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ON THE STRUCTURE OF THE QUADRATIC BOOLEAN PROBLEM POLYTOPE

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In this paper we give some results about the polytope associated with the quadratic boolean optimization problem. We introduce several classes of inequalities which are valid for this polytope and pay particular attention to inequalities defining facets.

I. Introduction

The quadratic boolean problem polytope (QBP-polytope) was put into consideration in [5]. Recall that the *QBP-polytope* is the convex hull $\mathrm{CH}(M_n)$ of the set of matrices

$$M_n = \{Y \in \{-1, 1\}^{n \times n} | y_{ij} = y_{ii} y_{jj},\ i \neq j\}.$$

The "natural" way of associating this polytope with the quadratic boolean problem

$$(1) \qquad \sum_{1 \leqslant i,j \leqslant n} a_{ij} x_i x_j + \sum_{1 \leqslant i \leqslant n} p_i x_i \to \mathrm{extr}, \qquad x_i \in \{-1, 1\}^n,$$

is the following. Let $y_{ij} = x_i x_j$ for $1 \leqslant i, j \leqslant n$, $i \neq j$, and $y_{ii} = x_i$ for $1 \leqslant i \leqslant n$. Then the optimization problem (1) is equivalent to the linear programming problem

$$(2) \qquad \sum_{\substack{1 \leqslant i,j \leqslant n \\ i \neq j}} a_{ij} y_{ij} + \sum_{1 \leqslant i \leqslant n} p_i y_{ii} \to \mathrm{extr}, \qquad Y = (y_{ij})_{n \times n} \in \mathrm{CH}(M_n).$$

It should be noted that many important combinatorial optimization problems, e.g. the matrix cover problem and the maximum cut problem [1], can be formulated as the problem (2). Of course, in order to apply linear programming techniques we need a complete description of the QBP-polytope by means of linear equations and inequalities. This may be impossible, because of the NP-complexity of the matrix cover problem and the maximum cut problem [1]. But we can hope that partial results can be of great computational help for the numerical solution of the problem (1) when used in conjunction with linear programming and branch-and-bound methods.

Some characteristics of the QBP-polytope were investigated in [5]. In particular, the following propositions were proved.

PROPOSITION 1.1. $\operatorname{vert} \mathrm{CH}(M_n) = M_n$.

PROPOSITION 1.2. $\dim \mathrm{CH}(M_n) = n(n+1)/2$.

PROPOSITION 1.3. $\operatorname{diam} \mathrm{CH}(M_n) = 1$.

Let (A, b) be the hyperplane defined by $\sum_{1 \leqslant i,j \leqslant n} a_{ij} y_{ij} = b$ and

$$F(A, b) = \{Y \in \mathrm{CH}(M_n) | \sum_{1 \leqslant i,j \leqslant n} a_{ij} y_{ij} = b\}.$$

PROPOSITION 1.4. *Let $F(A, b)$ be a facet of $\mathrm{CH}(M_n)$, $n \geqslant 2$. Then $a_{ij} \neq 0$ for some pair of indices (i, j), $i \neq j$.*

This paper studies the facet properties of the QBP-polytope. In Section 2 we investigate some trivial inequalities. In Section 3 we determine some classes of facets for $\mathrm{CH}(M_n)$. Note that a detailed treatment of the theory of polyhedra and polyhedral aspects of combinatorial optimization problems can be found in [2–4].

II. Trivial inequalities for the QBP-polytope

The polytope $\mathrm{CH}(M_n)$ is contained in the cube

$$\{Y \in \boldsymbol{R}^{n \times n} | y_{ij} = y_{ji},\ i \neq j,\ -1 \leqslant y_{ij} \leqslant 1,\ i \leqslant j\}.$$

Thus the cube constraints are valid inequalities for $\mathrm{CH}(M_n)$.

PROPOSITION 2.1. *Every inequality $y_{ij} \leqslant 1$, $y_{ij} \geqslant -1$, $i \leqslant j$, defines the $n(n-1)/2$-dimensional face of $\mathrm{CH}(M_n)$, $n \geqslant 2$, which is $\mathrm{CH}(M_{n-1})$.*

Proof. Let $E_n(i, j)$, $i \leqslant j$, be the $n \times n$-matrix with elements $y_{ij} = 1$, $y_{kp} = 0$, $(k, p) \neq (i, j)$. It is evident that $(E_n(i, j), 1)$ is a supporting hyperplane for $\mathrm{CH}(M_n)$ and therefore $F(E_n(i, j), 1)$ is a face of $\mathrm{CH}(M_n)$. Suppose that $i < j$. Every matrix $Y \in F(E_n(i, j), 1)$ must satisfy the following nonredundant system of equations:

$$\begin{gathered} y_{ij} = 1, \quad y_{ii} = y_{jj}, \quad y_{ki} = y_{kj}, \quad k = 1, \dots, i-1, \\ y_{i,i+p} = y_{i+p,j}, \quad p = 1, \dots, j-i-1, \quad y_{i,j+k} = y_{j,j+k}, \quad k = 1, \dots, n-j. \end{gathered} \tag{3}$$

Then by Proposition 1.2, $\dim F(E_n(i,j), 1) \leqslant n(n-1)/2$. Let $K_n(i_1, i_2; \ldots ; i_{s-1}, i_s)$ be the set of matrices from M_n with elements $y_{i_{2r-1}i_{2r}} = 1$, $r = 1, \ldots, s/2$. We show that $\dim F(E_n(i,j), 1) = n(n-1)/2$ by exhibiting $n(n-1)/2+1$ affinely independent matrices in $F(E_n(i,j), 1)$. This set of matrices is the following:

$$2^{-n+1} \sum_{K_n(i,j)} Y; \quad 2^{-n+2} \sum_{K_n(i,i;j,j;i,j)} Y;$$

$$2^{-n+2} \sum_{K_n(i,j;k,p)} Y, \ k \neq i, \ p \neq j; \quad 2^{-n+2} \sum_{K_n(i,j;k,i;k,j)} Y, \ k = 1, \ldots, i-1;$$

$$2^{-n+2} \sum_{K_n(i,j;i,i+p;i+p,j)} Y, \quad p = 1, \ldots, j-i-1;$$

$$2^{-n+2} \sum_{K_n(i,j;i,j+k;j,j+k)} Y, \quad k = 1, \ldots, n-j.$$

Therefore we have $\dim F(E_n(i,j), 1) = n(n-1)/2$. Clearly $F(E_n(i,j), 1)$ is the polytope $\mathrm{CH}(M_{n-1})$ in the linear subspace determined by the hyperplanes (3). The cases $i = j$ and $y_{ij} \geqslant -1$ can be proved similarly.

III. Facets of the QBP-polytope

We shall now consider facets of the QBP-polytope. We shall use the so-called lifting technique, which gives a good way of constructing new facets of $\mathrm{CH}(M_n)$ having a facet of $\mathrm{CH}(M_{n-1})$.

PROPOSITION 3.1. *Let $F(A, b)$ be a facet of $\mathrm{CH}(M_n)$, $n \geqslant 2$. Then the matrix A has at least three nonzero elements a_{ij}, $i \leqslant j$.*

Proof. First of all, it is easy to show that the zero matrix $0_{n\times n} \in \mathrm{int}\,\mathrm{CH}(M_n)$ [5] and therefore $b \neq 0$ for every facet of $\mathrm{CH}(M_n)$. Suppose that $F(A, b)$ is a facet of $\mathrm{CH}(M_n)$ with only one element $a_{ij} \neq 0$, $i \leqslant j$. Let $Y \in \mathrm{vert}\,F(A, b)$ and suppose $y_{ij} = 1$ (or $y_{ij} = -1$). Then we have $a_{ij} = b$ ($-a_{ij} = b$). Therefore the facet $F(A, b)$ is determined by the trivial inequality $y_{ij} \leqslant 1$ ($y_{ij} \geqslant -1$). But in this case by Proposition 2.1, $\dim F(A, b) = n(n-1)/2$.

Now suppose that only two elements of A are nonzero with $i \leqslant j$, say a_{ij}, a_{kp}, $(i,j) \neq (k,p)$. Let $Y' \in \mathrm{vert}\,F(A, b)$. We have $a_{ij}y'_{ij} + a_{kp}y'_{kp} = b$. If $\mathrm{sign}\,y'_{ij} = \mathrm{sign}\,y'_{kp}$ ($\mathrm{sign}\,y'_{ij} \neq \mathrm{sign}\,y'_{kp}$) then $y_{ij} = y_{kp}$ ($y_{ij} = -y_{kp}$) for every vertex of $F(A, b)$. Therefore $\dim F(A, b) \leqslant \dim \mathrm{CH}(M_n) - 2$, i.e. $F(A, b)$ is not a facet.

Let A be an $n \times n$-matrix and c an $(n+1)$-vector. Define the following matrices:

$$A_0(c) = \begin{bmatrix} c_1 & a_{11} & a_{12} & \cdots & a_{1,n-1} & a_{1n} \\ a_{11} & c_2 & a_{22} & \cdots & a_{2,n-1} & a_{2n} \\ a_{21} & a_{22} & c_3 & \cdots & a_{3,n-1} & a_{3n} \\ \cdots & \cdots & \cdots & \cdots & \cdots & \cdots \\ a_{n1} & a_{n2} & a_{n3} & \cdots & a_{nn} & c_{n+1} \end{bmatrix},$$

$$A_i(c) = \begin{bmatrix} a_{11} & \dots & a_{i,i-1} & c_1 & a_{1i} & \dots & a_{1n} \\ \dots & \dots & \dots & \dots & \dots & \dots & \dots \\ a_{i-1,1} & \dots & a_{i-1,i-1} & c_{i-1} & a_{i-1,i} & \dots & a_{i-1,n} \\ c_1 & \dots & c_{i-1} & c_i & c_{i+1} & & c_{n+1} \\ a_{i1} & \dots & a_{i,i-1} & c_{i+1} & a_{ii} & \dots & a_{in} \\ \dots & \dots & \dots & \dots & \dots & \dots & \dots \\ a_{n1} & & a_{n,i-1} & c_{n+1} & a_{ni} & & a_{nn} \end{bmatrix},$$

$$i = 1, \dots, n+1.$$

We say that the facet $F(B, b)$ of $\mathrm{CH}(M_{n+1})$ is a *lifting* of the facet $F(A, b)$ of $\mathrm{CH}(M_n)$ if $B = A_i(c)$ for some $0 \leqslant i \leqslant n+1$ and a vector c.

THEOREM 3.1. *Let $F(A, b)$ be a facet of the polytope $\mathrm{CH}(M_n)$, $n \geqslant 2$. Then $F(A_i(c), b)$ is a facet of the polytope $\mathrm{CH}(M_{n+1})$ if and only if $c = 0$.*

Proof. Let $F(A_i(c), b)$ be both a facet of the polytope $\mathrm{CH}(M_n)$ and a lifting of the facet $F(A, b)$ of $\mathrm{CH}(M_n)$. Suppose $Y \in \mathrm{vert} F(A, b)$ and $d = (y_{11}, y_{22}, \dots, y_{nn}, 1)$. Then $Y_i(d)$, $Y_i(-d) \in \mathrm{vert}\,\mathrm{CH}(M_{n+1})$. Therefore $Y_i(0) = \frac{1}{2} Y_i(d) + \frac{1}{2} Y_i(-d) \in \mathrm{CH}(M_n)$. Clearly, $Y_i(0) \in F(A_i(c), b)$ and we have by Proposition 1.3, $Y_i(d)$, $Y_i(-d) \in F(A_i(c), b)$. Let $Y^1, \dots, Y^k$ be a set of $k = (n+1)n/2$ linearly independent matrices of $F(A, b)$. By Proposition 1.4 we have $a_{ij} \neq 0$ for some $i < j$ and then

$$\det \begin{bmatrix} y_{11}^1 & \dots & y_{nn}^1 & b & y_{12}^1 & \dots & y_{i-1,j}^1 & y_{i+1,j}^1 & \dots & y_{n-1,n}^1 \\ y_{11}^2 & \dots & y_{nn}^2 & b & y_{12}^2 & \dots & y_{i-1,j}^2 & y_{i+1,j}^2 & \dots & y_{n-1,n}^2 \\ \dots & \dots & \dots & \dots & \dots & \dots & \dots & \dots & \dots & \dots \\ y_{11}^k & \dots & y_{nn}^k & b & y_{12}^k & \dots & y_{i-1,j}^k & y_{i+1,j}^k & & y_{n-1,n}^k \end{bmatrix} \neq 0.$$

Therefore the submatrix determined by the first $n+1$ columns of this determinant has at least one nonzero $(n+1) \times (n+1)$-minor, say

$$\begin{bmatrix} y_{11}^1 & y_{22}^1 & \dots & y_{nn}^1 & b \\ y_{11}^2 & y_{22}^2 & \dots & y_{nn}^2 & b \\ \dots & \dots & \dots & \dots & \dots \\ y_{11}^{n+1} & y_{22}^{n+1} & \dots & y_{nn}^{n+1} & b \end{bmatrix}.$$

Then we have the following system of linear equations for the vector c:

$$c_1 y_{11}^1 + c_2 y_{22}^1 + \dots + c_n y_{nn}^1 + c_{n+1} b = 0,$$
$$c_1 y_{11}^2 + c_2 y_{22}^2 + \dots + c_n y_{nn}^2 + c_{n+1} b = 0,$$
$$\dots\dots\dots\dots\dots\dots\dots\dots$$
$$c_1 y_{11}^{n+1} + c_2 y_{22}^{n+1} + \dots + c_n y_{nn}^{n+1} + c_{n+1} b = 0.$$

This means that $c = 0$.

Now let $F(A, b)$ be a facet of $\mathrm{CH}(M_n)$. Clearly $F(A_i(0), b)$ is a face of $\mathrm{CH}(M_{n+1})$. Suppose $\dim F(A_i(0), b) < (n+2)(n+1)/2-1$. Then there exists a facet $F(D, b)$ of $\mathrm{CH}(M_{n+1})$ such that $F(A_i(0), b) \subset F(D, b)$. But $Y_i(0) \in F(A_i(0), b)$ for every $Y \in F(A, b)$. Thus $Y_i(0) \in F(D, b)$ and we have $D = A_i(c)$. Therefore necessarily $c = 0$.

THEOREM 3.2. *Let* $n \geqslant 2$. *Then every inequality*

$$\left.\begin{aligned} y_{ij}+y_{ik}-y_{k-j+i,k} &\leqslant 1,\\ y_{ij}-y_{ik}+y_{k-j+i,k} &\leqslant 1,\\ -y_{ij}+y_{ik}+y_{k-j+i,k} &\leqslant 1,\\ -y_{ij}-y_{ik}-y_{k-j+i,k} &\leqslant 1, \end{aligned}\right. \qquad 1 \leqslant i \leqslant j < k \leqslant n,$$

defines a facet of $\mathrm{CH}(M_n)$.

Proof. This is trivial for $n = 2$, and for $n > 2$ follows from Theorem 3.1.

THEOREM 3.3. *Let* $n \geqslant 3$. *Then each of the inequalities*

$$(n-3)\sum_{1\leqslant k\leqslant n} y_{kk} - \sum_{1\leqslant p<j\leqslant n} y_{pj} \leqslant 1+(n-2)(n-3)/2,$$

$$-(n-3)\sum_{1\leqslant k\leqslant n} y_{kk} - \sum_{1\leqslant p<j\leqslant n} y_{pj} \leqslant 1+(n-2)(n-3)/2,$$

$$(n-3)\Big(\sum_{1\leqslant k\leqslant i} y_{ki} + \sum_{i<k\leqslant n} y_{ik}\Big) - \sum_{\substack{1\leqslant p\leqslant j\leqslant n\\ p,j\neq i}} y_{pj} \leqslant 1+(n-2)(n-3)/2, \qquad i = 1, \ldots, n,$$

$$-(n-3)\Big(\sum_{1\leqslant k\leqslant i} y_{ki} + \sum_{i<k\leqslant n} y_{ik}\Big) - \sum_{\substack{1\leqslant p\leqslant j\leqslant n\\ p,j\neq i}} y_{pj} \leqslant 1+(n-2)(n-3)/2, \qquad i = 1, \ldots, n,$$

defines a facet of $\mathrm{CH}(M_n)$.

Proof. Each of the above inequalities is valid in $\mathrm{CH}(M_n)$. Consider the $n(n+1)/2$ matrices in M_n with exactly one or two elements of the main diagonal equal to -1. These matrices are affinely independent and satisfy the first inequality of the theorem as equality. Similarly we can find affinely independent matrices corresponding to other inequalities of the theorem.

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