Unit vectors with non-negative inner products

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1. Introduction

In [1] W. Kruskal is credited with the following

Conjecture. 1.1. The squared length of the sum of n unit vectors in $\mathbb{R}^d$, having mutually non-negative inner products, is at least $\frac{n^2 + r(d-r)}{d}$, where $n \equiv r \pmod d$, $0 \le r < d$. Moreover, equality is attained if and only if the n vectors are spread as evenly as possible over an orthonormal set of d vectors.

For a number of cases we settle this conjecture in the affirmative. Moreover, we describe a setting for the problem which may lead to a general proof. However, the general conjecture remains open.

2. The problem (cf. [1]).

Suppose we have d + 1 observations of n standardized variables. Arrange them in an $(d+1) \times n$ matrix

$$X = [x_{ij}];\ i = 1,\dots,d+1\ ;\ j = 1,\dots,n,$$

and assume that they are nonnegatively correlated, that is, for $j,k = 1,\dots,n$ assume

$$r_{jk} := \frac{1}{d+1} \sum_{i=1}^{d+1} (x_{ij} - \bar{x}_j)(x_{ik} - \bar{x}_k) \ge 0,$$

where

$$\bar{x}_j = \frac{1}{d+1} \sum_{i=1}^{d+1} x_{ij}\ ,\ \frac{1}{d+1} \sum_{i=1}^{d+1} (x_{ij} - \bar{x}_j)^2 = 1.$$

The sum variable $y_i = \sum_{j=1}^{n} x_{ij}$ achieves its maximum possible variance n^2 if all correlations r_{jk} equal 1. It is natural to identify the "relatedness" of the variables with the variance of their sum and ask what is the minimum possible variance. Without changing the situation essentially we may assume that the column sums of X are 0, $\sum_{i=1}^{d+1} x_{ij} = 0$ for all j. If $\underline{x}_j$ denotes the j-th column, then the variance of $\underline{x}_j$ equals $\frac{1}{d+1}(\underline{x}_j,\underline{x}_j)$, which is 1 by assumption. Also the correlation $r_{jk} = \frac{1}{d+1}(\underline{x}_j,\underline{x}_k) \geq 0$, hence no angle between the $\underline{x}_j$'s exceeds $\pi/2$. The variance we wish to minimize can be written as

$$\frac{1}{d+1}\left(\sum_{j=1}^{n} \underline{x}_j, \sum_{j=1}^{n} \underline{x}_j\right) = \frac{1}{d+1}\left\| \sum_{j=1}^{n} \underline{x}_j \right\|^2 .$$

Now write $\underline{u}_j := \frac{1}{\sqrt{d+1}} \underline{x}_j$. These vectors are all perpendicular to $(1,1,\ldots,1)^t$. Hence we have n unit vectors $\underline{u}_1,\ldots,\underline{u}_n$ in $\mathbb{R}^d$ with nonnegative inner products, and the problem is to minimize $\left\| \sum_{j=1}^{n} \underline{u}_j \right\|^2$.

3. Inequalities

Let $S_{n,d}$ denote the collection of all sets of n unit vectors in $\mathbb{R}^d$ all of whose inner products are nonnegative. Let $n = qd + r$, $0 \leq r < d$. For any $S \in S_{n,d}$, let $G = [g_{ij}]$ denote the Gram matrix of S, and let $\pi = \lambda_1 \geq \lambda_2 \geq \ldots \geq \lambda_d$ denote the nonzero eigenvalues of G.

Lemma 3.1. $\frac{n^2}{d} + \frac{(\pi d-n)^2}{d(d-1)} \leq \sum g_{ij}^2 \leq \sum g_{ij} \leq \pi n.$

Proof. tr G = n and tr $G^2 = \sum g_{ij}^2$ read

$$\lambda_2+\ldots+\lambda_d = n - \pi, \quad \lambda_2^2+\ldots+\lambda_d^2 = \sum g_{ij}^2 - \pi^2,$$

whence

$$(n - \pi)^2 \leq (d - 1)(\sum g_{ij}^2 - \pi^2),$$

implying the first inequality. The second follows from $0 \le g_{ij} \le 1$, and the third one is implied by choosing $x = (1,1,...,1)$ in

$$\pi \ge (Gx,x)/(x,x). \qquad \square$$

When does equality hold? In the first inequality iff $\lambda_2 = ... = \lambda_d$ (= λ say), that is iff

$$G^2 - \lambda G = \pi(\pi - \lambda)P,$$

where $P = [p_i p_j]$ is the rank one matrix made up from the (positive) components p_i of the unit eigenvector of π. G is a (0,1) matrix iff equality holds in the second, and G has constant row sums iff equality holds in the third inequality.

Finally, our inequalities imply $n \le \pi d$, and equality holds if and only if $G = I_d \otimes J_{n/d}$, that is, iff S consists of d orthonormal vectors each repeated n/d times.

Part of the conjecture reads

Conjecture 3.2. $\sum g_{ij} \ge (n^2 + r(d-r))/d$, $S \in S_{n,d}$.
Clearly, lemma 3.1 implies that conjecture 3.2 is true for $n \equiv 0 \pmod d$. We observe that the right-hand side of the inequality equals the sum of the entries of

$$\begin{bmatrix} I_r \otimes J_{q+1} & O \\ O & I_{d-r} \otimes J_q \end{bmatrix},$$

the adjacency matrix of Turan's graph, cf. [2]. This illustrates the following lemma, by which conjecture 3.2 needs only be investigated for irreducible $S \in S_{n,d}$.

Lemma 3.3. If $n = n_1 + n_2$, $d = d_1 + d_2$, $n = qd + r$, $n_1 = q_1 d_1 + r_1$, $n_2 = q_2 d_2 + r_2$, $0 \le r < d$, $0 \le r_1 < d_1$, $0 \le r_2 < d_2$, then

$$\frac{n_1^2 + r_1(d_1 - r_1)}{d_1} + \frac{n_2^2 + r_2(d_2 - r_2)}{d_2} - \frac{n^2 + r(d - r)}{d} \ge 0.$$

Proof. Suppose $q_1 \le q_2$, then $q_1 \le q \le q_2$. Indeed,

$$n = q_1 d + (q_2 - q_1)d_2 + r_1 + r_2 = q_2 d - (q_2 - q_1)d_1 + r_1 + r_2,$$

hence $q_1 d \le n < (q_2 + 1)d$. Straightforward caluculation shows that the left-hand side of the inequality in the lemma equals

$$d_1((q - q_1)^2 + (q - q_1)) - 2r_1(q - q_1) + d_2((q_2 - q)^2 - (q_2 - q)) + 2r_2(q_2 - q).$$

Since $r_1 < d_1$ and $r_2 \ge 0$, this is not less than

$$d_1((q - q_1)^2 - (q - q_1)) + d_2((q_2 - q)^2 - (q_2 - q)),$$

which is nonnegative, since $q - q_1$ and $q - q_2$ are nonnegative integers.

Remark. In the lemma equality holds iff $q = q_1 = q_2$ or $q_1 = q$, $q_2 = q + 1$, $r_2 = 0$.

Remark. If conjecture 3.2 were true, then the Perron eigenvalue π of G would satisfy

$$\frac{n}{d} + \frac{r(d-r)}{nd} \le \pi.$$

4. The solution in a special case

Theorem 4.1. The conjecture is true for $S \in S_{n,d}$, S a two-distance set with inner products 0 and σ^{-1}.

Proof. Let $G = I + \sigma^{-1}A$ with a (0,1) matrix A having 2m ones. Thus, $-\sigma$ is the smallest eigenvalue of A. Assume the conjecture were not true for any irreducible $I + \sigma^{-1}A$. Lemma 3.1 and the assumption then yield

$$\frac{n^2}{d} \overset{(1)}{\le} n + \frac{2m}{\sigma^2} \overset{(2)}{\le} n + \frac{2m}{\sigma} \overset{(4)}{<} \frac{n^2 + r(d-r)}{d} .$$

From (1) and (4) we obtain

$$\sigma^2 n(n - d) \le 2md < \sigma(n - r)(n + r - d).$$

For $n \le d$ the right hand inequality yields a contradiction. For $d < n \le 2d$ we have $\sigma^2 nr \le 2md < \sigma d2r < 4dr < 2nd$, since $\sigma < \frac{2d}{d+r} < 2$, hence $m < n$ and A is the adjacency matrix of a tree. But $n - 1 = m < 2r < n$ is impossible. We are left with $n > 2d$, but then

$$\sigma < \frac{(n-r)(n-d+r)}{n(n-d)} = 1 + \frac{r(d-r)}{n(n-d)} \le 1 + \frac{\frac{1}{4}d^2}{2d^2} = \frac{9}{8} .$$

In [3] it is proved that any graph of diameter D has smallest eigenvalue

$$-\sigma \le -2 \cos \pi / (D + 2).$$

Hence our graph has diameter $D = 1$, $\sigma = 1$, $d = 1$, $r = 0$, contradicting (4). This proves the theorem.

<u>Corollary</u>. The adjacency matrix of a graph has

$$\text{Perron-eigenvalue} \ge \sigma(n - d + r)(n - r) / nd,$$

where $(-\sigma)$, of multiplicity $n - d$, is the smallest eigenvalue and $n = qd + r$, $0 \le r < d$.

5. Geometric methods

Let $S^{d-1} = \{x \in \mathbb{R}^d \mid (x,x) = 1\}$. The hyperplane perpendicular to any unit vector $z \in \mathbb{R}^d$ determines two closed hemispheres

$$H^+ = \{x \in S^{d-1} \mid (x,z) \geq 0\} \quad \text{and} \quad H^- = \{x \in S^{d-1} \mid (x,z) \leq 0\}.$$

For any finite set $X \in S^{d-1}$ the convex hull $C(X)$ is the set of all finite convex linear combinations of elements of X, that is,

$$C(X) := \{z \in S^{d-1} \mid z = \lambda_1 x_1 + \ldots + \lambda_n x_n, \; n \in \mathbb{N}, \; x_i \in X, \; \lambda_i \geq 0\}.$$

Its dual spherical polytope $D(X)$ is defined by

$$D(X) := \{z \in S^{d-1} \mid \forall_{x \in X} : (x,z) \geq 0\},$$

that is, the intersection of the positive hemispheres of the vectors of X. Let P and P^* be spherical polytopes. P^* is said to be dual to P if $\varphi : F(P) \to F(P^*)$ is a bijection from the set of faces of P to the set of faces of P^* such that $f \subseteq g \Leftrightarrow \varphi f \supseteq \varphi g$ for all $f,g \in F(P)$. P is called self-dual if $P^* = P$.

The polar set $\hat{P}$ of a spherical polytope P is defined by

$$\hat{P} := \{z \in S^{d-1} \mid \forall_{x \in P} : (x,z) \geq 0\}.$$

Clearly $\hat{P}$ is dual to P and $D(X) = C(\hat{X})$.

Theorem 5.1. Assume that X is such that

$$\Big\| \sum_{z \in X} z \Big\|^2 \leq \Big\| \sum_{z \in Y} z \Big\|^2$$

for all $Y \in S_{n,d}$. Then $X \in V(DX))$, where $V(P)$ is the set of vertices of P.

Proof. Suppose $x \in X$ is not a vertex of $D(X)$, that is, there exist $a,b \in D(X)$ such that $x = \alpha a + \beta b$, where $0 < \alpha, \beta < 1$ are related by $\alpha^2 + 2\alpha\beta(a,b) + \beta^2 = 1$. Now let $X' = X \setminus \{x\}$. Then

$$\left(\sum_{z\in X'} z, x\right) = \alpha\left(\sum_{z\in X'} z, a\right) + \beta\left(\sum_{z\in X'} z, b\right)$$

is, as we shall prove, a nonconstant concave function of α, thus reaching its mininum for $\alpha = 0$, say. But if $X'' = X' \cup \{a\}$, this contradicts the assumption, since then

$$\left\| \sum_{z\in X''} z \right\|^2 < \left\| \sum_{z\in X} z \right\|^2,$$

because

$$\left(\sum_{z\in X} z, \sum_{z\in X} z\right) = \left(\sum_{z\in X'} z, \sum_{z\in X'} z\right) + 2\left(\sum_{z\in X'} z, x\right) + 1 > \left(\sum_{z\in X'} z, \sum_{z\in X'} z\right) +$$

$$+ 2\left(\sum_{z\in X'} z, a\right) + 1 = \left(\sum_{z\in X''} z, \sum_{z\in X''} z\right).$$

$f(\alpha)$ is a concave function iff $\frac{d^2f}{d\alpha^2} \leq 0$. Hence the sum of two concave functions and the square root of a nonnegative concave function are again concave. Since

$$\beta = -\alpha(a,b) + \sqrt{\alpha^2(a,b)^2 + 1 - \alpha^2}$$

it remains to prove that $\alpha^2\{(a,b)^2 - 1\}$ is a concave function of α, and this is obvious since $(a,b)^2 \leq 1$.

Corollary 5.2.: For every $x \in X$, with X as in theorem 5.1, there exist $d - 1$ linearly independent $x_i \in X$ such that $(x,x_i) = 0$ for all $i = 1,2,\ldots,d - 1$.

Corollary 5.3. For d = 2 and $|X| = n \equiv 1 \pmod 2$,

$$\left\| \sum_{z\, X} z \right\|^2 \geq \frac{n^2+1}{2} .$$

Equality is attained iff X consists of two orthogonal vectors, each repeated $\frac{n-1}{2}$ and $\frac{n+1}{2}$ times respectively.

Corollary 5.4. If X contains a set of d orthonormal vectors, then D(X) = C(X) is the regular orthogonal spherical polytope spanned by these vectors and

$$\left\| \sum_{z \in X} z \right\|^2 \geq \frac{n^2 + r(d-r)}{d} .$$

Theorem 5.5. Assume that X is as in thm. 5.1, then a self-dual spherical polytope P exists with $X \subseteq V(P)$.

Proof: From the properties of X we know $C(X) \subseteq D(X)$ and further $V(C(X)) = X \subseteq V(D(X))$. Let L be the set of all polytopes P with $P \subseteq \hat{P}$ and $V(C(X)) \subseteq V(P) \subseteq V(D(X))$. Clearly $C(X) \in L$, so L is not empty. The set L is partially ordered by $P' < P$ iff $V(P) \subset V(P')$. L contains an upper bound of each totally ordered subset M of L, so, with the lemma of Zorn, L contains a maximal element, which has to be self-dual and which contains $X = V(C(X))$ as vertices.

6. Cases in which the conjecture holds

The conjecture holds for

i) $n \leq d$, all d. Equality holds iff all vectors are orthonormal;

ii) $n \equiv 0 \pmod d$, all d. See the observations after conjecture 3.2.;

iii) d = 2, all n. Corollary 5.3.;

iv) all n, all d, some special cases as in section 4 and corollary 5.4.

References

[1] J.B. Kruskal & H.J. Witsenhausen, An inequality for positively correlated variables, Journal Amer. Statistical Ass., 69 (1974), 540-542.

[2] P. Turan, On the Theory of graphs, Collog. Math. 3 (1954), 19-30.

[3] R. Zurmuhl, Matrizen, Ch. 17.5, Springer 1958.