The Sherman-Morrison Formula for the Determinant and its Application for Optimizing Quadratic Functions on Condition Sets Given by Extreme Generators

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Abstract. First a short survey is made of formulas, which deal with either the inverse, or the determinant of perturbed matrices, when a given matrix is modified with a scalar multiple of a dyad or a finite sum of dyads. By applying these formulas, an algorithmic solution will be developed for optimizing general (i. e. nonconcave, nonconvex) quadratic functions on condition sets given by extreme generators. (In other words: the condition set is given by its internal representation.) The main idea of our algorithm is testing copositivity of parametral matrices.

Key words: copositive matrix, determinant calculus, extreme generator, matrix inversion, matrix perturbation, optimization, parametral matrix, quadratic programming.

1. Introduction

If $A(h)$ is a parametral real symmetric matrix, we may be interested to seek the smallest value of h — provided that there is one — for which $v^T A(h) v \geq 0$ holds for all $v \geq 0$. Optimization of quadratic functions may lead to this type of problem, if the condition set is given by its internal representation.

Two special cases of parametral matrices are of special interest to us. The first is

$$A(h) = A + huu^T, \tag{1.1}$$

where A is a constant real symmetric matrix and u is a given vector. In this case $A(h)$ is obtained by adding a dyad to A.

The second case is the generalization of the first one, when the modification of a given matrix with a finite sum of dyads is under consideration. Then we have

$$A(h) = A + h \cdot \sum_{i=1}^{k} u_i u_i^T = A + hUU^T. \tag{1.2}$$

In the present paper some methods will be worked out for the above mentioned problem, where — as it will be seen — the determinant, as

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well as the adjoint of the parametral matrix $A(h)$ will play an important role. This is why our problem has a close connection to methods — known from the literature as the Sherman-Morrison formula or the Sherman-Morrison-Woodbury formula — which deal with the inversion of perturbed matrices of type $A(h) = A + uv^T$ or $A(h) = A + UV^T$. The probably first appearance of an identity of this type was found by Duncan [8] in 1944. Sherman and Morrison published their work [14] in 1949, Woodbury [17] in 1950.

Different formulations of this matrix identity have been cited e. g. by Householder [10] in 1964, by Ortega and Rheinboldt [13] in 1970. A special case of the formula is contained in Bodewig's book [1], 1956. This list of occurrences of the formula is far not complete. A simpler identity of this type is often mentioned in connection with basis changes in linear programming.

We shall deduce formulas not only for the inverse, but also for the determinant of parametral matrices given in the form (1.1) or (1.2). These formulas will be applied; however, for quadratics and not for LP.

Methods developed for testing copositivity of constant matrices will be applied for the determination of the critical value of h. The probably best applicable results towards this direction were achieved by Cottle, Habetler, and Lemke [4] in 1970. For a copositivity test it is enough to deal with determinants and adjoints of different principal submatrices, see Theorems 3.1 and 4.2 (Keller's theorem) in [4]. Later Hadeler [9] and Väliaho [15]-[16] gave some other criteria for the copositivity of quadratic matrices. For our purpose – i.e. for copositivity test of parametral matrices – the test involved in Keller's theorem seems to be the most applicable. As checking copositivity is an NP-hard problem (See e. g. Murty and Kabadi [12]), so it would be a vain hope to reduce the number of steps to polynomial in our algorithms; some kinds of reductions are possible, however.

Standardization of QP and using copositivity for checking global optimality in general QP problems occur e. g. in the papers of Bomze [2], Danninger [6], Bomze and Danninger [3], [7]. The same kind of standardization (without using this word) is also applied in a previous publication of the author of the present paper [11].

2. Definitions, notations, and abbreviations

Let R^r denote the Euclidean r-space, R^r_+ its nonnegative orthant, and C^r the Euclidean complex r-space.

DEFINITION 2.1 *A real symmetric $r \cdot r$ matrix A is copositive (abbreviated CP), if $x^T Ax \geq 0$ holds for every $x \in R^r_+$.*

The abbreviation *NCP* will be used for "noncopositive".

DEFINITION 2.2 *A real symmetric matrix A is copositive of order k (abbreviated kCP), if every $k \cdot k$ principal submatrix of A is CP.*

DEFINITION 2.3 *A real symmetric $r \cdot r$ matrix A is copositive of exact order k, if it is kCP, but not $(k+1)$CP.*

An important special case for *"copositive of exact order k"* comes forward in the following definition.

DEFINITION 2.4 *A real symmetric $r \cdot r$ matrix A is almost copositive if it is $(r-1)$CP, but not CP — provided that $r > 1$. A real symmetric matrix $A = [a]$ of order 1 is almost copositive if $a < 0$.*

The determinant of a quadratic matrix A will be denoted by $|A|$, its adjoint by $\operatorname{adj} A$. The element of the transposed matrix of $\operatorname{adj} A$ with coordinates (i, j) will be denoted by A_{ij}; this is the algebraic complement (otherwise co-factor) belonging to the entry a_{ij} of A. The adjoint of $A = [a]$ is defined the matrix $[1]$, regardless of the value of a.

When 0 or 1 will be used as vectors, that means they contain all zeros, or all ones, respectively, as their components.

We note that the concept of *"copositive matrix"* was first introduced by Motzkin in 1952, while *"almost copositive matrix"* by Väliaho in 1989.

3. The Sherman-Morrison formula and related topics

Throughout this whole section, let A, B denote real or complex $r \cdot r$ matrices, u, v denote r-vectors, U, V denote $r \cdot k$ matrices, $I^{(r)}$ denote the unit matrix of order r, and h denote an arbitrary real or complex number.

The Sherman-Morrison formula applies to inverting the modification of a given matrix with a dyad. If not a single dyad, but a finite sum of dyads (i. e. a matrix-product UV^T) is added to A, then the Sherman-Morrison-Woodbury formula is applicable as a more general matrix equality. Further, it is not very difficult to give similar formulas for determinants rather than inverses, which we shall call "the Sherman-Morrison formula for the determinant", and the "Sherman-Morrison-Woodbury formula for the determinant".

PROPOSITION 3.1 (Sherman-Morrison formula). *If A is invertible and $1 + hv^T A^{-1} u \neq 0$, then*

$$(A + huv^T)^{-1} = A^{-1} - h \cdot \frac{A^{-1} uv^T A^{-1}}{1 + hv^T A^{-1} u}. \tag{3.1}$$

We shall prove a more general formula that will occur in the next statement.

PROPOSITION 3.2 (Sherman-Morrison-Woodbury formula). *If* A *and* $D^{(k)}(h) = I^k + hV^TA^{-1}U$ *are invertible, then*

$$(A + hUV^T)^{-1} = A^{-1} - hA^{-1}U[D^{(k)}(h)]^{-1}V^TA^{-1}. \tag{3.2}$$

Proof.

$$\begin{aligned}(A+hUV^T)\{A^{-1} - hA^{-1}U[D^{(k)}(h)]^{-1}V^TA^{-1}\} = AA^{-1} + hUV^TA^{-1} - \\ -hAA^{-1}U[D^{(k)}(h)]^{-1}V^TA^{-1} - h^2 \cdot UV^TA^{-1}U[D^{(k)}(h)]^{-1}V^TA^{-1} = \\ = I^{(r)} + hUV^TA^{-1} - hU(I^{(k)} + hV^TA^{-1}U)[D^{(k)}(h)]^{-1}V^TA^{-1} = \\ = I^{(r)} + hUV^TA^{-1} - hU[D^{(k)}(h)][D^{(k)}(h)]^{-1}V^TA^{-1} = I^{(r)}.\end{aligned}$$

PROPOSITION 3.3 *For arbitrary square matrices* A *and* B,

$$|A + B| = \sum_{i_1=0}^{1} \sum_{i_2=0}^{1} \cdots \sum_{i_r=0}^{1} |C^{(i_1 i_2 \ldots i_r)}|, \tag{3.3}$$

where the j*-th column of* $C^{(i_1 i_2 \ldots i_r)}$ *is defined by*

$$c_j^{(i_1 i_2 \ldots i_r)} = \begin{cases} a_j, & \text{if } i_j = 0 \\ b_j, & \text{if } i_j = 1 \end{cases} \quad (j = 1, 2, \ldots, r).$$

We omit the proof, which is elementary and is known from the determinant calculus.

PROPOSITION 3.4 *If* $\operatorname{rank} B \le 1$, *then*

$$|A + B| = |A| + \sum_{i=1}^{r} \sum_{j=1}^{r} b_{ij} A_{ij}. \tag{3.4}$$

Proof. Let us consider the matrices $C^{(i_1 i_2 \ldots i_r)}$ introduced in the previous proposition. If $i_1 + i_2 + \cdots + i_r \ge 2$, then $C^{(i_1 i_2 \ldots i_r)}$ contains at least two columns selected from B, and therefore the assumption about the rank of B implies that

$$|C^{(i_1 i_2 \ldots i_r)}| = 0.$$

If $i_j = 1$ and $i_t = 0$ for $t \in \{1, 2, \ldots, r\} \setminus \{j\}$, then

$$|C^{(i_1 i_2 \ldots i_r)}| = |a_1\ a_2\ \ldots\ a_{j-1}\ b_j\ a_{j+1}\ \ldots\ a_r| = \sum_{i=1}^{r} b_{ij} A_{ij}$$

according to the determinant expansion theorem. Now we can write

$$|A+B| = |A| + \sum_{i_1+i_2+\cdots+i_r=1} |C^{(i_1 i_2 \dots i_r)}| = |A| + \sum_{j=1}^{r} \left(\sum_{i=1}^{r} b_{ij} A_{ij} \right).$$

COROLLARY 3.5 (Sherman-Morrison formula for the determinant).

$$|A + huv^T| = |A| + hv^T(\operatorname{adj} A)u. \tag{3.5}$$

Proof. The dyad huv^T is an $r \cdot r$ matrix with rank equal to 1. According to Proposition 3.4, we have

$$|A + huv^T| = |A| + \sum_{i=1}^{r}\sum_{j=1}^{r} hu_i v_j A_{ij} = |A| + hv^T(\operatorname{adj} A)u.$$

COROLLARY 3.6 *If A is invertible, then*

$$|A + huv^T| = |A| \cdot (1 + hv^T A^{-1} u). \tag{3.6}$$

The proof is obvious, if we take into account that $\operatorname{adj} A = |A| \cdot A^{-1}$.

COROLLARY 3.7 *If A and $A + huv^T$ are invertible, then*

$$1 + hv^T A^{-1} u \neq 0.$$

The proof is evident from (3.6).

For the more general case, where the vectors u and v are replaced by the matrices U and V, statements, parallel to Corollaries 3.6–3.7 will also be formulated. Before doing this, we state the following lemma, which will help us to prove the generalization of Corollary 3.6.

LEMMA 3.8 *Let $D = D^{(k)} = [d_{ij}]_{i,j=1,2,\dots,k}$ denote a real or complex $k \cdot k$ matrix, and denote*

$$D^{(t)} = [d_{ij}]_{i,j=1,2,\dots,t}$$

the leading principal submatrices of D. Then we state the following:

$$|D^{(k)}| = d_{kk} \cdot |D^{(k-1)}| - \sum_{i=1}^{k-1}\sum_{j=1}^{k-1} (\operatorname{adj} D^{(k-1)})_{ij} d_{ki} d_{jk}. \tag{3.7}$$

Proof. Expand the determinant $|D^{(k)}|$ according to its last row, and then expand the given smaller determinants — with the exception of $|D^{(k-1)}|$ — according to their last columns. Then we obtain the sum standing on the right hand side of (3.7).

THEOREM 3.9 (Sherman-Morrison-Woodbury formula for the determinant). *If A is invertible, then*

$$|A + hUV^T| = |A| \cdot |D^{(k)}(h)|, \tag{3.8}$$

where

$$D^{(k)}(h) = I^{(k)} + hV^T A^{-1} U. \tag{3.9}$$

Proof. We prove the theorem by induction on k. If $k = 1$, then the assertion reduces to the statement of Corollary 3.6.

Consider the modified matrix $A + hUV^T$ in the form

$$A + h \cdot \sum_{i=1}^{k} u_i v_i^T$$

where u_i and v_i are r-vectors, and assume that the assertion of the theorem is true for $k = 1$, i. e.

$$|A + h \cdot \sum_{i=1}^{k-1} u_i v_i^T| = |A| \cdot |D^{(k-1)}(h)|.$$

We suppose temporarily, that $D^{(k-1)}(h)$ is invertible. Then, according to Corollary 3.6,

$$|A + hUV^T| = |(A + h \cdot \sum_{i=1}^{k-1} u_i v_i^T) + hu_k v_k^T| =$$

$$= |A + h \cdot \sum_{i=1}^{k-1} u_i v_i^T| \cdot \{1 + hv_k^T (A + h \cdot \sum_{i=1}^{k-1} u_i v_i^T)^{-1} u_k\} =$$

$$= |A| \cdot |D^{(k-1)}(h)| \cdot \{1 + hv_k^T (A + h \cdot \sum_{i=1}^{k-1} u_i v_i^T)^{-1} u_k\}.$$

According to Proposition 3.2 we can obtain, that

$$(A + h \cdot \sum_{i=1}^{k-1} u_i v_i^T)^{-1} = A^{-1} - hA^{-1}[U^{(k-1)}][D^{(k-1)}(h)]^{-1}[V^{(k-1)}]^T A^{-1}$$

where

$$U^{(k-1)} = [u_1 \; u_2 \; \ldots \; u_{k-1}]$$

and similarly

$$V^{(k-1)} = [v_1 \; v_2 \; \ldots \; v_{k-1}].$$

Thus

$$hv_k^T(A + h \cdot \sum_{i=1}^{k-1} u_i v_i^T)^{-1} u_k =$$

$$= hv_k^T A^{-1} u_k - h^2 \cdot v_k^T A^{-1} [U^{(k-1)}][D^{(k-1)}(h)]^{-1}[V^{(k-1)}]^T A^{-1} u_k =$$

$$= hv_k^T A^{-1} u_k - \sum_{i=1}^{k-1}\sum_{j=1}^{k-1} (hv_k^T A^{-1} u_i)[D^{(k-1)}(h)]_{ij}^{-1}(hv_j^T A^{-1} u_k) =$$

$$= hv_k^T A^{-1} u_k - \sum_{i=1}^{k-1}\sum_{j=1}^{k-1} d_{ki}(h) \cdot \frac{(\operatorname{adj} D^{(k-1)}(h))_{ij}}{|D^{(k-1)}(h)|} \cdot d_{jk}(h).$$

Now we can write

$$|A + hUV^T| = |A| \cdot |D^{(k-1)}(h)| \cdot \{1 + hv_k^T A^{-1} u_k -$$

$$-\sum_{i=1}^{k-1}\sum_{j=1}^{k-1} \frac{(\operatorname{adj} D^{(k-1)}(h))_{ij}}{|D^{(k-1)}(h)|} \cdot d_{ki}(h) d_{jk}(h)\} =$$

$$= |A| \cdot \{d_{kk}(h) \cdot |D^{(k-1)}(h)| - \sum_{i=1}^{k-1}\sum_{j=1}^{k-1} (\operatorname{adj} D^{(k-1)}(h))_{ij} d_{ki}(h) d_{jk}(h)\}.$$

Finally, by applying Lemma 3.8 for $D^{(k)}(h)$, we obtain that (3.8) is valid, provided that $D^{(k-1)}(h)$ is invertible. As clearly $D^{(k-1)}(0) = I^{(k-1)}$, we can conclude that (3.8) is valid, if h is in a neighbourhood of zero. Since the expression

$$|A + hUV^T| - |A| \cdot |D^{(k)}(h)|$$

is a polynomial, i. e. analytical function of h, thus if it vanishes in a neighbourhood of zero, then it does so for any complex h. By this the proof is complete.

COROLLARY 3.10 *If both A and $A + hUV^T$ are invertible, then $I^{(k)} + hV^T A^{-1} U$ is invertible as well.*

Remark 3.11 The assertions of Proposition 3.2 and Corollary 3.10 can be united in the following way: Suppose that A is invertible. In this case $A + hUV^T$ is invertible if and only if $I^{(k)} + hV^T A^{-1} U$ is invertible, and then

$$(A + hUV^T)^{-1} = A^{-1} - hA^{-1} U (I^{(k)} + hV^T A^{-1} U)^{-1} V^T A^{-1}.$$

The Sherman-Morrison-Woodbury formula is cited in this form in [13], where $k \leq r$ is assumed. As we have seen, the restriction $k \leq r$ is not necessary to suppose.

4. Domain of copositivity of a parametral matrix

For the discussion of this section $A(h)$ will denote a real parametral $r \cdot r$ matrix, having the properties, we specify in the following definition.

DEFINITION 4.1 *A real parametral $r \cdot r$ matrix is proper parametral matrix, if it has the following features:*

(i) *$A(h)$ is symmetric for every real h.*

(ii) *$A(h)$ is a continuous function of h.*

(iii) *For any principal submatrix $B(h)$ of $A(h)$ it is true that if $B(h_1)$ is CP and $h_2 > h_1$, then $B(h_2)$ is also CP.*

(iv) *There exists some $h \in R$ such that $A(h)$ is NCP.*

The next statement contains examples for proper parametral matrices.

PROPOSITION 4.2 *If A is a real symmetric $r \cdot r$ matrix and U is a real nonzero $r \cdot k$ matrix, then $A(h) = A + hUU^T$ is a proper parametral matrix. As a special case, for a nonzero r-vector u, $A(h) = A + huu^T$ is a proper parametral matrix.*

Proof. The validity of (i) and (ii) is obvious. If $h_2 > h_1$, then $(h_2 - h_1)UU^T$ is positive semidefinite, therefore its principal submatrices are all *CP*. The sum of two *CP* matrices is also *CP*. This way, feature (iii) is established.

For the proof of feature (iv) it is enough to show that h may assume such values, for which $A(h)$ has a negative entry in its main diagonal. Indeed, let $\overline{u}_i$ be a nonzero row vector of U, then $a_{ii}(h) = a_{ii} + h\overline{u}_i\overline{u}_i^T < 0$ holds for any such h for which $h < -\frac{a_{ii}}{\overline{u}_i\overline{u}_i^T}$.

DEFINITION 4.3 *The domain of copositivity of a proper parametral matrix $A(h)$ is the set*

$$G = \{\, h : \ A(h) \text{ is } CP \,\}. \tag{4.1}$$

DEFINITION 4.4 *The threshold number of copositivity (briefly threshold) of a proper parametral matrix $A(h)$ is the number*

$$h^* = \inf G = \inf\{\, h : \ A(h) \text{ is } CP \,\}. \tag{4.2}$$

Remark 4.5 Because of the assumption involved in feature (iv) of Definition 4.1, only the following two possibilities may occur:

a) G is empty, and then $h^* = +\infty$;

b) G is a nonempty closed convex set, and then h^* is finite. Further, in this case $G = [h^*, +\infty)$.

5. Connection between quadratic optimization and copositivity of parametral matrices

Let us consider the following optimization problem:

$$\begin{aligned} &\text{minimize } f(x) = x^T Dx + 2g^T x \\ &\text{subject to } x \in K = \{Qy + Sz : y \geq 0, z \geq 0, 1^T z = 1\}, \end{aligned} \tag{5.1}$$

where D is a given real symmetric $n \cdot n$ matrix, g is a given n-vector, Q is a given $n \cdot r_1$ matrix, S is a given $n \cdot r_2$ matrix ($r_1 \geq 0$ and $r_2 \geq 1$).

On the matrix D, which determines the type of the objective function, there are no further conditions. That means that the objective function $f(x)$ can be nonconvex and also nonconcave.

The matrices Q and S contain the column vectors q_i and s_i respectively.

Now let us apply the following notations:

$$A = \begin{bmatrix} Q^T & 0 \\ S^T & 1 \end{bmatrix} \begin{bmatrix} D & g \\ g^T & 0 \end{bmatrix} \begin{bmatrix} Q & S \\ 0^T & 1^T \end{bmatrix} =$$

$$= \begin{bmatrix} Q^T DQ & Q^T DS + Q^T g 1^T \\ S^T DQ + 1 g^T Q & S^T DS + 1 g^T S + S^T g 1^T \end{bmatrix} \tag{5.2}$$

and

$$A(h) = \begin{bmatrix} Q^T & 0 \\ S^T & 1 \end{bmatrix} \begin{bmatrix} D & g \\ g^T & h \end{bmatrix} \begin{bmatrix} Q & S \\ 0^T & 1^T \end{bmatrix}. \tag{5.3}$$

Here A is a real symmetric $r \cdot r$ matrix with $r = r_1 + r_2$. Denoting by I the set, whose elements are the last r_2 row indices of matrix A, i. e.

$$I = \{r_1 + 1, r_1 + 2, \ldots, r_1 + r_2\}, \tag{5.4}$$

then the entries of the parametral matrix $A(h)$ are the following:

$$a_{ij}(h) = \begin{cases} a_{ij} & \text{if } i \notin I \text{ or } j \notin I \\ a_{ij} + h & \text{if } i \in I \text{ and } j \in I. \end{cases} \tag{5.5}$$

According to Proposition 4.2, $A(h)$ is a proper parametral matrix. With the newly introduced notations the objective function increased by the additive constant h can be written as follows:

$$f(x)+h=\begin{bmatrix} x^T & 1\end{bmatrix}\begin{bmatrix} D & g\\ g^T & h\end{bmatrix}\begin{bmatrix} x\\ 1\end{bmatrix}=$$

$$=\begin{bmatrix} y^TQ^T+z^TS^T & 1\end{bmatrix}\begin{bmatrix} D & g\\ g^T & h\end{bmatrix}\begin{bmatrix} Qy+Sz\\ 1\end{bmatrix}=$$

$$=\begin{bmatrix} y^T & z^T\end{bmatrix}\begin{bmatrix} Q^T & 0\\ S^T & 1\end{bmatrix}\begin{bmatrix} D & g\\ g^T & h\end{bmatrix}\begin{bmatrix} Q & S\\ 0^T & 1^T\end{bmatrix}\begin{bmatrix} y\\ z\end{bmatrix}= \tag{5.6}$$

$$=\begin{bmatrix} y^T & z^T\end{bmatrix}A(h)\begin{bmatrix} y\\ z\end{bmatrix}=v^TA(h)v.$$

At the last phase of the transformation we applied the notation

$$v=\begin{bmatrix} y\\ z\end{bmatrix}. \tag{5.7}$$

On the basis of equality (5.6) an interesting relationship between the optimum value of problem (5.1) and the domain of copositivity of $A(h)$ can be recognized. Namely, if h^* is the smallest value, for which $f(x)+h^*\geq 0$ for every $x\in K$, i. e. the optimum value of (5.1) is $-h^*$, then according to (5.6), h^* is also the smallest value for which the matrix $A(h^*)$ is copositive, i. e. the threshold of $A(h)$ is h^*.

Our last observation will be precisely described in the following two statements, which include also the case of the unbounded objective function:

PROPOSITION 5.1 *For the parametral matrix $A(h)$ specified at (5.3), its threshold is finite if and only if the function $f(x)$ is bounded from below on K.*

PROPOSITION 5.2 *If for the parametral matrix $A(h)$ specified at (5.3), its threshold is finite and equals h^*, then the optimum value of problem (5.1) is $-h^*$.*

On the basis of the observations made so far we can go even further and derive a conclusion for the optimal solutions of (5.1). Namely, a certain vector $x^*\in K$ is an optimal solution to problem (5.1) if and only if $f(x^*)+h^*=0$, i. e. for the corresponding v^* the equation $v^{*T}A(h^*)v^*=0$ holds. So the following statement is also true.

PROPOSITION 5.3 *If for the parametral matrix $A(h)$ specified at (5.3), its threshold is finite and equals h^*, moreover for a certain vector $v^* = \begin{bmatrix} y^* \\ z^* \end{bmatrix}$ conditions*

$$\begin{aligned} & v^* \in R_+^r, \\ & \sum_{i \in I} v_i^* = 1, \\ & v^{*T} A(h^*) v^* = 0 \end{aligned} \tag{5.8}$$

hold, then the vector

$$x^* = Qy^* + Sz^* \tag{5.9}$$

is an optimal solution of problem (5.1). Conversely, if the vector produced in the form of (5.9) is an optimal solution of (5.1), then (5.8) holds for $v^* = \begin{bmatrix} y^* \\ z^* \end{bmatrix}$.

From the above statements it follows that the quadratic programming problem (5.1) is equivalent to solving the following *derived problem* — a) and b) — for a proper parametral matrix.

a) *Determine the h^* threshold of $A(h)$. (More accurately: first decide whether it is finite or not. If it is finite, then compute its value.)*

b) *In the case when h^* is finite, find a vector v^* satisfying conditions (5.8).*

Remark 5.4 It can never occur that $h^* = -\infty$, because $A(-a_{ii} - 1)$ is NCP for any $i \in I$ (cf. Proposition 6.6).

On the contrary, $h^* = +\infty$ can occur, and according to Proposition 5.1 it does occur in every case when $f(x)$ is unbounded from below on set K. Now let us consider the following example:

$$\min\{x_1^2 - 2x_2 : x_1 \geq 0, x_2 \geq 0\}.$$

The application of (5.3) for this special case gives the matrix

$$A(h) = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 0 & -1 \\ 0 & -1 & h \end{bmatrix}.$$

This matrix cannot be *CP* for any real h, because in the case of non-positive h, taking the vector $v^T = \begin{bmatrix} 0 & 1 & 1 \end{bmatrix}$, and substituting it into the quadratic form with $A(h)$ results in

$$v^T A(h) v = -2 + h < 0,$$

while in the case of a positive h, taking $v^T = \left[\, 0 \;\; h \;\; 1 \,\right]$, we obtain that

$$v^T A(h) v = -h < 0.$$

Remark 5.5 If h^* is finite, then $A(h^*)$ is CP (cf. Proposition 6.4).

6. Algorithms for proper parametral matrices

Our next purpose is to develop algorithmic procedures for finding the threshold number h^* of a proper parametral matrix. In view of the definition of almost copositive matrices, h^* is the smallest such value, for which none of the principal submatrices of $A(h)$ is almost copositive. This fact suggests the following scheme as an algorithm skeleton (Algorithm I.).

Denote by $B_1(h), B_2(h), \ldots, B_N(h)$ the principal submatrices of $A(h)$ in a nondecreasing order of their size; i. e. the first r such submatrices $B_1(h), B_2(h), \ldots, B_r(h)$ are of order 1, while the last such submatrix $B_N(h)$ is identical to $A(h)$. The sequential order of submatrices of same algebraic order is optional.

Algorithm I.

Initialization:

A1) Let $t = 1$.

A2) Let h_0 be any real value for which $A(h_0)$ is NCP.

Main cycle of the algorithm: While $t \le N$, perform steps B1-B4.

B1) If $B_t(h_{t-1})$ is not almost copositive, then let $h_t = h_{t-1}$ and go to B4, else continue at B2.

B2) If the set $\{\, h : B_t(h)$ is not almost copositive, $h > h_{t-1} \,\}$ is empty, then stop. (In this case h^* is unbounded.)

B3) Let $h_t = \inf \{\, h : B_t(h)$ is not almost copositive, $h > h_{t-1} \,\}$.

B4) Let $t = t + 1$.

Normal termination

C1) Let $h^* = h_N$.

C2) Stop.

This formulation of the algorithm does not contain a copositivity test. It will be built into the algorithm after the proof of this simpler algorithm version, which can be done with the help of the following definition and lemma.

DEFINITION 6.1 *Let A denote a real symmetric $r \cdot r$ matrix, and $\beta = (B_1, B_2, \ldots, B_N)$ denote the ordered set of all principal submatrices of A in a nondecreasing order of their size. Then A is defined to be β-copositive of order t, if all of $B_1, B_2, \ldots, B_t$ are CP.*

Clearly, A is $1CP$ if and only if A is β-copositive of order r, A is $2CP$ if and only if A is β-copositive of order $r + \binom{r}{2}$, etc.

LEMMA 6.2 *If $A(h)$ is a proper parametral $r \cdot r$ matrix, h_1 is a real number such that $A(h_1)$ is β-copositive of order $t-1$, but not of order t, where $1 \leq t \leq N$, and*

$$h_2 = \inf \{ h : B_t(h) \textit{ is not almost copositive, } h > h_1 \}$$

is finite, then $A(h_2)$ is β-copositive of order t.

Proof. The copositivity of $B_1(h_2), B_2(h_2), \ldots, B_{t-1}(h_2)$ follows from feature (iii) of proper parametral matrices (Definition 4.1), while the copositivity of $B_t(h_2)$ follows from the definition of h_2.

Proof of Algorithm I. If the set, appearing at Step B2 is empty, then clearly $A(h)$ is NCP for any real h. Now let us suppose, that the algorithm ends with a normal termination. Then $B_1(h_1)$ is CP according to the definition of h_1 given in step B3 of the algorithm. Applying the assertion of Lemma 6.2, it follows by induction, that $A(h_t)$ is β-copositive of order t if $t \in \{1, 2, \ldots, N\}$. For $t = N$ this means that $A(h_N)$ is CP. Because $A(h_0)$ is NCP, there should be a $t \in \{1, 2, \ldots, N\}$, for which

$$h_{t-1} < h_t = h_N.$$

Then $B_t(h)$ is NCP for any $h < h_N$, and consequently so is $A(h)$. We have seen; however, that $A(h_N)$ is CP, thus h_N is equal to the threshold number of copositivity h^* of $A(h)$.

It is not very nice in the description of Algorithm I, that it contains certain clumsy details such as

- to determine if a submatrix is almost copositive or not;
- to find the smallest value of the parameter h, for which a given submatrix is not almost copositive.

Now we are going to make these details clearer. For this purpose, the first — and probably the most important — tool is the following theorem.

THEOREM 6.3 (Cottle-Habetler-Lemke's theorem). *Suppose that a real symmetric $r \cdot r$ matrix A is $(r-1)CP$. In this case A is NCP if and only if the following two conditions hold:*
(i) $|A| < 0$;
(ii) $\operatorname{adj} A \geq 0$.

For the proof of this theorem see [4], Theorem 3.1.

Next some properties of CP and almost copositive matrices as well as statements on the adjoint of real quadratic matrices will be listed. All of these can be proved very simply, in an elementary way, so their proofs will be omitted.

PROPOSITION 6.4 *The set of all CP matrices of order r is a closed convex cone.*

PROPOSITION 6.5 *Adding a nonnegative matrix to a CP matrix results in another CP matrix.*

PROPOSITION 6.6 *Every principal submatrix of a CP matrix is also CP. (As a special case, the elements of its main diagonal are nonnegative.)*

PROPOSITION 6.7 *An almost copositive matrix has at least one negative entry in each of its rows.*

PROPOSITION 6.8 *If a symmetrical row-column permutation is performed for a CP (or almost copositive) matrix, the result is also a CP (or almost copositive) matrix.*

PROPOSITION 6.9 *The product of a singular matrix and its adjoint always yields the zero matrix.*

PROPOSITION 6.10 *The rank of the adjoint of a singular matrix cannot be greater than 1. In other words, if A is a singular matrix, then all columns of* $\operatorname{adj} A$ *are proportional to each other.*

Now we are going to reformulate our general algorithm and build a copositivity test into it. Before doing that, we state two more lemmas.

LEMMA 6.11 *If $A(h)$ is a proper parametral matrix, then*

$$H = \{h : A(h) \text{ is almost copositive}\} \tag{6.1}$$

is convex (i. e. it is either finite or infinite interval).

Proof. Let us consider the sets

$$H_1 = \{h : A(h) \text{ is } (r-1)CP\} \tag{6.2}$$

and

$$H_2 = \{h : A(h) \text{ is } CP\}. \tag{6.3}$$

By the definition of almost copositive matrices,

$$H = H_1 \setminus H_2. \tag{6.4}$$

Obviously H_1 and H_2 are intervals on the real axis, both of them being infinite from right. From this it follows that H is also an interval.

LEMMA 6.12 *Let us suppose that for a proper parametral matrix $A(h)$, the set specified in (6.1) as set H is not empty, and $h_0 = \sup H$ has a finite value. Then $A(h_0)$ has the following two features:*

$$|A(h_0)| = 0,$$

$$\operatorname{adj} A(h_0) \geq 0. \tag{6.5}$$

Proof. Denote by h_1 an arbitrary element of H. According to Lemma 6.11, $A(h)$ is almost copositive for $h \in [h_1, h_0)$; therefore, according to Theorem 6.3, $|A(h)| < 0$ and $\operatorname{adj} A(h) \geq 0$ are also satisfied if $h \in [h_1, h_0)$. From this it follows by continuity that the second line of (6.5) is true and

$$|A(h_0)| \leq 0. \tag{6.6}$$

If $h > h_0$, then $A(h)$ is obviously $(r-1)CP$, but not almost copositive, so it must be CP. Then $A(h_0)$ is also CP, and therefore $|A(h_0)| < 0$ is not possible, according to Theorem 6.3, i. e. the first line of (6.5) holds as well.

By the help of Theorem 6.3 and Lemma 6.12 we can adjust the general Algorithm I into the following form (where a copositivity test is already built into the algorithm):

Algorithm I'.

Initialization:

A1) Let $t = 1$.

A2) Let h_0 *be any real value for which* $A(h_0)$ *is NCP.*

Main cycle of the algorithm: While $t \le N$, *perform steps B1-B4.*

B1) If $|B_t(h_{t-1})| \ge 0$ *or* $\operatorname{adj} B_t(h_{t-1})$ *has a negative entry, then let* $h_t = h_{t-1}$ *and go to B4, else continue at B2.*

B2) If the set $\{h : |B_t(h)| = 0, h > h_{t-1}\}$ *is empty, then stop. (In this case* h^* *is unbounded.)*

B3) Let $h_t = \min\{h : |B_t(h)| = 0, h > h_{t-1}\}$.

B4) Let $t = t + 1$.

Normal termination

C1) Let $h^* = h_N$.

C2) Stop.

In the next part of this section we turn our attention to two special cases, when $A(h) = A + hUU^T$ or $A(h) = A + huu^T$. In the first, more general case let V_t denote the submatrix of U consisting of all such row vectors of U, which correspond to a given submatrix B_t of A. With this notation

$$B_t(h) = B_t + hV_tV_t^T, \tag{6.7}$$

and Steps B2-B3 of Algorithm I' require the solution of the equation

$$|B_t + hV_tV_t^T| = 0. \tag{6.8}$$

This is an algebraic equation of order not greater than the rank of V_t. If B_t is invertible, then — according to Theorem 3.9 — (6.8) is equivalent to

$$|I + hV_t^T B_t^{-1} V_t| = 0, \tag{6.9}$$

i. e. (6.8) leads to seek the eigenvalues of $V_t^T B_t^{-1} V_t$. We shall prove the following assertion:

THEOREM 6.13 *Suppose, that* A *is a real symmetric* $r \cdot r$ *matrix,* U *is a real* $r \cdot k$ *matrix, and let* $A(h) = A + hUU^T$. *Further, suppose, that* $A(\hat{h})$ *is almost copositive for some* $\hat{h} \in R$. *Denote by* H *the set*

$$H = \{h : |A(h)| = 0, h > \hat{h}\}, \tag{6.10}$$

and by E *the spectrum of* $U^T[A(\hat{h})]^{-1}U$, *i. e.*

$$E = \{\lambda : |U^T[A(\hat{h})]^{-1}U - \lambda I^{(k)}| = 0\}. \tag{6.11}$$

Then we state the following:

$\inf H$ *is finite if and only if there exists a* $\lambda \in E$ *such that* $\lambda < 0$, *and then*

$$\inf H = \min\{\hat{h} - \frac{1}{\lambda} : \lambda \in E, \lambda < 0\}. \tag{6.12}$$

Proof will be given by referring to the following lemma.

LEMMA 6.14 *With the assumption of Theorem 6.13, we state that* $|A(h)| = 0$ *if and only if* $h \neq \hat{h}$ *and* $\frac{1}{\hat{h}-h} \in E$.

Proof. The almost copositive matrix $A(\hat{h})$ is invertible according to Theorem 6.3. Therefore Theorem 3.9 can be applied in the following way:

$$|A(h)| = |A + hUU^T| = |A(\hat{h}) + (h - \hat{h})UU^T| =$$

$$= |A(\hat{h})||I^{(k)} + (h - \hat{h})U^T[A(\hat{h})]^{-1}U|.$$

From this it follows that $|A(h)| = 0$ if and only if $h \neq \hat{h}$, and

$$\left|U^T[A(\hat{h})]^{-1}U - \frac{1}{\hat{h} - h}I^{(k)}\right| = 0.$$

Proof of Theorem 6.13

The value of $\inf H$ is finite if and only if H is nonempty. According to Lemma 6.14, H is nonempty if and only if $\frac{1}{\hat{h}-h} \in E$ for some $h > \hat{h}$, i. e. if E contains one or more negative elements. The roots of equation $|A(h)| = 0$ are the elements of the set

$$\left\{h : \frac{1}{\hat{h} - h} = \lambda, \lambda \in E\right\} = \left\{\hat{h} - \frac{1}{\lambda} : \lambda \in E\right\}$$

from which follows the validity of (6.12).

Now we are ready to concretize Algorithm I' for the special case where $A(h) = A + hUU^T$.

Algorithm II.

Replace steps B2)-B3) in Algorithm I' by the following:

B2) Let E_t *denote the spectrum of* $V_t^T[B_t(h_{t-1})]^{-1}V_t$. *If* E_t *contains only nonnegative elements, then stop. (In this case* h^* *is unbounded.)*

B3) Let $h_t = h_{t-1} - \frac{1}{\min\{\lambda:\lambda\in E_t,\lambda<0\}}$.

(All other steps are the same as in Algorithm I'.)

Now let us consider the simpler special case where $A(h) = A + huu^T$. In this case $|A(h)| = 0$ is a linear equation, the solution of which can be given explicitly by the help of Corollary 3.5. Moreover, in this case the set E introduced in (6.11) has a single element, namely

$$E = \{u^T[A(\hat{h})]^{-1}u\} = \left\{\frac{u^T \operatorname{adj} A(\hat{h})u}{|A(\hat{h})|}\right\}. \tag{6.13}$$

These observations make it possible, that Steps B2 and B3 of the algorithm become much simpler. We shall choose, however, a different approach, and apply the following assertion.

LEMMA 6.15 *Consider the proper parametral matrix* $A(h) = A + huu^T$, *and suppose that* $A(\hat{h})$ *is almost copositive for some* $\hat{h} \in R$. *Then we state the following:*

a) $|A(h)| = 0$ *if and only if*

$$u^T \operatorname{adj} A(\hat{h})u \neq 0 \tag{6.14}$$

and

$$h = \hat{h} - \frac{|A(\hat{h})|}{u^T \operatorname{adj} A(\hat{h})u}. \tag{6.15}$$

b) Let $\overline{h}$ *be an arbitrary real number. Then* $|A(h)| = 0$ *if and only if*

$$|A(\overline{h}+1)| - |A(\overline{h})| \neq 0 \tag{6.16}$$

and

$$h = \hat{h} - \frac{|A(\hat{h})|}{|A(\overline{h}+1)| - |A(\overline{h})|}. \tag{6.17}$$

c) For the solution of $|A(h)| = 0$, $h > \hat{h}$ *if and only if*

$$|A(\overline{h}+1)| - |A(\overline{h})| > 0. \tag{6.18}$$

d) If (6.18) holds, then denoting by h^* *the value obtained according to the right hand side expression of (6.15), and by* v^* *an arbitrary nonzero column vector of* adj $A(h^*)$, *the following are true:*

$$A(h^*)v^* = 0, v^* \geq 0, \text{ and } u^T v^* \neq 0.$$

Proof. By applying Corollary 3.5 we get

$$|A(h)| = |A(\hat{h})| + (h - \hat{h})u^T \operatorname{adj} A(\hat{h})u \tag{6.19}$$

where

$$|A(\hat{h})| < 0 \tag{6.20}$$

according to Theorem 6.3. This implies assertion a).

From (6.19) it follows that

$$|A(\overline{h}+1)| - |A(\overline{h})| = u^T \mathrm{adj}\, A(\hat{h})u \tag{6.21}$$

which validates assertion b). Assertion c) follows from (6.17) and (6.20). To prove assertion d), using the matrix identity

$$A\mathrm{adj}\, A = |A| \cdot I,$$

and applying Lemma 6.12, one can take the conclusion that $A(h^*)v^* = 0$ and $v^* \geq 0$. Clearly, (6.21) remains true when we substitute $\hat{h}$ by an arbitrary real number. Thus

$$u^T \mathrm{adj}\, A(h^*)\ u = |A(\overline{h}+1)| - |A(\overline{h})| > 0.$$

From this it follows that $u^T \mathrm{adj}\, A(h^*) \neq 0$. Because the rank of the adjoint of a singular matrix cannot be greater than 1, $u^T v^* = 0$ would imply that $u^T \mathrm{adj}\, A(h^*) = 0$. As this is not the case, consequently $u^T v^* \neq 0$ is true.

Finally we remark that the difference of two determinants standing on the left of (6.21) is generally easier to handle than a quadratic form like the expression of the right hand side of (6.21).

The assertions stated in Lemma 6.15 can be used for the adaptation of Algorithm I' to the case $A(h) = A + huu^T$:

Algorithm III.

Replace steps B2)-B3) in Algorithm I' by the following:

B2) If $|B_t(h_{t-1}+1)| - |B_t(h_{t-1})| \leq 0$, *then stop. (In this case* h^* *is unbounded.)*

B3) Let

$$h_t = h_{t-1} - \frac{|B_t(h_{t-1})|}{|B_t(h_{t-1}+1)| - |B_t(h_{t-1})|}\ .$$

(All other steps are the same as in Algorithm I'.)

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