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Hyperorthogonal family of vectors and the associated Gram matrix

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Abstract. A family of non-zero vectors in Euclidean n-space is termed hyperorthogonal if the angle between any two distinct vectors of the family is at least $\pi/2$. Any hyperorthogonal family is finite and contains at most $2n$ vectors. It decomposes uniquely into the union of mutually orthogonal irreducible subfamilies. An equivalent formulation in terms of the associated Gram matrix is given.

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Let n and p be natural numbers. The standard inner product of two vectors $v, w \in \mathbb{R}^n$ is denoted by $\langle v, w \rangle$, and the corresponding norm of v by $\|v\| = \langle v, v \rangle^{1/2}$.

Definition 1. A p-tuple $(v_1, \dots, v_p)$ of vectors in $\mathbb{R}^n \setminus \{0\}$ is said to be *hyperorthogonal* if

$$\langle v_i, v_j \rangle \le 0 \qquad \text{for any two distinct } i, j \in \{1, \dots, p\}.$$

The vectors of a hyperorthogonal p-tuple are of course distinct. A p-tuple $(v_1, \dots, v_p)$ [of vectors] in $\mathbb{R}^n \setminus \{0\}$ is hyperorthogonal if and only if the normalized vectors $v_i/\|v_i\|$, $i \in \{1, \dots, p\}$, form a hyperorthogonal p-tuple (of points) on the unit sphere Σ_n in $\mathbb{R}^n$, in the sense that the spherical distance $d(v_i, v_j) \ge \pi/2$ for any two distinct $i, j \in \{1, \dots, p\}$.

It is shown in Theorem 1 that an irreducible hyperorthogonal p-tuple in $\mathbb{R}^n \setminus \{0\}$ of rank r is maximal if and only if $p = r + 1$. According to Theorem 2 every hyperorthogonal p-tuple decomposes uniquely into the union of mutually orthogonal irreducible hyperorthogonal subtuples. A hyperorthogonal $2n$-tuple on Σ_n is the same as the union of an orthonormal basis $(v_1, \dots, v_n)$ for $\mathbb{R}^n$ and its negative $(-v_1, \dots, -v_n)$. Furthermore, there is no hyperorthogonal p-tuple in $\mathbb{R}^n \setminus \{0\}$ with $p > 2n$.

We close by considering the $p \times p$ matrix $A = (\langle v_i, v_j \rangle)$ associated with a hyperorthogonal p-tuple $(v_1, \dots, v_p)$. Such matrices are characterized by being positive semidefinite with diagonal entries > 0 and off-diagonal entries ≤ 0. In a corollary to Theorem 2, an equivalent decomposition of such a matrix A is obtained.

The concepts and results obtained in this paper naturally extend to the case of p-tuples of vectors in $E \setminus \{0\}$, where E denotes any n-dimensional vector space over $\mathbb{R}$, endowed with an inner product.

The present concept of hyperorthogonal p-tuples enters in an elementary proof of a characterization of certain positive projections related to Jordan algebras, given in [3].

Further related results are mentioned at the end of the paper.

Definition 2. A hyperorthogonal p-tuple $(v_1, \dots, v_p)$ in $\mathbb{R}^n \setminus \{0\}$ is termed *maximal hyperorthogonal,* or just *maximal*, if it cannot be extended to a hyperorthogonal $(p+1)$-tuple by adjoining a vector (necessarily non-zero) from the linear span $\mathrm{lin}(v_1, \dots, v_n)$ of $(v_1, \dots, v_n)$.

A single vector $v \in \mathbb{R}^n \setminus \{0\}$ trivially forms a hyperorthogonal 1-tuple. It is not maximal because the antipodal pair $(v, -v)$ is a hyperorthogonal 2-tuple in $\mathrm{lin}(v) = \mathbb{R}v$.

Definition 3. A p-tuple $(v_1, \dots, v_p)$ in $\mathbb{R}^n \setminus \{0\}$ is said to be *reducible* if some q among its vectors, with $q \in \{1, \dots, p-1\}$, are orthogonal to the remaining $p - q$ vectors.

Remark 1. An *irreducible* (i.e. not reducible) hyperorthogonal p-tuple $(v_1, \dots, v_p)$ in $\mathbb{R}^n \setminus \{0\}$ is maximal if (and only if) it cannot be extended to an *irreducible* hyperorthogonal $(p+1)$-tuple by adjoining a vector $v \in \mathrm{lin}(v_1, \dots, v_p)$. In fact, if $(v_1, \dots, v_p, v)$ were a reducible hyperorthogonal $(p+1)$-tuple then v would be orthogonal to $v_1, \dots, v_p$, and hence $v = 0$.

Example 1. The vertices $v_1, \dots, v_{n+1}$ of a regular n-simplex in $\mathbb{R}^n$ centered at 0 form a maximal irreducible hyperorthogonal $(n+1)$-tuple in $\mathbb{R}^n \setminus \{0\}$. Indeed, the angle between two of the vertices is $2 \arccos \frac{1}{n} > \frac{\pi}{2}$ (if $n \geq 2$), which also implies irreducibility. Maximality follows from the implication (i) $\wedge$ (iii) $\Longrightarrow$ (ii) in Theorem 1 below since $p = n + 1$ here and since $(v_1, \dots, v_{n+1})$ clearly has full rank n.

A pair of vectors (v, w) in $\mathbb{R}^n \setminus \{0\}$ is termed *antipodal* if there exists a real number $\alpha < 0$ such that $w = \alpha v$. An antipodal pair in $\mathbb{R}^n \setminus \{0\}$ is the same as a maximal hyperorthogonal 2-tuple in $\mathbb{R}^n \setminus \{0\}$, and is moreover irreducible.

Remark 2. If a hyperorthogonal p-tuple $(v_1, \dots, v_p)$ in $\mathbb{R}^n \setminus \{0\}$ contains an antipodal pair, say (v_1, v_2), then the remaining vectors $v_3, \dots, v_p$ are orthogonal to v_1 and v_2. If $(v_1, \dots, v_p)$ is moreover *irreducible* then $p = 2$, and we just have an antipodal pair.

Lemma 1. *Let $(v_1, \dots, v_p)$ be a hyperorthogonal p-tuple in $\mathbb{R}^n \setminus \{0\}$ of rank r and having no antipodal pair containing v_p. For any vector $v \in \mathbb{R}^n$ let v' denote the orthogonal projection of v on the orthogonal complement $(\mathbb{R}v_p)^\perp$ of $\mathbb{R}v_p$ in $\mathbb{R}^n$. Then $(v'_1, \dots, v'_{p-1})$ is hyperorthogonal of rank $r - 1$. If $(v_1, \dots, v_p)$ is*

(a) *maximal* *or* (b) *irreducible,*

then so is $(v'_1, \dots, v'_{p-1})$.

Proof. Clearly $n, p \geq r \geq 2$, for if $r = 1$ then (v_1, v_p) would be an antipodal pair. Assuming as we may that $\|v_p\| = 1$, we have

$$v'_i = v_i - \langle v_i, v_p \rangle v_p \quad \text{for } i < p. \tag{1}$$

In view of (1) the p-tuple $(v'_1, \dots, v'_{p-1}, v_p)$ has the same rank r as $(v_1, \dots, v_p)$. Being orthogonal to $v_p \neq 0$, $(v'_1, \dots, v'_{p-1})$ therefore has rank $r - 1$. Since $(v_1, \dots, v_p)$ is hyperorthogonal it follows from (1) that so is $(v'_1, \dots, v'_{p-1})$ because

$$\langle v'_i, v'_j \rangle = \langle v_i, v_j \rangle - \langle v_i, v_p \rangle \langle v_j, v_p \rangle \leq 0 \tag{2}$$

for distinct $i, j < p$.

(a) Suppose that $(v_1, \dots, v_p)$ is maximal. For maximality of the hyperorthogonal $(p-1)$-tuple $(v'_1, \dots, v'_{p-1})$, suppose that, on the contrary, there exists a non-zero vector $v \in \operatorname{lin}(v'_1, \dots, v'_{p-1})$ such that $(v'_1, \dots, v'_{p-1}, v)$ is hyperorthogonal. Then v is orthogonal to each $v_i - v'_i$ (which belongs to $\mathbb{R}v_p$, by (1)), and hence

$$\langle v, v_i \rangle = \langle v, v'_i \rangle \leq 0 \qquad \text{for } i \in \{1, \dots, p-1\},$$

by hyperorthogonality of $(v'_1, \dots, v'_{p-1}, v)$. Thus $(v_1, \dots, v_p, v)$ is hyperorthogonal in $\mathbb{R}^n \setminus \{0\}$ along with $(v_1, \dots, v_p)$ and $(v_1, \dots, v_{p-1}, v)$, in view of $\langle v_p, v \rangle = 0$. Furthermore,

$$v \in \operatorname{lin}(v'_1, \dots, v'_{p-1}, v_p) = \operatorname{lin}(v_1, \dots, v_{p-1}, v_p),$$

by (1). This contradicts the maximality of $(v_1, \dots, v_p)$.

(b) Suppose that $(v_1, \dots, v_p)$ is irreducible. If $(v'_1, \dots, v'_{p-1})$ is reducible we may assume that, for example, $v'_1, \dots, v'_q$ are orthogonal to $v'_{q+1}, \dots, v'_{p-1}$ for some $q \in \{1, \dots, p-2\}$. We then show that (when thus including v_p) either

$$(v_1, \dots, v_q) \perp (v_{q+1}, \dots, v_{p-1}, v_p) \tag{3}$$

or

$$(4) \qquad (v_1, \dots, v_q, v_p) \perp (v_{q+1}, \dots, v_{p-1}).$$

For $i \in \{1, \dots, q\}$ and $j \in \{q+1, \dots, p-1\}$ we have in fact in view of (1) by hyperorthogonality of $(v_1, \dots, v_p)$

$$(5) \qquad 0 \geq \langle v_i, v_j \rangle = \langle v_i', v_j' \rangle + \langle v_i, v_p \rangle \langle v_j, v_p \rangle \geq 0$$

because $v_i' \perp v_j'$ and that $\langle v_i, v_p \rangle \leq 0$ and $\langle v_j, v_p \rangle \leq 0$, again by hyperorthogonality of $(v_1, \dots, v_p)$. Thus the equality signs in (5) prevail, and so $\langle v_i, v_j \rangle = 0$ for $i \leq q < j \leq p-1$, and the non-negative number $\langle v_i, v_p \rangle \langle v_j, v_p \rangle$ therefore equals 0. Hence either $\langle v_i, v_p \rangle = 0$ for every $i \in \{1, \dots, q\}$, or else $\langle v_j, v_p \rangle = 0$ for every $j \in \{q+1, \dots, p-1\}$. In the former case, (3) holds in view of (5) with equality signs, as just established; and similarly in the latter case, (4) holds. In either case, this contradicts the irreducibility of $(v_1, \dots, v_p)$. $\square$

Remark 3. If $v_1, \dots, v_p$ are normalized, that is, if they lie on Σ_n, it is natural to replace the orthogonal projection v' of any $v \in \Sigma_n$ on $\mathbb{R}^{n-1} = (\mathbb{R} v_p)^\perp$ with $v \neq \pm v_p$ by the *spherical projection* v° (the point of the "equator" $\Sigma_{n-1} = (\mathbb{R} v_p)^\perp \cap \Sigma_n$ nearest to v). Clearly $v^\circ = v'/\|v'\|$, and hence Lemma 1 remains valid when v_i' is replaced by v_i°, $i < p$.

Theorem 1. *Let $(v_1, \dots, v_p)$ be a hyperorthogonal p-tuple in $\mathbb{R}^n \setminus \{0\}$ of rank r. Then $r \geq 1$, and if $(v_1, \dots, v_p)$ is irreducible then either $p = r$ or $p = r+1$. Any two of the following three properties imply the third:*

(i) $(v_1, \dots, v_p)$ *is irreducible,*

(ii) $(v_1, \dots, v_p)$ *is maximal,*

(iii) $p = r + 1$.

Proof. Clearly $p, n \geq r \geq 1$. It follows that, if $p = 1$, then $r = 1$ and hence $p = r$. Furthermore, the singleton (v_1) is not maximal, the antipodal pair $(v_1, -v_1) \subset \mathrm{lin}(v_1)$ being hyperorthogonal. Thus (ii) and (iii) fail, and there is nothing more to prove when $p = 1$. We therefore assume that $p \geq 2$.

Suppose that (i) holds. Assume for a moment that $(v_1, \dots, v_p)$ is a union of antipodal pairs. By Remark 2 these are mutually orthogonal, and by irreducibility there is just one antipodal pair. Such a pair is maximal, and $p = 2$, $r = 1$, whence (ii) and (iii) hold. We may therefore assume for example that (v_i, v_p) *is not an antipodal pair for any* $i \in \{1, \dots, p-1\}$. It follows that $r \geq 2$, for if $r = 1$ then (v_1, v_p) would be an antipodal pair. By Lemma 1 the projection $(v_1', \dots, v_{p-1}')$ of $(v_1, \dots, v_{p-1})$ on $(\mathbb{R} v_p)^\perp$ is an irreducible hyperorthogonal $(p-1)$-tuple of rank $r-1$. This shows by induction that $p-1$ equals either

$r-1$ or r because $p=2$ implies either $r=1$ or $r=2$, the former in case (v_1, v_2) is antipodal, and the latter if not. *Thus* (i) *implies that either* $p=r+1$ *or* $p=r$. If in addition $(v_1, \dots, v_p)$ is maximal then so is $(v_1', \dots, v_{p-1}')$ by Lemma 1(a), and hence by induction $p-1=(r-1)+1$, that is $p=r+1$. This is because $p=2$ now implies $r=1$, and hence $p=r+1$, a hyperorthogonal pair of rank 2 being clearly non-maximal. Thus (i) $\wedge$ (ii) $\Longrightarrow$ (iii).

To show that (i) $\wedge$ (iii) $\Longrightarrow$ (ii), suppose that, on the contrary, $(v_1, \dots, v_p)$ is not maximal. We shall then prove that $p \neq r+1$, that is, $p=r$. There exists a non-zero vector $v \in \operatorname{lin}(v_1, \dots, v_p)$ such that $(v_1, \dots, v_p, v)$ is an *irreducible* hyperorthogonal $(p+1)$-tuple, cf. Remark 1. In particular, $\langle v, v_p \rangle \leq 0$. Clearly $(v_1, \dots, v_p, v)$ has unchanged rank r. If (v, v_p) were an antipodal pair then $\langle v_i, v_p \rangle = 0$ for $i \in \{1, \dots, p-1\}$, cf. Remark 2, in contradiction with the irreducibility of $(v_1, \dots, v_p)$ since $p \geq 2$. Thus actually (v, v_p) is not antipodal, nor is (v_i, v_p) for any $i \in \{1, \dots, p-1\}$, for then $p+1=2$ by Remark 2 applied to the irreducible $(p+1)$-tuple $(v_1, \dots, v_p, v)$. Consequently, Lemma 1 applies to the hyperorthogonal $(p+1)$-tuple $(v_1, \dots, v_{p-1}, v, v_p)$ of rank r, while keeping v_p. It thus follows by Lemma 1 that $(v_1', \dots, v_{p-1}', v')$ is hyperorthogonal. Because $v \in \operatorname{lin}(v_1, \dots, v_p)$ and that $v_p' = 0$ we have $v' \in \operatorname{lin}(v_1', \dots, v_{p-1}')$, and we conclude from the supposed non-maximality of $(v_1, \dots, v_p)$ that $(v_1', \dots, v_{p-1}')$ likewise is not maximal. According to Lemma 1 as it stands it follows from (i) that $(v_1', \dots, v_{p-1}')$ is irreducible and has rank $r-1$. By induction, $p-1=r-1$, and hence indeed $p=r$. This is because $p=2$ now implies $r=2=p$, a hyperorthogonal pair (v_1, v_2) of rank 1 being antipodal and hence maximal. The conclusion $p=r$ contradicts (iii), and so $(v_1, \dots, v_p)$ must actually be maximal, that is, (i) $\wedge$ (iii) $\Longrightarrow$ (ii).

The remaining implication (ii)$\wedge$(iii) $\Longrightarrow$ (i) will be established after the proof of (7) below. □

For Assertion (d) of the following theorem, see alternatively [3], Theorem 2. Assertion (c) shows that $p \leq 2n$ holds for any hyperorthogonal p-tuple in $\mathbb{R}^n \setminus \{0\}$. In particular, there is no infinite hyperorthogonal family, as is also clear because Σ_n is compact.

Theorem 2. *Let* $(v_1, \dots, v_p)$ *be a hyperorthogonal* p*-tuple in* $\mathbb{R}^n \setminus \{0\}$ *of rank* r.

(a) *There exists a decomposition of* $\{1, \dots, p\}$, *unique up to permutation, into nonvoid subsets* $J_1, \dots, J_m$ *with* $m \in \{1, \dots, p\}$ *such that the corresponding hyperorthogonal subtuples* $(v_j \colon j \in J_k)$ *with* $k \in \{1, \dots, m\}$ *are irreducible and (if* $m \geq 2$*) mutually orthogonal in* $\mathbb{R}^n$.

(b) *These hyperorthogonal subtuples are all maximal if and only if* $(v_1, \dots, v_p)$ *itself is maximal.*

(c) *We have*

$$p \le r + m \quad \textit{and} \quad p \le 2r \le 2n. \tag{6}$$

Furthermore, $(v_1, \dots, v_p)$ *is maximal if and only if* $p = r + m$ *and hence* $p \ge 2$.

(d) *If* $p = 2n$ *and hence* $r = m = n$ *then* $(v_1, \dots, v_p)$ *is maximal, and is the union of* n *antipodal pairs (necessarily mutually orthogonal if* $n \ge 2$*). If, in addition, each* v_i *is normalized then* $(v_1, \dots, v_{2n})$ *is the union of an orthonormal base for* $\mathbb{R}^n$*, say* $(v_1, \dots, v_n)$*, and its opposite orthonormal base* $(-v_1, \dots, -v_n)$*. Conversely, any such union is maximal hyperorthogonal on* Σ_n *and has rank* n.

Proof. (a) The existence part follows right away in view of Definition 3. For uniqueness of the decomposition, write briefly V for $(v_1, \dots, v_p)$, and V_k for $(v_j : j \in J_k)$, so that we have a decomposition $V = \bigcup_{k=1}^m V_k$ of V into mutually orthogonal subtuples V_k. For any other such decomposition $V = \bigcup_l W_l$ of V into mutually orthogonal subtuples W_l of V, suppose for some k and l that $V_k \cap W_l \neq \varnothing$. Then

$$W_l = (V_k \cap W_l) \cup ((V \setminus V_k) \cap W_l)$$

defines a decomposition of W_l into two mutually orthogonal subtuples $V_k \cap W_l$ and $(V \setminus V_k) \cap W_l$ of W_l and hence of V because $V_k \perp V \setminus V_k$. Since W_l is irreducible and $V_k \cap W_l \neq \varnothing$ we must have $(V \setminus V_k) \cap W_l = \varnothing$, that is $W_l \subset V_k$. By interchanging the roles of V_k and W_l in this argument we also have $V_k \subset W_l$, and so $V_k = W_l$. Thus any two V_k and W_l are either disjoint or identical. This means, however, that the two decompositions $V = \bigcup_k V_k$ and $V = \bigcup_l W_l$ must be the same (up to permutation).

(b) With the above abbreviations we show by contradiction that V is maximal if and only if each V_k is so. For the "only if" part, suppose that some V_k is not maximal. There exists then $v \in \operatorname{lin} V_k$ such that $(v) \cup V_k$ remains hyperorthogonal, that is, $v \neq 0$ and $\langle v, v_j \rangle \le 0$ for all $j \in J_k$. This contradicts the maximality of V because $v \in \operatorname{lin} V$ and that $(v) \cup V$ remains hyperorthogonal. Indeed, for any $l \in \{1, \dots, m\}$ with $l \neq k$, V_l is orthogonal to V_k and therefore $v \in \operatorname{lin} V_k$, whence $\langle v_j, v \rangle = 0$ for every $j \in J_l$, and altogether $\langle v_j, v \rangle \le 0$ for any $j \in \{1, \dots, p\}$. – For the "if" part, suppose that V is not maximal. Then there exists $v \in \operatorname{lin} V$ such that $(v) \cup V$ remains hyperorthogonal, that is, $\langle v, v_j \rangle \le 0$ for all $j \in \{1, \dots, p\}$. For any $k \in \{1, \dots, m\}$ denote by v' the orthogonal projection of v on $\operatorname{lin} V_k$. Then $(v') \cup V_k$ remains hyperorthogonal, in contradiction with the maximality of V_k. Indeed, for any $j \in J_k$ we have $v_j \in V_k$, hence $v - v' \perp v_j$, and so $\langle v', v_j \rangle = \langle v, v_j \rangle \le 0$. Furthermore $v' \neq 0$, for otherwise $v = v - v' \perp v_j$, hence $v \perp \operatorname{lin}(v_j : j \in J_k) = \operatorname{lin} V_k$, and so $v = v'$ by definition of v', in contradiction with $v \neq 0$.

(c) For the second inequality (6), denote $p_k = \# J_k$ and $r_k = \operatorname{rk} V_k$. Clearly $p = \sum_k p_k$ and $r = \sum_k r_k$, the latter because the V_k are mutually orthogonal. Since V_k is irreducible it follows by Theorem 1 that $p_k \leq r_k + 1$, and hence

$$(7) \qquad p = \sum_{k=1}^{m} p_k \leq m + \sum_{k=1}^{m} r_k = m + r \leq 2r,$$

the latter inequality because each $r_k \geq 1$ and hence $r \geq m$. By Theorem 1, all the irreducible subtuples V_k are maximal if and only if $p_k = r_k + 1$ for all $k \leq m$, which in turn, by addition, is equivalent to $p = r + m$ since anyway $p_k \leq r_k + 1$, as already noted. Thus, by (b), V *is maximal if and only if* $p = r + m$. And if V is maximal and reducible then $m > 1$ and hence $p = r + m > r + 1$, thus establishing by contradiction the remaining implication (ii) $\wedge$ (iii) $\Longrightarrow$ (i) in Theorem 1.

(d) If $p = 2n$, and hence $n = r \leq m$ by (6), then by (7) with equality it follows from (c) that V is maximal, and we have $m = r$, hence $r_k = 1$ for every $k \in \{1, \ldots, m\}$; furthermore, $p_k = r_k + 1 = 2$ for every k because V_k is irreducible and maximal, by (b), and thus each of the $m = r = n$ subtuples V_k is an antipodal pair, as noted after Example 1. The final assertion in (d) is easily verified. □

Exercise 1. Determine all hyperorthogonal $(2n-1)$-tuples on Σ_n, for example for $n = 3$. (*Hint:* begin by determining the non-maximal ones.)

We continue identifying a p-tuple $(v_1, \ldots, v_p)$ of vectors in $\mathbb{R}^n$ with the $n \times p$ matrix V with columns $v_1, \ldots, v_p$. We only consider matrices with real entries. The transpose of a matrix V is denoted by V^t. The following lemma concerning the associated Gram matrix $V^t V$ is well known.

Lemma 2. (a) *For any* $n \times p$ *matrix* $V = (v_1, \ldots, v_p)$ *of rank* r, *the* $p \times p$ *matrix*

$$(8) \qquad A \overset{\text{def}}{=} V^t V = (\langle v_i, v_j \rangle)_{i,j \in \{1,\ldots,p\}}$$

is positive semidefinite and has rank r.

(b) *Conversely, every positive semidefinite* $p \times p$ *matrix* A *of rank* r *has the form* (8) *with* V *an* $r \times p$ *matrix, necessarily of rank* r.

Proof. (a) A is obviously symmetric: $\langle v_i, v_j \rangle = \langle v_j, v_i \rangle$, and positive semidefinite:

$$\sum_{i,j=1}^{p} \langle v_i, v_j \rangle x_i x_j = \Big\langle \sum_{i=1}^{p} x_i v_i, \sum_{j=1}^{p} x_j v_j \Big\rangle = \Big\| \sum_{i=1}^{p} x_i v_i \Big\|^2 \geq 0$$

for $x_1, \dots, x_p \in \mathbb{R}$. Clearly $\operatorname{rk} A \le \operatorname{rk} V = r$. For the proof that $\operatorname{rk} A \ge r$ we may assume for example that $v_1, \dots, v_r$ are linearly independent. The principal submatrix

$$B \overset{\text{def}}{=} (\langle v_i, v_j \rangle)_{i,j \le r}$$

of A then has full rank r. Otherwise there would be an r-tuple $(c_1, \dots, c_r) \in \mathbb{R}^r \setminus \{0\}$ such that $\sum_{j=1}^r c_j \langle v_i, v_j \rangle = 0$ for every $i \le r$, and hence $\left\langle \sum_{i=1}^r c_i v_i, \sum_{j=1}^r c_j v_j \right\rangle = 0$, that is, $\sum_{i=1}^r c_i v_i = 0$, in contradiction with the linear independence of $v_1, \dots, v_r$.

(b) There exists an orthogonal $p \times p$ matrix Ω such that

$$\Omega^t A \Omega = \Lambda \overset{\text{def}}{=} \operatorname{diag}(\lambda_1, \dots, \lambda_p),$$

with $\lambda_i > 0$ for $i \le r$ and $\lambda_i = 0$ for $i > r$ because $\operatorname{rk} \Lambda = \operatorname{rk} A = r$. Consider the $r \times p$ matrix U obtained from $\operatorname{diag}(\sqrt{\lambda_1}, \dots, \sqrt{\lambda_r})$ by adjoining after it $p - r$ columns equal to 0. Then $U^t U = \Lambda$, and the $r \times p$ matrix

$$V \overset{\text{def}}{=} U \Omega$$

has the same rank r as U, and satisfies $V^t V = \Omega^t U^t U \Omega = \Omega^t \Lambda \Omega = A$. $\square$

Remark 4. For any $n \ge r$, (8) of course remains valid after the $r \times p$ matrix V in the proof of Lemma 2 has been extended by adjoining $n - r$ new rows equal to 0, whereby $\operatorname{rk} V$ remains equal to r. Also note that it was shown in the proof of Lemma 2 that every positive semidefinite $p \times p$ matrix A of rank r has a *principal* submatrix B of full rank r.

Lemma 3. *For $n, p \ge 1$ let $V = (v_1, \dots, v_p)$ be an $n \times p$ matrix with column vectors $v_1, \dots, v_p$ in $\mathbb{R}^n \setminus \{0\}$. Let*

$$A = (a_{ij})_{i,j \in \{1,\dots,p\}} \overset{\text{def}}{=} V^t V$$

be the associated Gram matrix, cf. Lemma 2, obviously with diagonal entries > 0. Then

(a) *V is hyperorthogonal if and only if the off-diagonal entries of A are all ≤ 0.*

(b) *V is irreducible if and only if A is irreducible in the sense that one cannot decompose $\{1, \dots, p\}$ into two nonvoid disjoint parts J_1 and J_2 such that $a_{ij} = 0$ for $i \in J_1$ and $j \in J_2$.*

(c) *V is maximal (hyperorthogonal) if and only if A (with all off-diagonal entries ≤ 0) is maximal in the sense that one cannot adjoin to A a new last column $a \in \mathbb{R}^{n+1}$ and the corresponding last row a^t in such a way that the extended $(p+1) \times (p+1)$ matrix has all diagonal entries > 0, all off-diagonal entries ≤ 0, and is positive semidefinite with the same rank as A.*

Proof. Assertions (a) and (b) are easily verified. For (c), suppose first that V is hyperorthogonal, but not maximal. There is then a column vector $v \in \mathbb{R}^n \backslash \{0\}$ such that the $n \times (p+1)$ matrix W with columns $v_1, \ldots, v_p, v$ remains hyperorthogonal with unchanged rank r (namely $v \in \text{lin}(v_1, \ldots, v_p)$). In view of Lemma 2,

$$B \stackrel{\text{def}}{=} W^t W$$

is an extension of A to a positive semidefinite $(p+1) \times (p+1)$ matrix of rank r with diagonal entries > 0 and off-diagonal entries ≤ 0, by (a). This shows that A is not maximal in the stated sense.

Conversely, suppose that A is not maximal. There is then a column vector $b \in \mathbb{R}^p$ with coordinates $b_i \leq 0$, and a number $c > 0$, such that the symmetric $(p+1) \times (p+1)$ matrix

$$\begin{pmatrix} a & b \\ c & d \end{pmatrix}$$

remains positive semidefinite with rank r. In particular, the first p rows of B have rank r (not just rank $\leq r$ because $\text{rk}\, A = r$). The system of linear equations

$$\sum_{j=1}^{p} a_{ij} x_j = b_i,$$

$i \in \{1, \ldots, p\}$, therefore has a solution $(x_1, \ldots, x_p)$. The linear combination $v = \sum_{j=1}^{p} x_j v_j$ satisfies

$$(9) \qquad \langle v_i, v \rangle = \sum_{j=1}^{p} \langle v_i, v_j \rangle x_j = \sum_{j=1}^{p} a_{ij} x_j = b_i \leq 0$$

for $i \in \{1, \ldots, p\}$, showing that the $(p+1)$-tuple $(v_1, \ldots, v_p, v)$ is hyperorthogonal along with $(v_1, \ldots, v_p)$. Note at this point that $v \neq 0$, for if $v = 0$ then $b = 0$, by (9), and since $c > 0$ this would imply that $\text{rk}\, B = 1 + \text{rk}\, A$, which is false. We have thus shown that indeed $(v_1, \ldots, v_p)$ is non-maximal if A is so, thereby completing the proof of (c). □

In view of Lemma 3 we have the following equivalent version of Theorem 2.

Corollary 1. *Let* $A = (a_{ij})_{i,j \in \{1,\ldots,p\}}$ *be a positive semidefinite* $p \times p$ *matrix of rank* r *with diagonal entries* > 0 *and off-diagonal entries* ≤ 0.

(a) *There exists a decomposition of* $\{1, \ldots, p\}$, *unique up to permutation, into nonvoid subsets* $J_1, \ldots, J_m$ *with* $m \in \{1, \ldots, p\}$ *such that the corresponding positive semidefinite principal submatrices* $A_k = (a_{ij})_{i,j \in J_k}$ *with* $k \in \{1, \ldots, m\}$ *are irreducible and (if* $m \geq 2$*) mutually orthogonal in* $\mathbb{R}^n$, *in the sense that* $a_{ij} = 0$ *for all* $(i, j) \in J_k \times J_l$ *and distinct* $k, l \in \{1, \ldots, m\}$.

(b) *These positive semidefinite principal submatrices* A_k *are all maximal if and only if* A *is itself maximal.*

(c) *We have*

$$p \leq r + m \quad \textit{and} \quad p \leq 2r.$$

Furthermore, A *is maximal if and only if* $p = r + m$ *and hence* $p \geq 2$.

(d) *If* $p = 2n$, *and hence* $r = m = n$, *and if the diagonal entries of* A *equal* 1, *then* A *is maximal, and (up to a permutation of rows and the same permutation of columns)* A *equals the block matrix*

$$A = \begin{pmatrix} I_n & -I_n \\ -I_n & I_n \end{pmatrix}, \tag{10}$$

where I_n *denotes the* $n \times n$ *unit matrix. Conversely, this block matrix* A *has rank* n *and is maximal with diagonal entries 1 and off-diagonal entries* 0 *or* -1.

In (d), the requirement that the diagonal entries of A equal 1 of course amounts to the columns of V from Lemma 2 being normalized. For (10) note that, by Theorem 2, the columns of V therefore are $v_1, \dots, v_n, -v_1, \dots, -v_n$ in terms of an orthonormal base $(v_1, \dots, v_n)$ for $\mathbb{R}^n$. If instead we order the columns of V as $v_1, -v_1, v_2, -v_2, \dots, v_n, -v_n$ then A becomes the diagonal block matrix

$$A = \operatorname{diag}(E, E, \dots, E) \quad \text{with } E = \begin{pmatrix} 1 & -1 \\ -1 & 1 \end{pmatrix}.$$

Exercise 2. Determine all positive semidefinite $(2n-1) \times (2n-1)$ matrices of rank n with diagonal entries 1 and off-diagonal entries ≤ 0.

Related results. The author owes to the Editors the following observations.

The inequality $r \geq p - m$ of the last corollary is contained in Lemma 4 of Section 3.5, Chapter 5 of [1].

Unit vectors $v_1, \dots, v_p$ in $\mathbb{R}^n$ with *equal* inner products $\langle v_i, v_j \rangle$ for distinct i, j in $\{1, \dots, p\}$ have been studied in [4]. For example, given an integer $d \geq 1$, if $\langle v_i, v_i \rangle = 1$ and $\langle v_i, v_j \rangle = -1/d$ for $i \neq j$, then $p \leq n + [n/d]$; see [4], Theorem 4.2.

Given a subset S of the real interval $[-1, 1]$, a *spherical* S*-code* is a subset V of the unit sphere in $\mathbb{R}^n$ such that $\langle v, v' \rangle \in S$ for any pair (v, v') of distinct vectors in V. In particular, a spherical $[-1, 0]$-code is precisely a hyperorthogonal set of unit vectors. Bounds on cardinalities of spherical S-codes have been established in [2] and more recent papers.

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