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Monomials in Quadratic Forms

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Abstract—We obtain some constraints on the zero-nonzero pattern of entries in the matrix of a real quadratic form which attains a minimum on a large set of vertices in the multidimensional cube centered at the origin whose edges are parallel to the coordinate axes. In particular, if the graph of the matrix contains an articulation point then the set of the minima of the corresponding quadratic form is not maximal (with respect to set inclusion) among all such sets for various quadratic forms.

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The search of the minimum points of a real quadratic polynomial on the vertices of a multidimensional cube is algorithmically complex. Efficient algorithms are known only in special cases. For example, if the quadratic terms constitute a tridiagonal symmetric matrix then the minimum can be found by pseudo-Boolean programming [1]. For the square of a linear function with integer coefficients, the search of the minimum is reduced to finding the maximum of a linear functional on the set of vertices of a cube with one linear constraint, which can be done by dynamic programming. The last problem admits a fully polynomial approximation scheme [11, 20]; an overview of the linear programming methods for its solving is given in [17]; see [5] for another approach. Replacing the quadratic functional without changing the positions of the minima on the vertices of the cube can sometimes reduce computational complexity [16]. Other examples of exactly solvable problems and heuristic algorithms can be found in [1–3,12, 21].

We obtain some constraints on the zero-nonzero pattern in the matrices of quadratic forms attaining a minimum on an inclusion maximal proper subset of ± 1-points. A point in the linear space $\mathbb{R}^{n+1}$ with fixed basis is identified with the column $x = (x_0, \dots, x_n)^*$, where * stands for transposition. A symmetric matrix A of order $n + 1$ defines a quadratic form $A(x) = x^*Ax$ on $\mathbb{R}^{n+1}$. A monomial x_jx_k occurs in the representation of the quadratic form with matrix A if and only if $A_{jk} \neq 0$.

Define the mapping $\lambda : \mathbb{R}^{n+1} \to \mathbb{R}^N$, where $N = \frac{n(n+1)}{2}$, by the formula

$$\lambda(x) = (x_0x_1, \dots, x_0x_n, x_1x_2, \dots, x_{n-1}x_n)^*.$$

In other words, the components of $\lambda(x)$ are entries in the square matrix xx^* lying above the principal diagonal. Obviously, $\lambda(-x) = \lambda(x)$. The convex hull of the images of the ± 1-points under this mapping is called the *polytope* BQP_n. The polytope BQP_n is combinatorially equivalent to the polytope QP^n in [19]. For example, BQP_2 is a simplex with four vertices.

The entries lying above the principal diagonal of a matrix A are the coefficients of a linear form $A(x)$ on $\mathbb{R}^N$. Given a symmetric matrix A of order $n + 1$, denote by Φ_A the face of BQP_n on which $A(x)$ attains its minimum. The face Φ_A coincides with the whole of BQP_n if and only if the matrix A is diagonal [10]. A *facet* is a face of codimension one. Since each facet belongs to a unique supporting hyperplane, the symmetric matrix of the coefficients of a quadratic form $A(x)$ is defined by the facet Φ_A in BQP_n up to a change of the principal diagonal and multiplication by a nonzero number.

To a symmetric matrix A of order $n + 1$, there is assigned a simple nonoriented graph $G(A)$ with $n + 1$ vertices such that the vertices with numbers j and k are adjacent if $A_{jk} \neq 0$. The entries on the principal

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diagonal do not influence the form of the graph. Call a vertex in a graph an *articulation point* if its removal increases the number of the connected components of the graph. A set of vertices in a graph is called *independent* if every two of these vertices are nonadjacent. If Φ_A is a facet then the graph A is defined uniquely.

Let $A[i, \dots, j]$ denote the submatrix in A situated in the rows and columns with the indicated numbers, and let $A[i] = A_{ii}$ stand for a diagonal entry. Denote by $\pi[i, \dots, j]$ the projection of $\mathbb{R}^{n+1}$ onto the coordiante subspace for the coordinates $x_i, \dots, x_j$. If a symmetric matrix $A = A' \oplus A''$ is decomposable as the direct sum of two matrices A' and A'' then the face Φ_A is embedded in the intersection of the faces $\Phi_{A'\oplus 0} \cap \Phi_{0 \oplus A''}$ [9].

Lemma. *Suppose that the vertex in the graph $G(A)$ with number i is the articulation point of the generated subgraphs $G(A[0, \dots, i])$ and $G(A[i, \dots, n])$ and $\check{A} = A[0, \dots, i] \oplus 0$ is a decomposable matrix. Then the faces Φ_A and $\Phi_{\check{A}}$ of the polytope* BQP_n *are embedded in one another*: $\Phi_A \subseteq \Phi_{\check{A}}$.

Proof. The symmetric matrix A has the form

$$A = \begin{pmatrix} A[0, \dots, i-1] & B & 0 \\ B^* & A[i] & C^* \\ 0 & C & A[i+1, \dots, n] \end{pmatrix},$$

where B and C are column containing at least one nonzero entry. Consider the restriction of $A(x)$ to the $(i+1)$-dimensional linear subspace H defined by the system of equations $x_j = x_i$ or $x_j = -x_i$, where $j > i$. This is a quadratic form $A_H(\pi[0, \dots, i]x)$ with matrix of the kind

$$A_H = \begin{pmatrix} A[0, \dots, i-1] & B \\ B^* & d_H \end{pmatrix},$$

in which only one entry d_H depends on the choice of H, and the rest of the entries coincide with the elements in a submatrix in A.

The form $A_H(\pi[0, \dots, i]x)$ attains a minimum on H at those ± 1-points of the ambient space whose projections $\pi[0, \dots, i]x$ are independent of the choice of H. Moreover, the minimal value on H linearly depends on d_H. Consider the form on $\mathbb{R}^{n+1}$ with the matrix

$$\check{A} = \begin{pmatrix} A[0, \dots, i-1] & B & 0 \\ B^* & A[i] & 0 \\ 0 & 0 & 0 \end{pmatrix}.$$

If $A(x)$ attains its minimum at a ± 1-points then so does $\check{A}(x)$. □

Theorem. *Given a symmetric matrix A of order $n+1$ defining a facet Φ_A in* BQP_n, *removing from $G(A)$ any independent set of its vertices does not increase the number of connected components. In particular, $G(A)$ has no articulation points.*

Proof. Suppose that the set of vertices with numbers from i to j is independent; i.e., the matrix $D = A[i, \dots, j]$ is diagonal. Assume that removing all vertices with numbers from i to j from $G(A)$ increases the number of connected components. Then A has the form

$$A = \begin{pmatrix} A[0, \dots, i-1] & B & 0 \\ B^* & D & C^* \\ 0 & C & A[j+1, \dots, n] \end{pmatrix},$$

where $1 \leqslant i \leqslant j \leqslant n-1$, the matrix $D = A[i, \ldots, j]$ is diagonal, while B and C are rectangular matrices.

Consider the restriction of $A(x)$ to the $(n+i+1-j)$-dimensional linear subspace in H defined by the system of equations $x_k = x_i$ or $x_k = -x_i$ for each k, $i+1 \leqslant k \leqslant j$. This restriction is a quadratic form $A_H(\pi[0, \ldots, i, j+1, \ldots, n]x)$ for which the graph $G(A_H)$ has an articulation point. By Lemma 1, this form attains a minimum at each ± 1-point where so does the form with the matrix

$$\breve{A}_H = \begin{pmatrix} A[0, \ldots, i-1] & B_H & 0 \\ B_H^* & d_H & 0 \\ 0 & 0 & 0 \end{pmatrix}.$$

Define the decomposable matrix $\breve{A} = A[0, \ldots, j] \oplus 0$. All matrices $\breve{A}_H$ are restrictions of the same matrix $\breve{A}$ to H. Therefore, $\breve{A}(x)$ attains its minimum at each ± 1-point where so does $A(x)$. Since A defines a facet in BQP_n, this is possible only if the matrices A and $\breve{A}$ differ only by entries on the principal diagonal and positive factor. But the matrix C contains a nonzero entry; a contradiction.

The proof of the theorem is complete. $\square$

The facets of the polytopes BQP_n for $n \leqslant 6$ were computed by lrs Version 4.2c [13, 14] (see http://cgm.cs.mcgill.ca). BQP_1 has two facets; BQP_2 has four facets; BQP_3 has 16 facets; BQP_4 has 56 facets; BQP_5 has 368 facets; and BQP_6 has 116764 facets. The graph of the matrix defining the facet of BQP_n for $n \leqslant 5$ is either complete or is a union of a clique or several isolated vertices. Choosing entries on the principal diagonal, we can reduce the rank of such matrix to 1. On the other hand, for any values on the principal diagonal, the rank of the matrix

$$A = \begin{pmatrix} * & 0 & 0 & -1 & 1 & 1 & -1 \\ 0 & * & -1 & -1 & 0 & 1 & 1 \\ 0 & -1 & * & 0 & -1 & 1 & 1 \\ -1 & -1 & 0 & * & 1 & 1 & 0 \\ 1 & 0 & -1 & 1 & * & 0 & 1 \\ 1 & 1 & 1 & 1 & 0 & * & 0 \\ -1 & 1 & 1 & 0 & 1 & 0 & * \end{pmatrix}$$

is at least three, and the face Φ_A is a facet in BQP_6. This facet is a simplex with 21 vertices.

The polytopes BQP_n are defined via an explicit description of their vertices. For some series of facets of these polytopes, there was obtained an explicit description [18, 19]. There is a well-known constraint on the mutual disposition of vertices in a face [4, 8]. Nevertheless, for large n, the problem of the recognition of supporting hyperplanes to BQP_n remains algorithmically complex. Such problems for different polytopes are reduced to each other [6, 7, 15].

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