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Letter

Remarks on the numerical solution of certain linear complementarity problems

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Abstract

In a recent paper, J.K. Aitchison and N.K. Upton have proposed a mathematical model of the behaviour of a cloud formed immediately after the sudden release of a pollutant, together with an algorithm for determining numerical solutions of the resulting system of constrained nonlinear equations and complementarity relations. This algorithm requires, at each step, the solution of a special linear complementarity problem, which is solved by an iterative method. In this note, it is argued that the robustness and reliability of the solution procedure can be improved by the use of standard linear programming techniques.

Keywords: Linear Complementarity Problem; Z-matrices; Cryer's algorithm; Linear programming

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1. Introduction

In this note we make a few remarks concerning an algorithm for solving systems of nonlinear equations with simple constraints and complementarity relations arising in the study of air-pollutant cloud models, see [1]. The algorithm proposed in [1] consists of an inner–outer procedure which involves the solution of several linear inequalities and one unconstrained nonlinear equation. At each outer step, a nonlinear equation in a single unknown is solved by some root-finding technique. The remaining unknowns are shown to be the solution of a symmetric linear complementarity problem (LCP) having a very special structure. Once a solution to this LCP is computed, the approximations found for the unknowns are used as input for the next outer

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step. In this note, we consider only the solution of the LCPs, which is likely to account for the bulk of the work in the overall computation, especially for realistic problems. Here the problem size, n, is given by the number of different chemical components present in the cloud. In their paper [1], Aitchison and Upton suggest to use the *modified Gauss–Seidel* method (see [4]) for the solution of the LCP problem arising at each outer step. In our opinion, this method has little to recommend it in the present context. In particular, we are concerned about the indefiniteness of the quadratic programming problem associated with the LCP. Under these circumstances, there is no reason to expect that the modified Gauss–Seidel method will converge and, in fact, examples can be given to show that the iteration may fail to converge, or even converge to an infeasible point (see below). Clearly, these possibilities seriously undermine the robustness of the overall algorithm. In this note we argue that these and other difficulties can be circumvented by using standard linear programming techniques in solving the LCPs, resulting in a more robust and reliable algorithm.

2. The linear complementarity problem

Let A be a real $n \times n$ matrix and let $\boldsymbol{b}$ be a real n-vector. The linear complementarity problem for $\boldsymbol{b}$ and A, denoted by $(\boldsymbol{b}, A)$, consists in finding (if it exists) a real n-vector $\boldsymbol{x}$ such that

$$\boldsymbol{x}^{\mathrm{T}}[A\boldsymbol{x} - \boldsymbol{b}] = 0, \quad \boldsymbol{x} \geqslant \boldsymbol{0},\ A\boldsymbol{x} \geqslant \boldsymbol{b}, \tag{1}$$

where the inequalities are understood to be componentwise. For a general matrix A, this is a rather hard problem (see e.g. [3, 2, Ch. 10]). When A is a symmetric, it is well-known that (1) are the Karush–Kuhn–Tucker optimality conditions for the quadratic program over the nonnegative orthant:

$$\text{minimize}\, f(\boldsymbol{x}) = \tfrac{1}{2}\boldsymbol{x}^{\mathrm{T}}A\boldsymbol{x} - \boldsymbol{x}^{\mathrm{T}}\boldsymbol{b}, \quad \text{subject to}\ \boldsymbol{x} \geqslant \boldsymbol{0}. \tag{2}$$

When A is positive semidefinite, then the quadratic objective function is convex, and problems (1) and (2) are completely equivalent. When A is positive definite, problem (1) (or (2)) has a unique solution $\boldsymbol{x}$ which can be approximated by Cryer's projected SOR method, see [4]. For convenience, we recall that Cryer's method consists in generating a sequence of vectors $\{\boldsymbol{x}^{(k)}\}$ $(k = 0, 1, \dots,)$ where $\boldsymbol{x}^{(0)} \geqslant \boldsymbol{0}$ is an initial guess and

$$x_i^{(k+1)} = \max\left\{0, x_i^{(k)} + \left(\frac{\omega}{a_{ii}}\right)\left(b_i - \sum_{j<i} a_{ij}x_j^{(k+1)} - \sum_{j \geqslant i} a_{ij}x_j^{(k)}\right)\right\}, \quad 1 \leqslant i \leqslant n, \tag{3}$$

for all $k \geqslant 0$. Here, a_{ij} and b_i are the entries of matrix A and vector $\boldsymbol{b}$, respectively, and ω is a relaxation factor. It should be remarked that Cryer proposed this method for solving very large, sparse, strictly convex quadratic programming problems arising from the numerical solution of variational inequalities. Subsequently, various authors studied the convergence of the projected SOR method under weaker assumptions on A (see e.g. [6] for a good survey). As a result, it has been known for a long time that positive definiteness is not necessary for the convergence of the iteration. In particular, Pang proved the following result [6, p. 388]. Assume that A has nonzero principal minors and positive diagonal entries. Then, for any choice of $\boldsymbol{x}^{(0)} \geqslant \boldsymbol{0}$, Cryer's method (3) is convergent for all $0 < \omega < 2$ and for all right-hand sides $\boldsymbol{b}$ if and only if A is *copositive*, i.e., the following condition holds:

$$\boldsymbol{x}^{\mathrm{T}} \boldsymbol{A}\boldsymbol{x} \geqslant 0 \quad \text{for all } \boldsymbol{x} \geqslant \boldsymbol{0}.$$

It follows that if A fails to be copositive, there exist choices of $\boldsymbol{x}^{(0)}$ for which Cryer's method does not converge for all choices of ω and/or for all right-hand sides $\boldsymbol{b}$. We will give examples of this below.

After these general remarks, we now turn to the LCPs arising in the model of Aitchison and Upton. Here the matrix A has the following form:

$$\boldsymbol{A} = \begin{bmatrix} a_1 & -1 & -1 & \cdots & -1 \\ -1 & a_2 & -1 & \cdots & -1 \\ -1 & -1 & a_3 & \cdots & -1 \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ -1 & -1 & -1 & \cdots & a_n \end{bmatrix}, \tag{4}$$

where the diagonal entries a_i change from one outer iteration to the next. This (symmetric) matrix has several important properties. Note that $A \in Z^{n\times n}$ where $Z^{n\times n}$ denotes, as is customary, the class of $n \times n$ matrices with nonpositive off-diagonal entries. Such matrices (referred to as Z-matrices) have been thoroughly studied by researchers in many fields, and especially by the mathematical programming community. One basic fact about symmetric Z-matrices is the following (see e.g. [2, Ch. 6]): a symmetric Z-matrix is positive definite if and only if it is invertible with a (componentwise) nonnegative inverse, $A^{-1} \geqslant \boldsymbol{0}$. In this case A is said to be a symmetric nonsingular M-matrix, or a *Stieltjes* matrix. Because Cryer's method is guaranteed to converge to the unique solution of $(\boldsymbol{b}, A)$ when A is positive definite, it is important to determine when A is a Stieltjes matrix. By virtue of the above result, it is sufficient to check when A is invertible with a nonnegative inverse. A remarkable feature of matrix (4) is that its inverse is easily computed explicitly. The diagonal entries of A can be written as $a_i = c_i - 1$ with $c_i > 0$ (see [1]). If we introduce the diagonal matrix

$$\boldsymbol{C} = \mathrm{diag}(c_1, c_2, \ldots, c_n),$$

then, we can rewrite A as

$$\boldsymbol{A} = \boldsymbol{C} - \boldsymbol{e}\boldsymbol{e}^{\mathrm{T}},$$

where $\boldsymbol{e}$ denotes the column n-vector all of whose components are equal to one. We can then use the well-known Sherman–Morrison–Woodbury inversion formula (see [5, p. 51]) and write the inverse of A as

$$\boldsymbol{A}^{-1} = \boldsymbol{C}^{-1} + \frac{\boldsymbol{C}^{-1}\boldsymbol{e}(\boldsymbol{C}^{-1}\boldsymbol{e})^{\mathrm{T}}}{1 - \boldsymbol{e}^{\mathrm{T}}\boldsymbol{C}^{-1}\boldsymbol{e}}.$$

Clearly, $\boldsymbol{A}$ is invertible if and only if $\boldsymbol{e}^{\mathrm{T}}\boldsymbol{C}^{-1}\boldsymbol{e} \neq 1$, or $\sum_{i=1}^{n} \frac{1}{c_i} \neq 1$. Moreover, letting $z = 1 - \sum_{i=1}^{n} \frac{1}{c_i}$, we can write $\boldsymbol{A}^{-1}$ explicitly as

$$\boldsymbol{A}^{-1} = \begin{bmatrix} \frac{1}{c_1} + \frac{1}{c_1^2 z} & \frac{1}{c_1 c_2 z} & \frac{1}{c_1 c_3 z} & \cdots & \cdots & \frac{1}{c_1 c_n z} \\ \frac{1}{c_1 c_2 z} & \frac{1}{c_2} + \frac{1}{c_2^2 z} & \frac{1}{c_2 c_3 z} & \cdots & \cdots & \frac{1}{c_2 c_n z} \\ \frac{1}{c_1 c_3 n} & \frac{1}{c_2 c_3 z} & \frac{1}{c_3} + \frac{1}{c_3^2 z} & \cdots & \cdots & \frac{c}{c_3 c_n z} \\ \vdots & \vdots & \vdots & \ddots & & \vdots \\ \vdots & \vdots & \vdots & & \ddots & \vdots \\ \frac{1}{c_1 c_n z} & \frac{1}{c_2 c_n z} & \frac{1}{c_3 c_n z} & \cdots & \cdots & \frac{1}{c_n} + \frac{1}{c_n^2 z} \end{bmatrix}$$

from which we immediately conclude that $\boldsymbol{A}^{-1} \geqslant \boldsymbol{0}$ if and only if $z > 0$, or $\sum_{i=1}^{n} \frac{1}{c_i} < 1$. In particular, $\boldsymbol{A}$ is positive definite if and only if $\sum_{i=1}^{n} \frac{1}{c_i} < 1$. This result was proved by Aitchison and Upton using determinants (see [1, Theorem 1]). Here we have established the same result in an alternative fashion, and there are many other possible proofs.

Note that if $\boldsymbol{A}^{-1} \geqslant \boldsymbol{0}$ and $\boldsymbol{b} \geqslant \boldsymbol{0}$ then the LCP reduces to the linear system $\boldsymbol{Ax} = \boldsymbol{b}$ and the solution can be explicitly computed as $\boldsymbol{x} = \boldsymbol{A}^{-1}\boldsymbol{b}$. There are, however, more fundamental properties of Z-matrices which are important for the solvability of the LCP and that should be recalled here. The set of feasible vectors associated with $(\boldsymbol{b}, \boldsymbol{A})$ is defined as

$$X(\boldsymbol{b}, \boldsymbol{A}) = \{\boldsymbol{x} \geqslant \boldsymbol{0}; \boldsymbol{Ax} \geqslant \boldsymbol{0}\}$$

(see [2, p. 271]). If X is any set in n-dimensional space, we say that a vector $\boldsymbol{z} \in X$ is a *least element* of X if $\boldsymbol{z} \leqslant \boldsymbol{x}$ for all $\boldsymbol{x} \in X$. Note that if X has a least element then it is unique. Then the following facts are true (see [2, Ch. 10]):

- $\boldsymbol{A}$ is a Z-matrix if and only if $X(\boldsymbol{b}, \boldsymbol{A})$ has a least element which is a solution of $(\boldsymbol{b}, \boldsymbol{A})$ for each $\boldsymbol{b}$ such that $X(\boldsymbol{b}, \boldsymbol{A}) \neq \emptyset$;
- $\boldsymbol{A}$ is a nonsingular M-matrix if and only if for each $\boldsymbol{b}$, $X(\boldsymbol{b}, \boldsymbol{A})$ has a least element which is the unique solution of $(\boldsymbol{b}, \boldsymbol{A})$.

Furthermore, if a LCP with a Z-matrix if feasible, it can be solved by one linear program. We discuss this in the next section.

3. Remarks on the choice of the solution algorithm

Generally speaking, the matrices arising from the model of Aitchison and Upton will not be positive definite or even semidefinite. Under these circumstances it is difficult even to know, a priori, whether a solution to $(\boldsymbol{b}, \boldsymbol{A})$ exists, and if it is unique. Aitchison and Upton give a simple example where

$$A = \begin{bmatrix} 4.762 & -1 \\ -1 & 0.119 \end{bmatrix}$$

and observe that this matrix is indefinite. Nevertheless, Cryer's method with $\boldsymbol{x}^{(0)} = \boldsymbol{0}$ and $\omega = 1$ converged. It can be easily verified that this matrix is not copositive. It follows from Pang's above-mentioned result that the convergence of Cryer's method was in a sense a lucky coincidence, for there are right-hand sides $\boldsymbol{b}$ and choices of $\boldsymbol{x}^{(0)}$ and ω for which the iteration will fail to converge.

We will now give simple examples where Cryer's method does not converge or otherwise fails. Consider the LCP $(\boldsymbol{b}, \boldsymbol{A})$ where

$$A = \begin{bmatrix} 1 & -1 \\ -1 & \frac{1}{2} \end{bmatrix} \quad \text{and} \quad b = \begin{bmatrix} -3 \\ 1 \end{bmatrix}.$$

Here A is indefinite, and it is not copositive. Note that the LCP has the solution

$$x = A^{-1}b = \begin{bmatrix} 1 \\ 4 \end{bmatrix}.$$

This solution is not unique; another solution is given by $\boldsymbol{x} = [0, 2]^{\mathrm{T}}$. If we apply to this LCP the modified Gauss–Seidel algorithm (i.e. Cryer's method with $\omega = 1$) starting with the initial guess $\boldsymbol{x}^{(0)} = 0$, then we obtain the constant sequence $\boldsymbol{x}^{(k)} = \boldsymbol{0}$ for all $k = 0, 1, \ldots$. In other words, the sequence generated by the modified Gauss–Seidel method converges to an infeasible vector (in fact, it never reaches the feasible set $X(\boldsymbol{b}, \boldsymbol{A})$).

Another simple example of a troublesome situation is the following: consider the LCP $(\boldsymbol{b}, \boldsymbol{A})$ where

$$A = \begin{bmatrix} 1 & -1 \\ -1 & 1 \end{bmatrix} \quad \text{and} \quad b = \begin{bmatrix} 1 \\ -1 \end{bmatrix}.$$

Here A is positive semidefinite, singular. Obviously, every vector of the form $[\alpha + 1, \alpha]^{\mathrm{T}}$ with $\alpha \geqslant 0$ is a solution of $(\boldsymbol{b}, \boldsymbol{A})$. If we apply the modified Gauss–Seidel method with $\boldsymbol{x}^{(0)} = \boldsymbol{0}$ we find the particular solution $\boldsymbol{x} = [1, 0]^{\mathrm{T}}$ in one step, whereas starting from $\boldsymbol{x}^{(0)} = [0, 1]^{\mathrm{T}}$ we find the particular solution $\boldsymbol{x} = [2, 1]^{\mathrm{T}}$. More generally starting from the initial guess $\boldsymbol{x}^{(0)} = [0, \alpha]^{\mathrm{T}}$, $\alpha \geqslant 0$, we converge to the solution $[\alpha + 1, \alpha]^{\mathrm{T}}$ in one step. Hence, the computed solution depends on the initial guess.

Let us consider one more simple example:

$$A = \begin{bmatrix} \frac{1}{2} & -1 \\ -1 & \frac{1}{2} \end{bmatrix} \quad \text{and} \quad b = \begin{bmatrix} \frac{1}{2} \\ -1 \end{bmatrix}.$$

In this case $(\boldsymbol{b}, \boldsymbol{A})$ has the unique solution $\boldsymbol{x} = [1, 0]^{\mathrm{T}}$ and Cryer's method converges to it in one step with the initial choice $\boldsymbol{x}^{(0)} = \boldsymbol{0}$; on the other hand, the initial choice $\boldsymbol{x}^{(0)} = [0, 1]^{\mathrm{T}}$ yields a divergent sequence.

In addition, it is possible to give examples of infeasible problems for which Cryer's method is either divergent or, worse yet, convergent (to a necessarily infeasible point), depending on the choice of $\boldsymbol{x}^{(0)}$. In summary, for general LCPs Cryer's method is liable to exhibit virtually any type of misbehaviour. The fact that the computed solutions and even the convergence depend on the initial guess is very disturbing. If the infeasibility or the presence of multiple solutions do not correspond to a precise physical situation but are due to deficiencies of the model or to errors in the input data, the modified Gauss–Seidel algorithm would not be able to detect the trouble, which can be quite dangerous in practice.

We have provided evidence that using (3) for solving the (generally indefinite) LCPs arising from this particular application cannot possibly result in a robust implementation. Besides these fundamental difficulties, in our opinion Cryer's algorithm (3) is also not a very good choice from the point of view of efficiency. For instance, even if the problem is strictly convex and the conditions for applicability of Cryer's method apply, the number of iterations required for convergence may be very high. This happens, for example, if $\sum_{i=1}^{n} \frac{1}{c_i} \approx 1$, in which case A is nearly singular, and painfully slow convergence was actually observed in computer experiments performed on artificially generated problems. The only advantage of Cryer's method in this context is that it is trivial to implement and requires very little storage, thanks to the particular form of the coefficient matrix. However, these advantages are not sufficient to compensate for the lack of robustness of the algorithm, which in the present context should be the highest priority.

Fortunately, the situation can be greatly improved if the LCPs which arise at each outer iteration are solved by linear programming (LP) techniques rather than by (3). This is a consequence of the fact that the coefficient matrix A is a Z-matrix. We have already recalled that if A is a Z-matrix and $X(\boldsymbol{b}, A) \neq \emptyset$, then $X(\boldsymbol{b}, A)$ has a least element $\boldsymbol{x}$ which solves $(\boldsymbol{b}, A)$. It immediately follows that for every positive vector $\boldsymbol{c}$, this least element is the optimal solution of the linear program

$$\text{minimize} \quad \boldsymbol{c}^{\mathrm{T}}\boldsymbol{x} \quad \text{subject to} \quad A\boldsymbol{x} \geqslant \boldsymbol{b},\ \boldsymbol{x} \geqslant \boldsymbol{0}. \tag{5}$$

In other terms, if the LCP is solvable, it is LP-solvable. For example, one can take $\boldsymbol{c} = \boldsymbol{e}$ (say) and solve the LP problem (5) by any of the established techniques (and software) available, such as the two-phase simplex method, which can be found described in any textbook (e.g. [7]). This approach requires more storage than the one based on Cryer's method, since A must now be explicitly stored. However, standard and easily accessible LP software is able to handle efficiently and reliably a very wide range of problems even of large size. Moreover, it appears from the simulations reported in [1] that the problem size n for this application is usually moderate.

What is more important, the LP approach is guaranteed to compute a solution each time the problem is feasible, and will detect infeasibility whenever this occurs. As we have pointed out, Cryer's method may fail in both situations. The LP approach does not permit to detect the presence of multiple solutions to the LCP problem (1), but it computes the least element $\boldsymbol{x} \in X(\boldsymbol{b}, A)$ and this is unique. This is possible when solving the LCP with one linear program but, in general, not using Cryer's method. We also mention the existence of special algorithms for solving (1) for general A, for instance those developed by Cottle and Dantzig and by Lemke (see [3, 2]), but the point here is that (1) can be solved by the standard simplex method via the formulation (5) because A is a Z-matrix.

In conclusion, we believe that the robustness and reliability, and possibly even the efficiency, of the algorithm proposed by Aitchison and Upton would be substantially increased if the solution of the Linear Complementarity Problem arising at each step of the outer iteration is found by solving the corresponding linear program by well-established computational techniques rather than by Cryer's method.

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