Hyperorthogonal family of vectors and the associated Gram matrix

L'Enseignement Mathématique (2) 60 (2014), 31–41 DOI 10.4171/LEM/60-1/2-3

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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.

Mathematics Subject Classification (2010). 15A03, 15A63.

Keywords. Gram matrix, hyperorthogonal, spherical S-code.

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

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

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 $d(v_i, v_j) \geq \pi/2$ 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 $\operatorname{lin}(v_1, \dots, v_n)$ 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 $\operatorname{lin}(v) = \mathbb{R}v$.

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

Lemma 1. *Let $(v_1, \ldots, v_p)$ 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 $(v'_1, \ldots, v'_{p-1})$ is hyperorthogonal of rank $r - 1$. If $(v_1, \ldots, v_p)$ is*

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

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

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 $(v'_1, \ldots, v'_{p-1}, v_p)$ has the same rank r as $(v_1, \ldots, v_p)$. Being orthogonal to $v_p \neq 0$, $(v'_1, \ldots, v'_{p-1})$ therefore has rank $r - 1$. Since $(v_1, \ldots, v_p)$ is hyperorthogonal it follows from (1) that so is $(v'_1, \ldots, v'_{p-1})$ 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 $(v_1, \ldots, v_p)$ is maximal. For maximality of the hyperorthogonal $(p-1)$-tuple $(v'_1, \ldots, v'_{p-1})$, suppose that, on the contrary, there exists a non-zero vector $v \in \mathrm{lin}(v'_1, \ldots, v'_{p-1})$ such that $(v'_1, \ldots, v'_{p-1}, v)$ is hyperorthogonal. Then v is orthogonal to each $v_i - v'_i$ (which belongs to $\mathbb{R}v_p$, by (1)), and hence

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

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

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

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

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

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

or

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

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 $(v_1, \dots, v_p)$

$$0 \geq \langle v_i, v_j \rangle = \langle v_i', v_j' \rangle + \langle v_i, v_p \rangle \langle v_j, v_p \rangle \geq 0 \tag{5}$$

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 $(v_1, \dots, v_p)$. □

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*

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

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 $p_k \le r_k + 1$, and hence

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

the latter inequality because each $r_k \ge 1$ and hence $r \ge m$. By Theorem 1, all the irreducible subtuples V_k are maximal if and only if $p_k = r_k + 1$ for all $k \le m$, which in turn, by addition, is equivalent to $p = r + m$ since anyway $p_k \le r_k + 1$, 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 $n = r \le m$ 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 $k \in \{1, \dots, m\}$; 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 $(v_1, \dots, v_p)$ of vectors in $\mathbb{R}^n$ with the $n \times p$ matrix V with columns $v_1, \dots, v_p$. 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 $V = (v_1, \dots, v_p)$ of rank r, the $p \times p$ matrix*

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

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:

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

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 $v \in \mathbb{R}^n \setminus \{0\}$ such that the $n \times (p+1)$ matrix W with columns $v_1, \dots, v_p, v$ remains hyperorthogonal with unchanged rank r (namely $v \in \mathrm{lin}(v_1, \dots, v_p)$). 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 $b_i \le 0$, 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 $\le r$ because $\mathrm{rk}\, A = r$). The system of linear equations

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

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

$$\langle v_i, v \rangle = \sum_{j=1}^{p} \langle v_i, v_j \rangle x_j = \sum_{j=1}^{p} a_{ij} x_j = b_i \le 0 \tag{9}$$

for $i \in \{1, \dots, p\}$, showing that the $(p+1)$-tuple $(v_1, \dots, v_p, v)$ is hyperorthogonal along with $(v_1, \dots, v_p)$. Note at this point that $v \ne 0$, for if $v = 0$ then $b = 0$, by (9), and since $c > 0$ this would imply that $\mathrm{rk}\, B = 1 + \mathrm{rk}\, A$, which is false. We have thus shown that indeed $(v_1, \dots, v_p)$ 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* $A = (a_{ij})_{i,j \in \{1,\dots,p\}}$ *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* $\{1, \dots, p\}$, *unique up to permutation, into nonvoid subsets* $J_1, \dots, J_m$ *with* $m \in \{1, \dots, p\}$ *such that the corresponding positive semidefinite principal submatrices* $A_k = (a_{ij})_{i,j \in J_k}$ *with* $k \in \{1, \dots, m\}$ *are irreducible and (if* $m \ge 2$*) 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* $k, l \in \{1, \dots, m\}$.

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

(c) *We have*

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

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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(*Reçu le 9 octobre 2012*)

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