Pré-Publicações do Departamento de Matemática
Universidade de Coimbra
Preprint Number 19–38

ON SUMS OF SQUARES OF k-NOMIALS

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ABSTRACT: In 2005, Boman et al introduced the concept of Factor Width for a real symmetric positive semidefinite matrix. This is the smallest positive integer k for which the matrix A can be written as $A = VV^T$ with each column of V containing at most k non-zeros. The cones of matrices of bounded factor width give a hierarchy of inner approximations to the PSD cone. In the polynomial optimization context, a Gram matrix of a polynomial having factor width k corresponds to the polynomial being a sum of squares of polynomials of support at most k. Recently, Ahmadi and Majumdar [1], explored this connection for case $k = 2$ and proposed to relax the reliance on sum of squares polynomials in semidefinite programming to sum of binomial squares polynomials (sobs; which they call sdsos), for which semidefinite programming can be reduced to second order programming to gain scalability at the cost of some tolerable loss of precision. In fact, the study of sobs goes back to Reznick [10, 11] and Hurwitz [6]. In this paper, we will prove some results on the geometry of the cones of matrices with bounded factor widths and their duals, and use them to derive new results on the limitations of certificates of nonnegativity of polynomials by sums of k-nomial squares using standard multipliers.

KEYWORDS: factor width, sums of squares, positive semidefinite, k-nomials, SD-SOS.
MATH. SUBJECT CLASSIFICATION (2010): 13J30, 12D15, 90C30.

1. Motivation and introduction

Ahmadi and Majumdar in their recent paper [1] propose a new subclass of polynomials for semidefinite programming. They note that although semidefinite programming has been highly successful in being able to address the question of good approximations even to NP-complete or NP-hard optimization problems it lacks good scalability, that is, programs tend to grow rapidly in size as we attempt better approximations. They further observe that, in many practical problems, resorting to the full power of semidefinite programming is unnecessarily time or memory consuming and polynomial

Received November 29, 2019.
All authors were supported by Centro de Matemática da Universidade de Coimbra – UID/MAT/00324/2019, funded by the Portuguese Government through FCT/MEC and co-funded by the European Regional Development Fund through the Partnership Agreement PT2020. JG was partially supported by FCT under Grant P2020 SAICTPAC/0011/2015. MS was supported by a PhD scholarship from FCT, grant PD/BD/128060/2016.

optimization problems involving polynomials of degrees four to six and more than a dozen variables are currently unpractical to tackle with standard sums of squares techniques. To obviate these shortcomings, instead of working with the full class of sum-of-squares polynomials they propose to work with polynomials they call diagonally dominant (dsos) or scaled diagonally dominant (sdsos) sums of squares, respectively, obtaining problems that are linear programs (LP) and second order cone programs (SOCP), respectively. As proven in [3], scaled diagonally dominant (sdd) matrices are precisely the matrices with factor width at most two. In their paper Ahmadi and Majumdar already point out that a natural generalization would be to study certificates given by matrices with factor width greater or equal than 2. In this paper we advance in that direction, studying the geometry of the cones of matrices of bounded factor width and using the fact that these cones provide a hierarchy of inner approximations to the PSD cone, to establish new certificates for checking nonegativity of a polynomial, and simultaneously showing their limitations.

We organize the paper as follows: In Section 2 we give some basic definitions and notations that will be used throughout the paper. In Section 3 we present the concept of factor width for positive semidefinite matrices. Then in Section 4 we give some geometric properties of the cone of bounded factor width matrices. In particular we characterize some of the extreme rays of their duals which will be used later to derive the main results of the paper. Section 5 follows the study of an example given by Ahmadi and Majumdar in [1]. They considered the polynomial $p_n^a = (\sum_{i=1}^n x_i)^2 + (a-1)\sum_{i=1}^n x_i^2$ and proved that for $n = 3$, if $a < 2$, then no nonnegative integer r can be chosen so that $(x_1^2 + x_2^2 + x_3^2)^r p_3^a$ is a sum of squares of binomials (sobs or so2s), although it is clearly nonnegative for $a \geq 1$. In other words, p_3^a is not r-so2s for any r. We complete the study of this example for the strengthened certificates proposed, obtaining further negative results along the same direction. We first characterize when p_n^a is a sum of k-nomial squares (soks), then we show that $p_{n,r}^a$, that is, the multiplication of p_n^a with $(\sum_{i=1}^n x_i^2)^r$, is a sum of k-nomial squares (r-so$k$s) if and only if this is the case for $r = 0$. In the following Sections, we show that the behaviour found in Ahmadi and Majumdar's example is actually the rule in many cases. More precisely, in Section 6, we prove that if a quadratic form is not sobs, then it is not r-sobs for any r and in Section 7 we show that if a 4-variable quadratic form is not so3s, then it is not r-so3s for any r. To complete the paper, in

Section 8 we give an example which shows that our results are complete, as they cannot be extended in the most natural way to five or more variables. To that end, we give a quadratic form in five variables which is not so4s but which becomes so4s after multiplication with $\sum_{i=1}^{5} x_i^2$.

2. Definitions and notations

All our matrices are understood to be real. We denote by $\mathcal{S}^n$, the $n \times n$ (real) symmetric matrices. A symmetric matrix A is positive semidefinite (psd) if $x^T A x \geq 0$ for all $x \in \mathbb{R}^n$. This property will be denoted by the standard notation $A \succeq 0$. By $\mathcal{S}^n_+$ we denote the subset of real symmetric positive semidefinite matrices. The Frobenius inner product for matrices $A, B \in \mathcal{S}^n$ is given by $\langle A, B \rangle = \mathrm{trace}(\mathrm{AB}^\top) = \sum_{\mathrm{i,j}} \mathrm{A_{ij} B_{ij}}$. For a cone K of matrices in $\mathcal{S}^n$, we define its dual cone K^* as $\{Y \in \mathcal{S}^n : \langle Y, X \rangle \geq 0, \ \forall X \in K\}$.

If $X = (x_{ij})$ is an $n \times n$ matrix and $K \subseteq \{1, 2, ..., n\}$, then X_K denotes the (principal) submatrix of X composed from rows and columns of X with indices in K; $\mathrm{supp}(X) = \{(i, j) \in \{1, 2, ..., n\}^2 : x_{ij} \neq 0\}$ is the support of X.

If B is a $k \times k$ matrix and $K \subseteq \{1, 2, ..., n\}$, a k element subset of $\{1, 2, ..., n\}$, then $\iota_K(B)$ means the $n \times n$ matrix X which has zeros everywhere, except that $X_K = B$.

We denote by $\mathbb{R}[x_{1:n}] = \mathbb{R}[x_1, ..., x_n]$ the algebra of polynomials in n variables $x_1, x_2, \ldots, x_n$ over $\mathbb{R}$. A *monomial* in $\mathbb{R}[x_{1:n}]$ is an expression of the form $x^\alpha = x_1^{\alpha_1} x_2^{\alpha_2} \cdots x_n^{\alpha_n}$ and a polynomial p in $\mathbb{R}[x_{1:n}]$ is a finite linear combination of monomials; so $p = \sum_\alpha c_\alpha x^\alpha$. A polynomial $p \in \mathbb{R}[x_{1:n}]$ is nonnegative if it takes only nonnegative values, i.e., $p(x) \geq 0$, for all $x \in \mathbb{R}^n$ and a polynomial $p \in \mathbb{R}[x_{1:n}]$ is a *sum of squares (sos)* polynomial, if it has a representation $p = \sum_{i=1}^{m} q_i^2$ with polynomials $q_i \in \mathbb{R}[x_{1:n}]$. Of course every sum-of-squares polynomial is nonnegative and every nonnegative polynomial has necessarily even degree, $2d$, say. A useful introduction to polynomial optimization using sums of squares is found in [2].

A polynomial p is called a *scaled diagonally dominant sum of squares* (sdsos) if it can be written as a nonnegative linear combination of squares of monomials and binomials; that is, p is a sum of expressions of the form αm^2 and $\alpha(\beta_1 m_1 + \beta_2 m_2)^2$ with all the αs> 0, and βs real. A polynomial p is called a *diagonally dominant sum of squares* (dsos) if it can be written in this form using only the combinations $\beta_1 = \beta_2 = 1$ or $\beta_1 = 1 = -\beta_2$. A *k-nomial* is an expression of the form $\alpha_1 m_1 + \cdots + \alpha_k m_k$ with $\alpha_1, ..., \alpha_k$ reals and $m_1, ..., m_k$ monomials. Note that every $k-1$-nomial is also k-nomial. We call a sum of squares of k-nomials a *soks*-expression. A polynomial $p \in P_n$ is then called *r-soks* if $(\sum_{i=1}^n x_i^2)^r p$ is so$k$s.

For smooth reading the reader should keep in mind the following basic facts found in texts about convex sets, for example in [5], or in [9, Sections 1.3 and 1.4].

· If C is a closed convex cone then $C = C^{**}$.
· $\langle A, S_1 B S_2\rangle = \langle S_1^\top A S_2^\top, B\rangle$, whenever the matrix products are defined.
· The cone of real symmetric psd matrices is selfdual, i.e. $\mathcal{S}_+^n = (\mathcal{S}_+^n)^*$.
· If $A \in \mathcal{S}_+^n$ and for some $x \in \mathbb{R}^n$, $x^\top A x = 0$, then $Ax = 0$. See [5, p. 463].
· If $A \in \mathcal{S}^n$ then A is psd iff for all psd matrices B, $\langle A, B\rangle \geq 0$.
− In particular if $A, B \succeq 0$, then $\langle A, B\rangle \geq 0$.
· If $A, B \succeq 0$, then $\langle A, B\rangle = 0$ iff $AB = 0$.

3. On the factor width of a matrix

The concept of *factor width* of a real symmetric positive semidefinite matrix A was introduced by Boman et al. in [3] as the smallest integer k such that there exists a real (rectangular) matrix V such that $A = VV^\top$ and each column of V contains at most k non-zeros. We let

$FW_k^n = \{$symmetric positive semidefinite $n\times n$ matrices of factor width $\leq k.\}$.

We have of course

$$FW_1^n \subset FW_2^n \subset FW_3^n \subset \cdots \subset FW_n^n = \mathcal{S}_+^n.$$

Next assume $A = VV^T$ is a symmetric positive semidefinite matrix where each column of V has at most k nonzero entries. By the rules of matrix multiplication, for any $i, j \in \{1, ..., n\}$, and writing $V_{*\nu}$ and $V_{\nu *}$ for the ν-th column or row of a matrix V, respectively, we have

$$(VV^T)_{ij} = \sum_{\nu=1}^m V_{i\nu}(V^T)_{\nu j} = \sum_{\nu=1}^m (V_{*\nu} V^T_{\ \ \nu *})_{ij} = \sum_{\nu=1}^m (V_{*\nu} {V_{*\nu}}^T)_{ij}.$$

Write $A = \sum_{\nu=1}^m (V_{*\nu}{V_{*\nu}}^T)$. Note that each $V_{*\nu}{V_{*\nu}}^T$ is a symmetric positive semidefinite $n\times n$ rank 1 matrix whose support lies within a cartesian product $K^2 = K \times K$ for some $K \subseteq \{1, 2, ..., n\}$ of cardinality k. Since every $n \times n$ matrix with the latter properties can be written as vv^T for some v with at most k nonzero entries, we have the following

Proposition 3.1. *Let A be an $n \times n$ symmetric positive semidefinite matrix, and assume $k \in \mathbb{Z}_{\geq 1}$. Then $A \in FW_k^n$ if and only if A is the sum of a finite* *family of symmetric positive semidefinite $n \times n$ matrices whose supports are all contained in sets $K \times K$ with $|K| = k$.*

From this proposition it follows immediately that each set FW_k^n is a convex closed subcone of $\mathcal{S}_+^n$. We will now focus on the dual cone of FW_k^n. From [8, Lemma 5 + Subsection 3.2.5] we have the following result.

Proposition 3.2. *The dual of FW_k^n is given by*

$$(FW_k^n)^* = \{X \in \mathcal{S}^n \mid X_K \in \mathcal{S}_+^k \text{ for all } K \subseteq \{1, 2, ..., n\} \text{ with } |K| = k\}.$$

Furthermore the following inclusions and identity hold

$$FW_k^n \subseteq \mathcal{S}_+^n \subseteq (FW_k^n)^* \text{ and } FW_k^n = (FW_k^n)^{**}.$$

4. On the geometry of bounded factor width matrices

In this section, we give some geometric properties of the cone of bounded factor width matrices. In particular, we characterize some of the extreme rays of their duals.

We start with the following lemma about exposedness of the extreme rays of $(FW_k^n)^*$.

Lemma 4.1. *The cone $(FW_k^n)^*$ is (linearly equivalent to) a spectrahedron. Therefore a matrix in $(FW_k^n)^*$ which spans an extreme ray is an exposed ray.*

Proof: Let $E_{\{i,j\}}$ be the symmetric $n \times n$ matrix which has zeros everywhere except at the entries (i, j) and (j, i) where it has 1s. Denote by $I_1, I_2, \ldots, I_{\binom{n}{k}}$ the $\binom{n}{k}$ distinct k element subsets of $\{1, 2, \ldots, n\}$ and define for $l = 1, 2, \ldots, \binom{n}{k}$ the matrix

$$E_{\{i,j\}}^l = \begin{cases} E_{\{i,j\}} & \text{if } i, j \text{ are both contained in the } l\text{th of the sets } I_1, I_2, \ldots, I_{\binom{n}{k}}. \\ 0 & \text{otherwise.} \end{cases}$$

Consider now the condition

$$\sum_{1 \le i \le j \le \binom{n}{k}} b_{ij}(E_{\{i,j\}}^1 \oplus E_{\{i,j\}}^2 \oplus \cdots \oplus E_{\{i,j\}}^n) \succeq 0.$$

Since a direct sum of matrices is positive semidefinite if and only if each of its summands is positive semidefinite, the attentive reader finds that this condition expresses precisely that the submatrices B_{I_r}, $r = 1, \ldots, \binom{n}{k}$ with $|I_r| = k, I_r \subseteq \{1, \ldots, n\}$ of $B = (b_{ij}) \in \mathcal{S}^n$ should be positive semidefinite. Since this is the defining property of B to be in $(FW_k^n)^*$ we find that $(FW_k^n)^*$

is a spectrahedron. The second part is a consequence of the theorem that every face of a spectrahedron is exposed. This is proved in [9, p.11]. ■

Our first result about the extreme rays of the cone $(FW_k^n)^*$ is as follows.

Lemma 4.2. *The matrix $A \in \mathcal{S}_+^n$ spans an extreme ray of $(FW_k^n)^*$ if and only if it has rank 1.*

Proof: Let $A \in \mathcal{S}_+^n$ span an extreme ray of $(FW_k^n)^*$ and assume $\operatorname{rank}(A) = r \geq 2$. Then, as $A \in \mathcal{S}_+^n$, one can write $A = x_1x_1^T + \cdots + x_rx_r^T$ with real pairwise orthogonal x_i. Since $x_ix_i^T \in \mathcal{S}_+^n$, $i = 1, ..., r$, , these $x_ix_i^T$ are elements of $(FW_k^n)^*$ - recall $FW_k^n \subset \mathcal{S}_+^n \subset (FW_k^n)^*$ - and since they are not multiples of each other, A is not an extreme ray. So for extremality of A rank equal to 1 is necessary.

Now we prove that if the matrix A has rank 1, then it spans an extreme ray of $(FW_k^n)^*$. So let $A = xx^T$. Assume now $A = X + Y$ with some $X, Y \in (FW_k^n)^*$ and some $x \in \mathbb{R}^n$. Then for any k element subset $I \subseteq \{1, 2, \ldots, n\}$, $x_Ix_I^T = X_I + Y_I$. By the characterization of $(FW_k^n)^*$, X_I, Y_I are positive semidefinite; that is we have found in $\mathcal{S}_+^n$ a representation of a rank 1 matrix as a sum of two other matrices. Since the null space of a sum of two psd matrices is contained in the nullspace of each, we infer that X_I, Y_I are multiples of $x_Ix_I^T$: for some real λ_I, $X_I = \lambda_I x_I x_I^T$, $Y_I = (1 - \lambda_I)x_Ix_I^T$. Now, considering any two $k \times k$ submatrices of X indexed by I and J, we have if $i \in I \cap J$, then $x_{ii} = \lambda_I x_i^2 = \lambda_J x_i^2$ so if $x_{ii} \neq 0$ then $\lambda_I = \lambda_J$. Note that if $x_{ii} = 0$, the entire i-th row and column of X must be zero. For any I and J such that $i \in I$ and $j \in J$ with $x_{ii} \neq 0$ and $x_{jj} \neq 0$, we can pick a k-element set K such that $i, j \in K$ and the above argument gives $\lambda_I = \lambda_J = \lambda_K$. So all are equal to some λ and $X = \lambda xx^T$. ■

Next, we present a simple fact which will help us in the next theorem to characterize the extreme rays of $(FW_{n-1}^n)^*$.

Lemma 4.3. *Assume that $A \in (FW_{n-1}^n)^*$ and let A_I be an $n-1 \times n-1$ principal submatrix of A for some I with $I \subseteq \{1, 2, \ldots, n\}$. If $\operatorname{rank}(A_I) \leq n-3$, then A is psd.*

Proof: Since $A \in (FW_{n-1}^n)^*$, all its proper principal minors are nonnegative. So A is psd if and only if $\det(A) \geq 0$. But by Cauchy's interlacing theorem, see [5, p. 185], if $\beta_1, \ldots, \beta_{n-1}$ are the (nonnegative) eigenvalues of A_I and $\gamma_1, \ldots, \gamma_n$ are the eigenvalues of A, then

$$\gamma_1 \leq \beta_1 \leq \gamma_2 \leq \beta_2 \leq \ldots \leq \beta_{n-1} \leq \gamma_n.$$

Now, since $\operatorname{rank}(A_I) \leq n-3$, β_1 and β_2 should be zero which leads to $\gamma_2 = 0$ and so $\det(A) = 0$, hence A is psd. ■

Theorem 4.4. *If the matrix $A \in (FW^n_{n-1})^*$ is not psd, the matrix A spans an extreme ray of $(FW^n_{n-1})^*$, if and only if all of its $(n-1)\times(n-1)$ principal submatrices have rank $n-2$.*

Proof: We first prove that if the matrix A spans an extreme ray of $(FW^n_{n-1})^*$, then all of its $(n-1)\times(n-1)$ principal submatrices have rank $n-2$. Assume that this does not happen, which means there is one $(n-1)\times(n-1)$ principal submatrix which is full rank, otherwise by Lemma 4.3 A will be psd. Suppose $A_{\{1,2,\ldots,n-1\}}$ is such a principal submatrix of full rank. Since the cone $(FW^n_{n-1})^*$ is a spectrahedron, by Lemma 4.1 every of its faces is exposed. Hence A is an exposed extreme ray of $(FW^n_{n-1})^*$. So, there exists a $B \in (FW^n_{n-1})^{**} = FW^n_{n-1}$ such that $\langle B, A\rangle = 0$ and $\langle B, X\rangle > 0$ for all $X \in (FW^n_{n-1})^* \setminus \{\lambda A \mid \lambda \geq 0\}$.

This $B \in FW^n_{n-1}$, and so it can be written as

$$B = \sum_{I\subseteq\{1,2,\ldots,n\},|I|=n-1} \iota_I(B_I), \quad \text{for } B_I \in \mathcal{S}^{n-1}_+.$$

We thus get

$$0 = \langle B, A\rangle = \sum_{I\subseteq\{1,2,\ldots,n\},|I|=n-1} \langle \iota_I(B_I), A\rangle = \sum_{I\subseteq\{1,2,\ldots,n\},|I|=n-1} \langle B_I, A_I\rangle.$$

Since the $(n-1)\times(n-1)$ principal submatrices of A are all positive semidefinite, we get that all the inner products are nonnegative and hence must be 0. Which means $\langle B_I, A_I\rangle = 0$ for all I.

Under the current supposition that $A_{\{1,2,\ldots,n-1\}}$ is not singular, we conclude that $B_{\{1,2,\ldots,n-1\}} = 0$.

Let now a be the n-th column of A and let $\tilde{A} = aa^T$. Of course $\tilde{A} \in \mathcal{S}^n_+$ and so $\tilde{A} \in (FW^n_{n-1})^*$. We have

$$\langle \iota_I(B_I), \tilde{A}\rangle = \langle \iota_I(B_I), aa^T\rangle = \langle B_I, a_I a_I^T\rangle.$$

But note that a_I is a column of A_I for $I \neq \{1,2,\ldots,n-1\}$, so $A_I = a_I a_I^T + A'_I$ for some $A'_I \succeq 0$ and $\langle B_I, A_I\rangle = 0$ implies $\langle B_I, a_I a_I^T\rangle = 0$. Since we know already $B_{\{1,2,\ldots,n-1\}} = 0$ we get $\langle B, \tilde{A}\rangle = 0$. Now evidently $\tilde{A}$ is not a multiple of A so it does not span the same ray and we have a contradiction to our assumption that $A_{\{1,2,\ldots,n-1\}}$ has full rank. Therefore $A_{\{1,2,\ldots,n-1\}}$ has rank at most $n-2$ and similarly any other principal $(n-1)\times(n-1)$ submatrix has rank at most $n-2$.

For the reverse direction, assume that A does not span an extreme ray of $(FW^n_{n-1})^*$. This means that we can write it as

$$A = \gamma X + (1-\gamma)Y \text{ for some } X, Y \in (\widetilde{FW}^n_{n-1})^* \text{ and } \gamma \in]0,1[,$$

where $(\widetilde{FW}^n_{n-1})^*$ is the compact section of the cone $(FW^n_{n-1})^*$ consisting of the matrices that have the same trace as matrix A.

Let $X_\lambda = \lambda X + (1-\lambda)Y,\ \lambda \in \mathbb{R}_+$. Given some I, we know that $(X_\lambda)_I$ has rank at most $n-2$: in fact, there is a 2 dimensional space, $\ker(A_I)$, which is always contained in $\ker(X_\lambda)_I$. Then the set $L = \{\lambda | X_\lambda \in (FW^n_{n-1})^*\} = [\lambda_{min}, \lambda_{max}]$ since $L \cap (FW^n_{n-1})^* \subseteq (\widetilde{FW}^n_{n-1})^*$ which is compact. The eigenvalues and eigenvectors of $(X_\lambda)_I$ change continuously with λ. Since two zero eigenvalues correspond to fixed eigenvectors, the only way for $(X_\lambda)_I$ to stop being psd is if a third eigenvalue switches from positive to negative, which implies that for some I, $\operatorname{rank}((X_{\lambda_{max}})_I) \leq n-3$ and the same for $(X_{\lambda_{min}})_I$ and this means by Lemma 4.3 that both are psd. Hence A is psd since it is a convex combination of both. This is a contradiction to the hypothesis. ■

In the following observation, we observe that conjugating by a permutation and scaling of a matrix does not affect extreme rays.

Observation. Let D be a positive definite $n\times n$ diagonal matrix and P a $n \times n$ permutation matrix. Then

a. The operation $\bullet \mapsto D \bullet D$ defines a bijection from $\mathbb{R}^{n\times n}$ onto itself which induces also bijections of from $\mathcal{S}^n$ onto itself and from $\mathcal{S}^n_+$ onto itself and similarly bijections of the families of extreme rays of these cones onto themselves.
b. The cones FW^n_k and $(FW^n_k)^*$ are by $\bullet \mapsto D\bullet D$ also bijectively mapped onto themselves and analogous claims are true for the families of respective extreme rays.
c. The claims of parts a and b remain literally true if we replace in them the corresponding operation by $\bullet \mapsto P^T \bullet P$.

Proof: Note that the operations $\bullet \mapsto D\bullet D$ and $\bullet \mapsto P^T\bullet P$ are clearly linear maps and since D and P are invertible, they are bijections. This means that they map extreme rays to extreme rays, and we just have to show that they let the cones of interest invariant.

Note that $A \in \mathcal{S}_+^n$, if and only if we can write it as VV^T, and both DVV^TD^T and P^TVV^TP can be directly seen to be still positive semidefinite. Moreover, if V has at most k nonzero entries per column, so do DV and P^TV, so the operations also preserve FW_k^n. To see that it preserves $(FW_k^n)^*$ just note that the $k \times k$ submatrices of the image of A are just images of the $k \times k$ submatrices of A by maps of these types, so if all were positive semidefinite in A they will all be positive semidefinite in the image of A, showing invariance of $(FW_k^n)^*$.

■

4.1. Characterizing extreme rays of $(FW_3^4)^*$. We start this section with the following lemma.

Lemma 4.5. *If Q is positive semidefinite 4×4 and $Q \notin FW_3^4$ then there exists a symmetric 4×4 matrix B and a positive definite diagonal matrix D such that*

i. *B spans an extreme ray in $(FW_3^4)^*$;*
ii. *B has the diagonal entries all equal to 1;*
iii. *$\langle DQD, B\rangle < 0$.*

Proof: Suppose first that for all $B \in (FW_3^4)^*$ we had $\langle Q, B\rangle \geq 0$. This would show by definition of dual cones, that $Q \in (FW_3^4)^{**}$. But we know by Proposition 3.2 that $(FW_3^4)^{**} = FW_3^4$. So we get a contradiction. So there exists a matrix $B \in (FW_3^4)^*$ such that $\langle Q, B\rangle < 0$. Now every matrix in $(FW_3^4)^*$ is a finite positive linear combination of some matrices that span extreme rays of $(FW_3^4)^*$. Hence for at least one of these extreme-ray-defining matrices we again must have the inequality. We call this extremal matrix now B.

By hypothesis $Q \in \mathcal{S}_+^4$; so $\langle Q, B\rangle < 0$, implies $B \notin \mathcal{S}_+^4$. Since every diagonal entry of B is a diagonal entry of some principal 3×3 submatrix of B, and these are positive semidefinite, the diagonal entries of B are all nonnegative. Assume now that some diagonal entry, say $b_{11} = 0$. Then by a standard argument, see e.g. [5, p. 400], all the entries of column 1 and row 1 would be 0. The nonzero entries of B are thus found in B_{234}, which is positive semidefinite. Hence B is psd, a contradiction.

Thus we have $b_{11}, b_{22}, b_{33}, b_{44} > 0$ and the diagonal matrix

$$D = \mathrm{Diag}(b_{11}^{-1/2}, b_{22}^{-1/2}, b_{33}^{-1/2}, b_{44}^{-1/2})$$

is well defined. By the observation before, the matrix $B' = DBD$ will be again an extreme ray of $(FW_3^4)^*$ and it is clear that $B' = (b_{ii}^{-1/2} b_{ij} b_{jj}^{-1/2})_{i,j=1}^4$ is a matrix which has only ones on the diagonal. Finally $\langle D^{-1}QD^{-1}, B'\rangle = \langle Q, B\rangle < 0$. Thus renaming D^{-1}, B' to D, B, respectively, we get the claim. ■

Based on the results that we have proven so far, we can fully characterize the extreme rays of $(FW_3^4)^*$.

Proposition 4.6. *Let B be a symmetric 4×4 not positive semidefinite matrix which spans an extreme ray of $(FW_3^4)^*$, then for some $a, c \in]-\pi, \pi[\setminus\{0\}$ some permutation P and some nonsingular diagonal matrix D, the matrix B has the following form*

$$DPBP^TD^T = \begin{bmatrix} 1 & \cos(a) & \cos(a-c) & \cos(c) \\ \cos(a) & 1 & \cos(c) & \cos(a-c) \\ \cos(a-c) & \cos(c) & 1 & \cos(a) \\ \cos(c) & \cos(a-c) & \cos(a) & 1 \end{bmatrix}.$$

Proof: First note that by the considerations of the previous lemma, we can always assume a scaling that takes all diagonal entries of B to 1. Furthermore, by assumption, $B \in (FW_3^4)^*$ which means all of its 3×3 and accordingly its 2×2 principal submatrices are psd, hence for all $i, j \in \{1, 2, 3, 4\}$, $0 \leq b_{ii}b_{jj} - b_{ij}^2 = 1 - b_{ij}^2$ and hence $b_{ij}^2 \leq 1$ for all pairs (i, j). Therefore, using that the image of the cosine function is $[-1, 1]$, we can write B as

$$B = \begin{bmatrix} 1 & \cos(a) & \cos(b) & \cos(c) \\ \cos(a) & 1 & b_{23} & b_{24} \\ \cos(b) & b_{23} & 1 & b_{34} \\ \cos(c) & b_{24} & b_{34} & 1 \end{bmatrix},$$

for some $a, b, c \in [-\pi, \pi]$. The possibilities, $a, b, c \in \{-\pi, 0, \pi\}$ will be excluded below. Now since B spans an extreme ray of $(FW_3^4)^*$, by Theorem 4.4 all of its 3×3 principal submatrices have rank 2 and hence have zero determinant. Hence by starting with principal submatrix B_{123}, we have

$$0 = \det\left(\begin{bmatrix} 1 & \cos(a) & \cos(b) \\ \cos(a) & 1 & b_{23} \\ \cos(b) & b_{23} & 1 \end{bmatrix}\right) = 1 - b_{23}^2 - \cos(a)^2 + 2b_{23}\cos(a)\cos(b) - \cos(b)^2.$$

By solving this quadratic equation for b_{23} one finds

$$\begin{aligned} b_{23} &\in \{\cos(a)\cos(b) \pm \sqrt{1-\cos(a)^2-\cos(b)^2+\cos(a)^2\cos(b)^2}\} \\ &= \{\cos(a)\cos(b) \pm \sqrt{(1-\cos(a))^2(1-\cos(b)^2}\} \\ &= \{\cos(a)\cos(b) \pm \sin(a)\sin(b)\} \\ &= \{\cos(a \mp b)\}. \end{aligned}$$

We do completely analogous calculations for principal submatrices B_{134} and B_{124} and obtain $b_{34} \in \{\cos(b \pm c)\}$ and $b_{24} \in \{\cos(a \pm c)\}$, respectively. Now we have eight matrices that emerge from choosing one of the symbols $+$ or $-$ in each of the patterns $a \pm b, a \pm c, b \pm c$ existent in the matrix below by taking care that the symmetry of the matrix is preserved.

$$\begin{bmatrix} 1 & \cos(a) & \cos(b) & \cos(c) \\ \cos(a) & 1 & \cos(a \pm b) & \cos(a \pm c) \\ \cos(b) & \cos(a \pm b) & 1 & \cos(b \pm c) \\ \cos(c) & \cos(a \pm c) & \cos(b \pm c) & 1 \end{bmatrix}.$$

The following table indicates in the first column the possible selections of signs in $a \pm b, a \pm c, b \pm c$, respectively; and in the second column and the third column the determinants of the respective matrices B_{234} and B.

$x \pm y$	$\det(B_{234})$	$\det(B)$
$+,+,+$	$4\sin(a)\sin(b)\sin(c)\sin(a+b+c)$	$-4\sin(a)^2\sin(b)^2\sin(c)^2$
$+,+,-$	0	0
$+,-,+$	0	0
$+,-,-$	$-4\sin(a)\sin(b)\sin(a+b-c)\sin(c)$	$-4\sin(a)^2\sin(b)^2\sin(c)^2$
$-,+,+$	0	0
$-,+,-$	$-4\sin(a)\sin(b)\sin(c)\sin(a-b+c)$	$-4\sin(a)^2\sin(b)^2\sin(c)^2$
$-,-,+$	$4\sin(a)\sin(b)\sin(a-b-c)\sin(c)$	$-4\sin(a)^2\sin(b)^2\sin(c)^2$
$-,-,-$	0	0

Now assume one of the reals a, b, c is 0 or π. Then the table shows that all entries in columns two and three vanish. Hence the matrix B in this case is positive semidefinite. Thus in order that B, as required, is not positive semidefinite it is necessary that $a, b, c \neq \{-\pi, 0, \pi\}$. In this case column 3 guarantees we get a not positive semidefinite matrix B in exactly the cases of the sign choices $+++, +--, -+-, --+$ for $a \pm b, a \pm c, b \pm c$, respectively. The matrices corresponding to rows, 2,3,5,8 of the table are positive semidefinite independent of choices a, b, c.. Explicitly this means that B must be one of the following four matrices

$$\begin{bmatrix} 1 & \cos(a) & \cos(b) & \cos(c) \\ \cos(a) & 1 & \cos(a+b) & \cos(a+c) \\ \cos(b) & \cos(a+b) & 1 & \cos(b+c) \\ \cos(c) & \cos(a+c) & \cos(b+c) & 1 \end{bmatrix}, \begin{bmatrix} 1 & \cos(a) & \cos(b) & \cos(c) \\ \cos(a) & 1 & \cos(a+b) & \cos(a-c) \\ \cos(b) & \cos(a+b) & 1 & \cos(b-c) \\ \cos(c) & \cos(a-c) & \cos(b-c) & 1 \end{bmatrix},$$

$$\begin{bmatrix} 1 & \cos(a) & \cos(b) & \cos(c) \\ \cos(a) & 1 & \cos(a-b) & \cos(a+c) \\ \cos(b) & \cos(a-b) & 1 & \cos(b-c) \\ \cos(c) & \cos(a+c) & \cos(b-c) & 1 \end{bmatrix}, \begin{bmatrix} 1 & \cos(a) & \cos(b) & \cos(c) \\ \cos(a) & 1 & \cos(a-b) & \cos(a-c) \\ \cos(b) & \cos(a-b) & 1 & \cos(b+c) \\ \cos(c) & \cos(a-c) & \cos(b+c) & 1 \end{bmatrix}.$$

Note by substituting the letter c by $-c$ in the left upper matrix we get the right upper matrix because $\cos(-c) = \cos(c)$. Exactly the same remark leads from the left lower matrix to the right lower matrix. Finally note that after doing the transpositions of rows and columns $3, 4$, the upper left matrix shown takes the form

$$\begin{bmatrix} 1 & \cos(a) & \cos(c) & \cos(b) \\ \cos(a) & 1 & \cos(a+c) & \cos(a+b) \\ \cos(c) & \cos(a+c) & 1 & \cos(b+c) \\ \cos(b) & \cos(a+b) & \cos(b+c) & 1 \end{bmatrix}$$

and after changing the name of variable c to $-b$ and of variable b to c and noting that $\cos(b-c) = \cos(c-b)$ we see we have obtained the following matrix, which is the left lower matrix.

$$\begin{bmatrix} 1 & \cos(a) & \cos(b) & \cos(c) \\ \cos(a) & 1 & \cos(a-b) & \cos(a+c) \\ \cos(b) & \cos(a-b) & 1 & \cos(c-b) \\ \cos(c) & \cos(a+c) & \cos(c-b) & 1 \end{bmatrix}.$$

Hence we have one form and its possible permutations. We focus at the right lower matrix as the standard. Now we know that the determinant of the submatrix B_{234} is $4\sin(a)\sin(b)\sin(a-b-c)\sin(c)$. We know by Theorem 4.4 that all 3×3 principal minors must vanish, so $\det(B_{234}) = 0$ which happens if and only if $b = a - c + k\pi$. Substituting this in the start matrix B we get the following two forms

$$\begin{bmatrix} 1 & \cos(a) & \delta\cos(a-c) & \cos(c) \\ \cos(a) & 1 & \delta\cos(c) & \cos(a-c) \\ \delta\cos(a-c) & \delta\cos(c) & 1 & \delta\cos(a) \\ \cos(c) & \cos(a-c) & \delta\cos(a) & 1 \end{bmatrix},$$

with $\delta = \pm 1$. But note that these are the same up to scaling by the diagonal matrix Diag$(1, 1, -1, 1)$. So we may assume $\delta = 1$, finishing the proof. ∎

5. Factor width k matrices and sums of k-nomial squares polynomials

Ahmadi and Majumdar in [1] considered the polynomial

$$p_n^a = (\sum_{i=1}^{n} x_i)^2 + (a-1)\sum_{i=1}^{n} x_i^2$$

when $n = 3$ and proved that if $a < 2$ then no nonnegative integer r can be chosen so that $(x_1^2 + x_2^2 + x_3^2)^r p_3^a$ is a sum of squares of binomials, although it is clearly nonnegative for $a \geq 1$.

In this section, we give negative results along the same lines. We first characterize when p_n^a is a sum of k-nomial squares, then we show that $p_{n,r}^a$, that is, the multiplication of p_n^a with $(\sum_{i=1}^{n} x_i^2)^r$, is a sum of k-nomial squares if and only if this is the case for $r = 0$. Before presenting our proof, we make the connection between factor width k matrices and sums of k-nomial squares polynomials which will be used along the proof. In the following proposition $z(x)_d$ is the vector of all monomials of degree d, arranged in some order, in the variables figuring in x.

Proposition 5.1. *A multivariate polynomial $p(x)$ of degree $2d$ is a sum of k-nomial squares (soks) if and only if it can be written in the form $p(x) = z(x)_d^T Q z(x)_d$ with matrix $Q \in FW_k^{\binom{n+d-1}{d}}$.*

Proof: Consider an expression $a_1 m_1 + \cdots + a_k m_k$ with reals $a_1, \ldots, a_k$ and monomials $m_1, \ldots, m_k$. Note that monomials $m_1, \ldots, m_k$ occur necessarily in the column $z(x)_d$ at positions $i_1, \ldots, i_k$, say. Construct a column q of size $\binom{n+d}{d}$ by putting into positions $i_1, \ldots, i_k$ respectively the reals $a_1, \ldots, a_k$, and into all other positions 0s. Then evidently $z(x)_d^T q = a_1 m_1 + \cdots + a_k m_k$, and consequently $z(x)_d^T q q^T z(x)_d = (a_1 m_1 + \cdots + a_k m_k)^2$. Consequently, a polynomial which is a sum of, say, t squares of k-nomials can be written as $z(x)_d^T Q z(x)_d$, where $Q = \sum_{\nu=1}^{t} q_\nu q_\nu^T$, with suitable columns $q_1, \ldots, q_t$ of size $\binom{n+d}{d}$ each of which has at most k nonzero entries. It follows that Q is a matrix of factor width k. Conversely if Q is of factor width k, then we already know from the beginning of Section 3 that we can write $Q = \sum_{\nu=1}^{t} q_\nu q_\nu^T$ where each column q_ν has at most k nonzero real entries. Clearly from the arguments above follows now that $z(x)_d^T Q z(x)_d$ yields a polynomial which is a finite sum of k-nomial squares. ■

We shall also need the following lemma.

Lemma 5.2. *Consider a quadratic form* $q(x) = x^T Q x$ *and a polynomial* p *related to* q *by* $p = (\sum_{i=1}^{n} (\lambda_i x_i)^2)^r q$. *Then every monomial of* p *has at most two odd degree variables and we have* $p_{(i,j)} = 2(\sum_{i=1}^{n} \lambda_i^2)^r q_{ij}$ *and* $p_0 = (\sum_{i=1}^{n} \lambda_i^2)^r \mathrm{trace(Q)}$ *where* $p_{(i,j)}$ *is the sum of coefficients of the monomials in which* x_i *and* x_j *have odd degree,* p_0 *is the sum of coefficients of even monomials of* p *and* q_{ij} *is the entry* (i,j) *of* Q.

Proof: The quadratic form is

$$q(x) = \sum_{1 \le i,j \le n} x_i q_{ij} x_j = \sum_{i=1}^{n} q_{ii} x_i^2 + \sum_{1 \le i < j \le n} 2 q_{ij} x_i x_j,$$

while by the multinomial theorem we have

$$((\lambda_1 x_1)^2 + \cdots + (\lambda_n x_n)^2)^r = \sum_{i_1 + \cdots + i_n = r} \binom{r}{i_1, \ldots, i_n} (\lambda_1 x_1)^{2i_1} (\lambda_2 x_2)^{2i_2} \ldots (\lambda_n x_n)^{2i_n}.$$

Thus, putting the λs into evidence, by definition of p, we get

$$\begin{aligned} p = & \sum_{(i,\underline{i}) \in J_1} q_{ii} \binom{r}{\underline{i}} \lambda_1^{2i_1} \cdots \lambda_n^{2i_n} \cdot x_1^{2i_1} \cdots x_i^{2i_i+2} \cdots x_n^{2i_n} \\ & + \sum_{((i,j),\underline{i}) \in J_2} 2 q_{ij} \binom{r}{\underline{i}} \lambda_1^{2i_1} \cdots \lambda_i^{2i_n} \cdot x_1^{2i_1} \ldots x_i^{2i_i+1} \ldots x_j^{2i_j+1} \ldots x_n^{2i_n}, \end{aligned}$$

where $\underline{i} = (i_1, \ldots, i_n)$ and, with $|\underline{i}| = i_1 + \cdots + i_n$,

$$\begin{aligned} J_1 &= \{(i, \underline{i}) : i \in \{1, \ldots, n\}, \underline{i} \in \mathbb{Z}^n_{\ge 0}, |\underline{i}| = r\}, \\ J_2 &= \{((i,j), \underline{i}) : 1 \le i < j \le n, \underline{i} \in \mathbb{Z}^n_{\ge 0}, |\underline{i}| = r\}. \end{aligned}$$

From the above equation for p , we recognize that

$$p_{(i,j)} = 2 q_{ij} \sum_{i_1 + \cdots + i_n = r} \binom{r}{i_1, \ldots, i_n} \lambda_1^{2i_1} \cdots \lambda_i^{2i_n} = 2 q_{ij} (\lambda_1^2 + \cdots + \lambda_n^2)^r,$$

again by the multinomial theorem; and similarly we have

$$\begin{aligned} p_0 &= \sum_{i=1}^{n} \sum_{i_1+\cdots+i_n=r} q_{ii} \binom{r}{i_1,\ldots,i_n} \lambda_1^{2i_1}\cdots\lambda_n^{2i_n} \\ &= \sum_{i=1}^{n} q_{ii} \sum_{i_1+\cdots+i_n=r} \binom{r}{i_1,\ldots,i_n} \lambda_i^{2i_1}\cdots\lambda_n^{2i_n} \\ &= (\lambda_1^2+\cdots+\lambda_n^2)^r \mathrm{trace(Q)}. \end{aligned}$$ ∎

In addition, we will make use of the following fact proved in Muir's treatise [7, p 61].

Lemma 5.3. *For the determinant at the left hand side below which has only letters a except on the diagonal, we have*

$$\begin{vmatrix} b_1 & a & \ldots & a \\ a & b_2 & \ldots & a \\ \vdots & \vdots & \ddots & \vdots \\ a & a & \ldots & b_n \end{vmatrix} = \prod_{i=1}^{n}(b_i-a) + a\sum_{j=1}^{n}\prod_{i:i\neq j}^{n}(b_i-a)$$

Now we are ready to prove our results regarding Ahmadi and Majumdar's example.

Proposition 5.4. *If $a \geq \frac{n-1}{k-1}$, then p_n^a is a sum of k-nomial squares.*

Proof: The quadratic form p_n^a, can be written as $a\sum_{i=1}^{n} x_i^2 + 2\sum_{i<j} x_i x_j$, so $p = z(x)^T Q z(x)$ by means of the $n\times n$ matrix Q shown.

$$Q = \begin{bmatrix} a & 1 & \cdots & 1 & 1 \\ 1 & a & \cdots & 1 & 1 \\ \vdots & & \ddots & & \vdots \\ 1 & & & & 1 \\ 1 & 1 & \cdots & 1 & a \end{bmatrix}.$$

Now there exist $\binom{n}{k}$ subsets K of cardinality k of the set $\{1,2,\ldots,n\}$. Let $i,j\in\{1,2,\ldots,n\}$. A pair (i,i) lies in exactly $\binom{n-1}{k-1}$ of the sets $K\times K$ while a pair (i,j) with $i\neq j$ lies in $K\times K$ if and only if $\{i,j\}\subseteq K$. It hence lies in exactly $\binom{n-2}{k-2}$ sets $K \times K$. Consider the $k \times k$ matrix B as following

$$B = \binom{n-2}{k-2}^{-1} \begin{bmatrix} \frac{(k-1)a}{n-1} & 1 & \cdots & 1 & 1 \\ 1 & \frac{(k-1)a}{n-1} & \cdots & 1 & 1 \\ \vdots & & \ddots & & \vdots \\ 1 & & & & 1 \\ 1 & 1 & \cdots & 1 & \frac{(k-1)a}{n-1} \end{bmatrix},$$

and define $\iota_K(B)$ to be the $n \times n$ matrix of support $K \times K$ which carries on it the matrix B. Then our arguments yield that $\sum_{K:|K|=k} \iota_K(B) = Q$.

Take an arbitrary $l \times l$ submatrix of the matrix factor of B. By the previous lemma , this submatrix has determinant $(\frac{(k-1)a}{n-1} - 1)^{-1+l})(\frac{(k-1)a}{n-1} - 1 + l)$. It follows from the hypothesis for a that this determinant is nonnegative. So B, and thus $\iota_K(B)$, is a positive semidefinite matrix and Q hence a matrix of factor width $\leq k$ by Proposition 3.1. This means by Proposition 5.1 that p_n^a is a sum of k-nomial squares. ■

Theorem 5.5. *For integers $n \geq 0$ and $r \geq 0$, define*

$$p_{n,r}^a = (\sum_{i=1}^n x_i^2)^r \, p_n^a = (\sum_{i=1}^n x_i^2)^r \cdot \left((\sum_{i=1}^n x_i)^2 + (a-1) \sum_{i=1}^n x_i^2 \right).$$

Then $p_{n,r}^a$ is a sum of k-nomial squares if and only if $p_n^a = p_{n,0}^a$ is a sum of k-nomial squares.

Proof: Clearly, if p_n^a is a so$k$s then $p_{n,r}^a$ is a so$k$s. So we need to show the inverse. Assume that the degree $2(r+1)$ polynomial $p_{n,r}^a$ is a so$k$s. Let $I_{n,r+1} = \{(i_1, \ldots, i_n) \text{ } s.t. \text{ } i_k \in \mathbb{N}_0, \sum_{k=1}^n i_k = r+1\}$ be the set of vectors of exponents in $\mathbb{Z}_{\geq 0}^n$ that occurs in the family of monomials of a homogeneous polynomial of degree $r+1$ in variables $x_1, ..., x_n$. Let this family of monomials be also the one that occurs in $z(x)_{r+1}$.

By Proposition 5.1, we can write

$$p_{n,r}^a = z(x)_{r+1}^T H_{n,r} z(x)_{r+1} \text{ for some } H_{n,r} \in FW_k^{\binom{n+r}{r+1}}.$$

Call an $i \in \mathbb{Z}_{\geq 0}^n$ *even* if it has only even entries and consider now the matrix $B_{n,r} \in \mathbb{R}^{I_{n,r+1} \times I_{n,r+1}}$ given by

$$(B_{n,r})_{ij} = \begin{cases} k-1 & \text{if } i+j \text{ is even,} \\ -1 & \text{otherwise.} \end{cases}$$

We will show now that $B_{n,r} \in (FW_k^{\binom{n+r}{r+1}})^*$; that is we shall prove that every $k \times k$ principal submatrix of $B_{n,r}$ is positive semidefinite, see Proposition 3.2. Since n, r are fixed, we write B and H for matrices $B_{n,r}, H_{n,r}$ respectively.

Note that a sum $i + j$ of such n-uples is even if and only if the sets of positions in i where odd entries occur equals the corresponding set in j. (Example: The 5-uple $i = (1, 0, 0, 3, 2)$ has $\{1, 4\}$ as the set of positions of odd entries.)

So take a $k \times k$ submatrix M of B with rows and columns indexed by the n-uples $i_1, \ldots, i_k$, say. Determine for each n-uple its set of positions of odd entries. Let $S_1, \ldots, S_l$ $(l \leq k)$ be the distinct non empty sets of such positions. Now rearrange the n-uples so that the first few n-uples each have S_1 as set of positions of odd entries, the next few have S_2 as such set of positions, etc. Let $s_1, \ldots, s_l$ be the sizes of these sets. To the rearrangement of the n-uples corresponds a $k \times k$ permutation matrix P such that PMP^T is 'a direct sum of blocks of sizes $s_1 \times s_1, \ldots, s_l \times s_l$ with entries $k - 1$ over a background of -1s'. Formally, for suitable P we can express this as

$$PMP^T = (-1)J_k + k(J_{s_1} \oplus J_{s_2} \oplus \cdots \oplus J_{s_l})$$

This same matrix can be produced as follows. Define $l \times l$ matrix N and $l \times k$ matrix C by

$$N = (-1)J_l + kI_l = \begin{bmatrix} k-1 & -1 & \ldots & -1 \\ -1 & k-1 & \ldots & -1 \\ \vdots & & \ddots & \\ -1 & & \ldots & k-1 \end{bmatrix},$$

$$C = \begin{pmatrix} 1 & 1 & \cdots & 1 & & & & & & & & \\ & & & & 1 & 1 & \cdots & 1 & & & & \\ & & & & & & & & .... & & & \\ & & & & & & & & & 1 & 1 & \cdots & 1 \end{pmatrix}$$

where rows, $1, 2, ..., l$ of C have, respectively, $s_1, s_2, ..., s_l$ entries equal to 1. Check that then $PMP^T = C^T NC$. Now, again by Lemma 5.3, N is positive semidefinite, Hence M will be psd. Since the $k \times k$ submatrix M of B was arbitrary, we are done with proving that $B \in (FW_k^{\binom{n+r}{r+1}})^*$. By definition of the concept of a dual cone, we have $\langle B, H \rangle \geq 0$, and by the definitions of

$\langle , \rangle$, H, and B, hence

$$\langle B, H\rangle = (k-1)\sum_{i,j:i+j \text{ even}} h_{ij} + (-1)\sum_{i,j:i+j \text{ non-even}} h_{ij} \geq 0.$$

Since the quadratic form underlying our construction of $p^a_{n,r}$ is $p^a_n = a\sum_{i=1}^n x_i^2 + 2\sum_{i<j} x_i x_j$, and it has the defining matrix Q mentioned in the previous proposition, we get by Lemma 5.2 that

$$\begin{aligned}\sum_{i,j:i+j \text{ even}} h_{ij} &= n^r \mathrm{trace\,Q} = \mathrm{n^{r+1}a};\\ \sum_{i,j:i+j \text{ non}-\text{even}} h_{ij} &= 2n^r \times \sum_{1\leq i<j\leq n} q_{ij} = 2n^r\frac{1}{2}n(n-1) = n^{r+1}(n-1).\end{aligned}$$

Hence the inequality above reads $(k-1)n^{r+1}a \geq n^{r+1}(n-1)$ or $a \geq \frac{n-1}{k-1}$, which means by the previous proposition that p^a_n is a sum of k-nomial squares. ■

6. A quadratic form that is not sum of squares of binomials (so2s) is not r-so2s for any r

For the case of $k = 2$, sums of squares of k-nomials are also known as sums of binomial squares [4] or scaled diagonally dominant sums of squares (SDSOS) [1]. In this section we will try to generalize Ahmadi And Majumdar's counterexample in this setting. More concretely we will prove that the standard multipliers are useless for certifying nonnegativity of quadratics using sobs, as we prove that a quadratic form is r-sobs, if and only if it is sobs. But before we proceed further, we shall need the following proposition.

Proposition 6.1. [4, Corollary 2.8]. *Given a quadratic form*

$$q(x) = \sum_{i=1}^n q_i x_i^2 + \sum_{i<j} q_{ij} x_i x_j,$$

then if $\hat{q}(x) = \sum_{i=1}^n q_i x_i^2 - \sum_{i<j} |q_{ij}| x_i x_j$ *is nonnegative,* $q(x)$ *is a sum of binomial squares.*

This is enough to show the previously announced result.

Theorem 6.2. *Let* $q(x) = q(x_1, \ldots, x_n)$ *be a real quadratic form and let* $r \in \mathbb{Z}_{\geq 0}$. *Then if* $q(x)(x_1^2 + \cdots + x_n^2)^r$ *is a sum of binomial squares, so is* $q(x)$ *itself.*

Proof: Assume that $q(x)(x_1^2 + \cdots + x_n^2)^r$ is a sum of binomial squares. We will prove that $q(x)$ is a sum of binomial squares. Write

$$q(x) = \sum_{i=1}^{n} a_i x_i^2 + \sum_{1 \le i < j \le n} d_{ij} x_i x_j,$$

say. Then considerations as in the proof of Lemma 5.2 yield

$$\begin{aligned} q(x).(x_1^2 + \cdots + x_n^2)^r = & \sum_{(i,\underline{i}) \in J_1} a_i \binom{r}{\underline{i}} x_1^{2i_1} \cdots x_i^{2i_i+2} \cdots x_n^{2i_n} \\ & + \sum_{((i,j),\underline{i}) \in J_2} d_{ij} \binom{r}{\underline{i}} x_1^{2i_1} \cdots x_i^{2i_i+1} \cdots x_j^{2i_j+1} \cdots x_n^{2i_n}, \end{aligned}$$

where again,

$$J_1 = \{(i, \underline{i}) : i \in \{1, \ldots, n\}, \underline{i} \in \mathbb{Z}^n_{\ge 0}, |\underline{i}| = r\},$$

$$J_2 = \{((i,j), \underline{i}) : 1 \le i < j \le n, \underline{i} \in \mathbb{Z}^n_{\ge 0}, |\underline{i}| = r\}.$$

Now the monomials of degree r are of the form $x_1^{i_1} x_2^{i_2} \ldots x_n^{i_n}$ with $i_1 + \cdots + i_n = r$. There are as we know $L = \binom{r+n-1}{r}$ such monomials. We order these and denote them by $m_1, \ldots, m_L$. Every binomial is of the form $(\alpha_{ij} m_i + \beta_{ij} m_j)$ with some selection of i, j with $1 \le i < j \le L$. By defining suitable α_{ii}, we can thus assume the binomials are of the form $\alpha_{ii} m_i$, $1 \le i \le L$ or $(\alpha_{ij} m_i + \beta_{ij} m_j)$ with $1 \le i < j \le L$. A sum of binomial squares is thus given as

$$\begin{aligned} & \sum_{i=1}^{L} \alpha_{ii}^2 m_i^2 + \sum_{1 \le i < j \le L} (\alpha_{ij} m_i + \beta_{ij} m_j)^2 \\ = & \sum_{i=1}^{L} \alpha_{ii}^2 m_i^2 + \sum_{i<j} \alpha_{ij}^2 m_i^2 + \sum_{i<j} \beta_{ij}^2 m_j^2 + \sum_{1 \le i < j \le L} 2\alpha_{ij} \beta_{ij} m_i m_j \\ = & \sum_{i=1}^{L} (\alpha_{ii}^2 + \alpha_{i,i+1}^2 + \ldots + \alpha_{iL}^2 + \beta_{1i}^2 + \ldots \beta_{i-1,i}^2) m_i^2 + \sum_{1 \le i < j \le L} 2\alpha_{ij} \beta_{ij} m_i m_j. \end{aligned}$$

Now assuming, as we do, that $q(x)(x_1^2 + \cdots + x_n^2)^r$ is a sobs, by means of comparison of coefficients, we get a system of $|J_1| + |J_2|$ equations between reals. It is easily seen that these equations can be obtained as follows: For each $(i, \underline{i}) \in J_1$ define

$$T(i, \underline{i}) = \{\text{indices } t \in \{1, \ldots, L\} \text{ for which } m_t^2 = x_1^{2i_1} \cdots x_i^{2i_i+2} \cdots x_n^{2i_n}\},$$

$$S(i, \underline{i}) = \{\text{pairs } s_1 < s_2 \text{ so that } m_{s_1} m_{s_2} = x_1^{2i_1} \cdots x_i^{2i_i+2} \cdots x_n^{2i_n}\}$$

and write the equation

$$a_i \binom{r}{\underline{i}} = \sum_{t \in T(i,\underline{i})} (\alpha_{tt}^2 + \ldots + \alpha_{tL}^2 + \beta_{1t}^2 + \ldots + \beta_{t-1,t}^2) + \sum_{(s_1,s_2) \in S(i,\underline{i})} 2\alpha_{s_1 s_2} \beta_{s_1 s_2}$$

for each $((i,j), \underline{i}) \in J_2$, let

$$S'((i,j), \underline{i}) = \{\text{pairs } s'_1 < s'_2 \text{ so that } m_{s'_1} m_{s'_2} = x_1^{2i_1} \ldots x_i^{2i_i+1} \ldots x_j^{2i_j+1} \ldots x_n^{2i_n}\},$$

and write the equation

$$d_{ij} \binom{r}{\underline{i}} = \sum_{s'_1, s'_2 \in S'((i,j),\underline{i})} 2\alpha_{s'_1 s'_2} \beta_{s'_1 s'_2}.$$

Every system of reals

$$(\{a_i\}_{i=1}^n, \{d_{ij}\}_{i,j=1}^n, \{\alpha_{ij}\}_{1 \le i \le j \le L}, \{\beta_{ij}\}_{1 \le i < j \le L})$$

which satisfies the system of equations gives rise to a quadratic form q and binomials so that $q(x)(x_1^2 + \cdots + x_n^2)^r$ is a sum of squares of these binomials. Now if we have a system of reals satisfying the system, then we can find a particular new solution by replacing the d_{ij} which are positive by $-d_{ij}$ and simultaneously replacing the $\beta_{s'_1 s'_2}$ for which $s'_1, s'_2 \in S'((i,j), \underline{i})$ by $-\beta_{s'_1 s'_2}$. Indeed note that the sets $S'((i,j), \underline{i})$ are disjoint from the sets $S(i, \underline{i})$ and $(-\beta_{s'_1 s'_2})^2 = (\beta_{s'_1 s'_2})^2$, hence the first set of $|J_1|$ equations will again be satisfied. What concerns the second set of equations we note that the sets $S'((i,j), \underline{i})$ are also mutually disjoint, because a choice (s'_1, s'_2) defines via forming $m_{s'_1} m_{s'_2}$ a unique power product

$$x_1^{2i_1} \ldots x_i^{2i_i+1} \ldots x_j^{2i_j+1} \ldots x_n^{2i_n}$$

with exactly two odd exponents determining i, j and then $\underline{i}$. In other words (s'_1, s'_2) lives in only one of the sets $S'((i,j), \underline{i})$ hence carrying through the replacements indicated we change the sign at the left hand side of equation if and only if we change the sign of the corresponding right hand side. We therefore satisfy also the second group of equations.

The new solution tells us that $\hat{q}(x)(x_1^2 + \cdots + x_n^2)^r$ is a sum of squares of binomials where

$$\hat{q}(x) = \sum_{i=1}^{n} a_i x_i^2 - \sum_{1\le i<j\le n} |d_{ij}| x_i x_j.$$

Now since the multiplier is evidently positive definite, $\hat{q}$ is nonnegative. Hence by Proposition 6.1, q is a sum of squares of binomials. ■

7. Factor width 3 matrices and sums of trinomial squares

The purpose of this section is to show that if a quarternary quadratic form $q(w, x, y, z)$ is not a sum of squares of trinomials then, given any positive integer r, the form $(w^2+x^2+y^2+z^2)^r \cdot q$ is not a sum of squares of trinomials. In fact it will be necessary to show more generally that for nonzero reals $\lambda_1, \lambda_2, \lambda_3, \lambda_4$, the form $(\lambda_1^2 w^2 + \lambda_2^2 x^2 + \lambda_3^2 y^2 + \lambda_4^2 z^2)^r \cdot q$ is not a sum of squares of trinomials.

Proposition 7.1. *Let $\underline{x} = [w, x, y, z]^\top$ and let $q = \underline{x}^T Q \underline{x}$ be a psd quadratic form and B a matrix such that B spans an extreme ray in $(FW_3^4)^*$ and $\langle Q, B\rangle < 0$. Then the degree $(2r+2)$ form $p = (\lambda_1^2 w^2 + \lambda_2^2 x^2 + \lambda_3^2 y^2 + \lambda_4^2 z^2)^r q$ is not a sum of trinomial squares, for any, not all zero, reals $\lambda_1, \lambda_2, \lambda_3, \lambda_4$.*

Proof: The inequality in the hypothesis implies that B is not psd. In addition, it spans an extreme ray, hence by Proposition 4.6, for some permutation P and non singular matrix D and some $a, c \in]-\pi, \pi[\setminus\{0\}$ it has the following form

$$B_2 = DPBP^TD^T = \begin{bmatrix} 1 & \cos(a) & \cos(a-c) & \cos(c) \\ \cos(a) & 1 & \cos(c) & \cos(a-c) \\ \cos(a-c) & \cos(c) & 1 & \cos(a) \\ \cos(c) & \cos(a-c) & \cos(a) & 1 \end{bmatrix}.$$

We now have the inequality $0 > \langle Q, B\rangle = \langle P^TD^TQDP, B_2\rangle$. We work with the new quadratic form q_{new} defined by $q_{\mathrm{new}} = x^TP^TD^TQDPx$ and show that given any $\lambda \in (\mathbb{R}^*)^4 \setminus \{0\}$, we have that the associated quartic form $p_{\mathrm{new}} = (\lambda_1^2 w^2 + \lambda_2^2 x^2 + \lambda_3^2 y^2 + \lambda_4^2 z^2)^r q_{\mathrm{new}}$, for any $\lambda_1, \lambda_2, \lambda_3, \lambda_4$ is not a sum of trinomial squares. Since the property 'not being a sum of trinomial squares for any λ' is invariant under permutations and scalings of the variables in q_{new}, we shall get the claim concerning the original p, q. For simplicity of notation be aware that *we redefine* $(Q, B) := (P^TD^TQDP, B_2)$ and $(p, q) := (p_{\mathrm{new}}, q_{\mathrm{new}})$. The original Q, B, p, q will not play any further role in this proof.

The polynomial p is of degree $2r+2$. From Theorem 5.1 we know that p has a, usually nonunique, representation $p = z(x)_{r+1}^T Q' z(x)_{r+1}$, where $z(x)_{r+1}$ collects all monomials of degree $r+1$ and hence Q' is an $\binom{r+4}{3} \times \binom{r+4}{3}$ matrix. We define the matrix $B' = (b'_{ij})$ as follows (where we use for the moment as the most natural indexation, the one given by the vectors of exponents of the monomials), where $i, j \in \mathbb{Z}^4_{\geq 0}$ are uples with $|i| = |j| = r+1$ so that B' is also an $\binom{r+4}{3} \times \binom{r+4}{3}$ matrix:

$$b'_{ij} = \begin{cases} b_{kl} & \text{iff } i+j \text{ has two odd entries exactly in positions } k \neq l \\ 1 & \text{iff } i+j \text{ has only even entries} \\ 0 & \text{iff } i+j \text{ has 1 or 3 odd entries} \\ \omega & \text{iff } i+j \text{ has only odd entries} \end{cases}$$

(The case that $i+j$ has exactly 1 or 3 odd entries can actually not happen in case $|i| = |j|$, but we will need the given rules below also in cases where $|i| \neq |j|$.) We will show that $B' \in (FW_3^{\binom{r+4}{3}})^*$, and then that $\langle B', Q' \rangle < 0$, thus showing $Q' \notin FW_3^{\binom{r+4}{3}}$, and hence showing by Propositions 3.2 and 5.1 that p is not a sum of squares of trinomials. We will then see from the fact that being a sum of squares of trinomials is invariant under permutations, that the original p is also not a sum of squares of trinomials.

To any string of exponents $i = (i_1, i_2, i_3, i_4) \in \mathbb{Z}^4_{\geq 0}$ we can associate a unique 4-uple $\varepsilon = \varepsilon(i) = (\varepsilon_1, \varepsilon_2, \varepsilon_3, \varepsilon_4) \in \{0,1\}^4$ defined by $i_\nu \equiv \varepsilon_\nu \mod 2$.

To prove that $B' \in (FW_3^{\binom{r+4}{3}})^*$, note that its entries depend only on $\varepsilon(i + j) = \varepsilon(i) + \varepsilon(j)$ (computed in $\mathbb{Z}_2$).

If $|i|$ is even then the only 4-uples possible for $\varepsilon(i)$ are:

$$0000, 1100, 1010, 1001, 0110, 0101, 0011, 1111.$$

If $|i|$ is odd then the only 4-uples possible for $\varepsilon(i)$ are:

$$1000, 0100, 0010, 0001, 1110, 1101, 1011, 0111.$$

The table below is the modulo 2 addition table for 4-uples $\varepsilon(i)$ with $|i|$ even (for example $1100 + 1001 = 0101$). The reader verifies that precisely the same addition table would be obtained when the first line and the first column would be replaced by the 4-uples $\varepsilon(i)$ for which $|i|$ is odd. If we replace the 4-uples of the inner part of this table according to the rules given for the construction of matrix B' we get the matrix that follows the table. For example to 0101 corresponds b_{24}. That matrix can serve as a look-up table for the construction of (sub)matrices of B'.

+	0000	1100	1010	1001	0110	0101	0011	1111
0000	0000	1100	1010	1001	0110	0101	0011	1111
1100	1100	0000	0110	0101	1010	1001	1111	0011
1010	1010	0110	0000	0011	1100	1111	1001	0101
1001	1001	0101	0011	0000	1111	1100	1010	0110
0110	0110	1010	1100	1111	0000	0011	0101	1001
0101	0101	1001	1111	1100	0011	0000	0110	1010
0011	0011	1111	1001	1010	0101	0110	0000	1100
1111	1111	0011	0101	0110	1001	1010	1100	0000

$$\begin{array}{cccccccc}
1 & b_{12} & b_{13} & b_{14} & b_{23} & b_{24} & b_{34} & \omega \\
b_{12} & 1 & b_{23} & b_{24} & b_{13} & b_{14} & \omega & b_{34} \\
b_{13} & b_{23} & 1 & b_{34} & b_{12} & \omega & b_{14} & b_{24} \\
b_{14} & b_{24} & b_{34} & 1 & \omega & b_{12} & b_{13} & b_{23} \\
b_{23} & b_{13} & b_{12} & \omega & 1 & b_{34} & b_{24} & b_{14} \\
b_{24} & b_{14} & \omega & b_{12} & b_{34} & 1 & b_{23} & b_{13} \\
b_{34} & \omega & b_{14} & b_{13} & b_{24} & b_{23} & 1 & b_{12} \\
\omega & b_{34} & b_{24} & b_{23} & b_{14} & b_{13} & b_{12} & 1
\end{array}$$

After having imposed some order on the set of 4-uples i of 1-norm $|i| = 1+r$ one can construct the matrix B'. Consider now selecting three distinct 4-uples i, j, k of 1-norm $1 + r$ and selecting in the matrix B' the 3×3 submatrix determined by this selection. If i precedes j precedes k in the ordering of the 4-uples the obtained 3×3 matrix is the matrix at the left. Its entries are, as mentioned, completely determined by the matrix at the right

$$\begin{pmatrix} b'_{ii} & b'_{ij} & b'_{ik} \\ b'_{ji} & b'_{jj} & b'_{jk} \\ b'_{ki} & b'_{kj} & b'_{kk} \end{pmatrix} \qquad \begin{pmatrix} \varepsilon(i+i) & \varepsilon(i+j) & \varepsilon(i+k) \\ \varepsilon(j+i) & \varepsilon(j+j) & \varepsilon(j+k) \\ \varepsilon(k+i) & \varepsilon(k+j) & \varepsilon(k+k) \end{pmatrix},$$

from which it can be constructed using the above look-up table. Hence the 3×3 submatrix of B' is simply permutation equivalent to a principal 3×3 submatrix and it is sufficient to show that all principal 3×3 submatrices of the look-up table are positive semidefinite. To see this note first that the left upper 4×4 matrix of the look-up table coincides with B. More generally all principal 3×3 submatrices of the look up table which do not contain an ω are permutation equivalent to 3×3 principal submatrices of B and hence are automatically positive semidefinite. The 3×3 principal submatrices containing ω stem from selecting sets of three line indices which contain one of the sets $\{1,8\},\{2,7\},\{3,6\},\{4,5\}$. These matrices are permutation equivalent to one of the following matrices:

$$\begin{bmatrix} 1 & \omega & b_{12} \\ \omega & 1 & b_{34} \\ b_{12} & b_{34} & 1 \end{bmatrix}, \quad \begin{bmatrix} 1 & \omega & b_{14} \\ \omega & 1 & b_{23} \\ b_{14} & b_{23} & 1 \end{bmatrix}, \quad \begin{bmatrix} 1 & \omega & b_{13} \\ \omega & 1 & b_{24} \\ b_{13} & b_{24} & 1 \end{bmatrix}.$$

So it is sufficient to find an $\omega \in \mathbb{R}$ such that these matrices are positive semidefinite. To see this, the easiest choice is to put $\omega = 1$. This is a universal choice valid for all $0 < a, c < \pi$ that result in determinants equal to 0. If one is given explicit real numbers for a, b, c, then putting $\omega = 1-\varepsilon)$ for sufficiently small $\varepsilon > 0$, one will obtain strictly positive definite (sub)determinants. With these checks we have proved that $B' \in (FW_3^{\binom{r+4}{3}})^*$.

We now show the other claim we made for B'.

Claim: There holds $\langle B', Q' \rangle = (\sum_{i=1}^4 \lambda_i^2)^r \langle B, Q \rangle$. Thus $\langle Q', B' \rangle < 0$.

By the definition of the inner product in matrix space, we have to show

$$\sum \{ b'_{ij} q'_{ij} : \ i, j \in \mathbb{Z}^4_{\geq 0}, |i| = |j| = 1 + r \} = (\sum_{i=1}^{4} \lambda_i^2)^r \sum_{i,j=1}^{4} b_{ij} q_{ij}.$$

Now, given $i, j \in \mathbb{Z}^4_{\geq 0}$, $|i| = |j| = 1 + r$, we have of course $|i + j| = 2r + 2$. Furthermore for any such sum $s = i + j$ we have *a priori* exactly one of the following possibilities: all entries are even; exactly two entries are odd; one or three entries are odd; all entries are odd.

Since for an $s \in \mathbb{Z}^4_{\geq 0}$ for which $|s|$ is even it is impossible that s has exactly one or three odd entries, we can write the left side above as follows:

$$\sum_{\substack{|s| = 2r+2 \\ s \text{ has four} \\ \text{even entries}}} \ \sum_{\substack{|i| = |j| = r+1 \\ i+j=s}} b'_{ij} q'_{ij} + \sum_{\substack{|s| = 2r+2 \\ s \text{ has two} \\ \text{odd entries}}} \ \sum_{\substack{|i| = |j| = r+1 \\ i+j=s}} b'_{ij} q'_{ij} + \sum_{\substack{|s| = 2r+2 \\ s \text{ has four} \\ \text{odd entries}}} \ \sum_{\substack{|i| = |j| = r+1 \\ i+j=s}} b'_{ij} q'_{ij}.$$

By the definition of B' given, this is equal to

$$\sum_{\substack{|s| = 2r+2 \\ s \text{ has four} \\ \text{even entries}}} \ \sum_{\substack{|i| = |j| = r+1 \\ i+j=s}} q'_{ij} + \sum_{1 \leq k < l \leq 4} \ \sum_{\substack{|s| = 2r+2 \\ s \text{ has odd} \\ \text{entries at } k,l}} \ \sum_{\substack{|i| = |j| = r+1 \\ i+j=s}} b_{kl} q'_{ij} + \sum_{\substack{|s| = 2r+2 \\ s \text{ has four} \\ \text{odd entries}}} \ \sum_{\substack{|i| = |j| = r+1 \\ i+j=s}} \omega q'_{ij}.$$

Now we remember that by its construction, polynomial p cannot have a monomial with only odd exponents so the third sum is 0. The sum of the coefficients of monomials whose variables have only even powers in p is given by Lemma 5.2 by

$$(\sum_{i=1}^{4} \lambda_i^2)^r (q_{11} + q_{22} + q_{33} + q_{44});$$

while the second sum is

$$\sum_{1 \le k < l \le 4} b_{kl} \sum_{\substack{|s| = 2r+2 \\ s \text{ has odd} \\ \text{entries at } k,l}} \sum_{\substack{|i| = |j| = r+1 \\ i+j=s}} q'_{ij}$$

The inner double sum here can be described exactly as the sum of the coefficients of the monomials of p which have two odd entries at distinct k, l. Hence again by Lemma 5.2 the inner double sum is equal to $2(\sum \lambda_i^2)^r q_{kl}$ and so the sum is

$$2(\sum_{i=1}^{4} \lambda_i^2)^r \sum_{1 \le k < l \le 4} b_{kl} q_{kl} = (\sum_{i=1}^{4} \lambda_i^2)^r \sum_{\substack{1 \le k, l \le 4, \\ k \ne l}} b_{kl} q_{kl}.$$

The claim now follows because $\sum_{i=1}^{4} \lambda_i^2 > 0$.

To conclude the proof we detail an idea we mentioned at the beginning. We have till now shown that whatever the reals $\lambda_1, ..., \lambda_4$, (not all zeros) are, if the polynomial $q_{\text{new}} = x^\top P'^\top Q P' x$, (with Q satisfying the hypotheses) then the polynomial $p_{\text{new}} = (\lambda_1^2 w^2 + \lambda_2^2 x^2 + \lambda_3^2 y^2 + \lambda_4^2 z^2)^r q_{\text{new}}$ is not sum of trinomial squares. Now by its definition $q_{\text{new}}(w, x, y, z) = q(\pi(w), \pi(x), \pi(y), \pi(z))$ where π embodies the permutation matrix P'. Since the property 'to be a sum of squares of trinomials' is evidently invariant under permutations, it follows that $(\lambda_1^2 \pi^{-1}(w)^2 + \lambda_2^2 \pi^{-1}(x)^2 + \lambda_3^2 \pi^{-1}(y)^2 + \lambda_4^2 \pi^{-1}(z)^2)^r q(w, x, y, z)$ is not a sum of trinomial squares for any $\lambda_1, ..., \lambda_4$. Since $\{\pi^{-1}(w), \pi^{-1}(x), \pi^{-1}(y), \pi^{-1}(z)\} = \{w, x, y, z\}$ it follows that $(\lambda_1^2 w^2 + \lambda_2^2 x^2 + \lambda_3^2 y^2 + \lambda_4^2 z^2)^r q(w, x, y, z)$ is not a sum of trinomial squares. ■

We can now extract from the previous result a new theorem of the same general form of Theorems 5.5 and 6.2.

Theorem 7.2. *Assume $r \in \mathbb{Z}_{\ge 0}$. If the quadratic form $q(\underline{x}) = q(w, x, y, z)$ is not a sum of squares of trinomials, then the quarternary form $(w^2 + x^2 + y^2 + z^2)^r q(\underline{x})$ is not a sum of squares of trinomials.*

Proof: If the quadratic form is not positive semidefinite then the claim is trivial. So assume now q is positive semidefinite and let it be written as $q = x^T Qx$. Then Q is positive semidefinite and by Proposition 5.1, $Q \notin FW_3^4$. So there exists $B \in (FW_3^4)^*$ spanning an extreme ray such that $\langle B, Q\rangle < 0$. By Proposition 7.1 it follows that $(\lambda_1^2 w^2+\lambda_2^2 x^2+\lambda_3^2 y^2+\lambda_4^2 z^2)^r q(\underline{x})$ is not a sum of squares of trinomials for any $\lambda_1, \lambda_2, \lambda_3, \lambda_4$. In particular, $(w^2+x^2+y^2+z^2)q(x)$ is not a sum of squares of trinomials. ∎

8. A counterexample

Up to now we established three results (Theorems 5.5, 6.2 and 7.2) that show that quadratics on n variables are r-so$k$s if and only if they are so$k$s under certain assumptions, namely that they are symmetric, that $k = 2$ or that $n \leq 4$. A natural belief that may occur to the reader is that in fact the same would hold without such assumptions. In this section we give a counterexample to that natural conjecture. We give a quadratic form in 5 variables which is not so4s but that becomes so4s after multiplication with $x_1^2 + \cdots + x_5^2$.

Example 8.1. Consider the matrix M given by

$$M = \begin{bmatrix} 49 & -21 & 37 & -37 & -21 \\ -21 & 17 & -21 & 21 & 29 \\ 37 & -21 & 41 & -25 & -33 \\ -37 & 21 & -25 & 41 & 33 \\ -21 & 29 & -33 & 33 & 73 \end{bmatrix}.$$

This matrix is not in FW_4^5. To see this just verify that the matrix

$$A = \begin{bmatrix} 3 & 1 & -2 & 2 & -1 \\ 1 & 3 & 0 & 0 & -1 \\ -2 & 0 & 2 & -1 & 1 \\ 2 & 0 & -1 & 2 & -1 \\ -1 & -1 & 1 & -1 & 1 \end{bmatrix}$$

is in $(FW_4^5)^*$, by checking that all its 4×4 principal submatrices are psd, and note that $\langle A, M\rangle = -1 < 0$.

Consider the quadratic form $q_M = x^T Mx$. By our previous observation, q_M is not so4s. Let then $p_M = (x_1^2 + x_2^2 + x_3^2 + x_4^2 + x_5^2) \cdot q_M$. We claim that p_M is so4s, hence, q_M is 1-so4s. To prove it one would have to provide an exact certificate. One can easily check that $p_M = z(x)_2^T Q z(x)_2$ where

$$Q = \begin{bmatrix}
49 & -21 & 0 & 37 & 0 & 0 & -37 & 0 & -5 & 0 & -21 & 0 & 0 & 0 & 0 \\
-21 & 66 & -21 & -21 & 37 & -11/5 & 21 & -37 & 0 & -17/5 & 29 & -21 & 0 & 0 & 0 \\
0 & -21 & 17 & 0 & -21 & 0 & 0 & 21 & 0 & 0 & 0 & 29 & 0 & 0 & 0 \\
37 & -21 & 0 & 90 & -94/5 & 37 & -20 & 0 & -37 & 0 & -33 & 0 & -14 & 0 & 0 \\
0 & 37 & -21 & -94/5 & 58 & -21 & 0 & -25 & 21 & 0 & 0 & -33 & 29 & 0 & -4 \\
0 & -11/5 & 0 & 37 & -21 & 41 & 0 & 0 & -25 & 0 & -7 & 0 & -33 & 0 & 0 \\
-37 & 21 & 0 & -20 & 0 & 0 & 90 & -88/5 & 37 & -37 & 33 & 0 & 0 & 12 & 0 \\
0 & -37 & 21 & 0 & -25 & 0 & -88/5 & 58 & -21 & 21 & 0 & 33 & 0 & 29 & 17/5 \\
-5 & 0 & 0 & -37 & 21 & -25 & 37 & -21 & 82 & -25 & 0 & 0 & 33 & -33 & -23/5 \\
0 & -17/5 & 0 & 0 & 0 & 0 & -37 & 21 & -25 & 41 & -9 & 0 & 0 & 33 & 0 \\
-21 & 29 & 0 & -33 & 0 & -7 & 33 & 0 & 0 & -9 & 122 & -21 & 37 & -37 & -21 \\
0 & -21 & 29 & 0 & -33 & 0 & 0 & 33 & 0 & 0 & -21 & 90 & -17 & 88/5 & 29 \\
0 & 0 & 0 & -14 & 29 & -33 & 0 & 0 & 33 & 0 & 37 & -17 & 114 & -102/5 & -33 \\
0 & 0 & 0 & 0 & 0 & 0 & -12 & 29 & -33 & 33 & -37 & 88/5 & -102/5 & 114 & 33 \\
0 & 0 & 0 & 0 & -4 & 0 & 0 & 17/5 & -23/5 & 0 & -21 & 29 & -33 & 33 & 73
\end{bmatrix}.$$

It remains to show that this matrix is in fact in FW_4^{15}. In general, such matrices are sums of up to $\binom{15}{4} = 1365$ matrices with 4×4 support, and generating rational decompositions is certainly not trivial. In this case the example was chosen in such a way that numerically we can do it using only 27 such matrices (in fact possibly all with rank one) with supports $K \times K$ with K as follows; we write $1, 2, 4, 7$ instead of $\{1, 2, 4, 7\}$, etc.:

1,2,4,7	1, 2, 4, 11	1, 2, 7, 11	1, 4, 7, 9	2, 3, 5, 8	2, 3, 5, 12
2, 3, 8, 12	2,4,5,6	2, 5, 8, 12	2, 7, 8, 10	3, 5, 8, 12	4, 5, 6, 9
4, 5, 6, 13	4, 5, 9, 13	4,6,11,13	5, 6, 9, 13	5, 12, 13, 15	7, 8, 9, 10
7, 8, 9, 14	7, 10, 11, 14	8, 9, 10, 14	8, 12, 14, 15	9, 13, 14, 15	11, 12, 13, 14
11, 12, 13, 15	11, 12, 14, 15	11, 13, 14, 15			

Since to put the 27 matrices with their floating point entries themselves at this place would be too space consuming, the reader interested to check the example can obtain them by request from the first author.

We did simply a numerical verification, but due to the small size of the calculation we have confidence in the example. Further work would involve rationalizing this certificate, in order to eliminate any remaining doubts.

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