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Rank of Hadamard powers of Euclidean distance matrices

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Abstract In mathematical chemistry and computational biology, eigenvalues of distance matrices are also used as descriptors for determining the degree of similarity between different chemical structures or biological sequences. Since observed structures can vary in size, the spectra of corresponding distance matrices can be of different size, which makes the comparison of such structures difficult. In this paper we introduce a mathematical theory needed to support novel graphical (qualitative and visual) and numerical (quantitative and computational) representation of biological sequences. As the main result, we derive a formula for the rank of the Hadamard power of an Euclidean distance matrix.

Keywords Rank · Hadamard product · Hadamard power · Euclidean distance matrix · Eigenvalues · Similarity of DNA sequences · DNA descriptors

Mathematics Subject Classification 05C10 · 92B05 · 15A16 · 15A18 · 15A42

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1 Introduction

In applications of graph theory to chemistry and biology, often one considers objects of different size, such as molecules having different number of atoms or proteins or DNA of different length. One is interested in numerical characterizations of such objects that can offer an estimate of the degree of similarity between them. If such objects are represented by matrices one faces the problem of comparing matrices of different order. In such situation most of the invariants of such matrices [8,9], as a rule, will be size-dependent, which may cause bias for the calculated similarity/dissimilarity magnitudes. Hence, one has both, the conceptual and the computational difficulties, which need to be resolved if one is to obtain reliable results free of biased preferences for objects of the same size.

One way to proceed in such situations is, after selecting a set of invariants, to normalize them with respect to the size of the object considered. For example, in the case of graphs, if one selects the leading eigenvalues of several of matrices of graphs considered as object descriptors, e.g., the the leading eigenvalues of adjacency matrix, the leading eigenvalues of the distance matrix, the leading eigenvalue of the distance matrix having only the maximal elements in each row and columns [11], and the leading eigenvalue of the common vertex matrix [10] and divides them by $\frac{1}{\sqrt{n}}$, where n is the number of vertices, one obtains values of the same order of magnitude. But it has been known in mathematics for some time [1,2,13] that matrices of squared distance between points in planar case (not on a sphere) regardless of the matrix size, have only four non-zero eigenvalues. Hence, if one is to use matrix of squared distances for objects of different size one would automatically arrive at vectors of the same size representing objects which could be of variable sizes.

Leading eigenvalues of several matrices have been of interest in chemistry because of their interpretations in structural concepts. Thus Lovaz and Pelikan [6] have interpreted the leading eigenvalue of the adjacency matrix as an index of molecular branching. Later Randić et al. [5] introduced a matrix with elements based on path counts, the leading eigenvalue of which appeared even better descriptor of molecular branching. In another publication Randić et al. [3] have interpreted the leading eigenvalue of the D/D matrix as an index that gives numerical measure of the degree of bending of a unbranched chain structures. On the other hand in early 1930's Hückel [4] introduced a simplified model of interaction of π-electrons in benzenoid hydrocarbons, which allowed benzenoid hydrocarbons to be represented by adjacency matrix of molecular graphs. This model has lead to the interpretation of the eigenvalues of the adjacency matrix as π-electron orbital energies in the so called Hückel Molecular Orbital (HMO) theory of quantum chemistry. More recently, Šali et al. [12] have outlined how the eigenvalues of weighted adjacency matrix associated with amino acid contacts for conformations of proteins embedded on $3D$ Cartesian grid of cubes allowed calculation of the total energy of such conformations.

As we have seen, the adjacency matrix and the distances between vertices have been of considerable interest in chemistry. An *Euclidean distance matrix* or shorter EDM is a matrix $D \in \mathbb{R}^{m \times m}$ with components

$$d_{ij} = \left\| \boldsymbol{x}_i - \boldsymbol{x}_j \right\|^2$$

for some points $\boldsymbol{x}_1, \ldots, \boldsymbol{x}_m \in \mathbb{R}^d$.

The formula for the rank of an EDM is well known [2, pp. 385–485]: if the points $\boldsymbol{x}_1, \ldots, \boldsymbol{x}_m \in \mathbb{R}^d$ don't lie on a common sphere then

$$\operatorname{rank} \ D = d + 2$$

otherwise

$$\operatorname{rank} \ D = d + 1.$$

In this paper we extend the results to the n-th Hadamard power of D.

2 Preliminaries

The Hadamard product of matrices $A, B \in \mathbb{R}^{m \times n}$, denoted by $A \circ B \in \mathbb{R}^{m \times n}$ is the entry-wise product

$$A \circ B = \begin{bmatrix} a_{11}b_{11} & \ldots & a_{1n}b_{1n} \\ \vdots & \ddots & \vdots \\ a_{m1}b_{m1} & \ldots & a_{mn}b_{mn} \end{bmatrix} \in \mathbb{R}^{m \times n}.$$

The space $\mathbb{R}^{m \times n}$ is commutative unital algebra for the Hadamard product. The unit element is the matrix $E_{mn} \in \mathbb{R}^{m \times n}$ with all elements equal to 1. We also define the k-th Hadamard power as the repeated Hadamard product

$$\begin{aligned} A^{(0)} &= E_{mn}, \\ A^{(k)} &= \underbrace{A \circ A \circ \ldots \circ A}_{k}, \qquad k > 0 \end{aligned}$$

In general, the Hadamard product doesn't mix well with the ordinary matrix product. However, if $L \in \mathbb{R}^{m \times m}$ and $R \in \mathbb{R}^{n \times n}$ are diagonal, then the two products commute [7]

$$LAR \circ B = L(A \circ B)R.$$

For the purposes of this paper we define the *Kronecker column product* of matrices $A = [a_{ij}]_{ij} \in \mathbb{R}^{m \times n}$ and $B = \begin{bmatrix} \boldsymbol{b}_1 & \boldsymbol{b}_2 & \ldots & \boldsymbol{b}_n \end{bmatrix} \in \mathbb{R}^{m' \times n}$ as a block matrix

$$A \otimes_c B = \begin{bmatrix} a_{11}\boldsymbol{b}_1 & \ldots & a_{1n}\boldsymbol{b}_n \\ \vdots & \ddots & \vdots \\ a_{n1}\boldsymbol{b}_1 & \ldots & a_{nn}\boldsymbol{b}_n \end{bmatrix} \in \mathbb{R}^{mm' \times n},$$

where $\boldsymbol{b}_i$ denotes i-th column of B.[1]

Kronecker column product is bilinear and associative, but not commutative. The neutral element for Kronecker column product on the set of all real matrices with n columns is the matrix $E_{1n} \in \mathbb{R}^{1\times n}$, a row of all ones.

We also define Kronecker column power

$$\begin{aligned} A^{\otimes_c 0} &= E_{1n} \in \mathbb{R}^{1\times n}, \\ A^{\otimes_c k} &= \underbrace{A \otimes_c A \otimes_c \ldots \otimes_c A}_{k} \in \mathbb{R}^{m^k \times n}, \qquad k > 0. \end{aligned}$$

The reason we will need Kronecker column product is the following observation that connects it to the Hadamard product.

Proposition 1 *For any matrices $A \in \mathbb{R}^{m\times r}$, $B \in \mathbb{R}^{n\times r}$, $C \in \mathbb{R}^{m\times r'}$, $D \in \mathbb{R}^{n\times r'}$, the following equalities hold*

$$(A^T B) \circ (C^T D) = (A \otimes_c C)^T (B \otimes_c D) \tag{1}$$

$$(A^T B)^{(n)} = (A^{\otimes_c n})^T (B^{\otimes_c n}) \tag{2}$$

Proof The (i, j)-th matrix entry on the left side is

$$\big((A^T B) \circ (C^T D)\big)_{ij} = \left(\sum_{k=1}^{r} a_{ki} b_{kj}\right)\left(\sum_{l=1}^{r'} c_{li} d_{lj}\right)$$

and on the right side

$$\big((A \otimes_c C)^T (B \otimes_c D)\big)_{ij} = \sum_{k=1}^{r} a_{ki} \boldsymbol{c}_i^T b_{kj} \boldsymbol{d}_j = \sum_{k=1}^{r} a_{ki} b_{kj} \Big(\sum_{l=1}^{r'} c_{li} d_{lj}\Big).$$

The two are obviously equal. Formula (2) follows by induction on the number of factors. □

One consequence of Proposition 1 is a simple proof of the well known Schur Theorem:

Theorem (Schur) *If $A, B \in \mathbb{R}^{n\times n}$ are positive semidefinite, then $A \circ B$ is positive semidefinite.*

[1] We call it this way because of the similarity to Kronecker product, which is defined for matrices $A \in \mathbb{R}^{m\times n}$ and $B \in \mathbb{R}^{m'\times n'}$ as a block matrix by the following formula

$$A \otimes B = \begin{bmatrix} a_{11}B & \ldots & a_{1n}B \\ \vdots & \ddots & \vdots \\ a_{n1}B & \ldots & a_{nn}B \end{bmatrix} \in \mathbb{R}^{mm'\times nn'}.$$

Proof If A and B are positive semidefinite, there exist matrices X and Y, such that $A = X^T X$ and $B = Y^T Y$ (e.g. by Cholesky decomposition). By above proposition $A \circ B = (X \otimes_c Y)^T (X \otimes_c Y)$, which is positive semidefinite. □

Proposition 2 *For any matrices* $A, B \in \mathbb{R}^{n\times n}$, $\mathrm{im}\,(A+B) \subseteq \mathrm{im}\ A + \mathrm{im}\ B$. *If in addition any of the following two conditions holds*

(a) A and B are both positive semidefinite,
(b) A and B are normal and $\mathrm{im}\ A \cap \mathrm{im}\ B = 0$,

then $\mathrm{im}\,(A+B) = \mathrm{im}\ A + \mathrm{im}\ B$.

Proof It can be found in any linear algebra book □

We will denote the space of all polynomials with real coefficients on $\mathbb{R}^d$ by $\mathbf{P}_{\mathbb{R}^d}$ and the space of all polynomials of degree at most n by $\mathbf{P}^n_{\mathbb{R}^d}$. The space of all homogeneous polynomials of degree n will be denoted by $\mathbf{H}^n_{\mathbb{R}^d}$. When the dimension d is known from the context, we will sometimes shorten the notation to $\mathbf{P}$, $\mathbf{P}^n$ or $\mathbf{H}^n$.

The spaces $\mathbf{P}^n$ and $\mathbf{H}^n$ are finite-dimensional real vector spaces. The dimension of $\mathbf{H}^n$ is $\binom{n+d-1}{d-1}$, the number of combinations with repetition of size n for d elements (since this is the number of different monomials of degree n). The space $\mathbf{P}^n$ is the direct sum of $\mathbf{H}^0, \ldots, \mathbf{H}^n$, hence its dimension is $\sum_{k=0}^n \binom{k+d-1}{d} = \binom{n+d}{d}$.

Lemma 1 *Let* $X = \left[\boldsymbol{x}_1\ \boldsymbol{x}_2\ \ldots\ \boldsymbol{x}_n\right] \in \mathbb{R}^{d\times n}$. *Then*

$$\mathrm{im}\,(X^{\otimes_c n})^T = \left\{ \left[\, p(\boldsymbol{x}_1)\ p(\boldsymbol{x}_2)\ \ldots\ p(\boldsymbol{x}_m) \right]^T \,\middle|\, p \in \mathbf{H}^n_{\mathbb{R}^d} \right\}$$

Proof Let x_{ij} be the j-th component of the vector $\boldsymbol{x}_i$. The i-th column of $X^{\otimes_c n}$ is $\boldsymbol{x}_i^{\otimes_c n}$. Its components are all products of the form $x_{ij_1} x_{ij_2} \ldots x_{ij_n}$. Combining repeated factors, these are all products of the form $x_{i1}^{k_1} x_{i2}^{k_2} \ldots x_{id}^{k_d} = \boldsymbol{x}_i^{\boldsymbol{k}}$ where $\boldsymbol{k} = [k_j]_{j=1\ldots d} \geq 0$ and $|k| = k_1 + k_2 + \ldots k_d = n$. These are exactly all the monomials of degree n in $\boldsymbol{x}_i$ (please note that every mixed monomial appears several times).

For any $y \in \mathbb{R}^{d^n}$, $\left((X^{\otimes_c n})^T a\right)_i = (\boldsymbol{x}_i^{\otimes_c n})^T y$. This is a linear combination of monomials of degree n in $\boldsymbol{x}_i$, hence it equals $p(\boldsymbol{x}_i)$ for some $p \in H_n$ (which depends only on y, not on i). It's obvious that for every p a corresponding y exists. □

For polynomial $p \in \mathbf{P}_{\mathbb{R}^d}$ and matrix $X = \left[\boldsymbol{x}_1\ \boldsymbol{x}_2\ \ldots\ \boldsymbol{x}_m\right] \in \mathbb{R}^{d\times m}$ we define

$$\mathrm{ev}_X(p) = \left[\, p(\boldsymbol{x}_1)\ p(\boldsymbol{x}_2)\ \ldots\ p(\boldsymbol{x}_m) \right]^T .$$

(The transposition is there to turn the result into a vector in $\mathbb{R}^m$.) The map $ev_X : \mathbf{P}_{\mathbb{R}^d} \to \mathbb{R}^m$ is linear. As usual we define image of a subspace $P \subseteq \mathbf{P}_{\mathbb{R}^d}$

$$\mathrm{ev}_X(P) = \{\mathrm{ev}_X(p) \mid p \in P\}.$$

With this notation, the above proposition can be restated simply

$$\mathrm{im}\,(X^{\otimes_c n})^T = \mathrm{ev}_X(\mathbf{H}^n_{\mathbb{R}^d}).$$

For any space of polynomials $P \leq \mathbf{P}_{\mathbb{R}^d}$, the kernel of restriction $\mathrm{ev}_X|_P$ consists of all polynomials from P that are simultaneously zero on all columns $\boldsymbol{x}_1, \ldots, \boldsymbol{x}_m$. In particular, if P contains no such polynomial, then $\dim \mathrm{ev}_X(P) = \dim P$.

3 The spherical case

The case of spherical EDM seems to be simpler than the generic one, that's why we will consider it first.

Theorem 1 *Let D be an Euclidean distance matrix corresponding to the points $\boldsymbol{x}_1, \ldots, \boldsymbol{x}_m \in S \subseteq \mathbb{R}^d$, where S is a $(d-1)$-dimensional sphere with center $\boldsymbol{c}$ and radius r. Define*

$$S_d^n := \binom{d+n-1}{d-1} + \binom{d+n-2}{d-1}.$$

Then

$$\operatorname{rank} D^{(n)} \leq S_d^n,$$

where equality holds iff there is no nonzero polynomial p on $\mathbb{R}^d$ with all terms of degree either n or $n-1$ such that $p\big(\frac{1}{r}(\boldsymbol{x}_i - c)\big) = 0$ for all $i = 1, \ldots, m$.

Proof Since the EDM D is invariant to common translations of $\boldsymbol{x}_1, \ldots, \boldsymbol{x}_m$ and since the rank of a matrix is invariant to scaling, we may assume without loss of generality that all $\boldsymbol{x}_i$ lie on the sphere $S(0, 1)$, i.e. $\|\boldsymbol{x}_i\|^2 = 1$ for all i. The only change is that the condition $p\big(\frac{1}{r}(\boldsymbol{x}_i - c)\big) = 0$ reduces to the simpler condition $p(\boldsymbol{x}_i) = 0$.

The ij-th element of matrix D can be calculated as follows

$$d_{ij} = \left\|\boldsymbol{x}_i - \boldsymbol{x}_j\right\|^2 = \|\boldsymbol{x}_i\|^2 - 2\boldsymbol{x}_i^T\boldsymbol{x}_j + \left\|\boldsymbol{x}_j\right\|^2 = 2(1 - \boldsymbol{x}_i^T\boldsymbol{x}_j).$$

Defining $X = \left[\boldsymbol{x}_1\ \boldsymbol{x}_2\ \ldots\ \boldsymbol{x}_m\right] \in \mathbb{R}^{d\times m}$ and $E = E_{mm} \in \mathbb{R}^{m\times m}$, the above can be written in matrix form

$$D = 2(E - X^T X).$$

By Binomial theorem and since E is the unit for Hadamard product

$$D^{(n)} = \sum_{k=0}^{n} (-1)^k \binom{n}{k} (X^T X)^{(k)}.$$

Finally, by Proposition 1

$$\begin{aligned} D^{(n)} &= \sum_{k=0}^{n} (-1)^k \binom{n}{k} (X^{\otimes_c k})^T (X^{\otimes_c k}) \\ &= \underbrace{\sum_{k \text{ even}} \binom{n}{k} (X^{\otimes_c k})^T (X^{\otimes_c k})}_{D_+} - \underbrace{\sum_{k \text{ odd}} \binom{n}{k} (X^{\otimes_c k})^T (X^{\otimes_c k})}_{D_-}. \end{aligned}$$

According to Lemma 1

$$\mathrm{im}\,(X^{\otimes_c k})^T (X^{\otimes_c k}) = \mathrm{im}\,(X^{\otimes_c k})^T = \mathrm{ev}_X(\mathbf{H}^k_{\mathbb{R}^d}).$$

Since both D_+ and D_- are sums of positive semidefinite terms, we can replace image of sums with sum of images by Proposition 2

$$\mathrm{im}\ D_+ = \sum_{k\ \text{even}} \mathrm{ev}_X(\mathbf{H}^k_{\mathbb{R}^d}) \qquad \text{and} \qquad \mathrm{im}\ D_- = \sum_{k\ \text{odd}} \mathrm{ev}_X(\mathbf{H}^k_{\mathbb{R}^d})$$

For any column $\boldsymbol{x}_i$ of X, $\|\boldsymbol{x}_i\|^2 = 1$. For any $p \in \mathbf{H}^k_{\mathbb{R}^d}$ it follows that

$$p(\boldsymbol{x}_i) = \|\boldsymbol{x}_i\|^2\, p(\boldsymbol{x}_i) =: q(\boldsymbol{x}_i).$$

Hence $\mathrm{ev}_X(p) = \mathrm{ev}_X(q)$ and since $q \in \mathbf{H}^{k+2}_{\mathbb{R}^d}$ it follows that $\mathrm{ev}_X(\mathbf{H}^k_{\mathbb{R}^d}) \subseteq \mathrm{ev}_X(\mathbf{H}^{k+2}_{\mathbb{R}^d})$. The above sums therefore collapse and we obtain simply

$$\mathrm{im}\ D_+ = \mathrm{ev}_X(\mathbf{H}^n_{\mathbb{R}^d}) \qquad \text{and} \qquad \mathrm{im}\ D_- = \mathrm{ev}_X(\mathbf{H}^{n-1}_{\mathbb{R}^d})$$

in case n is even, otherwise n and $n-1$ are exchanged. Now from

$$\mathrm{im}\ D^{(n)} = \mathrm{im}\,(D_+ - D_-) \subseteq \mathrm{im}\ D_+ + \mathrm{im}\ D_-$$

and

$$\begin{aligned}\mathrm{im}\ D_+ + \mathrm{im}\ D_- &= \mathrm{ev}_X(\mathbf{H}^n_{\mathbb{R}^d}) + \mathrm{ev}_X(\mathbf{H}^{n-1}_{\mathbb{R}^d})\\ &= \mathrm{ev}_X(\mathbf{H}^n_{\mathbb{R}^d} + \mathbf{H}^{n-1}_{\mathbb{R}^d})\end{aligned}$$

it is easy to see the inequality

$$\mathrm{rank}\ D^{(n)} \leq \dim(\mathbf{H}^n_{\mathbb{R}^d} + \mathbf{H}^{n-1}_{\mathbb{R}^d}) = S^n_d.$$

To check when equality holds we proceed as follows. First, assume that there exists a nonzero polynomial p with all terms having degree n or $n-1$ that annihilates all $\boldsymbol{x}_i$. In other words, such polynomial is an element of the space $\mathbf{H}^n_{\mathbb{R}^d} + \mathbf{H}^{n-1}_{\mathbb{R}^d} \subseteq \mathbf{P}_{\mathbb{R}^d}$. Since $\mathrm{ev}_X(p) = 0$, the kernel of $\mathrm{ev}_X : \mathbf{H}^n_{\mathbb{R}^d} + \mathbf{H}^{n-1}_{\mathbb{R}^d} \to \mathbb{R}^m$ is nontrivial. Therefore

$$\begin{aligned}\mathrm{rank}\ D^{(n)} &\leq \dim\big(\mathrm{ev}_X(\mathbf{H}^n_{\mathbb{R}^d} + \mathbf{H}^{n-1}_{\mathbb{R}^d})\big)\\ &< \dim(\mathbf{H}^n_{\mathbb{R}^d} + \mathbf{H}^{n-1}_{\mathbb{R}^d}) = S^n_d.\end{aligned}$$

On the other hand, if there is no polynomial in $\mathbf{H}^n_{\mathbb{R}^d} + \mathbf{H}^{n-1}_{\mathbb{R}^d}$ that annihilates X, then $\mathrm{im}\ D_+ \cap \mathrm{im}\ D_- = \mathrm{ev}_X(\mathbf{H}^n_{\mathbb{R}^d}) \cap \mathrm{ev}_X(\mathbf{H}^{n-1}_{\mathbb{R}^d}) = 0$; otherwise there would be nonzero polynomials $p_1 \in \mathbf{H}^n_{\mathbb{R}^d}$ and $p_2 \in \mathbf{H}^{n-1}_{\mathbb{R}^d}$ such that $\mathrm{ev}_X(p_1) = \mathrm{ev}_X(p_2)$, hence $\mathrm{ev}_X(p_1 - p_2) = 0$. From Proposition 2 it follows that

$$\mathrm{im}\,(D_+ - D_-) = \mathrm{im}\ D_+ + \mathrm{im}\ D_- = \mathrm{ev}_X(\mathbf{H}^n_{\mathbb{R}^d} + \mathbf{H}^{n-1}_{\mathbb{R}^d}).$$

And since kernel of ev_X on $\mathbf{H}^n_{\mathbb{R}^d} + \mathbf{H}^{n-1}_{\mathbb{R}^d}$ is trivial, the dimension of its image equals S^n_d. □

Remark Using the theorem for spherical case, we can obtain the correct upper bound for the rank of EDM in generic case. Take EDM D corresponding to the points $\boldsymbol{x}_1, \ldots, \boldsymbol{x}_m \in \mathbb{R}^d$. Embed $\mathbb{R}^d$ in $\mathbb{R}^{d+1}$ as $\mathbb{R}^d \times \{0\}$ and let $\boldsymbol{x}'_i = (\boldsymbol{x}_i, 0)$ be the images of points under this embedding (which is isometric and therefore preserves the EDM). Consider a series of d-spheres $\{S_k\}_{k\in\mathbb{N}}$ in $\mathbb{R}^{d+1}$ where $S_k = S\big((0^d, k), k\big)$. These spheres all touch the plane $\mathbb{R}^d \times \{0\}$ at point 0. Let $\boldsymbol{x}^{[k]}_i$ be the nearest point to $\boldsymbol{x}_i$ on the sphere S_k and let D_k be the EDM corresponding to the points $\boldsymbol{x}^{[k]}_1, \ldots, \boldsymbol{x}^{[k]}_m$. Because the radii of S_k increase towards infinity, points $\boldsymbol{x}^{[k]}_i$ converge towards $\boldsymbol{x}_i$ for all i, hence D_k converges towards D. Because the rank is subcontinuous

$$\mathrm{rank}\ D^{(n)} \le \lim_{k\to\infty} \mathrm{rank}\ D^{(n)}_k = S^n_{d+1} = \binom{d+n}{d} + \binom{d+n-1}{d}.$$

Unfortunately, the conditions for equality cannot be obtained in this way. For this reason we consider it separately in the next section.

4 The generic case

Theorem 2 *Let D be an Euclidean distance matrix corresponding to the points $\boldsymbol{x}_1, \ldots, \boldsymbol{x}_m \in \mathbb{R}^d$. Define*

$$R^n_d := \binom{d+n}{d} + \binom{d+n-1}{d}.$$

Then

$$\mathrm{rank}\ D^{(n)} \le R^n_d,$$

the inequality is strict if there exist nonzero polynomials $p \in \mathbf{P}^n_{\mathbb{R}^d}$ and $q \in \mathbf{P}^{n-1}_{\mathbb{R}^d}$ such that

$$p(\boldsymbol{x}_i) + \|\boldsymbol{x}_i\|^{2n}\, q\left(\frac{\boldsymbol{x}_i}{\|\boldsymbol{x}_i\|^2}\right) = 0$$

for all $i = 1, \ldots, m$.

Proof We will assume that $\boldsymbol{x}_i \neq i$ for al i. If some of the points are zero, translate points a bit so that all are nonzero (however, the condition for equality must then be considered for translated points).

The ij-th element of the matrix D is expressed as

$$d_{ij} = \left\|\boldsymbol{x}_i - \boldsymbol{x}_j\right\|^2 = \|\boldsymbol{x}_i\|^2 - 2\boldsymbol{x}_i^T\boldsymbol{x}_j + \left\|\boldsymbol{x}_j\right\|^2.$$

Defining $X = \left[\boldsymbol{x}_1\ \boldsymbol{x}_2\ \ldots\ \boldsymbol{x}_m\right] \in \mathbb{R}^{d\times m},\ E = E_{mm} \in \mathbb{R}^{m\times m}$, and

$$N = \begin{bmatrix} \|\boldsymbol{x}_1\|^2 & & & \\ & \|\boldsymbol{x}_2\|^2 & & \\ & & \ddots & \\ & & & \|\boldsymbol{x}_n\|^2 \end{bmatrix} \in \mathbb{R}^{m\times m}$$

one can easily check that the above can be written in matrix form as

$$D = NE - 2X^TX + EN.$$

To calculate the power we have to use binomial theorem for three terms

$$D^{(n)} = \sum_{\substack{r+s+t=n\\ r,s,t\geq 0}} (-1)^s 2^s \frac{n!}{r!s!t!}(NE)^{(r)} \circ (X^TX)^{(s)} \circ (EN)^{(t)}$$

Because N is diagonal matrix, the interesting part reduces to

$$\begin{aligned}(NE)^{(r)} \circ (X^TX)^{(s)} \circ (EN)^{(t)} &= (N^rE) \circ (X^TX)^{(s)} \circ (EN^t)\\ &= N^r(X^TX)^{(s)}N^t\end{aligned}$$

Which by Proposition 1 is further equal to

$$N^r(X^TX)^{(s)}N^t = N^r(X^{\otimes_c s})^T(X^{\otimes_c s})N^t.$$

We introduce new index $k = 2r+s$ and from this and $r+s+t = n$ express $t = r+n-k$ (Explanation for the apparently arbitrary choice: k is the degree of the corresponding polynomial term in the image of $D^{(n)}$)

$$D^{(n)} = \sum_{k=0}^{2n} \sum_{\substack{2r+s=k\\ r+s\leq n\\ r,s\geq 0}} (-1)^s \frac{2^s n!}{r!s!t!} N^r(X^{\otimes_c s})^T(X^{\otimes_c s})N^{r+n-k}.$$

Because k and s differ by even number, we can replace $(-1)^s$ with equal factor $(-1)^k$. Factoring out everything that doesn't depend on r or s we produce

$$D^{(n)} = \sum_{k=0}^{2n}(-1)^k D_k N^{n-k}$$

where

$$D_k = \sum_{\substack{2r+s=k\\ r+s\leq n\\ r,s\geq 0}} \frac{2^s n!}{r!s!t!} N^r(X^{\otimes_c s})^T(X^{\otimes_c s})N^r.$$

Since D_k is a sum of positive definite terms, its image is

$$\mathrm{im}\ D_k = \sum_{\substack{2r+s=k\\ r+s\leq n\\ r,s\geq 0}} \mathrm{im}\,(X^{\otimes_c s} N^r)^T. \tag{3}$$

Consider a subspace of homogeneous polynomials

$$\|\boldsymbol{x}\|^{2r}\,\mathbf{H}^s_{\mathbb{R}^d} = \left\{(x_1^2+\cdots+x_d^2)^r p(\boldsymbol{x}) \,\middle|\, p \in \mathbf{H}^s_{\mathbb{R}^d}\right\} \leq \mathbf{H}^{2r+s}_{\mathbb{R}^d}.$$

Due to Lemma 1, it is elementary to see

$$\mathrm{im}\,(X^{\otimes_c s} N^r)^T = \mathrm{ev}_X\big(\|\boldsymbol{x}\|^{2r}\,\mathbf{H}^s_{\mathbb{R}^d}\big).$$

It is also easy to check that $\|\boldsymbol{x}\|^{2r}\,\mathbf{H}^s_{\mathbb{R}^d} \subseteq \|\boldsymbol{x}\|^{2(r-1)}\,\mathbf{H}^{s+2}_{\mathbb{R}^d}$ and therefore

$$\mathrm{im}\,(X^{\otimes_c s} N^r)^T \subseteq \mathrm{im}\,(X^{\otimes_c s+2} N^{r-1})^T.$$

This means that the sum in (3) reduces to the subspace term with the largest s. However, we must be careful that k may go up to $2n$ while r and s only go up to n. Thus (3) simplifies to

$$\mathrm{im}\ D_k = \begin{cases} \mathrm{im}\,(X^{\otimes_c k} N^0) = \mathrm{ev}_X\big(\mathbf{H}^k_{\mathbb{R}^d}\big) & k \leq n,\\ \mathrm{im}\,(X^{\otimes_c l} N^{n-l} = \mathrm{ev}_X\big(\|\boldsymbol{x}\|^{2(n-l)}\,\mathbf{H}^l_{\mathbb{R}^d}\big) & k > n. \end{cases}$$

In the second case we introduced $l = 2n-k$, which ranges from 0 to $n-1$. The value comes from the fact that $2n-k$ is the maximum value of s given the constraints $k > n,\ 2r+s = k,\ r+s \leq n$ and $r, s \geq 0$.

Since $\mathrm{im}\,(D_k N^{n-k}) = \mathrm{im}\ D_k$ we see

$$\mathrm{im}\ D^{(n)} \subseteq \sum_{k=0}^{2n} \mathrm{im}\ D_k = \mathrm{ev}_X\left(\sum_{k=0}^{n} \mathbf{H}^k_{\mathbb{R}^d} + \sum_{l=0}^{n-1} \|\boldsymbol{x}\|^{2(n-l)}\,\mathbf{H}^l_{\mathbb{R}^d}\right) \tag{4}$$

Obviously, $\dim\big(\|\boldsymbol{x}\|^{2(n-l)}\,\mathbf{H}^l_{\mathbb{R}^d}\big) = \dim \mathbf{H}^l_{\mathbb{R}^d}$. Therefore

$$\mathrm{rank}\ D^{(n)} \leq \sum_{k=0}^{n} \dim \mathbf{H}^k_{\mathbb{R}^d} + \sum_{l=0}^{n-1} \dim \mathbf{H}^l_{\mathbb{R}^d} \tag{5}$$

and since

$$\sum_{k=0}^{n} \dim \mathbf{H}^k_{\mathbb{R}^d} = \sum_{k=0}^{n} \binom{k+d-1}{d-1} = \binom{n+d}{d},$$

we finally get $\mathrm{rank}\ D^{(n)} \leq \binom{n+d}{d} + \binom{n-1+d}{d} = R^n_d$.

When do we get strict inequality? We need to find the case when the kernel of ev_X restricted to the space

$$V := \sum_{k=0}^{n} \mathbf{H}^k_{\mathbb{R}^d} + \sum_{l=0}^{n-1} \|\boldsymbol{x}\|^{2(n-l)}\, \mathbf{H}^l_{\mathbb{R}^d}$$

is nontrivial. The first sum in this expression is just $\mathbf{P}^n_{\mathbb{R}^d}$, the space of all polynomials of degree at most n. How about the second part?

Every $p \in \|\boldsymbol{x}\|^{2(n-l)}\, \mathbf{H}^l_{\mathbb{R}^d}$ has the form $p(\boldsymbol{x}) = \|\boldsymbol{x}\|^{2(n-l)}\, q(\boldsymbol{x})$ for some $q \in \mathbf{H}^l_{\mathbb{R}^d}$. Since q is homogeneous with degree l,

$$p(\boldsymbol{x}) = \frac{\|\boldsymbol{x}\|^{2n}}{\|\boldsymbol{x}\|^{2l}} q(\boldsymbol{x}) = \|\boldsymbol{x}\|^{2n}\, q\left(\frac{\boldsymbol{x}}{\|\boldsymbol{x}\|^2}\right)$$

Now if $p \in \sum_{l=0}^{n-1} \|\boldsymbol{x}\|^{2(n-l)}\, \mathbf{H}^l_{\mathbb{R}^d}$ there exist $q_l \in \mathbf{H}^l_{\mathbb{R}^d}$ for $l = 1, \ldots, n-1$

$$p(\boldsymbol{x}) = \sum_{l=0}^{n-1} \|\boldsymbol{x}\|^{2n}\, q_l\left(\frac{\boldsymbol{x}}{\|\boldsymbol{x}\|^2}\right) = \|\boldsymbol{x}\|^{2n}\, q\left(\frac{\boldsymbol{x}}{\|\boldsymbol{x}\|^2}\right)$$

where $q = \sum l = 0^{n-1} q_l \in \mathbf{P}^{n-1}_{\mathbb{R}^d}$ is an arbitrary polynomial in $\mathbf{P}^{n-1}_{\mathbb{R}^d}$. In this way we obtain necessity of the condition in the statement of the theorem: if there exist $p \in \mathbf{P}^n_{\mathbb{R}^d}$ and $q \in \mathbf{P}^{n-1}_{\mathbb{R}^d}$ such that

$$p(\boldsymbol{x}_i) + q\left(\frac{\boldsymbol{x}_i}{\|\boldsymbol{x}_i\|^2}\right) = 0$$

for all i, then ev_X has nontrivial kernel on V. This means that there is a strict inequality in (5); consequently rank $D^{(n)} < R^n_d$. □

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