Detailed description

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Problem description

The subject of investigation are *copositive forms*, i.e., real symmetric matrices A such that $x^T Ax \geq 0$ for every vector x with nonnegative entries. The set of copositive matrices of size $n \times n$ forms a closed convex cone $\mathcal{C}^n$ in the space of all real symmetric matrices of size $n \times n$. The goal is to determine the *extreme rays* of $\mathcal{C}^n$. A copositive matrix A lies on an extreme ray if it cannot be decomposed as a sum $A = B + C$ of two other, linearly independent, copositive matrices. The extreme rays of $\mathcal{C}^n$ are known for $n \leq 5$. Here we consider the case $n = 6$.

A real symmetric matrix P such that $x^T Px \geq 0$ for all vectors x is called *positive semi-definite*. The set of $n \times n$ positive semi-definite matrices forms also a closed convex cone $\mathcal{S}_+^n$. A real symmetric matrix N is called *nonnegative* if all its entries are nonnegative numbers. The set of $n \times n$ nonnegative matrices forms a closed convex cone $\mathcal{N}^n$. Clearly every positive semi-definite and every nonnegative matrix are also copositive. This means that the inclusion $\mathcal{S}_+^n + \mathcal{N}^n \subset \mathcal{C}^n$ holds for all n. Diananda has found [3] that this inclusion is an equality for $n \leq 4$, and Prof. Alfred Horn has constructed a copositive matrix in $\mathcal{C}^5$ which is not in $\mathcal{S}_+^5 + \mathcal{N}^5$, the *Horn form*

$$H = \begin{pmatrix} 1 & -1 & 1 & 1 & -1 \\ -1 & 1 & -1 & 1 & 1 \\ 1 & -1 & 1 & -1 & 1 \\ 1 & 1 & -1 & 1 & -1 \\ -1 & 1 & 1 & -1 & 1 \end{pmatrix}.$$

Thus the inclusion is strict for $n \geq 5$.

The extreme rays of $\mathcal{C}^n$ which are in $\mathcal{S}_+^n + \mathcal{N}^n$ have been described by Hall and Newman [6]. We shall hence concentrate on the *exceptional* matrices in $\mathcal{C}^6$, i.e., those which lie on an extreme ray and which are not in $\mathcal{S}_+^6 + \mathcal{N}^6$. We also assume that the diagonal elements of such a matrix are positive, as otherwise it is effectively a copositive form on a space of lower dimension.

The approach proposed here to study copositive matrices $A \in \mathcal{C}^n$ is based on a consideration of those nonnegative vectors x which satisfy $x^T Ax = 0$. A nonzero such vector x is called a *zero* of A. The set of indices $i \in \{1, \dots, n\}$ such that the i-th entry x_i of x is *positive* is called the *support* of the zero x and is denoted by $\operatorname{supp} x$. A zero x of A is called *minimal* if there exists no zero y of A such that $\operatorname{supp} y \subset \operatorname{supp} x$ strictly. For example, the Horn form has zeros with supports

$$\{1,2\}, \{2,3\}, \{3,4\}, \{4,5\}, \{1,5\}, \{1,2,3\}, \{2,3,4\}, \{3,4,5\}, \{1,4,5\}, \{1,2,5\}.$$

Of these, only the supports consisting of two indices correspond to minimal zeros. We shall call the set of all supports of minimal zeros of A the *minimal zero support set*. The minimal zero support set of an exceptional copositive matrix is subject to restrictions [9]. For $n = 6$, these restrictions lead to 44 possible different equivalence classes of minimal zero support sets[1]. Here two such sets are considered to be equivalent if there exists a permutation of the indices $1, \dots, 6$ which induces a map taking one set to the other. In the table on the site, one representative of each equivalence class is listed.

Solution strategy

We shall describe here how copositive matrices with a given minimal zero support set can be analyzed.

[1] In an earlier version, the number of equivalence classes was 80 (see `http://arxiv.org/abs/1401.0134`). We have adapted the table of equivalence classes to comply with the table in the published version [9].

Restrictions on the elements of A

By the transformation $A \mapsto DAD$, where D is a diagonal matrix with positive diagonal elements, the diagonal elements of A can be normalized to 1. We shall hence assume that $A_{ii} = 1$ for $i = 1, \dots, 6$. There are 15 off-diagonal elements A_{ij}, $1 \le i < j \le 6$, to determine. By a result of Hall and Newman [6], we may assume that $A_{ij} \in [-1, 1]$ for all i, j.

The analysis proceeds using equality and inequality relations generated by the minimal zeros corresponding to the given supports. If u is a zero of A, then the matrix-vector product Au has nonnegative entries. Moreover, since $u^T Au = 0$ is a scalar product of two nonnegative vectors, the i-th entry of Au is zero whenever $u_i > 0$, and vice versa.

There are minimal zeros with supports consisting of 2,3, and 4 indices. We shall now consider the restrictions imposed by these zeros.

Zeros with two positive elements: Suppose A has a minimal zero u with support $\{i, j\}$. We thus have $u_i > 0$, $u_j > 0$, and $u_k = 0$ for $k \ne i, j$. Since $A_{ii} = A_{jj} = 1$ and $A_{ii}u_i^2 + 2A_{ij}u_iu_j + A_{jj}u_j^2 = 0$, we obtain that $u_i = u_j$ and $A_{ij} = -1$. Thus each minimal zero with two positive entries determines one off-diagonal element of A. Moreover, if $A_{ij} = A_{jk} = -1$ are determined in such a way, then $A_{ik} = 1$. This follows from the condition $v^T Av \ge 0$, where v is a vector defined by $v_i = v_k = 1$, $v_j = 2$, and $v_l = 0$ for $l \ne i, j, k$. Therefore, if several minimal zeros with two positive elements are present, additional off-diagonal elements may be determined. If all elements of A are determined this way, it can be told by the criteria of Haynsworth and Hoffman [7] whether A is copositive or extremal, see also [2].

Zeros with three positive elements: Suppose A has a minimal zero u with support $\{i, j, k\}$. Then there exist angles $\varphi_{ij}, \varphi_{ik}, \varphi_{jk} > 0$ such that $\varphi_{ij} + \varphi_{ik} + \varphi_{jk} = \pi$, $A_{ij} = -\cos\varphi_{ij}$, $A_{ik} = -\cos\varphi_{ik}$, $A_{jk} = -\cos\varphi_{jk}$, and the zero u can be normalized such that $u_i = \sin\varphi_{jk}$, $u_j = \sin\varphi_{ik}$, $u_k = \sin\varphi_{ij}$. A derivation of this condition can be found in [5], which is also available at `http://www.optimization-online.org/DB_HTML/2012/03/3383.html`.

Zeros with four positive elements: Suppose A has a minimal zero u with support $\{i, j, k, l\}$. Then the determinant of the submatrix

$$\begin{pmatrix} 1 & A_{ij} & A_{ik} & A_{il} \\ A_{ij} & 1 & A_{jk} & A_{jl} \\ A_{ik} & A_{jk} & 1 & A_{kl} \\ A_{il} & A_{jl} & A_{kl} & 1 \end{pmatrix}$$

vanishes, it has a kernel vector whose entries are all positive, and every proper principal submatrix of this submatrix is positive definite. The last condition can be rewritten as follows. If we set $A_{ij} = -\cos\varphi_{ij}, \dots, A_{kl} = -\cos\varphi_{kl}$, then the angles $\varphi_{ij}, \dots, \varphi_{kl}$ are contained in the open interval $(0, \pi)$ and satisfy the inequalities $\varphi_{ij} + \varphi_{ik} + \varphi_{jk} > \pi$, $\varphi_{ij} - \varphi_{ik} - \varphi_{jk} > -\pi$ and all similar inequalities which can be obtained by permuting the indices i, j, k or substituting another triple of indices chosen of the set $\{i, j, k, l\}$.

T-matrices: The conditions imposed by the presence of minimal zeros with supports consisting of 2 or 3 elements may lead to the presence of a principal submatrix of order 5 which can be brought by a permutation of rows and columns to the form

$$T(\phi) = \begin{pmatrix} 1 & -\cos\phi_4 & \cos(\phi_4+\phi_5) & \cos(\phi_2+\phi_3) & -\cos\phi_3 \\ -\cos\phi_4 & 1 & -\cos\phi_5 & \cos(\phi_1+\phi_5) & \cos(\phi_3+\phi_4) \\ \cos(\phi_4+\phi_5) & -\cos\phi_5 & 1 & -\cos\phi_1 & \cos(\phi_1+\phi_2) \\ \cos(\phi_2+\phi_3) & \cos(\phi_1+\phi_5) & -\cos\phi_1 & 1 & -\cos\phi_2 \\ -\cos\phi_3 & \cos(\phi_3+\phi_4) & \cos(\phi_1+\phi_2) & -\cos\phi_2 & 1 \end{pmatrix}$$

with $\phi_k \in [0, \pi]$. Copositivity of the submatrix is equivalent to the condition $\sum_{k=1}^5 \phi_k \le \pi$ [8, 5]. If $\sum_{k=1}^5 \phi_k = \pi$, then $T(\phi)$ is positive semi-definite and hence A cannot be exceptional [5]. Thus we obtain the restriction $\sum_{k=1}^5 \phi_k < \pi$.

Suppose there exist indices i, j such that there is no minimal zero u with $u_iu_j > 0$. Then there must exist a zero u with support consisting of either two or three indices such that $u_i + u_j > 0$, and both the i-th and the j-th entry of Au is zero. For a derivation see [5].

Checking copositivity

Once the values of the off-diagonal elements A_{ij} have been found, possibly containing some free parameters, it must be checked whether the corresponding matrices A are indeed copositive. In principle, this can be accomplished by checking whether there exists a principal submatrix of A which has a single negative eigenvalue such that the corresponding eigenvector has only positive elements. Copositivity of a matrix is equivalent to the absence of such a principal submatrix. However, in practice this approach may not always be easy to implement.

Hoffman and Pereira [10] have established that for a matrix A with unit diagonal elements, it is sufficient to check only those principal submatrices which do not contain off-diagonal entries equal to 1.

Convexity of the cone $\mathcal{C}^n$ can also be employed. If A can be represented as a sum of matrices which are known to be copositive, then A is also copositive.

If a principal submatrix is copositive, and A is obtained from this submatrix by repeating a row and the corresponding column, then A is also copositive.

Checking extremality

Given a copositive matrix A, it can be determined whether it is extremal by computing the *face* of A in the cone $\mathcal{C}^n$. The face of A is the intersection of $\mathcal{C}^n$ with the linear subspace spanned by all real symmetric $n \times n$ matrices Δ such that there exists $\varepsilon > 0$ satisfying $A \pm \varepsilon\Delta \in \mathcal{C}^n$.

Let u be a zero of A and B a matrix in the face of A. Then u has to be also a zero of B, i.e., $u^T B u = 0$, and the i-th element of the matrix-vector product Bu is zero whenever the i-th element of Au is zero. Every zero u gives rise to linear conditions on B in this way. If the solution space of the corresponding linear system of equations is 1-dimensional (and then necessarily generated by A), then A is extremal. In [4, Theorem 17] it has been shown that this is also a necessary condition for extremality.

If a principal submatrix is extremal, and A is obtained from this submatrix by repeating a row and the corresponding column, then A is also extremal by a criterion of Baumert [1, Theorem 3.8].

On the other hand, if there exists a real symmetric matrix Δ which is linear independent of A, and $A \pm \varepsilon\Delta \in \mathcal{C}^n$ for some $\varepsilon > 0$, then A is not extremal.

References

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