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ACTIVE SET METHODS FOR INVERSE LINEAR COMPLEMENTARITY PROBLEMS

Stefan Scholtes[1]

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Abstract

Inverse complementarity problems play an increasingly important role. They arise naturally in data estimation or design optimization for equilibrium or optimization processes. A typical example is the estimation of origin-destination demand from traffic counts in congested networks. We suggest an extension of the standard active set approaches to linear and quadratic programming to inverse linear complementarity problems with linear or quadratic objectives. The obtained methods produce locally optimal solutions of the inverse problems and can be used to improve on heuristics or as building blocks in a branch-and-bound process for global optimization.

Keywords. Active Set Method, Inverse Complementarity Problem, Mathematical Program with Equilibrium Constraints, OD-demand Estimation, Simplex Method

[1]Department of Engineering and Judge Institute of Management Studies, University of Cambridge, Cambridge CB2 1AG, England, E-mail: ss248@eng.cam.ac.uk

1 Introduction

Optimization and equilibrium models are among the most useful tools of Operations Research and arguably form the backbone for process optimization. It is therefore quite surprising that most of the literature on optimization models concentrates on the direct problem of finding an optimal solution to a model. Indeed, in particular in equilibrium models we often observe solutions or consequences thereof and are more interested in either calibrating our model by estimating unknown data on the basis of the observed equilibrium or changing model parameters so that the equilibrium has some desired properties. Such questions belong to the realm of inverse problems, where observed solutions or desired properties of solutions are given and corresponding data or model parameters are sought.

Traffic assignment models, for instance, have been developed to explain the arc flow pattern induced by given origin-destination (OD-) demand in a congested network. The direct problem associated with this model is to predict traffic flow, given OD-demand. We can, however, observe traffic flow fairly easily - so why predict it? The argument is then that we wish to change some network characteristics and use the model to predict the corresponding equilibrium flow. This is a problem of optimal network design and an inverse problem of the traffic assignment problem as we are primarily looking for model parameters which produce an equilibrium assignment with some desirable property. Alternatively, we may wish to use the model to obtain realistic estimates of the OD-demand from traffic counts. Again this is a typical inverse problem which has been recently suggested in the transportation literature, e.g. [2, 3, 4, 8, 13, 21, 24], along with heuristics for its solution. Our aim here is to complement these approaches by suggesting a methodology that is guaranteed to produce at least a local optimum of such an inverse problem.

Inverse problems that stem from optimization or equilibrium processes are typically characterized by the presence of a complementarity condition in their constraints. These conditions can stem from Kuhn-Tucker type optimality conditions or can be a consequence of a general complementarity principle. A typical example of the latter is Wardrop's law for equilibrium traffic assignments which states that in equilibrium a possible path between an origin and a destination is unused, unless it realises the minimal travel time between the origin and the destination. Such complementarity constraints lead to nonconvex optimization problems but they posess a combinatorial nature which makes them amenable to branch-and-bound type methods as well as to active set methods. The latter approach has not been given much attention in the literature although, as a local optimization method, it bears the promise to be applicable to large problem instances and can be a useful addition to problem dependent heuristics or bounding processes in a branch-and-bound framework. They are particularly relevant for inverse linear complementarity problems as an alternative to more elaborate methods which were designed to apply to nonlinear problems, e.g. the PIPA method of [12] or the implicit programming method of [14]. The main purpose of this paper is to demonstrate that the standard active set approaches to linear and quadratic programming extend to inverse linear complementarity problems with linear and quadratic objectives, respectively. The paper is organized as follows. In the next section we explain in more detail the inverse complementarity problem associated with the demand estimation in congested networks on the basis of traffic counts. We then present the general inverse complementarity problem, review some results from the literature that we shall use in the sequel, and present a canonical branch-and-bound scheme. In Section 4 we explain the simplex method for inverse linear complementarity problems with linear objectives, while Section 5 is devoted to an active set method for quadratic objectives. The final section contains some obvious extensions which we have not included in the paper for the sake of its readability.

2 Demand estimation in traffic assignment models: A motivating example

To motivate our study of inverse complementarity problems, we review in this section the complementarity formulation of the traffic assignment problem and the associated inverse complementarity formulation of the OD-demand estimation problem. Consider a network $N = (V, A)$ with nodes V and arcs A and a set P of paths through the network. Let $O \subset A \times A$ be the set of origins and destinations of the paths $p \in P$. The network is used by many users, each of which chooses a path $p \in P$ that leads from her origin to her destination and minimizes her travel time or some other objective function. Obviously, in a congested network the travel time along a path depends on the choices of paths by the other users. In equilibrium the assignment of traffic to the network is governed by a behavioural principle known as Wardrop's law: *Every user will only use paths that realize the minimum travel time from her origin to her destination*, [23]. In other words,

> all utilized paths between an origin-destination pair (o, d) will have the same travel time (the minimum travel time u_{od}) and
>
> a path that requires more than the minimum travel time will not be used.

Wardrop's law is a classical example of a complementarity condition. It states that for each path either the flow on the path is zero or the difference between the travel time along the path and the minimal realizable travel time from its origin to its destination is zero, [1]. In mathematical terms this can be rephrased as[2]

$$\begin{aligned} \min\{h, C(h) - \Lambda^\top u\} &= 0 \\ \Lambda h - T(u) &= 0 \\ u &\geq 0. \end{aligned}$$

[2] Here and in the sequel the minimum $\min\{x, y\}$ of two vectors x, y of the same dimension denotes the vector with components $\min\{x_i, y_i\}$.

The variables in this model are the path flow vector $h \in \mathbb{R}^P$ and the vector of minimal travel times $u \in \mathbb{R}^O$ between OD-pairs and the data are the OD-path incidence matrix Λ, the path travel time mapping $C : \mathbb{R}^P \to \mathbb{R}^P$ and the demand function $T : \mathbb{R}^O \to \mathbb{R}^O$. The induced arc flow in the network is readily obtained by $f = \Delta h$, where Δ is the arc-path incidence matrix[3].

A natural inverse of the traffic assignment problem is the OD-demand estimation problem: Given observed arc flow $\hat{f}$, estimate the OD-demand T that induced this arc flow. In addition to the observed arc flow one may have a coarse estimate $\hat{T}$ of the demand matrix, possibly an old demand matrix that one wishes to update. Estimates $\hat{u}$ of the minimal travel times between various OD-pairs in the network may also be available. The inverse problem is therefore characterized by the data

observed arc flows $\hat{f}$

(possibly) estimated minimal travel times $\hat{u}$

(possibly) estimated OD-demand $\hat{T}$ (e.g. past demand)

and a natural estimation model for the OD-demand T is of the form

$$\begin{array}{ll} \min\limits_{(h,u,T)} & d([\Delta h, u, T], [\hat{f}, \hat{u}, \hat{T}]) \\ \text{s.t.} & \min\{h, C(h) - \Lambda^\top u\} = 0 \\ & \Lambda h - T = 0 \\ & u \geq 0 \end{array}$$

where $d(.,.)$ is a suitable distance function, e.g.,

$$d([\Delta h, u, T], [\hat{f}, \hat{u}, \hat{T}]) = \alpha\|\Delta h - \hat{f}\| + \beta\|u - \hat{u}\| + \gamma\|T - \hat{T}\|,$$

with suitable nonnegative constants α, β, γ not all of which are vanishing. Such estimation models have been suggested by various authors in the transportation literature, cf.

[3] Notice that, discounting for the typically strictly satisfied nonnegativity condition on the minimal travel time, there are as many equations as there are unknowns in the above system. This suggests that the traffic assignment problem should typically have isolated solutions which is indeed the case if perturbations of the mappings T and C by constants are allowed, i.e. if $C : R^p \to R^p$ and $T : R^d \to R^d$ are smooth functions then for almost all a, b all roots of

$$F(h,u) = \begin{pmatrix} \min\{h, C(h) - a - \Lambda^\top u\} \\ \Lambda h - T(u) - b \end{pmatrix}$$

are isolated (cf. Proposition 6 in the appendix). However, while constant perturbations of the demand T seem natural, constant perturbations of the travel time C are rather artificial. Indeed, the travel time along a path is typically the sum of the travel times on its arcs, i.e. $C(h) = \Delta^\top c(\Delta h)$, where $c(f)$ is the vector of arc travel times which depends on the arc flow f in the network. A straight-forward extension of the latter genericity result to perturbations of arc travel times c is possible if the arc-path incidence matrix Δ has full column rank. This, however, is often not the case in practical situations. Indeed, given the paths (A,B,C), (A,D,C), (A,B,E), (A,D,E) it is impossible to say which flow on arcs (A,B) and (A,D) is destined for node C or E, respectively, cf. [1].

e.g. [2, 3, 4, 13, 21, 24]. The aim is to find a demand matrix and a corresponding equilibrium assignment so that the observed arc flow is best explained in the assignment model. The inverse traffic assignment problem is computationally challenging, due to the inherent nonconvexity induced by the combinatorial nature of the complementarity constraint. Notice that the inverse problem is feasible with $(h, u, T) = (0, 0, 0)$ being a feasible solution. Alternatively, given demand T, e.g. the coarse estimate $T = \hat{T}$ of the OD-demand, one can, under suitable assumptions, compute a corresponding feasible path flow vector h and minimal travel time vector u as the solution of the corresponding complementarity problem, cf. [11, 18]. The latter feasible point may be used as a starting point for a local optimization procedure for the inverse problem. Such local optimization procedures are the object of this paper. We demonstrate that the well-known active set methodology for standard linear and quadratic programming extends to inverse complementarity problems like the inverse traffic assignment problem and provides a local solutions. If the problem size is large then a local solution close to a starting point determined by a suitable heuristic, cf. [9, 24, 25], may indeed be the best one can hope for. A local optimization procedure can also be a useful ingredient in a global optimization method for small problem sizes as it can be used to improve the bounding process in the canonical branch-and-bound scheme induced by the combinatorial structure of the complementarity constraints.

3 Inverse complementarity problems

The inverse problem of the last section is an instance of a complementarity constrained mathematical program with equilibrium constraints (MPEC), [12]. Its general form is

$$\begin{array}{ll} \min & f(z) \\ s.t. & g(z) \leq 0 \\ & h(z) = 0 \\ & \min\{G(z), H(z)\} = 0. \end{array} \tag{1}$$

We assume in the sequel that all functions f, g, h, G, H are smooth.

3.1 The patchwork picture

The arguably simplest way to study MPECs is to view them as a patchwork of nonlinear programs of the type

$$\begin{array}{lll} \min & f(z) & \\ s.t. & g(z) \leq 0 & \\ & h(z) = 0 & \\ & G_i(z) = 0 & i \in I_G \\ & H_j(z) \geq 0 & j \in I_H \\ & G_k(z) \geq 0 & k \notin I_G \\ & H_l(z) = 0 & l \notin I_H \end{array} \tag{2}$$

where I_G and I_H are index sets with $I_G \cup I_H = \{1, \ldots, r\}$ and r is the common dimension of $G(z)$ and $H(z)$. We say that an NLP piece (2) is adjacent to z if z is a feasible point of that piece. Obviously, z is a local minimizer of MPEC if and only if it is a local minimizer of all adjacent NLP pieces. A feasible point z of MPEC is called B-stationary if it is a stationary point of all adjacent NLP-pieces, cf. [16]. Here, we call z a stationary point of an NLP piece if the Karush-Kuhn-Tucker conditions are satisfied. Notice that all NLP pieces have the same Lagrangian

$$L(z, \lambda, \mu, \gamma, \nu) = f(z) + \lambda^\top g(z) + \mu^\top h(z) - \gamma^\top G(z) - \nu^\top H(z)$$

and therefore the multipliers at a stationary point satisfy in particular

$$\begin{array}{rcl} \nabla_z L(z, \lambda, \mu, \gamma, \nu) & = & 0 \\ \lambda_i & = & 0, \quad g_i(z) < 0 \\ \gamma_j & = & 0, \quad G_j(z) > 0 \\ \nu_k & = & 0, \quad H_k(z) > 0. \end{array}$$

We shall call a point z a *critical point* of MPEC if there exist multipliers $\lambda, \mu, \gamma, \nu$ that satisfy the latter set of equations. If the linear independence constraint qualification (LICQ) holds at z, i.e. the gradients of the vanishing constraint functions at z are linearly independent, then the multipliers are unique and the same for all adjacent NLP pieces. This makes it easy to verify stationarity for a point z, provided LICQ holds at z. Indeed, if LICQ holds at a stationary point z of an NLP piece then z is B-stationary for MPEC if and only if the multipliers corresponding to G_i and H_i are nonnegative for all i with $G_i(z) = H_i(z) = 0$, cf. [12]. This can be extended to local minimizers if the MPEC has convexity properties. To this end we call an MPEC *convex* if the functions f and g_i are convex and the functions h, G, H are affine.

Proposition 1 *Let z be a feasible point of a convex MPEC and suppose LICQ holds at z. Then z is a local minimizer of the MPEC if and only if z is a stationary point of some adjacent NLP piece and the corresponding unique multipliers $\lambda, \mu, \gamma, \nu$ satisfy $\lambda \geq 0$ and $\gamma_k, \nu_k \geq 0$ for every k such that $G_k(z) = H_k(z) = 0$.*

In the sequel we shall be concerned with particular types of convex MPECs, called LPECs and QPECs, where f is a linear or quadratic function, respectively, and g, h, G, H are affine mappings. In other words, a QPEC is a program of the form

$$\begin{array}{ll} \min & q^\top z + \frac{1}{2} z^\top Q z \\ s.t. & Az \leq a \\ & Bz = b \\ & \min\{Cz - c, Dz - d\} = 0 \end{array} \tag{3}$$

where Q is an $n \times n$-matrix, A and B are $p \times n$- and $q \times n$-matrices, respectively, and C, D are $r \times n$-matrices and an LPEC is a QPEC with $Q = 0$. LPECs and convex QPECs arise typically as inverse problems, like the inverse traffic assignment problem, if weighted l_1, l_∞, or l_2-norms induce the distance functions.

3.2 A branch-and-bound process

The patchwork interpretation (2) of the MPEC (1) lends itself naturally to a branch-and-bound scheme with index pairs (I_G, I_H) and corresponding programs (2) associated with the nodes of the branch-and-bound tree. The apex of the tree corresponds to $(\emptyset, \emptyset)$. At a given node (I_G, I_H), program (2) is evaluated. If the optimal solution is feasible for MPEC then one checks whether the current upper bound for the optimal objective value can be improved upon. If the optimal solution is not feasible for the MPEC then there exists an index j with $H_j(z) > 0$ and $G_j(z) > 0$ and one branches by including j either in I_G or I_H. This approach is very similar to the standard branch-and-bound methodology for integer programming with one substantial difference: the feasible set of MPEC is not discrete. Therefore, if a feasible point is reached it may well be improved upon by employing a local optimization method. This will generally lead to better bounds and, if the local optimization method is efficient, is likely to have a benefitial effect on the overall efficiency of the branch-and-bound method. In the remainder of this paper we will focus on the active set methodology for the local solution of LPECs and QPECs under the assumption that a feasible point is known.

4 The LPEC simplex method

We consider the problem of finding a local minimizer of the LPEC

$$\begin{array}{ll} \min & q^\top z \\ & Az \leq a \\ & Bz = b \\ & \min\{Cz - c, Dz - d\} = 0. \end{array} \tag{4}$$

The following two examples illustrate typical feasible regions of LPECs:

$$\begin{aligned} \mathcal{F}^1 &= \{z \mid \min\{z_1, z_2\} = 0, \min\{z_3, -z_1 - z_2 - z_3 + 1\} = 0\}\} \\ \mathcal{F}^2 &= \{z \mid z_3 \geq 0, \min\{z_1, z_2\} = 0, \min\{z_1, -z_1 - z_2 - z_3 + 1\}\} = 0\}. \end{aligned}$$

Both feasible sets are subsets of a three-dimensional simplex, the convex hull of the origin o and the three standard unit vectors e_1, e_2, e_3. The set $\mathcal{F}^1$ consists of the four edges $[o, e_1], [e_1, e_3], [e_3, e_2], [e_2, o]$, while $\mathcal{F}^2$ consists of the face $[o, e_2, e_3]$ and the edge $[o, e_1]$. The underlying three-dimensional simplex itself is the feasible set of a relaxed linear program (RLP) which, in general, is defined by

$$\begin{array}{ll} \min & q^\top z \\ & Az \leq a \\ & Bz = b \\ & Cz \geq c \\ & Dz \geq d. \end{array} \tag{5}$$

The feasible set of LPEC is the union of all sets of the form

$$\mathcal{F}_I = \{z \mid Az \le a, Bz = b, C_I z = c_I, D_I z \ge d_I, C_{I^c} z \ge c_{I^c}, D_{I^c} z = d_{I^c}\},$$

where $I \subseteq \{1, \ldots, m\}$ and I^c is the complement of I. Each set $\mathcal{F}_I$ is a face of the feasible set of RLP and thus the feasible set of LPEC is a nonconvex polyhedral subset of the feasible set of RLP. In particular, the face lattice of the feasible set of LPEC is a subset of the face lattice of RLP and we may therefore speak unambiguously of extremal points, edges, faces, lineality space, etc., of the feasible set of LPEC. This observation gives rise to the following proposition which is the basis for the LPEC Simplex method.

Proposition 2 *Suppose the feasible set of RLP is pointed.*

1. *If the objective function is bounded below on the feasible set of LPEC then there exists an extremal point which is a global optimizer of LPEC.*
2. *An extremal point z of LPEC is a local minimizer if and only if there exists no LPEC feasible edge adjacent to z along which the objective function decreases.*

The example

$$\begin{array}{ll} \min & -z_1 \\ s.t. & z_1 \le 1 \\ & \min\{z_1, z_2\} = 0 \end{array}$$

shows that the set of local minimizers which are not global minimizers - in this case the positive z_2-axis - does not necessarily contain an extremal point.

The above proposition suggests to modify the simplex method to find a local minimizer of LPEC. Notice that an extremal point z of RLP is feasible for LPEC if and only if there is a corresponding basis matrix[4]

$$M = \begin{pmatrix} A_I \\ B \\ C_J \\ D_K \end{pmatrix}$$

with $J \cup K = \{1, \ldots, m\}$. To apply the simplex method with a given initial extremal point z of LPEC we allow only basis changes which leave the latter condition valid. In the case of unbounded edges, we only consider those which are LPEC feasible, in which case they indicate unboundedness of the objective function over the LPEC feasible set. Notice that, in the case of a nondegenerate extremal point z the edge directions for RLP are precisely those columns of M^{-1} which do not correspond to the equation matrix B and that column l is a feasible edge direction for LPEC if and only if $\{l\} \in J \cap K$. If the simplex method is modified in this way then it either stops at a local minimizer, with suitable precautions for degeneracy, or it produces a feasible edge along which the

[4] Here and in the sequel we denote by N_I the submatrix of a matrix N consisting of the rows with indices in I.

objective function is unbounded. Notice that the LPEC simplex does occasionally escape local minimizers. Indeed, if we choose the objective function $z_1 + z_2 - z_3$ in the foregoing example of the feasible set $\mathcal{F}^1$, then the origin is a locally optimal extremal point since the edge $[o, e_3]$ is not LPEC feasible. Nevertheless, the simplex method would move from the origin to the global solution e_3 since it is a neighbouring LPEC feasible extremal point[5].

The above procedure relies on the availability of an LPEC feasible extremal point. Notice that the branch-and-bound scheme of Section 3.2 would produce such an extremal point if the simplex method was used to solve the intermediate linear programs. An alternative arises if the LPEC stems from a bilevel problem which allows to fix some variables z_i - the design variables - and solve a fairly simple problem, e.g. a monotone linear complementarity problem, in the remaining so-called state variables. This will result in a feasible point of LPEC which will be a point of some set $\mathcal{F}_I$ from which, by successive projection of the objective gradient, one can find an extremal point of $\mathcal{F}_I$ with at least as good a function value as the original point, provided the objective function is bounded on $\mathcal{F}_I$ and the feasible set of RLP is pointed.

Feasible regions of pointed LPs are intersections of simplicial cones with different vertices. The link between the geometry and the linear algebra of the simplex method is the fact that the edge directions of a simplicial cone $Ax \leq 0$ are precisely the columns of the matrix A^{-1}. The situation is complicated if vertices of some of the simplicial cones coincide. Such vertices are called degenerate. Special pivot procedures are needed in the standard simplex method to escape from such a degenerate vertex or prove that it is optimal. Such procedures may, in the worst case, amount to an enumeration of all simplicial cones whose vertices coincide with the current iterate. Any such enumeration procedure can, in principle, be adopted to LPECs by imposing the additional requirement on the edge directions that they not only increase the objective function but either lead to an LPEC-feasible neighbouring vertex or, in the case of unbounded edges, are LPEC-feasible. There is an indication, however, that degeneracy may causes more problems for LPECs than in ordinary linear programming. Checking local optimality for LPECs at a degenerate vertex is - in contrast to linear programming - NP-hard, [22], even in the presence of strictly feasible solutions of RLP.

[5] Indeed, all extremal points of RLP are feasible for LPEC in this example and this is always the case if $m < \frac{n-l}{2} + 1$ since for an infeasible extremal point we need $p + q + r = n$ with $p, q \leq m - 1$ and $r \leq l$ and therefore $2(m-1) + l \geq n$. In this case, the LPEC simplex finds a global solution if one exists. The condition is, however, very restrictive. If $z = (x, y) \in \mathbb{R}^s \times \mathbb{R}^t$ and the constraints are of standard linear complementarity type $\min\{C_1 x + C_2 y - c, x\} = 0$ with no further inequality constraints then the condition $m < \frac{n-l}{2} + 1$ amounts to $s \leq t + 1$ while the pointedness condition requires $s \geq t$.

5 An active set method for QPECs

In this section we consider QPECs of the form

$$\begin{array}{ll} \min & q^\top z + \frac{1}{2} z^\top Q z \\ & Az \leq a \\ & Bz = b \\ & \min\{Cz - c, Dz - d\} = 0. \end{array} \tag{6}$$

In the same way as LPECs lend themselves naturally to the Simplex method, QPECs are amenable to the active set methodology from standard quadratic programming. As in the case of the LPEC simplex method we assume that we have a feasible starting point z of the QPEC (6). Given this feasible starting point, we apply a standard active set method to the QP that arises from the QPEC (6) by relaxing the equations $\min\{Cz - c, Dz - d\} = 0$ to the two inequalities $Cz \geq c, Dz \geq d$. However, during the course of the method, we consider only search directions that are feasible for the QPEC (6). This can be done in the active set framework by ensuring that at each iteration at least one of each pair of complementary inequalities $C_i z \geq c_i$ and $D_i z \geq d_i$ is contained in the active set.

The method that we describe in the sequel is closely related to the active set method for QPs of [5], Chapter 10. We assume that a feasible point z of the QPEC (6) is known and that three active index sets I, J, L are given which satisfy

$$L \subseteq \{l \mid A_l z = a_l\}, \quad I \subseteq \{i \mid C_i z = c_i\}, \quad J \subseteq \{j \mid D_j z = d_j\}, \quad I \cup J = \{1, \ldots, r\}, \tag{7}$$

where r is the number of rows of C. With (I, J, L) we associate the equality constrained QP

$$\begin{array}{ll} \min & q^\top \zeta + \frac{1}{2} \zeta^\top Q \zeta \\ s.t. & A_l \zeta = a_l, \quad l \in L \\ & B\zeta = b \\ & C_i \zeta = c_i, \quad i \in I \\ & D_j \zeta = d_j, \quad j \in J. \end{array} \tag{8}$$

Let us assume that we are given index sets L^k, I^k, J^k with $I^k \cup J^k = \{1, \ldots, r\}$ and a feasible point z^k of the corresponding QP (8). We assume that the constraints of (8) are linearly independent. To update z^k and the index sets we attempt to find a stationary point of (8). We consider two possible outcomes of this attempt:

1. If the point z^k is stationary for (8) then there are unique multipliers $\lambda, \mu, \gamma, \nu$ with

$$q + Qz^k + \sum_{l \in L} \lambda_l A_l + B^\top \mu - \sum_{i \in I} \gamma_i C_i - \sum_{j \in J} \nu_j D_j = 0.$$

   (a) If $\lambda \geq 0$ and $\gamma_i, \nu_i \geq 0$ for every $i \in I \cap J$ then z^k is B-stationary for the QPEC since the given multipliers are multipliers for each adjacent NLP piece. We terminate with the B-stationary point z^k.

(b) Otherwise, set $z^{k+1} = z^k$, $L^{k+1} = L^k$, $I^{k+1} = I^k$, $J^{k+1} = J^k$ and we do exactly one of the following:

   i. Remove an index $l \in L^{k+1}$ with $\lambda_l < 0$ from L^{k+1}.

   ii. Remove an index $i \in I^{k+1} \cap J^{k+1}$ with $\gamma_i < 0$ from I^{k+1}.

   iii. Remove an index $j \in I^{k+1} \cap J^{k+1}$ with $\nu_j < 0$ from J^{k+1}.

2. If the point z^k is not stationary for (8) then

   (a) **either** find a stationary point ζ of (8) with a lower objective function value and choose the search direction $s^k = \zeta - z^k$ and a maximal step size $\alpha^k_{\max} = 1$

   (b) **or** find a search direction s^k, feasible for (8), along which the objective function decreases monotonically to $-\infty$ and set $\alpha^k_{\max} = \infty$.

   To stay feasible for QPEC we bound the stepsize by

$$\alpha_k = \min\{\alpha^k_{\max}, \min_{\substack{l:l\notin L^k \\ A_l s^k > 0}} \frac{a_l - A_l z^k}{A_l s^k}, \min_{\substack{i:i\notin I^k \\ C_i s^k < 0}} \frac{c_i - C_i z^k}{C_i s^k}, \min_{\substack{j:j\notin J^k \\ D_j s^k < 0}} \frac{d_j - D_j z^k}{D_j s^k}\}.$$

   If $\alpha^k = \infty$ then terminate and report that the QPEC has no optimal solution. Otherwise set $z^{k+1} = z^k + \alpha_k s^k$ and $L^{k+1} = L^k, I^{k+1} = I^k, J^{k+1} = J^k$. If $\alpha_k < \alpha^k_{\max}$ then we have hit a new constraint and we do exactly one of the following:

   (a) Add an index $l \notin L^k$ with $A_l s^k > 0$ and $A_l z^{k+1} = a_l$ to L^{k+1}.

   (b) Add an index $i \notin I^k$ with $C_i s^k < 0$ and $C_i z^{k+1} = c_i$ to I^{k+1}.

   (c) Add an index $j \notin J^k$ with $D_j s^k < 0$ and $D_j z^{k+1} = d_j$ to J^{k+1}.

   Notice that s^k is orthogonal to all the old constraints and therefore the new QP (8) will have linearly independent constraints as well.

The next lemma guarantees that a suitable search direction can be found in step 2. Its proof in the appendix is based on the suggested choice of s^k in [5], Chapter 10.4.

Lemma 3 *If z^k is a feasible but non-stationary point of (8) and there exists no stationary point of (8) with lower objective function value then there exists a feasible direction s^k at z^k along which the objective function decreases monotonically to $-\infty$.*

The following proposition summarizes some properties of the above active set method and extends results known from active set methods for QPs to QPECs, cf. e.g. Chapter 10 of [5].

Proposition 4 *Suppose the active set method is started with index sets L^0, I^0, J^0 and a feasible point z^0 of the QPEC such that*

1. $I^0 \cup J^0 = \{1, \ldots, r\}$

2. *(8) has linearly independent constraints*

3. *z^0 is feasible for the corresponding QP (8).*

The method produces a possibly infinite sequence of index sets L^k, I^k, J^k and feasible points z^k for the corresponding QPs (8) and the following statements hold:

1. *The constraints of all QPs (8) are linearly independent.*

2. *The method produces a sequence of feasible points z^k for the QPEC. If $z^{k+1} \neq z^k$ then the former has a lower objective function value.*

3. *If the method terminates then it either reports correctly that there is no optimal solution of the QPEC or its final point z^k is B-stationary for the QPEC.*

4. *If the sequence is infinite then for every sufficiently large k we have $z^k = z^{k+1}$.*

5. *If LICQ holds at z^k and z^k is not B-stationary for the QPEC then there exists j with $z^{k+j} \neq z^k$.*

As a consequence of the last statement, the method will always terminate if LICQ is satisfied at all critical points of QPEC since any point of step 1 of the method is critical. The method can be readily applied to positive definite matrices Q since stationary points of (8) exist and are unique. Positive semidefinite matrices can be handled by adding a small multiple of the unit matrix to Q or, alternatively, by perturbing zero diagonal elements of the $LL^\top$ factors of the reduced Hessian. In the positive semidefinite case the method produces local minimizers, in view of Proposition 1, provided it terminates. Indefinite matrices Q are more difficult to deal with and the efficiency of the method depends on the choice of the search direction s^k in step (2b). We refer the interested reader to [7] for a discussion of this issue in ordinary quadratic programming.

5.1 Upgrading an existing active set QP solver

Following the active set approach, an existing active set QP solver can be easily upgraded to a QPEC solver, provided a feasible point for the QPEC is known. If that is not the case then one may have to use the branch and bound approach to find such a feasible point. We assume that at the beginning of iteration k we are given a feasible point z^k and index sets I^k, J^k with $I^k \cup J^k = \{1, \ldots, r\}$. We use the QP solver to solver the problem

$$\begin{array}{ll} \min & q^\top \zeta + \frac{1}{2}\zeta^\top Q \zeta \\ s.t. & A\zeta \leq a \\ & B\zeta = b \\ & C_i\zeta = c_i, \quad i \in I^k \\ & C_i\zeta \geq c_i, \quad i \notin I^k \\ & D_j\zeta = d_j, \quad j \in J^k \\ & D_j\zeta \geq d_j, \quad j \notin J^k. \end{array} \tag{9}$$

If the QP solver reports unboundedness, then the QPEC is unbounded as well since the feasible set of the QP is a subset of the feasible set of the QPEC. Otherwise we obtain a locally optimal solution z^{k+1} of the QP, associated multipliers $\lambda, \mu, \gamma, \nu$ with

$$q + Qz^k + A^\top \lambda + B^\top \mu - C^\top \gamma - D^\top \nu = 0,$$

and active index sets I^{k+1}, J^{k+1} for the constraints involving the matrices C and D, respectively. We presume that the latter index sets contain the index sets I^k and J^k. If all multipliers γ_i, ν_i corresponding to indices in $I^{k+1} \cap J^{k+1}$ are nonnegative then we have arrived at a B-stationary point of the QPEC and terminate. Otherwise we do exactly one of the following:

1. Remove an index $i \in I^{k+1} \cap J^{k+1}$ with $\gamma_i < 0$ from I^{k+1}.
2. Remove an index $j \in I^{k+1} \cap J^{k+1}$ with $\nu_j < 0$ from J^{k+1}.

After this we reiterate. If the QP solver fits the active set description given in the foregoing section with complementarity constraints removed, then the upgraded QP solver is nothing else but the QPEC solver of the foregoing section with the additional requirement that in step (1b) an index $l \in L^{k+1}$ is chosen whenever that is possible. The QP solver stops if that is not possible and requires a specification of how to proceed according to step (1b) of the method. In view of this, the statements of Proposition 4 remain valid for the upgraded QP solver.

5.2 Finding a feasible solution

In applications, one may wish to start a local minimization procedure for the QPEC (6) at an infeasible point z^0 which is thought to be a good estimate of the global minimizer. For example, past data could serve as a solution estimate for the application discussed in Section 2. In such cases, one needs to find, in a first phase, a feasible point of the QPEC (6) close to z^0 which can serve as a starting point for the active set method of the preceding section. Notice that z is a feasible solution of the QPEC (6) if and only if it is a solution of the nonconvex QP

$$\begin{array}{ll} \min & (Cz - c)^\top (Dz - d) \\ & Az \leq a \\ & Bz = b \\ & Cz \geq c \\ & Dz \geq d \end{array} \tag{10}$$

with a vanishing objective value. This suggests the following two-step heuristic:

1. Given z^0, find a feasible point z^1 of (10) by solving the Euclidean projection problem

$$\begin{array}{ll} \min & (z - z^0)^\top (z - z^0) \\ & Az \leq a \\ & Bz = b \\ & Cz \geq c \\ & Dz \geq d. \end{array} \tag{11}$$

2. Starting at z^1, apply the active set method of the preceding section to find a local optimizer of the QP (10).

In general, this procedure is only a heuristic, due to the local optimization in the second step. However, it is guaranteed to produce a feasible point of the QPEC (6) if the starting point z^0 is sufficiently close to the feasible region of the QPEC (6).

Proposition 5 *For each feasible point z of the QPEC (6) there exists an $\epsilon > 0$ such that the above heuristic, if started at a point z^0 within distance ϵ from z, will produce a feasible point of the QPEC (6).*

6 The OD-demand model revisted

The main difficulty in using the developed methodology for OD-demand estimation is the nonlinearity of the travel time function $C(h)$. This function is generally of the form $C(h) = \Delta^\top c(\Delta h)$, where Δ is the arc-path incidence matrix and $c_a(f)$ is the travel time along arc $a \in A$, given arc flow f. We will assume that the arc travel time function c_a is separable in the sense that c_a depends only on the flow f_a on arc a. It seems to be natural to approximate the arc travel time $c_a(f_a)$ by a piecewise linear convex function. The simplest such function is of the form

$$c_a(f_a) = \begin{cases} \alpha_a & \text{if } f_a \le l_a \\ \alpha_a + \beta_a(f_a - l_a) & \text{if } l_a \le f_a \le u_a \\ \infty & \text{if } f_a > u_a. \end{cases}$$

Here α_a is the non-congested travel time on arc a, l_a is a congestion threshold of the arc and u_a is a maximal capacity of arc a. We can express the function c_a as

$$c_a(f_a) = \max\{\alpha_a, \alpha_a + \beta_a(f_a - l_a)\}$$

with the provision that $0 \le f_a \le u_a$. If we denote by Δ_a the a-th row of the arc-path incidence matrix Δ, then the travel time along path p turns into a function of the form

$$\begin{aligned} C_p(h) &= \sum_{a \in p} c_a(\Delta_a h) \\ &= \sum_{a \in p} \max\{\alpha_a, \alpha_a + \beta_a(\Delta_a h - l_a)\} \end{aligned}$$

with the constraint $\Delta_a h \le u_a$. Recall that the complementarity constraints in the OD-demand estimation problem is of the form

$$\min\{h_p, C_p(h) - u_{(o(p),d(p))}\} = 0, \quad p \in P,$$

where $o(p)$ and $d(p)$ are the origin and destination, respectively, of path p. Using a new variable $\zeta_p = C_p(h)$ and the above form of C_p we can reformulate these equations as

$$\begin{aligned} \min\{h_p, \zeta_p - u_{(o(p),d(p))}\} &= 0 \\ \zeta_p - \sum_{a \in p} \max\{\alpha_a, \alpha_a + \beta_a(\Delta_a h - l_a)\} &= 0. \end{aligned}$$

We now introduce auxiliary variable v_a for each summand in the last sum and arrive at the equivalent pair of equations

$$\begin{aligned} \min\{h_p, \zeta_p - u_{(o(p),d(p))}\} &= 0 \\ \min\{v_a - \alpha_a, v_a - \alpha_a - \beta_a(\Delta_a h - l_a)\} &= 0 \\ \zeta_p - \sum_{a \in p} v_a &= 0. \end{aligned}$$

In this way we can turn the OD-demand estimation problem into an inverse linear complementarity problem of the type that we have discussed in the previous sections, provided the arc costs are separable, convex, and piecewise linear.

7 Conclusions and extensions

We have demonstrated that standard active set type methods for linear and quadratic programming extend to inverse linear complementarity problems with linear or quadratic objectives and that these methods deliver local minimizers. The methods can be used for local optimization of large problems if a reasonable starting point is known or be built into a canonical branch-and-bound method for a global optimization of small problems. The active set approach extends to more general optimization problems, provided the constraints are of a complementarity nature, i.e. they specify finitely many combinations of either fixing certain constraint functions to certain values or allowing them to vary over certain ranges. Typical examples of such more general inverse problems are inverse box-contrained variational inequalities which can be expressed as mixed complementarity contraints of the form[6]

$$F_i(z) \geq 0, \quad G_i(z) \geq 0, \quad F_i(z)H_i(z) \geq 0, \quad G_i(z)H_i(z) \leq 0, \quad \forall i = 1, \ldots, r.$$

It is further possible to extend the active set approach for QPECs to other types of objective functions, e.g. maximal entropy models. The main criterion for such an extension is that the problem corresponding to a fixed combination of the complementarity conditions can be solved in a finite number of steps. For more general nonlinear problems one cannot expect a finite method. An interesting extension of the active set framework to linearly constrained inverse complementarity problems with general nonlinear objective functions has been recently proposed in [10]; it is shown that this method converges globally to B-stationary points under appropriate assumptions. For nonlinear constraints, a trust region SQP method, close in spririt to the active set approach, has been suggested and analysed in [17, 19]. As in the case of the active set methods discussed here, this SQP type method retains, under appropriate assumptions, the desirable properties of the underlying NLP method: global convergence and local superlinear convergence of the iteration sequence to a B-stationary point.

[6]If $z = (x, y)$, $F(x, y) = b - y$, $G(x, y) = y - a$ with $a \leq b$ then these constraints correspond to a parametric variational inequality in y induced by the parametric vector field $H(x, .)$ over the box $a \leq y \leq b$.

8 Appendix: Proofs of propositions

Proposition 1 *Let z be a feasible point of a smooth convex MPEC and suppose LICQ holds at z. Then z is a local minimizer of the MPEC if and only if z is a critical point and the (unique) multipliers $\lambda, \mu, \gamma, \nu$ satisfy $\lambda \geq 0$ and $\gamma_k, \nu_k \geq 0$ for every k such that $G_k(z) = H_k(z) = 0$.*

Proof. We have already argued that the given conditions are necessary optimality conditions for a local minimizer in the presence of LICQ. They are also sufficient since they are sufficient for z to be a minimizer of the convex problem

$$
\begin{array}{ll}
\min & f(\zeta) \\
s.t. & g(\zeta) \leq 0 \\
 & h(\zeta) = 0 \\
 & G_i(\zeta) = 0, i : H_i(z) > 0 \\
 & H_j(\zeta) = 0, j : G_j(z) > 0 \\
 & G_k(\zeta) \geq 0, k : G_k(z) = H_k(z) = 0 \\
 & H_k(\zeta) \geq 0, k : G_k(z) = H_k(z) = 0
\end{array}
$$

and there exists a neighbourhood of z such that in this neighbourhood any feasible point of the original MPEC is also feasible for the latter convex program. □

Proposition 2 *Suppose the feasible set of RLP is pointed.*

1. *If the objective function is bounded below on the feasible set of LPEC then there exists an extremal point which is a global optimizer of LPEC.*
2. *An extremal point z of LPEC is a local minimizer if and only if there exists no LPEC feasible edge adjacent to z along which the objective function decreases.*

Proof. The first part is trivial. Indeed, the global optimizer is an optimizer of the linear objective over some set $\mathcal{F}_I$ which is a face of the pointed feasible region of RLP and therefore the optimum is obtained at an extremal point of $\mathcal{F}_I$. The "only if" part of the second statement is equally trivial. To see the "if" part, suppose the extremal point z is not a local minimizer. Then z is feasible for some $\mathcal{F}_I$ for which it is not a minimizer and hence there exists a neighbouring extremal point in $\mathcal{F}_I$ with an improved objective value. These two extreme points are joined by an LPEC feasible edge within $\mathcal{F}_I$. □

Lemma 3 *If z^k is a feasible but non-stationary point of (8) and there exists no stationary point of (8) with lower objective function value then there exists a feasible direction s^k at z^k along which the objective function decreases monotonically to $-\infty$.*

Proof. In suitable coordinates (v,w) of the tangent space, the objective function, reduced to the feasible set of (8), takes on the form

$$q(z^k+(v,w)) = q_k + a^\top v + b^\top w + \frac{1}{2} w^\top D w,$$

where D is a nonsingular diagonal matrix and q_k is the objective value at z^k. If, on the one hand, $a \neq 0$ then $(v,w) = (-a,0)$ is a descent direction along which the objective function decreases to $-\infty$. If, on the other hand, $a = 0$ then $b \neq 0$ since z^k is not a stationary point of (8). Moreover, D must have a negative diagonal element since for positive definite D the point $z^k + (0, -D^{-1}b)$ is a stationary point of (8) with lower objective function value. If e_k is a unit vector corresponding to a negative entry on the diagonal of D then the function q tends monotonically to $-\infty$ in either the direction $(0, e_k)$ or $(0, -e_k)$.□

Proposition 4 *Suppose the active set method is started with index sets L^0, I^0, J^0 and a feasible point z^0 of the QPEC such that*

1. $I^0 \cup J^0 = \{1, \dots, r\}$
2. *(8) has linearly independent constraints*
3. *z^0 is feasible for the corresponding QP (8).*

The method produces a possibly infinite sequence of index sets L^k, I^k, J^k and feasible points z^k for the corresponding QPs (8) and the following statements hold:

1. *The constraints of all QPs (8) are linearly independent.*
2. *The method produces a sequence of feasible points z^k for the QPEC. If $z^{k+1} \neq z^k$ then the former has a lower objective function value.*
3. *If the method terminates then it either reports correctly that there is no optimal solution of the QPEC or its final point z^k is B-stationary for the QPEC.*
4. *If the sequence is infinite then for every sufficiently large k we have $z^k = z^{k+1}$.*
5. *If LICQ holds at z^k and z^k is not B-stationary for the QPEC then there exists j with $z^{k+j} \neq z^k$.*

Proof. Statements 1 has already been explained during the presentation of the method. To prove statement 2, we distinguish between step (2a) and (2b). In step (2a) the new value z^{k+1} is on the line segment between z^k and a stationary point with a lower objective function value. Any quadratic function decreases strictly on this line segment, i.e. the function value of z^{k+1} is lower than the function value of z^k. For step (2b) the required monotonicity of the objective along the search line yields the same result. Statement 3 is obvious; if the method terminates then it either reports that it has found a B-stationary point for the QPEC in step (1a) or the whole ray in the direction s^k determined in step (2b) is feasible for QPEC, in which case the objective function is unbounded. To see statement 4 suppose the sequence z^k is infinite. Notice first that if z^k is not stationary for (8) then either the QP (8) remains unchanged and z^{k+1} is stationary in the next iteration or a constraint is added. Since adding a constraint can only be done a finite number of times, we conclude that there is an infinite subsequence z^{k_i} of stationary points of the corresponding QP (8). Notice that all stationary points of an equality constrained quadratic program have the same objective value. Hence, if z^{k_i} is changed then the objective function decreases and therefore none of the subsequent points $z^{k_{i+j}}$ is stationary for the QP corresponding to z^{k_i}. Since there are only finitely many equality constrained QPs we conclude that z^{k_i} will eventually be constant. To see the last statement, suppose, by way of contradiction, that $z^k = z$ is constant for all sufficiently large k and not B-stationary for QPEC. Let us first show that step 1 of the method will eventually be reached. Indeed, in step 2 the method would always generate a zero steplength α_k for otherwise z^k would change. Hence a new constraint is added and since there are only finitely many constraints we will eventually reach step 1. In view of the LICQ assumption, we then have a *unique* multiplier vector u with

$$q + Qz + M^\top u \;=\; 0$$

where M contains all rows of A and B and negatives of all rows of C and D that are active at iteration k. Since the condition of step (1a) is necessary and sufficient for B-stationarity in the presence of LICQ we enter step (1b) and a constraint, say $M_1 z = b_1$, with negative multiplier $u_1 < 0$ is removed from the active set. Now z becomes non-stationary for the new QP (8) since the multipliers at z are unique. Hence step 2 is performed with zero step lengths until the removed constraint is added to the active set again. Suppose this is done in iteration $k + l$ where the search direction is $s = s^{k+l}$. Then, on the one hand, $M_1 s > 0$ by definition of the method. On the other hand we know that the objective function is decreasing in the search direction s. Differentiating the objective function on the line along the direction s we thus obtain

$$0 \geq q^\top s + s^\top Qz + \alpha s^\top Qs$$

for all $\alpha > 0$. With the stationarity condition $Qz = -q - M^\top u$ the latter inequality turns into

$$u \top Ms \geq \alpha s^\top Qs.$$

Since we have not yet entered step 1, no further constraint has been deleted between iterations k and $k + l$ and hence $M_i s = 0$ for all but the first row of the matrix M. Since $u_1 < 0$ we thus obtain $M_1 s \leq \alpha s^\top Qs$ for each $\alpha > 0$ and conclude that $M_1 s \leq 0$. This yields the required contradiction. □

Proposition 5 *For each feasible point z of the QPEC (6) there exists an $\epsilon > 0$ such that the above heuristic, if started at a point z^0 within distance ϵ from z, will produce a feasible point of the QPEC (6).*

Proof. Notice that the objective function of (10) at z is zero. Therefore, for any $\delta > 0$ there is a number $\epsilon > 0$ such that the objective function of (10) at z^1 will be less than δ, provided z^0 is within distance ϵ of the feasible point z. Now suppose the active set method of the preceding section is started at a feasible point z^1 of (10) to solve (10). If $\delta > 0$ is chosen sufficiently small then the constraints of the active index set at z^1 are also active at z. We therefore find a descent direction at z^1 in the currently active face and this descent direction will move us to a feasible point of (10) with an even smaller objective value. The procedure will thus converge to a feasible point. □

We finally give a proof of the statement in Footnote 3.

Proposition 6 *Let $C : R^p \to R^p$ and $T : R^d \to R^d$ be smooth functions and define*

$$F(h,u) = \begin{pmatrix} \min\{h, C(h) - a - \Lambda^\top u\} \\ \Lambda h - T(u) - b \end{pmatrix}.$$

For almost all a, b all roots of F are isolated.

Proof. The function F is a piecewise smooth function in the sense of [15] with selection functions F_I indexed by index sets $I \subseteq \{1, \ldots, p\}$ and defined by

$$(F_I)_i(h,u) = \begin{cases} h_i, & i \in I \\ C_i(h) - a_i - (\Lambda^\top u)_i, & i \in \{1, \ldots, p\} \backslash I \\ (\Lambda h - T(u) - b)_i & \text{otherwise.} \end{cases}$$

We will show that for almost all (a, b) every F_I has a non-singular Jacobian at any of its roots. Hence these roots are isolated. It then follows immediately that the roots of F are isolated since they form a subset of the union of the roots of the finitely many functions F_I. Now fix an index set I and let h_I be the vector obtained from h by setting $h_i = 0$ for $i \in I$. Notice that, in view of the special structure of F_I, the Jacobian of F_I is nonsingular if and only if the Jacobian with respect to (h_I, u) of the right-hand side of the equation

$$\begin{aligned} (C_i(h_I) - (\Lambda^\top u)_i &= a_i, \quad i \in \{1, \ldots, p\} \backslash I \\ \Lambda_I h_I - T(u) &= b \end{aligned}$$

is non-singular. In view of Sard's theorem, the Jacobian of the latter equation is indeed non-singular at all solutions for almost all a, b. Since there are only finitely many selection functions F_I and the union of a finite number of null sets is null, we conclude that for almost all (a, b) the Jacobian of every function F_I is non-singular at the roots of F_I. □

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