

Unit vectors with non-negative inner products

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TECHNOLOGICAL UNIVERSITY EINDHOVEN

Department of Mathematics

The Netherlands

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Unit vectors with non-negative inner products

by

A. Bos and J.J. Seidel

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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 $n \equiv r \pmod{d}$, $0 \leq r < d$. 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

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

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

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

where

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

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 situ-

ation 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

$(1, 1, \dots, 1)^t$. Hence we have n unit vectors $\underline{u}_1, \dots, \underline{u}_n$ in \mathbb{R}^d with non-

negative 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

$\pi = \lambda_1 \geq \lambda_2 \geq \dots \geq \lambda_d$ 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. $\text{tr } G = n$ and $\text{tr } G^2 = \sum g_{ij}^2$ read

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

whence

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

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

$$\pi \geq (Gx, x) / (x, x). \quad \square$$

When does equality hold? In the first inequality iff $\lambda_2 = \dots = \lambda_d (= \lambda \text{ say})$, 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 $n \leq \pi d$, 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. $\sum g_{ij} \geq (n^2 + r(d-r))/d, S \in S_{n,d}$.

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 $n = n_1 + n_2, d = d_1 + d_2, n = qd + r, n_1 = q_1 d_1 + r_1, n_2 = q_2 d_2 + r_2, 0 \leq r < d, 0 \leq r_1 < d_1, 0 \leq r_2 < d_2$, then

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

Proof. Suppose $q_1 \leq q_2$, then $q_1 \leq q \leq q_2$. 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 $q_1 d \leq n < (q_2 + 1) d$. Straightforward calculation 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 $r_2 \geq 0$, 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

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

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

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

From (1) and (4) we obtain

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

For $n \leq d$ the right hand inequality yields a contradiction. For $d < n \leq 2d$ we have $\sigma^2 nr \leq 2md < \sigma d 2r < 4dr < 2nd$, 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

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

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

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

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

Corollary. The adjacency matrix of a graph has

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

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

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,

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

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 $\varphi : F(P) \rightarrow F(P^*)$ 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

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

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 minimum 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

$$\begin{aligned} \left(\sum_{z \in X} z, \sum_{z \in X} z \right) &= \left(\sum_{z \in X'} z, \sum_{z \in X'} z \right) + 2 \left(\sum_{z \in X'} z, x \right) + 1 > \left(\sum_{z \in X'} z, \sum_{z \in X'} z \right) + \\ &+ 2 \left(\sum_{z \in X'} z, a \right) + 1 = \left(\sum_{z \in X''} z, \sum_{z \in X''} z \right). \end{aligned}$$

$f(\alpha)$ is a concave function iff $\frac{d^2 f}{d\alpha^2} \leq 0$. 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 $i = 1, 2, \dots, d - 1$.

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

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

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

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- [3] R. Zurmühl, *Matrizen*, Ch. 17.5, Springer 1958.