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## Hyperorthogonal family of vectors and the associated Gram matrix

Bent FUGLEDE

**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

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

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  $\Sigma_n$  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  $\Sigma_n$  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  $\leq 0$ . 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  $\text{lin}(v_1, \dots, v_p)$  of  $(v_1, \dots, v_p)$ .

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  $\text{lin}(v) = \mathbb{R}v$ .

**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  $v \in \text{lin}(v_1, \dots, v_p)$ . 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)  $\implies$  (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

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

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

$$(2) \quad \langle v'_i, v'_j \rangle = \langle v_i, v_j \rangle - \langle v_i, v_p \rangle \langle v_j, v_p \rangle \leq 0$$

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  $v \in \text{lin}(v'_1, \dots, v'_{p-1})$  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

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

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,

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

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

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

or

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

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  $(v_1, \dots, v_p)$

$$(5) \quad 0 \geq \langle v_i, v_j \rangle = \langle v'_i, v'_j \rangle + \langle v_i, v_p \rangle \langle v_j, v_p \rangle \geq 0$$

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  $\Sigma_n$ , 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*  $v^\circ$  (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  $v_i^\circ$ ,  $i < p$ .

**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  $(v_1, -v_1) \subset \text{lin}(v_1)$  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)  $\implies$  (iii).

To show that (i)  $\wedge$  (iii)  $\implies$  (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  $v \in \text{lin}(v_1, \dots, v_p)$  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  $v \in \text{lin}(v_1, \dots, v_p)$  and that  $v'_p = 0$  we have  $v' \in \text{lin}(v'_1, \dots, v'_{p-1})$ , 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)  $\implies$  (ii).

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

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  $\Sigma_n$  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  $(v_j: j \in J_k)$  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

$$(6) \quad p \leq r + m \quad \text{and} \quad p \leq 2r \leq 2n.$$

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

(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  $n \geq 2$ ). 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  $\Sigma_n$  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  $V_k \cap W_l \neq \emptyset$ . 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  $V_k \cap W_l \neq \emptyset$  we must have  $(V \setminus V_k) \cap W_l = \emptyset$ , 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  $v \in \text{lin } V_k$  such that  $(v) \cup V_k$  remains hyperorthogonal, that is,  $v \neq 0$  and  $\langle v, v_j \rangle \leq 0$  for all  $j \in J_k$ . This contradicts the maximality of  $V$  because  $v \in \text{lin } V$  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  $v \in \text{lin } V_k$ , whence  $\langle v_j, v \rangle = 0$  for every  $j \in J_l$ , and altogether  $\langle v_j, v \rangle \leq 0$  for any  $j \in \{1, \dots, p\}$ . – For the “if” part, suppose that  $V$  is not maximal. Then there exists  $v \in \text{lin } V$  such that  $(v) \cup V$  remains hyperorthogonal, that is,  $\langle v, v_j \rangle \leq 0$  for all  $j \in \{1, \dots, p\}$ . For any  $k \in \{1, \dots, m\}$  denote by  $v'$  the orthogonal projection of  $v$  on  $\text{lin } V_k$ . 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  $\langle v', v_j \rangle = \langle v, v_j \rangle \leq 0$ . Furthermore  $v' \neq 0$ , for otherwise  $v = v - v' \perp v_j$ , hence  $v \perp \text{lin}(v_j: j \in J_k) = \text{lin } V_k$ , 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  $r_k = \text{rk } V_k$ . 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

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

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)  $\implies$  (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  $k \in \{1, \dots, m\}$ ; 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.  $\square$

**Exercise 1.** Determine all hyperorthogonal  $(2n - 1)$ -tuples on  $\Sigma_n$ , 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

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

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:

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

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

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

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  $i \leq r$ , and hence  $\langle \sum_{i=1}^r c_i v_i, \sum_{j=1}^r c_j v_j \rangle = 0$ , 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  $\Omega$  such that

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

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

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

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  $n \geq r$ , (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  $\text{rk } V$  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  $n, p \geq 1$  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

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

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  $\leq 0$ .

(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  $\leq 0$ ) 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  $\leq 0$ , 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  $v \in \text{lin}(v_1, \dots, v_p)$ ). 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  $\leq 0$ , 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

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

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

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

for  $i \in \{1, \dots, p\}$ , 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  $v \neq 0$ , 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  $(v_1, \dots, v_p)$  is non-maximal if  $A$  is so, thereby completing the proof of (c).  $\square$

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  $\leq 0$ .*

(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  $m \geq 2$ ) 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  $k, l \in \{1, \dots, m\}$ .*

(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*

$$(10) \quad A = \begin{pmatrix} I_n & -I_n \\ -I_n & I_n \end{pmatrix},$$

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

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

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

**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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