Robust bilevel optimization models in transportation science

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Mathematical programs with equilibrium constraints (MPECs) constitute important modelling tools for network flow problems, as they place 'what-if' analyses in a proper mathematical framework. We consider a class of stochastic MPEC traffic models which explicitly incorporate possible uncertainties in travel costs and demands. In stochastic programming terminology, we consider 'here-and-now' models where decisions must be made before observing the uncertain parameter values and the responses of the network users; the objective is to minimize the expectation of the upper-level objective function. Such a model could, for example, be used to derive a fixed toll pricing scheme that provides the best revenue for a given network over a time period, where variations in traffic conditions and demand elasticities are described by distributions of parameters in the travel time and demand functions.

We present new results on the stability of globally optimal solutions to perturbations in the probability distribution, establishing the robustness of the model. We also discuss penalization and discretization algorithms, the latter enabling the utilization of standard MPEC algorithms, and provide many future research avenues.

Keywords: traffic and communication networks, stochastic mathematical program with equilibrium constraints, network design and pricing, solution stability, penalization, sample average approximation

1. Introduction and motivation

(*a*) *Motivation*

When addressing network design and pricing problems under user equilibrium, or any kind of traffic assignment model for that matter, in the form of a hierarchical (that is, bilevel) optimization model (or, mathematical programming problem with equilibrium constraints, MPEC) it is almost always understood that data is certain or that uncertain data can be given some deterministic representation, such as a mean value. It is at the same time understood by all who develop or utilize traffic equilibrium or assignment models, that this assumption is simplistic. Replacing a deterministic traffic equilibrium model by a stochastic one does not really solve the problem, because they also produce unique equilibrium solutions in general; hence the mapping from data to solution is not stochastic even in such models.

Since uncertainty in data *is* prevalent in traffic assignment models, and because bilevel models provide such an attractive modelling approach, there is a need for a bilevel model that can take into account the uncertainty in data. One possibility is to use a classic 'multi-load' approach, taken from the engineering sciences, in which several representative scenarios are included through an averaging in the upper-level objective function.

Inspiration for this work stems from work on structural optimization, the science of producing structures that carry loads optimally. Variations in, for example, loading conditions are often taken into account such that the effectiveness of a design is defined as the average value (or even the worst) of the effectiveness of several 'load cases'. Because of the anticipated fact that the 'real' probability model is never known, and the reported high sensitivity of solutions to stochastic structural optimization problems with respect to small changes in the probability measure, many probability-free worst-case ('pessimistic') models of uncertainty have been developed as alternatives to probabilistic ones (see further below).

This paper seeks to extend the scope of bilevel traffic models to take into account data variations in the form of a stochastic bilevel model, or SMPEC. In order to do so we must consider complications that do not arise in standard bilevel traffic models: SMPEC models are infinite-dimensional, so even the existence of optimal solutions is non-trivial to establish. The main focus of our study of the SMPEC traffic model of this paper is however one that, to some degree, can be used to validate the use of MPEC models in network design applications and in particular multi-load approaches and discretizations: we wish to establish conditions under which optimal designs change continuously with the probability distribution. We say that such solutions are stable, and the model therefore is 'robust' in some sense. Establishing the robustness of the stochastic bilevel model to be developed in this paper is also an alternative to the approach taken in some papers, where robust models are produced through reformulation.

(*b*) *Stochastic programming and robust optimization*

The problem of data uncertainty has been recognized as important for quite some time in the operations research community. The most well-known technique for dealing with uncertainty is stochastic programming (e.g., Birge & Louveaux 1997). Typically, one wants to minimize the expected cost of decisions, that must be made without the complete knowledge of data. In 'here-and-now' models decisions are made once, but in certain types of applications decisions can be made at one or several future recourse stages. The here-and-now decision then represents the first-stage decision which is made to properly hedge against future outcomes of the uncertain data. In these problems one assumes that the distribution of uncertainty is known, or, at least, can be well approximated.

The term 'robust optimization' (RO) has been and is used in a variety of contexts. An important aspect in most applications is the assumption that the distribution of data is known to be confined to certain (typically bounded) 'uncertainty sets'. For particular problems, such as linear and convex quadratic programming, and particular uncertainty sets, RO offers computationally tractable (i.e., polynomially solvable) robust versions. Because feasibility is required for every realization of the data, the robust counterparts include a semi-infinite system of constraints (whence tractability is only possible to obtain in the above instances). Importantly, it is at the same time a *worst-case* type of modelling approach.

Through the above modelling technique one imposes robustness on a model. Our main interest is to investigate the robustness of SMPEC models, in the hope that a reformulation is not necessary. As we shall see, it is in some circumstances possible to establish the robustness of an SMPEC model.

(*c*) *Stochastic mathematical programs with equilibrium constraints*

A mathematical program with equilibrium constraints (MPEC) is an optimization problem with two variables types: primary ones, or 'design' variables, and secondary variables, or 'responses'. The responses are evaluated as part of the constraints of the problem, often in the form of a secondary optimization problem (then often referred to as the 'lower-level problem'). The overall objective is optimized according to a criterion in terms of both design and response. In order to represent this framework in mathematical notation, suppose the design is represented by a vector $x \in \mathbb{R}^n$ and the response by a vector $y \in \mathbb{R}^m$. If the objective is to minimize the function $f : \mathbb{R}^n \times \mathbb{R}^m \to \mathbb{R}$ and the response can be described by the point-to-set mapping $S : \mathbb{R}^n \rightrightarrows \mathbb{R}^m$, then we can describe the MPEC problem as that to

$$\text{(MPEC)} \begin{cases} \underset{(x,y)}{\text{minimize}} \;\; f(x,y), \\ \text{subject to} \;\; (x,y) \in Z, \\ \qquad\qquad\qquad\quad y \in S(x), \end{cases}$$

where $Z \subseteq \mathbb{R}^n \times \mathbb{R}^m$ is the set of admissible designs and responses.

If the mapping $x \mapsto S(x)$ describes the solution of a variational inequality (VI), parameterized by x, then the inclusion $y \in S(x)$ holds if and only if

$$-F(x,y) \in N_{Y(x)}(y), \tag{1.1}$$

where $Y(x) \subseteq \mathbb{R}^m$ is the feasible set of the VI, $F(x,\cdot) : \mathbb{R}^m \to \mathbb{R}^m$ is the VI cost mapping, and $N_{Y(x)} : Y(x) \rightrightarrows \mathbb{R}^m$ is the normal cone mapping associated with the set $Y(x)$, all parameterized by x. We assume throughout that the set $Y(x)$ is closed and convex, whence its normal cone is the standard one in convex analysis: for $y \notin Y(x)$, $N_{Y(x)}(y) := \emptyset$, and for $y \in Y(x)$, $N_{Y(x)}(y) := \{\, z \in \mathbb{R}^m \mid z^{\mathrm{T}}(w - y) \leq 0,\ w \in Y(x)\,\}$. If $F(x,\cdot) = \nabla\varphi(x,\cdot)$ for some C^1 function $\varphi(x,\cdot) : \mathbb{R}^m \to \mathbb{R}$ then (1.1) is the first-order optimality conditions for the parameterized optimization problem to $\text{minimize}_{y \in Y(x)}\ \varphi(x,y)$. For general overviews of MPEC and VI models and their analysis, see Luo *et al.* (1996), and Facchinei & Pang (2003), respectively.

The existence of optimal solutions to the problem (MPEC) follows under standard assumptions that hark back to a version of Weierstrass' Theorem: if the set of feasible solutions to (MPEC) is non-empty and closed, and the objective function is lower semi-continuous and weakly coercive (this combination of properties is called 'inf-compact'), then there exists a closed and bounded set of optimal solutions (see, e.g., Zhang 1994). In particular, closedness of the feasible set follows in general from a closedness assumption on the mapping S and of the set Z. In the examples to follow, generally stronger properties still will hold.

We focus here on traffic and communication networks, whence x is the vector of design parameters, while the mapping S describes the solution to a traffic equilibrium (or, assignment) type model having y as the corresponding equilibrium traffic flows and (dis)utilities. The set Z could represent constraints on the available investments (or, tolls, etcetera), which then are independent on the response y (e.g., Marcotte 1986; and Patriksson and Rockafellar 2002); it could also represent maximum allowed travel times, exhaust emissions, or constraints defined by equity measures in a multi-class model (e.g., Eliasson & Mattsson 2006; and Stewart 2007), or on equilibrium travel times (e.g., Sumalee *et al.* 2006), which are examples of joint upper-level constraints.

The subject of rate control in computer communication networks is also related to congestion control in traffic networks, although the intrinsic existence of link flow capacity constraints in the former enforces the need to rephrase the Wardrop principle (cf. Larsson & Patriksson 1994). Ralph (2008) establishes the equivalence of rate flow equilibria for a model of the transmission rate protocol (TCP; see Kelly *et al.* 1998) to a mixed complementarity problem; various design and control problem of the MPEC type are then discussed. Robust such models that determine good transmission rates in the light of uncertainties in, e.g., link capacities, in the form of SMPECs are very natural extensions to study in the future.

We will in the following discuss in brief certain applications to structural (topology) optimization, wherein x refers to design variables describing an amount of material (thicknesses or volumes), while y refers to an equilibrium state (stresses and displacements); the equilibrium, described by the mapping S, corresponds to an energy minimization problem, parameterized by x. The set Z represents possible constraints on available material and/or on the (maximum) stresses. For an overview of structural (topology) optimization, see Bendsøe & Sigmund (2003).

The focus is on the analysis of a stochastic extension of the MPEC problem. It is known in the literature as stochastic MPEC, or SMPEC, a term coined in the paper by Patriksson & Wynter (1999). We suppose that $(\Omega, \Theta, \mathrm{P})$ is a complete probability space. When considering the space $\mathbb{R}^n \times \Omega$ we equip it always with the sigma algebra given by the product of the Borel sigma algebra of $\mathbb{R}^n$ and Θ.

The SMPEC problem then is that to

$$(\mathrm{SMPEC}_\Omega) \begin{cases} \underset{(x,y(\cdot))}{\text{minimize}} \ \mathrm{E}_\omega[f(x,y(\omega),\omega)] := \displaystyle\int_\Omega f(x,y(\omega),\omega)\,\mathrm{P}(d\omega), \\ \text{subject to } \ (x,y(\omega)) \in Z(\omega), \qquad \text{P-a.s.}, \\ \qquad\qquad\qquad\quad y(\omega) \in S(x,\omega), \qquad \text{P-a.s.} \end{cases}$$

where $y : \Omega \to \mathbb{R}^m$ is a random element of the probability space $(\Omega, \Theta, \mathrm{P})$, $Z : \Omega \rightrightarrows \mathbb{R}^n \times \mathbb{R}^m$ is a point-to-set mapping representing the upper-level constraints, and $S : \mathbb{R}^n \times \Omega \rightrightarrows \mathbb{R}^m$ defines the set of solutions to the lower-level parametric variational inequality problem,

$$S(x,\omega) := \{\, y \in \mathbb{R}^m \mid -F(x,y,\omega) \in N_{Y(x,\omega)}(y)\,\}. \tag{1.2}$$

The above lower-level problem is defined by a mapping $F : \mathbb{R}^n \times \mathbb{R}^m \times \Omega \to \mathbb{R}^m$ and a feasible set mapping $Y : \mathbb{R}^n \times \Omega \to \mathbb{R}^m$ having closed convex images with $N_{Y(x,\omega)} : \mathbb{R}^m \rightrightarrows \mathbb{R}^m$ denoting the normal cone mapping to the set $Y(x,\omega)$.

Patriksson & Wynter (1999) discuss toll setting problems under user equilibrium, as well as a pricing problem in a spatial-price equilibrium setting, where in both cases demand is stochastic. Evgrafov *et al.* (2002, 2003) analyze the continuously distributed case of topology optimization models. The paper by Evgrafov

& Patriksson (2004) provides the first existence analysis for the general SMPEC model as well as an inexact penalty method, while Evgrafov & Patriksson (2003*a*,*b*) investigated stability issues in the context of topology optimization; the latter two references established that in general the optimal design cannot be expected to vary continuously with the probability measure, but that continuity indeed could be established in some special circumstances for convex problems. We shall in this paper provide a corresponding analysis in the context of optimal design in networks, and reach stronger results in that they do not impose convexity on the model. Other applications of special cases of SMPEC include Stackelberg–Nash–Cournot equilibrium problems, in which case the lower-level problem is a nonlinear complementarity problem; the special SMPEC model is then referred to as SMPCC (stochastic program with complementarity constraints).

The next section provides a basic existence result for the problem (SMPEC_Ω), taken from Evgrafov & Patriksson (2004, theorem 2.1). Section 3 then introduces our traffic SMPEC model. Section 4 establishes the main result of this paper: that in the absence of joint upper-level constraints the optimal designs are continuous in the probability distribution; hence, we can conclude that globally optimal design solutions are stable, and the SMPEC traffic model is robust. Section 5 establishes the convergence of solution approaches to the SMPEC problem at hand. The first is a classic inexact exterior penalty method in which either the lower-level problem or any joint upper-level constraints are penalized. The second is a natural approach for the continuously distributed problem (SMPEC_Ω): we consider two related discretization approaches; the first is based on the method of mechanical quadratures, while the second is a straightforward application of sample average approximation. A final section discusses some interesting future research topics.

2. Existence of optimal solutions

Let X denote the projection of the feasible set of the problem (SMPEC_Ω) onto the space of x variables: $X := \{\, x \in \mathbb{R}^n \mid \exists y(\omega) : (x, y(\omega)) \in Z(\omega) \text{ for almost any } \omega \,\}$, and let $Z_x(\omega) := \{\, y \in \mathbb{R}^m \mid (x, y) \in Z(\omega) \,\}$. Let us also denote by $\Upsilon_x(\omega)$ the x-slice of the feasible set of (SMPEC_Ω), $\Upsilon_x(\omega) := Z_x(\omega) \cap S(x, \omega)$. The existence result is based on the measurability in ω for fixed x of this mapping. (A closed valued mapping $A : \Omega \rightrightarrows \mathbb{R}^n$ is said to be measurable if $A^{-1}(V) \in \Theta$ for every closed set $V \subset \mathbb{R}^n$.) We shall assume throughout that $Z_x(\omega)$ and $Y(x, \omega)$ are measurable in ω for any $x \in \mathbb{R}^n$; notice that this continuity type of assumption is not very restrictive. According to Evgrafov & Patriksson (2004, lemma 2.1), if in addition F is continuous in y and measurable in ω (which is referred to as the 'Carathéodory property') for any x, and Y has closed convex images for any x and almost any ω, then the mapping S is measurable in ω for any x.

The following result, quoted from Evgrafov & Patriksson (2004, theorem 2.1), establishes the existence of optimal solutions to the problem (SMPEC_Ω). This theorem, in turn, generalizes existence results for (MPEC) in a natural manner.

Theorem 2.1 (existence of optimal solutions). *Suppose that the mappings $Z_x(\cdot)$ and $S(x, \cdot)$ are measurable for any x; the set $Z(\omega)$ and the mapping $x \mapsto S(x, \omega)$ are closed for almost any $\omega \in \Omega$ and any x; the function f is continuous in (x, y), measurable in ω, uniformly weakly coercive with respect to x over the set*

X,† and bounded from below by a (Θ, P)-integrable function; for any $x \in X$, there is a neighbourhood $U_x \ni x$ such that the set $\cup_{\bar{x} \in U_x} Z_{\bar{x}}(\omega)$ is bounded for almost any $\omega \in \Omega$; and the set $\Upsilon_{x_0}(\omega)$ is nonempty for some $x_0 \in X$ and almost any $\omega \in \Omega$. Then, the problem (SMPEC$_\Omega$) *has at least one optimal solution.*

Clearly, the case of joint upper-level constraints is a complicating factor, and later discussions on robustness results and computations are discussed in a framework where Z is independent of y. A corollary to the above theorem illustrates how the analysis then simplifies.

Corollary 2.2 (existence of optimal solutions). *Suppose that the upper-level feasible set Z is independent of y, and hence can be written as $x \in X \subseteq \mathbb{R}^n$. Then, the assumptions of the theorem can be replaced by the following: the mapping $S(x, \cdot)$ is measurable for any x; the set X is closed, and the mapping $x \mapsto S(x, \omega)$ is closed for almost any $\omega \in \Omega$; the function f is continuous in (x, y), measurable in ω, uniformly weakly coercive with respect to x over the set X, and bounded from below by a (Θ, P)-integrable function; and the set $S(x_0, \omega)$ is nonempty for some $x_0 \in X$ and almost any $\omega \in \Omega$.*

In this latter case where the upper-level constraints are defined only in terms of x, we can provide a simple interpretation of the problem (SMPEC$_\Omega$). First, we recall that we select the response y for which we obtain the minimum value of the upper-level objective; we can then write the problem (SMPEC$_\Omega$) as the problem to

$$\underset{x \in X; y(\cdot) \in S(x, \cdot)}{\text{minimize}} \quad \mathrm{E}[f(x, y(\omega), \omega)], \tag{2.1}$$

where the optimization is performed over all $x \in X$ and all measurable selections $y(\omega) \in S(x, \omega)$. Equivalently, we may write the problem as that to minimize$_{x \in X}$ $w(x) := \mathrm{E}[v(x, \omega)]$, where $v(x, \omega) := \inf_{y \in S(x,\omega)} f(x, y, \omega)$. Notice that if for a given $x \in X$ the set $S(x, \omega)$ is empty with a positive probability we define $w(x) := \infty$; implicitly, therefore, the optimization over x is performed such that the set $S(x, \omega)$ is non-empty for almost any $\omega \in \Omega$.

A comparison is finally made with the case of a finite support of Ω. Suppose that $\Omega = \{\omega_1, \ldots, \omega_K\}$ is finite with probabilities $p_1, \ldots, p_K$. Then we may write the problem (2.1) as the problem to

$$(\mathrm{SMPEC}_K) \quad \begin{cases} \underset{(x, y_1, \ldots, y_K)}{\text{minimize}} & \displaystyle\sum_{k=1}^{K} p_k f(x, y_k, \omega_k), \\ \text{subject to} & x \in X, \\ & y_k \in S(x, \omega_k), \qquad k = 1, \ldots, K. \end{cases}$$

In the field of structural topology optimization this is a classic modelling approach. If, for example, the external load is stochastic, then (SMPEC$_K$) represents a 'multi-load case' model where K load scenarios are incorporated into the same design optimization model, together with their probabilities, resulting in a minimum average design 'cost'. We will return to this type of model later on when considering discretization approaches to the problem (SMPEC$_\Omega$).

† That is, that the set $\{x \in X \mid \exists y \in \mathbb{R}^m, \omega \in \Omega \text{ such that } f(x, y, \omega) \leq c\}$ is bounded for every $c \in \mathbb{R}$.

3. A representative SMPEC traffic model

(a) *Traffic equilibrium*

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, so 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 design parameter $x \in \mathbb{R}^n$. This parameter could be present in one or both of the travel cost and demand functions. We assume that the (continuous) travel cost function has the form $c(x, \cdot) : \mathbb{R}_+^{|\mathcal{R}|} \to \mathbb{R}^{|\mathcal{R}|}$ given a value of x, where $|\mathcal{R}|$ denotes the total number of routes in the network, and $\mathbb{R}_+ := \{\, x \in \mathbb{R} \mid x \geq 0 \,\}$. Further, the demand function is given by $g(x, \cdot) : \mathbb{R}^{|\mathcal{C}|} \to \mathbb{R}_+^{|\mathcal{C}|}$. Regarding the latter function we shall assume that either g is independent of the travel cost (hence a case of a fixed demand model) or is such that $-g(x, \cdot)$ is (at least) strictly monotone for each x; in the latter case we can then utilize the standard VI formulation based on the inverse of $g(x, \cdot)$.

We introduce the route–OD pair incidence matrix $\Gamma \in \mathbb{R}^{|\mathcal{R}| \times |\mathcal{C}|}$ (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 $h \in \mathbb{R}_+^{|\mathcal{R}|}$ and

$$\Gamma^{\mathrm{T}} h = g(x, \pi) \tag{3.1}$$

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

$$h_r > 0 \implies c_r(x, h) = \pi_{pq}, \qquad r \in \mathcal{R}_{pq}, \qquad (p, q) \in \mathcal{C}, \tag{3.2a}$$
$$h_r = 0 \implies c_r(x, h) \geq \pi_{pq}, \qquad r \in \mathcal{R}_{pq}, \qquad (p, q) \in \mathcal{C}, \tag{3.2b}$$

holds, where the value of $\pi_{pq} := \pi_{pq}(x, h)$ is the minimal (i.e., equilibrium) route cost in OD pair (p, q). By the non-negativity of the route flows, the system (3.1)–(3.2) can more compactly be written as the mixed complementarity problem (MCP)

$$0^{|\mathcal{R}|} \leq h \perp (c(x, h) - \Gamma\pi) \geq 0^{|\mathcal{R}|}, \tag{3.3a}$$
$$\Gamma^{\mathrm{T}} h = g(x, \pi), \tag{3.3b}$$

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

In general, we shall need to assume that the route cost is additive. For each link $l \in \mathcal{L}$, the travel cost has the form $t_l(x, v)$, where $v \in \mathbb{R}^{|\mathcal{L}|}$ 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 $c_r(x, h)$

if $c_r(x,h) = \sum_{l \in \mathcal{L}} \lambda_{lr} t_l(x,v)$. In short, then, $c(x,h) = \Lambda^{\mathrm{T}} t(x,v)$. 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: $v = \Lambda h$. In general, we shall assume that t is (at least) strictly monotone in v for any x. Notice, however, that it is in each of the results to follow possible for the function t to be only monotone for some values of v for any x, as long as it is strictly monotone around the equilibrium solution for any x; thus, so called "flat spots" of the travel cost are allowed, again as long as these are not situated near an equilibrium.

A more familiar representation of the parameterized Wardrop conditions (3.3) is that of a variational inequality,

$$-F(x,y) \in N_C(y), \tag{3.4}$$

where $y \in \mathbb{R}^m$, $C \subseteq \mathbb{R}^m$ is a closed and convex set, $F(x,\cdot) : C \to \mathbb{R}^m$ is smooth, and where the normal cone mapping is as defined in §1 *c*. Letting

$$y := \begin{pmatrix} h \\ \pi \\ v \end{pmatrix} \in \mathbb{R}^{|\mathcal{R}|} \times \mathbb{R}^{|\mathcal{C}|} \times \mathbb{R}^{|\mathcal{L}|}, \tag{3.5a}$$

$$F(x,y) := \begin{pmatrix} \Lambda^{\mathrm{T}} t(x,v) - \Gamma\pi \\ \Gamma^{\mathrm{T}} h - g(x,\pi) \\ v - \Lambda h \end{pmatrix}, \quad \text{and} \tag{3.5b}$$

$$C := \mathbb{R}_+^{|\mathcal{R}|} \times \mathbb{R}^{|\mathcal{C}|} \times \mathbb{R}^{|\mathcal{L}|}, \tag{3.5c}$$

we obtain an equivalent VI formulation from (3.3), where F is parameterized by x. Solutions exist to the problem (3.4), (3.5) whenever $t(x,\cdot)$ is continuous and $g(x,\cdot)$ is non-negative and upper bounded by some nonnegative vector (cf., e.g., Marcotte & Patriksson 2007, theorem 4).

We remarked above that the demand function is assumed to be of either of two different forms. In the case when the corresponding variational inequality models define first-order optimality conditions for an optimization problem, the two corresponding optimization formulations illustrate an important feature of the lower-level traffic equilibrium problem that we utilize heavily: its constraints do not depend on the design vector x; hence the equilibrium problem always exhibits feasible solutions, and according to the properties of the cost and demand functions assumed, equilibria will therefore also always exist.

In order to produce a hierarchical traffic model, we introduce finally a continuous function $f : \mathbb{R}^n \times \mathbb{R}^m \to \mathbb{R}$, and a possible set of jointly feasible designs and responses, $Z \subset \mathbb{R}^n \times \mathbb{R}^m$. The corresponding MPEC model then is to

$$\text{(HTM)} \quad \begin{cases} \underset{(x,y)}{\text{minimize}} \ f(x,y), \\ \text{subject to } \ (x,y) \in Z, \\ \qquad\qquad\qquad y \in S(x) := \{\, y \in \mathbb{R}^m \mid (3.4), (3.5) \text{ holds} \,\}. \end{cases}$$

The existence of solutions to the problem (HTM) follows under standard arguments, as it is an instance of (MPEC). The mapping S is closed as soon as t and g are continuous, which we have assumed. We further assume that the set Z

and the function f are so defined that there exist feasible solutions, and that f is inf-compact there. The most natural assumptions under which this is guaranteed to hold is that f is continuous, $t(x,\cdot)$ and $-g(x,\cdot)$ are strictly monotone, and the set Z is independent of y and compact; indeed, in most applications it is simply a box in x corresponding to investment bounds.

(b) An SMPEC traffic model

We introduce a stochastic extension of this model. Consider the problem to

$$(\mathrm{SHTM}_\Omega) \begin{cases} \underset{(x,y(\cdot))}{\text{minimize}} \ \mathrm{E}_\omega[f(x,y(\omega),\omega)] := \int_\Omega f(x,y(\omega),\omega)\,\mathrm{P}(d\omega), \\ \text{subject to } \ (x,y(\omega)) \in Z(\omega), \qquad \text{P-a.s.}, \\ \qquad\qquad\qquad y(\omega) \in S(x,\omega), \qquad \text{P-a.s.}, \end{cases}$$

where $y : \Omega \to \mathbb{R}^m$ is a random element of a complete probability space $(\Omega, \Theta, \mathrm{P})$, $Z : \Omega \rightrightarrows \mathbb{R}^n \times \mathbb{R}^m$ is a point-to-set mapping representing the upper-level constraints, and $S : \mathbb{R}^n \times \Omega \to \mathbb{R}^m$ now defines the set of solutions to a lower-level parametric variational inequality problem of the form

$$S(x,\omega) := \{\, y \in \mathbb{R}^m \mid -F(x,y,\omega) \in N_C(y) \,\}, \tag{3.6}$$

where

$$F(x,y,\omega) := \begin{pmatrix} \Lambda^{\mathrm{T}} t(x,v,\omega) - \Gamma\pi \\ \Gamma^{\mathrm{T}} h - g(x,\pi,\omega) \\ v - \Lambda h \end{pmatrix}. \tag{3.7}$$

In this model we take into account uncertainties in the modelling of the travel costs and/or demands when evaluating the upper-level objective function for a given value of the parameters in x; we take them into account by minimizing the expectation of these objective values over the uncertainty set.

Due to the fact that we study *stochastic* network models, we rule out from consideration such classic cases as 'first-best' toll pricing, where a desired link flow is fixed and the only variables are the tolls to be set, typically on every link, in order to reproduce this flow as a traffic equilibrium one; see Marcotte & Patriksson (2007) for a select bibliography on link toll pricing, especially for obtaining system (or, social) optimal flows. Our model, in the context of link tolls, therefore belongs to the 'second-best' school, as discussed, for example, by Yang *et al.* (2005).

We restate theorem 2.1 in the context of this problem.

Theorem 3.1 (existence of optimal solutions). *Suppose that the following assumptions are fulfilled: the mappings $t(x,\cdot)$, $g(x,\cdot)$ and $Z_x(\cdot)$ are measurable for any x; the set $Z(\omega)$ is closed for almost any $\omega \in \Omega$; the function f is continuous in (x,y), measurable in ω, uniformly weakly coercive with respect to x over the set X, and bounded from below by a (Θ,P)-integrable function; for any $x \in X$, there is a neighbourhood $U_x \ni x$ such that the set $\cup_{\bar{x}\in U_x} Z_{\bar{x}}(\omega)$ is bounded for almost any ω; and the set $\Upsilon_{x_0}(\omega)$ is nonempty for some $x_0 \in X$ and almost any ω. Then, the problem* (SHTM_Ω) *has at least one optimal solution.*

The absence of joint upper-level constraints makes life easier.

Corollary 3.2 (existence of optimal solutions). *Suppose that the upper-level feasible set Z is independent of y, and hence can be written as $x \in X \subseteq \mathbb{R}^n$. Then, the above assumptions can be replaced by the following: the mappings $t(x,\cdot)$ and $g(x,\cdot)$ are measurable for any x; the set X is closed; and the function f is continuous in (x,y), measurable in ω, uniformly weakly coercive with respect to x over the set X, and bounded from below by a (Θ,P)-integrable function.*

4. Solution stability

The question of the continuity of optimal solutions to (SMPEC_Ω) with respect to changes in the probability distribution is important. From the computational point of view, a positive answer to this question would allow us to solve the problem by approximating the underlying probability measure with a sequence of discrete probability measures, and hence approximating the original infinite-dimensional optimization problem with a sequence of finite-dimensional optimization problems. From the theoretical point of view, we would conclude the robustness of the resulting optimal solutions with respect to errors in the modelling of uncertainty.

As discussed in §1, the structural optimization community often utilize probability-free worst-case (pessimistic) models of uncertainty as alternatives to probabilistic models. These approaches do yield stable structures, but do not take into account the probability of occurrence of the different scenarios, thereby often resulting in unnecessarily costly designs. There are example problems where the optimal solutions do not change continuously even if the probability distribution measure changes only locally (that is, only the density of the probability measure changes); cf. Evgrafov *et al.* (2003). There are example models where no joint upper-level constraints are present, and whose optimal solutions *are* robust (Evgrafov *et al.* 2003), and there are also examples where a possible reformulation (that is, relaxation) of a non-robust problem yields a robust model (Evgrafov & Patriksson 2003*b*).

Certain convex problems in stochastic programming have been proven robust (e.g., Römisch 2003), in some cases with quantitative stability measures. Since stochastic programming is an instance of (SMPEC_Ω) (e.g., Patriksson & Wynter 1999, and Shapiro 2006) the latter clearly contains robust models. As remarked in Evgrafov & Patriksson (2004), however, no generic conditions on Z and S under which one can expect a continuous behaviour of the optimal solutions to non-convex models within the framework of (SMPEC_Ω) (or at least the continuous behaviour of the optimal values of the upper-level variables x) yet exist.

The main result in this section is that globally optimal solutions to (SHTM_Ω) are stable under natural conditions *when there are no joint upper-level constraints*. Due to space limitations, proofs of theorems will however be published elsewhere.

Consider a sequence $\{\mathrm{P}_k\}$ of probability measures defined on $\mathcal{B}(\Omega)$, together with the associated sequence of optimization problems:

$$(\mathrm{SHTM}_\Omega)^k \begin{cases} \underset{(x,y(\cdot))}{\text{minimize}} \ \mathrm{E}_\omega[f(x,y(\omega),\omega)] := \displaystyle\int_\Omega f(x,y(\omega),\omega)\,\mathrm{P}_k(d\omega), \\ \text{subject to} \quad x \in X, \\ \qquad\qquad y(\omega) \in S(x,\omega), \qquad \mathrm{P}_k\text{-a.s.} \end{cases}$$

We assume that each measure P_k has a density $p_k(\cdot)$ with respect to a Lebesgue measure on Ω and that the sequence $\{p_k(\cdot)\}$ converges to a density $p(\cdot)$ of P Lebesgue-almost everywhere. The existence of densities is not a very restrictive assumption from the theoretical point of view.

Theorem 4.1 (stability of globally optimal solutions). *In addition to the conditions of theorem 3.1 suppose that the mapping $t(x, \cdot, \omega)$ is strictly monotone for each $x \in X$ and $\omega \in \Omega$ and that g is either a constant mapping in π or $-g(x, \cdot, \omega)$ is strictly monotone for each $x \in X$ and $\omega \in \Omega$. Suppose that the sequence $\{\mathrm{P}_k\}$ of probability measures weakly converges to* P *and that $(x_k, y_k(\cdot))$ solves* $(\mathrm{SHTM}_\Omega)^k$ *for each k. Then, each limit point (and there is at least one) of the sequence $\{(x_k, y_k(\cdot))\}$ is an optimal solution to* (SHTM_Ω).

5. Solution approaches

(*a*) *Inexact penalization*

Compared to one-level problems, bilevel optimization algorithms are much less straightforward to develop owing to the non-convex nature of the problem and the absence of constraint qualifications for nonlinear programming (Luo *et al.* 1996). One approach is to move the equilibrium constraint as a penalty into the objective function. For examples of penalty functions leading to algorithmic constructions to MPEC, see Luo *et al.* (1996); and Ralph (2008). In particular, exact penalties are of great importance, since they lead to exact solutions while they do not require the penalty parameter to tend to infinity. However, one cannot expect to be able to construct an exact penalty for SMPEC problems, given an exact penalty for each ω, as an example in Evgrafov & Patriksson (2004) illustrates. Again, the reason is the presence of the coupling upper-level constraints.

Evgrafov & Patriksson (2004, theorem 4.1) establish the convergence of an inexact penalization method wherein the lower-level equilibrium problem is penalized. This result can be immediately transferred to the current situation. We have however argued that joint upper-level constraints imply complications and may therefore alternatively conclude that it is them that should be penalized, in order to turn the problem into a more 'standard' SMPEC model. (This has indeed been utilized; see, e.g., Evgrafov & Patriksson 2003*a*.) Providing a general theory of such an approach is a quite interesting avenue for future research. For now, we present a result within the transportation domain. In what follows, the notation val W refers to the optimal objective value of the problem W.

Theorem 5.1 (inexact penalization of upper-level constraints). *Suppose the conditions of theorem 4.1 are satisfied. Let also the function $(x, y, \omega) \mapsto G(x, y, \omega)$ be non-negative, continuous in (x, y) for almost any ω, measurable in ω for any $(x, y) \in \mathbb{R}^n \times \mathbb{R}^m$, and such that $Z(\omega) = \{\,(x, y) \in \mathbb{R}^n \times \mathbb{R}^m \mid G(x, y, \omega) = 0\,\}$. Then, the penalized problem*

$$(\mathrm{SHTM}_\Omega)^2_\mu \begin{cases} \underset{(x,y(\cdot))}{\text{minimize}} \ \mathrm{E}_\omega[f(x, y(\omega), \omega) + \mu G(x, y, \omega)], \\ \text{subject to } \ y(\omega) \in S(x, \omega), \qquad \text{P-a.s.}, \end{cases}$$

has an optimal solution for any $\mu \geq 0$ and

$$\sup_{\mu \geq 0} \mathrm{val}(\mathrm{SHTM}_\Omega)^2_\mu = \lim_{\mu \to \infty} \mathrm{val}(\mathrm{SHTM}_\Omega)^2_\mu = \mathrm{val}(\mathrm{SHTM}_\Omega).$$

Furthermore, any limit point of the sequence of optimal solutions $\{x_\mu\}$ to $(\mathrm{SHTM}_\Omega)^2_\mu$ *(and there is at least one) is an upper-level optimal solution to* (SHTM_Ω).

(*b*) *Discretization approaches*

A popular method for solving a stochastic programming problem involving a non-discrete probability measure is to approximate it with a sequence of finite-dimensional problems with discrete measures. For SMPEC models, such techniques are known as the sample path method, sample average approximation, stochastic counterpart method, and the simulated likelihood method (see, e.g., Robinson 1996; Gürkan *et al.* 1999; Shapiro & Xu 2005; Shapiro 2006; and the references therein). Using K random samples of the random vector ω, a problem of the form (SMPEC_K), with $p_k = 1/K$ for every k, is solved, for increased values of K.

Shapiro & Xu (2005) study the convergence of this method for $(\mathrm{SMPCC})_\Omega$ under conditions that are fulfilled if $y(\cdot, \omega)$ is unique and continuous for almost any ω, X is non-empty and compact, and the function $f(x, y(x, \cdot), \cdot)$ is bounded over X almost surely. Under additional conditions on S and f such that the expected value function is differentiable, it is also established that stationary points to discretizations converge to the set of stationary points to $(\mathrm{SMPCC})_\Omega$. Because of the smoothing effect of the averaging operation, it is remarked that differentiability of the expected value function may hold in many more cases than for the non-deterministic problem (MPCC). We expect the same to hold for $(\mathrm{SHTM})_\Omega$. The stronger conditions imposed in the work of Gürkan *et al.* (1999) in particular imply that the lower-level problem has strongly regular solutions (Robinson 1980), but on the other hand the results quite immediately extend to *inexact* solutions of the approximate problems $(\mathrm{SHTM})_K$.

In Birbil *et al.* (2006) the above sample path method was applied to a special case of $(\mathrm{SMPCC})_\Omega$ modelling a toll pricing problem under fixed demand traffic equilibrium. Suppose that tolls are to be set during the beginning of a fairly long time period, during which time the tolls cannot be altered. The parameters of the BPR formula are considered stochastic in order to represent varying road conditions during this time period, and the model $(\mathrm{SMPCC})_\Omega$ then represents a means to derive the best link tolls 'on average'. A test case using the Sioux Falls network is reported; in this example the exact solution can be computed before-hand, making it possible to establish, in this particular case, convergence to an optimal solution.

The main interest in the above techniques is of course that SMPEC models can be solved through a sequence of MPEC models, for which relatively efficient algorithms exist (e.g., Fletcher *et al.* 2006; Ralph 2008; and references therein). Shapiro (2006) establishes that convergence in some cases is exponential, which implies that relatively few samples may be needed to reach at least a near-optimal (or, near-stationary) solution; numerical experiments in Shapiro & Xu (2005) and Birbil *et al.* (2006) confirm this belief at least in small-scale examples. Therefore, there is a hope that SMPEC traffic models can be approximately solved with a computational effort that is not several orders of magnitude larger than for one instance of a discretized problem. In particular, a rough design solution that is at least a lot better than any individual MPEC solution can probably be achieved through the solution of one single problem of the form $(\mathrm{SHTM})^k$ or $(\mathrm{SHTM})^N$, provided of course that the samples are well chosen. The analysis performed in this paper in fact—to at least some degree—validates such a simple approach, through the combined results of theorem 4.1 and the convergence of discretization methods.

6. Final remarks and future research directions

While this work concerns a deterministic traffic equilibrium model, the above development can be performed in the context also of stochastic traffic equilibrium models. Indeed, the properties needed are not connected to the route-choice principles per se, but rather to the properties of the equilibrium solutions: that the lower-level optimal link flow and demand is closed, in some cases continuous, as a function of x and ω, which is a property present also for, say, the logit and probit based stochastic models. For a recent account of research on link tolling under stochastic user equilibrium, see Stewart (2007). As far as this author is aware, the present paper is the first that (essentially) covers an analysis of a stochastic MPEC model where the lower level model is a stochastic user equilibrium (SUE) model.

As mentioned already in §1 *c*, congestion control in communication networks is a very important topic; its relationships to traffic MPEC models were also alluded to. Several parameters in the definition of the problem through whose solution one determines the transmission rates are likely to be subject to random fluctuations and are also difficult to measure exactly, in particular the capacity of the links (in terms of flow rates). Therefore, it seems natural to study stochastic models of transmission control, which then would have the form of SMPEC problems.

A natural future research task is to investigate the possible convergence of *inexact* solutions to the subproblems in the algorithms investigated in this paper to (in)exact solutions to the original one. In this context it is interesting to note a result of Gürkan *et al.* (1999), stating that the maximum number of samples (K) required to reach a given accuracy of the final solution while also solving each subproblem inexactly grows linearly with the number n of design parameters. Another interesting question is whether convergence is achieved for the natural combination of penalization and discretization, as previously applied and established in structural topology optimization by Evgrafov & Patriksson (2003*a*).

A related issue regards the stability of optimal solutions to SMPEC traffic models with joint upper-level constraints. We have described the unlikehood of the existence of such a result for SMPEC traffic models in general, but we have also related to work that has showed that certain relaxations of joint upper-level constraints may in fact induce robustness. Their form is naturally highly dependent on the type of constraints considered. In topology optimization such relaxation algorithms are now quite well-known and established; see, e.g., Guo *et al.* (2001) and Evgrafov & Patriksson (2003*b*) for work on the 'stress singularity phenomenon' and specially designed relaxation methods for stress constraints. In relation to the negative result in Evgrafov & Patriksson (2003*b*) that one cannot expect convergence of a scheme in which $\{\mathrm{P}_k\}$ converges to P and the relaxation parameter tends to zero *simultaneously*, one must observe that in that application the objective function of the lower-level variational inequality is not everywhere finite; the situation in the SMPEC traffic context should be more favourable.

A possible relaxation of the constraint that $\mathrm{P}_\Omega[(x, y(\omega)) \in Z(\omega)] = 1$ holds is given by, for some $\alpha \in (0,1)$, $\mathrm{P}_\Omega[(x, y(\omega)) \in Z(\omega)] \geq \alpha$. This is the 'probabilistic' or 'chance constraint' of stochastic programming (e.g., Prékopa 2003) and the 'reliability constraint' from structural optimization. Whether interesting stability properties can be derived from an SMPEC model equipped with this relaxed joint upper-level constraint is an interesting future research question.

An interesting research issue related to the above is whether stability results extending that for globally optimal solutions can be verified also for locally optimal designs, and/or solutions to a suitably stated necessary condition for a local optimum. The latter conditions are interesting in their own right, as KKT-type optimality conditions for general SMPEC problems are not well developed yet.

Applications to toll pricing and design problems in traffic networks have been mentioned previously. SMPEC models can of course also be utilized to similarly model and analyze networks of other commodities. One example is optical data communication networks where, for example, revenue maximization models (known as *stochastic traffic engineering*) involving bandwidth provisioning in the face of stochastic elastic bandwidth demands are discussed in Mitra & Wang (2005). The analysis and numerical solution of this and other problems in communication networks within the framework of SMPEC, is a fruitful research avenue.

Finally, it would be interesting to investigate whether, in the context of network design and/or pricing the analysis of this paper may offer contributions to the study of reliability of traffic flows (see, e.g., Bell 2000; and Clark & Watling 2005).

The work leading to this paper was performed in association with the Gothenburg Mathematical Modelling Centre (GMMC) at Mathematical Sciences (Chalmers University of Technology and Göteborg University), whose main sponsor is the Swedish Foundation for Strategic Research (SSF). Five anonymous referees helped to improve the presentation.

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