant Jacobian matrices by numerical differencing requires many SUE evaluations and is prone to error due to the amplification of inaccuracies in the calculation of the SUE flows (see Connors et al. 2003). A sensitivity analysis of the SUE flows provides analytical expressions for the Jacobian of link flows that, in turn, are required to derive Jacobian matrices describing the gradients of any objective function in a network design optimisation (see MagnantiWong 1984).

Sensitivity analysis for the elastic demand UE case can be found in Yang (Yang 1997), for logit SUE in Davis (1994) and for single user class, fixed demand probit SUE in Clark & Watling (ClarkWatling 2002b). In this section, we calculate the sensitivity expressions for the multiple user-class variable demand probit SUE link flows.

The Taylor series expansion of the gap function (11) about the equilibrium flows at some initial setting, \mathbf{s}_0 , of the design parameters is

$$\mathbf{d}(\mathbf{x}; \mathbf{s}) \approx \mathbf{d}(\tilde{\mathbf{x}}(\mathbf{s}_0); \mathbf{s}_0) + \left[\nabla_{\mathbf{x}} \mathbf{d} \Big|_{\mathbf{d}(\tilde{\mathbf{x}}(\mathbf{s}_0); \mathbf{s}_0)} (\mathbf{x} - \tilde{\mathbf{x}}(\mathbf{s}_0)) \right] + \left[\nabla_{\mathbf{s}} \mathbf{d} \Big|_{\mathbf{d}(\tilde{\mathbf{x}}(\mathbf{s}_0); \mathbf{s}_0)} (\mathbf{s} - \mathbf{s}_0) \right] \quad (27)$$

We denote the ‘link flow Jacobian’ by $\mathbf{J}_{\mathbf{x}}$ and the ‘design parameter Jacobian’ by $\mathbf{J}_{\mathbf{s}}$; both are evaluated at the initial equilibrium flows. Evaluating $\mathbf{d}(\cdot)$ with the network flows at (the new) equilibrium, $\mathbf{x} = \tilde{\mathbf{x}}(\mathbf{s})$, by definition of the gap function, gives $\mathbf{d}(\tilde{\mathbf{x}}(\mathbf{s}), \mathbf{s}) = \mathbf{0}$ and, invoking the results of the previous section, the equilibrium flows at \mathbf{s} can be expressed in terms of those at \mathbf{s}_0 as

$$\tilde{\mathbf{x}}(\mathbf{s}) \approx \tilde{\mathbf{x}}(\mathbf{s}_0) - \mathbf{J}_{\mathbf{x}}^{-1} \mathbf{J}_{\mathbf{s}} \cdot (\mathbf{s} - \mathbf{s}_0). \quad (28)$$

This approximation is accurate in the neighbourhood of \mathbf{s}_0 where the neglected (curvature) terms in the Taylor expansion of $\mathbf{d}(\mathbf{x}; \mathbf{s})$ remain small. This approximation should be expected to break down where the variation in flows displays high curvature.

4.1 The link cost function prototype

In order to present explicit sensitivity expressions, the link cost functions that will be used in this paper (see DaganzoSheffi 1977) are of the form

$$t_a^m = \tau_a^m + \beta^m t_a(\mathbf{x}). \quad (29)$$

Here, $t_a(\cdot)$ is the common link cost. The parameter β^m is the value of time for user-class m and τ_a^m is a constant cost (toll) specific to this link and this user-class. The corresponding path costs are

$$c_k^{m,r}(\mathbf{x}) = \sum_a t_a^m \delta_{a,k}^{m,r} = \sum_a \left[\tau_a^m + \beta^m t_a(\mathbf{x}) \right] \cdot \delta_{a,k}^{m,r}. \quad (30)$$

For convenience (and to reduce the matrix sizes for numerical computation), we split the design parameters into various types: demand, class specific fixed link costs (tolls), value of time parameters and common link cost function parameters, so that $\mathbf{s} = [\mathbf{s}_q, \mathbf{s}_\tau, \mathbf{s}_\beta, \mathbf{s}_t]$ and

$$\nabla_{\mathbf{s}} \mathbf{d} \cdot (\mathbf{s} - \mathbf{s}_0) = \nabla_{\mathbf{s}_q} \mathbf{d} \cdot (\mathbf{s}_q - \mathbf{s}_{q0}) + \nabla_{\mathbf{s}_\tau} \mathbf{d} \cdot (\mathbf{s}_\tau - \mathbf{s}_{\tau0}) + \nabla_{\mathbf{s}_\beta} \mathbf{d} \cdot (\mathbf{s}_\beta - \mathbf{s}_{\beta0}) + \nabla_{\mathbf{s}_t} \mathbf{d} \cdot (\mathbf{s}_t - \mathbf{s}_t) \quad (31)$$

4.2 Link Flow Jacobian

We begin by invoking the chain rule to write $\mathbf{J}_x = \mathbf{I}_{MN} - \Delta \cdot \mathbf{q} \cdot \nabla_{\mathbf{c}} \mathbf{P} \cdot \nabla_{\mathbf{x}} \mathbf{c}$. We assume no inter-class nor inter-OD dependence of the path choice probabilities, *i.e.* $\partial P_k^{m,r} / \partial c_j^{n,s} = 0$ unless $n = m$ and $r = s$. This gives a block diagonal structure to the path choice probability Jacobian $\nabla_{\mathbf{c}} \mathbf{P}$ by class, within which it is block diagonal by OD movement.

$$\nabla_{\mathbf{c}} \mathbf{P} = \begin{bmatrix} \left[\begin{array}{ccc} (\nabla_{\mathbf{c}} \mathbf{P})^{1,1} & & 0 \\ & \ddots & \\ 0 & & (\nabla_{\mathbf{c}} \mathbf{P})^{1,R} \end{array} \right] & & 0 \\ & \ddots & \\ 0 & & \left[\begin{array}{ccc} (\nabla_{\mathbf{c}} \mathbf{P})^{M,1} & & 0 \\ & \ddots & \\ 0 & & (\nabla_{\mathbf{c}} \mathbf{P})^{M,R} \end{array} \right] \end{bmatrix}$$

with

$$(\nabla_{\mathbf{c}} \mathbf{P})^{m,r} = \begin{bmatrix} \frac{\partial P_1^{m,r}}{\partial c_1^{m,r}} & \dots & \frac{\partial P_1^{m,r}}{\partial c_{K^{m,r}}^{m,r}} \\ \vdots & \ddots & \vdots \\ \frac{\partial P_{K^{m,r}}^{m,r}}{\partial c_1^{m,r}} & \dots & \frac{\partial P_{K^{m,r}}^{m,r}}{\partial c_{K^{m,r}}^{m,r}} \end{bmatrix} \quad (32)$$

This allows us to write \mathbf{J}_x as

$$\mathbf{J}_x = \mathbf{I}_{MN} - \begin{bmatrix} \left[q^{1,1} \Delta^{1,1} (\nabla_{\mathbf{c}} \mathbf{P})^{1,1} \dots q^{1,R} \Delta^{1,R} (\nabla_{\mathbf{c}} \mathbf{P})^{1,R} \right] & 0 \\ 0 & \vdots \\ 0 & \left[q^{M,1} \Delta^{M,1} (\nabla_{\mathbf{c}} \mathbf{P})^{M,1} \dots q^{M,R} \Delta^{M,R} (\nabla_{\mathbf{c}} \mathbf{P})^{M,R} \right] \end{bmatrix} \cdot \nabla_{\mathbf{x}} \mathbf{c}$$

The path costs are defined to be $\mathbf{c} = \Delta^T \mathbf{t}$. With the function prototype (29), the link cost Jacobian comprises terms like $\partial(\tau_a^m + \beta^m t_a(\mathbf{x})) / \partial x_b^n = \beta^m \partial t_a(\mathbf{x}) / \partial x_b^n$, so that

$$\nabla_{\mathbf{x}} \mathbf{c} = \Delta^T \cdot \nabla_{\mathbf{x}} \mathbf{t} = \begin{bmatrix} \left[\begin{array}{ccc} \Delta^{1,1T} & & \\ \vdots & & \\ \Delta^{1,R^T} & & 0 \end{array} \right] & & \\ & \ddots & \\ \left[\begin{array}{ccc} \Delta^{2,1T} & & \\ \vdots & & \\ \Delta^{2,R^T} & & \end{array} \right] & & \\ & \ddots & \\ 0 & & \left[\begin{array}{ccc} \Delta^{M,1T} & & \\ \vdots & & \\ \Delta^{M,R^T} & & \end{array} \right] \end{bmatrix} \cdot \begin{bmatrix} \left[\begin{array}{ccc} \frac{\partial t_1}{\partial x_1^1} \dots \frac{\partial t_1}{\partial x_N^1} \\ \vdots & \ddots & \vdots \\ \frac{\partial t_N}{\partial x_1^1} \dots \frac{\partial t_N}{\partial x_N^1} \end{array} \right] & \dots & \left[\begin{array}{ccc} \frac{\partial t_1}{\partial x_1^M} \dots \frac{\partial t_1}{\partial x_N^M} \\ \vdots & \ddots & \vdots \\ \frac{\partial t_N}{\partial x_1^M} \dots \frac{\partial t_N}{\partial x_N^M} \end{array} \right] \\ \vdots & & \vdots \\ \left[\begin{array}{ccc} \frac{\partial t_1}{\partial x_1^1} \dots \frac{\partial t_1}{\partial x_N^1} \\ \vdots & \ddots & \vdots \\ \frac{\partial t_N}{\partial x_1^1} \dots \frac{\partial t_N}{\partial x_N^1} \end{array} \right] & \dots & \left[\begin{array}{ccc} \frac{\partial t_1}{\partial x_1^M} \dots \frac{\partial t_1}{\partial x_N^M} \\ \vdots & \ddots & \vdots \\ \frac{\partial t_N}{\partial x_1^M} \dots \frac{\partial t_N}{\partial x_N^M} \end{array} \right] \end{bmatrix} \quad (33)$$

The $[MN \times MN]$ link cost Jacobian is therefore

$$\mathbf{J}_x = \mathbf{I}_{MN} - \begin{bmatrix} \mathbf{J}_x^1 \\ \vdots \\ \mathbf{J}_x^M \end{bmatrix} \quad \text{where} \quad \mathbf{J}_x^m = \sum_r q^{m,r} \Delta^{m,r} (\nabla_{\mathbf{c}} \mathbf{P})^{m,r} \Delta^{m,r^T} \beta^m \begin{bmatrix} \frac{\partial t_1}{\partial x_1^1} \dots \frac{\partial t_1}{\partial x_N^1} \\ \vdots & \ddots & \vdots \\ \frac{\partial t_N}{\partial x_1^1} \dots \frac{\partial t_N}{\partial x_N^1} \end{bmatrix}$$

In the case of separable link costs that are functions of the total link flow (summed across classes) $\partial t_a^m(\mathbf{x})/\partial x_a^j = \beta^m t_a^m$ for all classes $j=1, \dots, M$, and the off-diagonal terms are zero.

$$\mathbf{J}_x^m = \sum_r q^{m,r} \Delta^{m,r} (\nabla_c \mathbf{P})^{m,r} \Delta^{m,rT} \beta^m \begin{bmatrix} t'_1 & 0 & 0 & t'_1 & 0 & 0 & \cdots & t'_1 & 0 & 0 \\ 0 & \ddots & 0 & 0 & \ddots & 0 & \cdots & 0 & \ddots & 0 \\ 0 & 0 & t'_N & 0 & 0 & t'_N & \cdots & 0 & 0 & t'_N \end{bmatrix} \quad (34)$$

4.3 Class-Specific Link Constant (link toll) Jacobian

For those design parameters, $\mathbf{s} = [s_1, \dots, s_L]$, changing the class-specific link constants, the $[MN \times L]$ Jacobian is $\mathbf{J}_\tau = -\Delta \cdot \mathbf{q} \cdot \nabla_c \mathbf{P} \cdot \nabla_\tau \mathbf{c}$

$$\mathbf{J}_\tau = - \begin{bmatrix} \left[\sum_r q^{1,r} \Delta^{1,r} (\nabla_c \mathbf{P})^{1,r} \Delta^{1,rT} \right] \mathbf{0} & & \mathbf{0} \\ & \ddots & \\ \mathbf{0} & & \mathbf{0} \left[\sum_r q^{M,r} \Delta^{M,r} (\nabla_c \mathbf{P})^{M,r} \Delta^{M,rT} \right] \end{bmatrix} \cdot \nabla_s \mathbf{t}. \quad (35)$$

The $[MN \times L]$ matrix, $\nabla_s \mathbf{t} = [\partial t_a^m / \partial s_j] = [\delta_{a,j}^m]$, where $\delta_{a,j}^m = 1$ when the design parameter s_j corresponds to the class-specific link constant, τ_a^m , for class m on link a ; each column has only one non-zero entry. Therefore the L columns of \mathbf{J}_τ are those picked by $\nabla_s \mathbf{t}$ directly from the block-diagonal matrix in (35).

4.4 Value of Time Jacobian

For those design parameters, $\mathbf{s} = [s_1, \dots, s_L]$, changing values of time for certain classes, the $[MN \times L]$ Jacobian is $\mathbf{J}_\beta = -\Delta \cdot \mathbf{q} \cdot \nabla_c \mathbf{P} \cdot \nabla_\beta \mathbf{c}$, as in (35). Here

$$\nabla_s \mathbf{t} = [\partial t_a^m / \partial s_j] = \begin{bmatrix} \frac{\partial t_1^1}{\partial s_1} & \cdots & \frac{\partial t_1^1}{\partial s_L} \\ \vdots & \ddots & \vdots \\ \frac{\partial t_N^M}{\partial s_1} & \cdots & \frac{\partial t_N^M}{\partial s_L} \end{bmatrix} = \begin{bmatrix} \mathbf{0} & \cdots & \mathbf{0} \\ \begin{bmatrix} t_1 \\ \vdots \\ t_N \end{bmatrix} & & \\ \mathbf{0} & \cdots & \mathbf{0} \\ & & \begin{bmatrix} t_1 \\ \vdots \\ t_N \end{bmatrix} \\ \mathbf{0} & \cdots & \mathbf{0} \end{bmatrix}$$

In each MN length column of $\nabla_s \mathbf{t}$, the vector of common link travel times, $\mathbf{t} = [t_1, \dots, t_N]^T$, occurs in the row-block of the class specified by the design parameter.

4.5 Common Link Cost Jacobian

For those design parameters, $\mathbf{s} = [s_1, \dots, s_L]$, changing constants in the shared link cost functions, the $[MN \times L]$ Jacobian is $\mathbf{J}_t = -\Delta \cdot \mathbf{q} \cdot \nabla_c \mathbf{P} \cdot \nabla_t \mathbf{c}$, as in (35). Here

$$\nabla_{\mathbf{s}} \mathbf{t} = \left[\frac{\partial t_a^m}{\partial s_j} \right] = \begin{bmatrix} \frac{\partial t_1^1}{\partial s_1} & \dots & \frac{\partial t_1^1}{\partial s_L} \\ \vdots & \ddots & \vdots \\ \frac{\partial t_N^M}{\partial s_1} & \dots & \frac{\partial t_N^M}{\partial s_L} \end{bmatrix} = \begin{bmatrix} \beta^1 \begin{bmatrix} \frac{\partial t_1}{\partial s_1} & \dots & \frac{\partial t_1}{\partial s_L} \\ \vdots & \vdots & \vdots \\ \frac{\partial t_N}{\partial s_1} & \dots & \frac{\partial t_N}{\partial s_L} \end{bmatrix} \\ \vdots \\ \beta^M \begin{bmatrix} \frac{\partial t_1}{\partial s_1} & \dots & \frac{\partial t_1}{\partial s_L} \\ \vdots & \vdots & \vdots \\ \frac{\partial t_N}{\partial s_1} & \dots & \frac{\partial t_N}{\partial s_L} \end{bmatrix} \end{bmatrix}$$

$$\text{So that } \mathbf{J}_t = \begin{bmatrix} \mathbf{J}_t^1 \\ \vdots \\ \mathbf{J}_t^M \end{bmatrix} \text{ where } \mathbf{J}_t^m = -\sum_r q^{m,r} \Delta^{m,r} (\nabla_c \mathbf{P})^{m,r} \Delta^{m,r,T} \beta^m \begin{bmatrix} \frac{\partial t_1}{\partial s_1} & \dots & \frac{\partial t_1}{\partial s_L} \\ \vdots & \vdots & \vdots \\ \frac{\partial t_N}{\partial s_1} & \dots & \frac{\partial t_N}{\partial s_L} \end{bmatrix}.$$

4.6 Demand Jacobian

For ease of notation, we rewrite the gap function, using (3), so that the OD demands appear as a vector:

$$\mathbf{d}(\mathbf{x}; \mathbf{s}_q) = \mathbf{x} - \Delta \cdot \text{diag}(\mathbf{P}) \cdot \Psi^T \cdot \hat{\mathbf{q}}(\mathbf{s}_q) \quad (36)$$

On differentiating with respect to the OD demands, $\mathbf{s} = [s_1, \dots, s_L]$, we find that the demand Jacobian, \mathbf{J}_q is composed of class-blocks

$$\mathbf{J}_q = \begin{bmatrix} \mathbf{J}_q^1 \\ \vdots \\ \mathbf{J}_q^M \end{bmatrix} \text{ where } \mathbf{J}_q^m = \begin{bmatrix} \frac{\partial d_1^m}{\partial s_1} & \dots & \frac{\partial d_1^m}{\partial s_L} \\ \vdots & \ddots & \vdots \\ \frac{\partial d_N^m}{\partial s_1} & \dots & \frac{\partial d_N^m}{\partial s_L} \end{bmatrix} = -\sum_r \Delta^{m,r} \cdot \begin{bmatrix} P_1^{m,r} \\ P_2^{m,r} \\ \vdots \\ P_{K^{m,r}}^{m,r} \end{bmatrix} \cdot \begin{bmatrix} \frac{\partial q^{m,r}}{\partial s_1} & \dots & \frac{\partial q^{m,r}}{\partial s_L} \end{bmatrix} \quad (37)$$

The design parameters simply designate those OD/class demands that are being perturbed and so the last matrix comprises zeros and ones, and simply picks out the path choice probabilities for the relevant class-OD pairs.

4.7 Gradient of the Equilibrium Link Flows

The Jacobians \mathbf{J}_x and \mathbf{J}_s describe the sensitivity of the SUE aggregate link flows to the network design parameters and hence provide gradient information for the NDP optimisation. From the sensitivity analysis, it easily follows that

$$\nabla_{\mathbf{s}} \tilde{\mathbf{x}}(\mathbf{s}) \approx -\mathbf{J}_x^{-1} \mathbf{J}_s \mathbf{I}_s$$

where \mathbf{I}_s is the identity matrix (of size equal to the number of design parameters).

5. Implementation and Computational Issues

Numerical computation of the SUE flows, and their sensitivities to changes in the design parameters, comprises several stages, each of which can be accomplished using a variety of methods. Given current path costs, the probit path choice probabilities need to be calculated. These probabilities are used within an iterative optimisation algorithm to determine the equilibrium flows; at each iteration, a search direction and step length are required. Once the equilibrium flows are known, the Jacobians must be computed to obtain the sensitivity expressions in the previous section.

There is no closed form expression for the probit path choice probabilities, which must therefore be computed either by numerical integration (e.g. Genz 1992), simulation (e.g. Monte Carlo as in SheffiPowell 1981), or by analytic approximation (review in Rosa 2003). Approximation by simulation (Monte Carlo or otherwise) introduces non-smooth variation in the equilibrium flows (as the design

parameters are smoothly varied) due to random sampling of the multivariate probability distribution; estimating the path choice probabilities via analytic approximation does not introduce such artefacts. In this paper, we follow the recommendation of Rosa (Rosa 2003) and use the Mendell-Elston analytic approximation method (MendellElston 1974). Monte Carlo simulation is not used anywhere in this paper

To calculate the equilibrium flows, we use an algorithm based on the ‘traditional’ method of successive averages (MSA), (see Wilde 1964). We seek to iteratively reduce the objective function of the SUE equivalent optimisation (Sheffi 1985) using the search direction from the MSA algorithm (moving toward the auxiliary flows). However, rather than using the prescribed, $1/n$, step length of MSA at each iteration, we calculate an optimised step length using a quadratic approximation (MaherHughes 1997), augmenting this with a bisection line search when necessary, to ensure improvement at every iteration.

Once the equilibrium flows have been determined, computation of their sensitivities to changes in the design parameters requires calculation of all the Jacobian matrices detailed in the previous section. One component in these formulae requires special effort: the Jacobian of path-choice probabilities with respect to path costs, $\nabla_{\mathbf{c}} \mathbf{P}$. A method to compute this Jacobian, which Daganzo (1979) attributes to McFadden, is described in Clark and Watling (2002b). The choice probabilities required within the calculation of $\nabla_{\mathbf{c}} \mathbf{P}$ are calculated using the method of Mendell-Elston.

The inverse of the path-covariance matrix appears in the definition of the probit path choice probabilities, and in the calculation of the path-choice probability Jacobian. Although the path-covariance matrix may be singular (see ClarkWatling 2002a) as it is, for example, in the figure-of-eight network, the network equilibrium flows are well-behaved and vary smoothly with the design parameters. Moreover, the probit model, that is to say the multivariate normal probability density function, can accommodate a singular variance-covariance matrix. However, our methods for computing the SUE flows and the sensitivity expressions presented in this paper do run into difficulties when the path-covariance matrix is not invertible. We therefore adopt a mechanism for avoiding this scenario, and construct the path set to avoid any rank deficiencies in the link-path incidence matrix for each OD pair that would result in such a non-invertible path-covariance matrix. In the standard MSA algorithm (Sheffi 1985), all paths are implicitly available. The active paths are generated incrementally, at each iteration, using auxiliary solutions generated by a stochastic shortest path method. While in an infinite number of iterations this algorithm would generate all conceivable paths, in practice (at the end of a finite number of iterations) the active path set simply comprises those paths generated thus far during the procedure. The alternative method for calculating probit SUE, as used in this paper, is to define the active path set upfront, avoiding degeneracies in the link-path incidence matrix for all OD pairs. The path set is generated heuristically in an attempt to include all paths that carry “significant” quantities of flow at equilibrium: this process begins with inclusion of the pseudo-links as the no-travel paths, and the shortest free flow path for each OD pair. With this initial path set, we iterate as follows: given the current path set, the equilibrium flows and resulting path costs are computed under ten times the normal demand, then new shortest and “non-degenerate” paths are added to the path set (as in the Sheffi MSA). Such iterations continue until no new paths are generated under the inflated demand and the resulting path set is then fixed.

While in theory, the probit model assigns strictly positive flows to every conceivable path in the network, in numerical computations this is limited by machine precision, and in reality is restricted by individuals’ rationality and limited network knowledge. In the standard implementation of MSA, the path set is limited in size by the number of iterations, and the set of active paths changes each time to equilibrium flows are calculated. Our alternative approach also restricts the size of the path set, although it is consistent for all calculations of the SUE flows at different settings of the design parameters. We confirm that at the extremes of the tested regime, no new shortest paths become attractive.

6. Numerical Experiments

We consider the Headingley network: 73 nodes, 240 OD movements (hence 240 pseudo-links) and 188 road links, with elastic demand and two user classes that have independent values of time, set to be 5.6 pence/minute and 10.5 p/m (see Department for Transport 2004). The path set is generated up front as described in the previous section, resulting in 1463 paths.

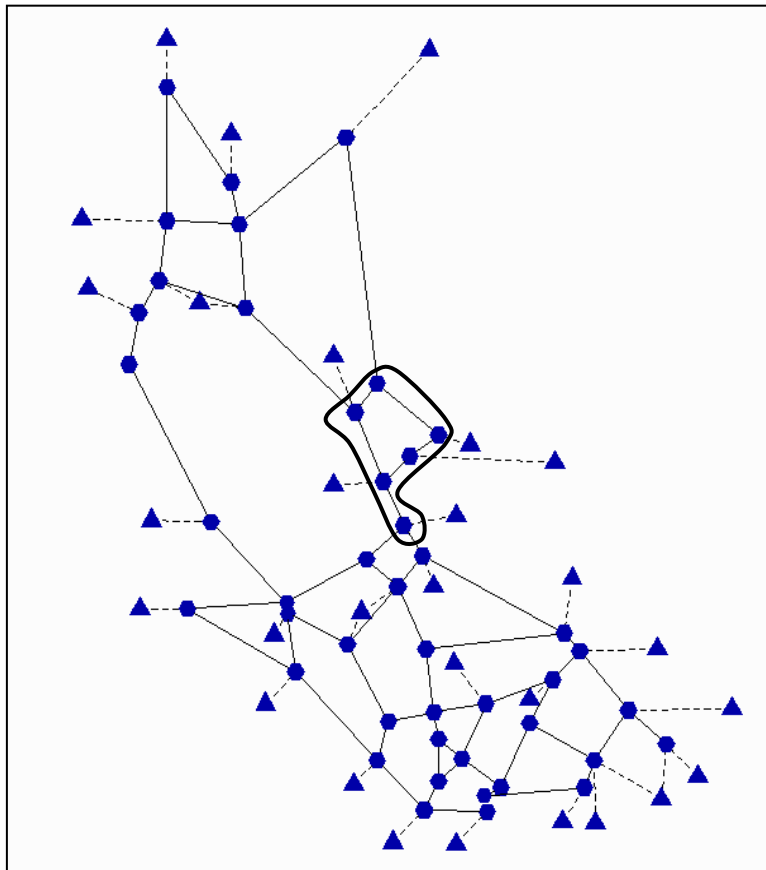


Figure 1: The Headingly Network

Appropriate costs for the pseudo-paths are calculated from a fixed demand assignment to the real links. For each OD movement, the pseudo-link cost is set equal to the maximum path cost. The probit variance for each link is set to be a multiple of the free flow time on that link. Since the pseudo-links have constant cost, they tend to have higher “free flow” times than other links in the network and hence are accorded relatively high variances, representing systematically higher variation in the travel/no travel decision than the perceived cost variation between alternative routes. Clearly, any other variance structure could be adopted with this model. Though the approach implemented is not substantiated by empirical evidence, it is convenient and seems reasonable.

The test network is shown in Figure 1. Origins and destinations are marked with triangles; the corresponding pseudo-links are not displayed in this figure. One scenario is investigated in this paper: a flat toll is imposed on the links within the marked area of the network. Sensitivity analysis of the equilibrium link flows is calculated at zero toll, and the new equilibrium flows are computed for various toll levels from -£5 to +£5.

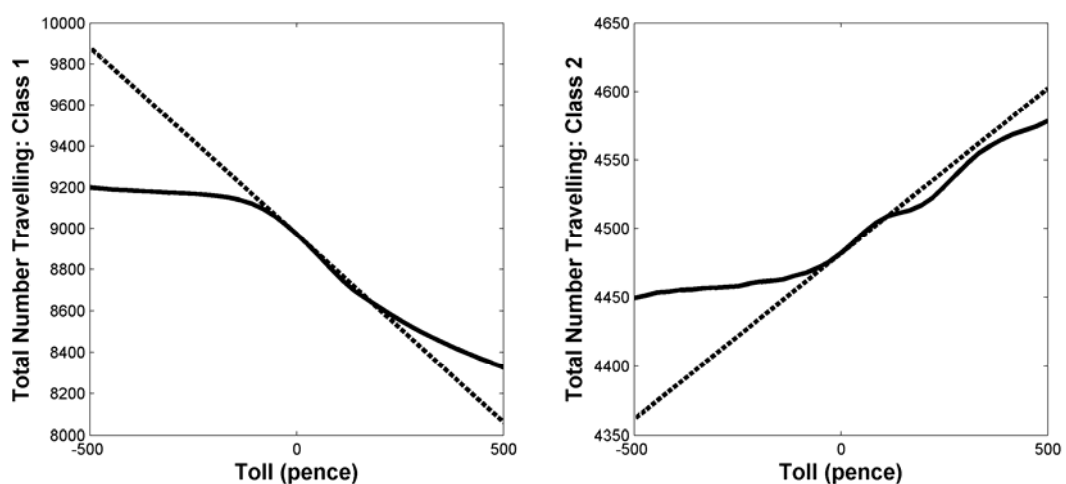


Figure 2: Variation in demand with toll, by user class.

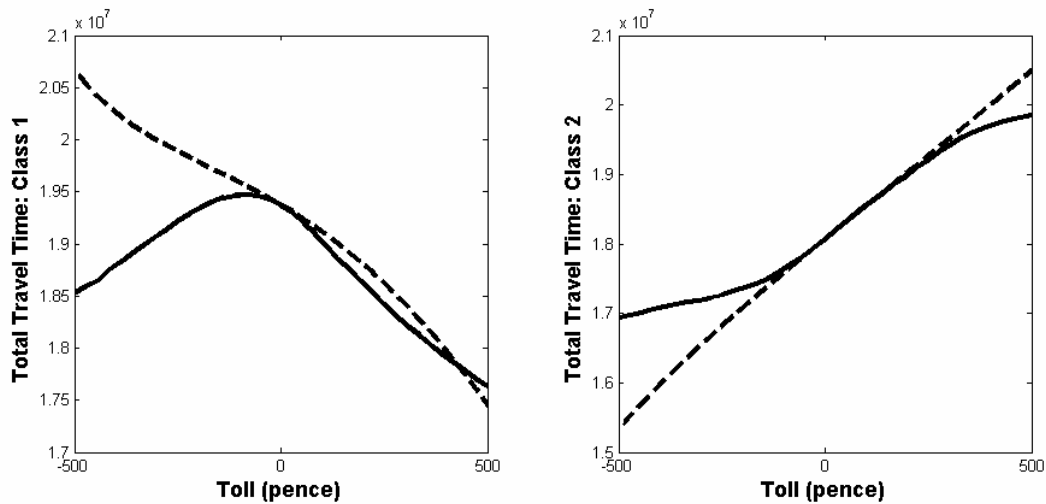


Figure 3: Variation in travel time with toll, by user class.

In Figures 2 and 3 the solid lines represent the equilibrium state of the network, with the SUE flows recomputed at each toll level. The dashed line is evaluated using the equilibrium flows that are predicted by the sensitivity analysis for this toll level. The approximations derived from the sensitivity expressions are tangential to the “true” (recomputed) equilibrium behaviour at zero toll, where the sensitivity analysis was conducted.

The sensitivity analysis gives a linear approximation to the SUE flows and hence to the total number travelling on the real network, since this is simply a sum of certain flows. Therefore, the dashed lines in Figure 2 are straight. However, travel time is not a linear function of flow, so the sensitivity analysis predictions in Figure 3 are not necessarily straight-line approximations.

The two user classes are distinguished by their value of time, and the toll imposed in this example is the same for all users. Figure 2 shows that demand for travel decreases with toll for users with a low value of time, removing congestion on the network, provoking an increase in the number of high value of time users choosing to travel. Figure 3 displays the total travel time by user class, calculated from those travelling on the real links in the network. As the toll increases, there is a decrease in total travel time for low value of time users; this is due to the decrease in number travelling. Similarly the increase in high value of time users choosing to travel results in an increases total travel time for this class.

7. Conclusions

In this paper we present a probit SUE model with multiple user classes and elastic demand, and establish conditions under which it the equilibrium flows are differentiable with respect to the design parameters. Sensitivity expressions are derived for the equilibrium flows under changes in demand and changes to the network design parameters. The constituent Jacobian matrices provide accurate and smooth gradient information regarding the impact of local perturbations to these parameters.

The method of implementation described, particularly the avoidance of simulation methods, avoids the difficulties in interpreting Monte Carlo error and is shown to be applicable to a realistic sized network.

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