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Distance Matrices and Isometric Embeddings

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We review the relations between distance matrices and isometric embeddings and give simple proofs that distance matrices defined on euclidean and spherical spaces have all eigenvalues except one nonpositive. Several generalizations are discussed.

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1. Introduction

Matrices with random (or pseudorandom) elements appear naturally in different physical problems and their statistical properties have been thoroughly studied (see e.g. [1]). A special case of random matrices, called distance matrices, has been recently proposed in [2]. They are defined for any metric space X with a probability measure μ on it as follows. Choose N points $\vec{x}_j \in X$ randomly distributed according to the measure μ. The matrix element M_{ij} of the $N \times N$ distance matrix M equals the distance on X between points $\vec{x}_i$ and $\vec{x}_j$

$$M_{ij} = \text{distance}(\vec{x}_i, \vec{x}_j), \quad i, j = 1, \dots, N \ . \tag{1}$$

In [3] we discussed the eigenvalue density for distance matrices defined on certain manifolds. When first numerical calculations were performed, an intriguing fact was observed, namely, all eigenvalues (except one) of distance matrices on euclidean and spherical manifolds were nonpositive. However, this property was not fulfilled e.g. for points on a torus. Typically, the eigenvalues of generic random matrices occupy the whole available energy space. To have all of them but one nonpositive one needs to control the signs of all principal minors (see Sect. 3.) which is usually difficult to do. While studying this fact we found a direct proof that for distance matrices over manifolds embedded into the euclidean space this property is automatically fulfilled. The relation between very basic geometrical properties of a manifold and spectral properties of its distance matrix was unexpected for us but analyzing the literature we found that it was proved by Schoenberg in the thirties [4, 5]. In [3] we noted this fact without details. Nevertheless, after many discussions on different occasions it became clear that this type of problems is practically unknown in the physics community and we think that it is of interest to present simple proofs of the main statements. The material in this note is not new (general references are [6–8]) but it seems that it has not been discussed in the random matrix community.

By definition of distance the matrix elements of a distance matrix have the following properties:

a) positivity

$$M_{ij} \geq 0 \text{ and } M_{ij} = 0 \text{ only when } i = j, \tag{2}$$

b) symmetry

$$M_{ij} = M_{ji}, \tag{3}$$

c) triangular inequalities

$$M_{ij} \leq M_{ik} + M_{kj} \quad \text{for all } i,\ j,\ k. \tag{4}$$

Eigenvalues Λ_p and eigenvectors $u_j^{(p)}$ of distance matrices are defined in the usual way

$$\sum_{j=1}^{N} M_{ij} u_j^{(p)} = \Lambda_p u_i^{(p)}. \tag{5}$$

Distance matrices (1) are real symmetric matrices and their eigenvalues are real. As all matrix elements of distance matrices are nonnegative, the application of the Perron–Frobenius theorem ([9, v. 2 p. 49]) states that these matrices have one special positive eigenvalue $\Lambda_0 > 0$ with the largest modulus. All other eigenvalues obey the inequality

$$|\Lambda_j| \leq \Lambda_0. \tag{6}$$

As distance matrices have only real eigenvalues the equality is possible only if there is a negative eigenvalue $\Lambda' = -\Lambda_0$.

The subject of this note is to show that the eigenvalues of distance matrices defined on the euclidean or a spherical space* are all nonpositive

$$\Lambda_i \leq 0, \quad i = 1, \ldots, N-1, \tag{7}$$

except the above-mentioned Perron–Frobenius eigenvalue Λ_0 and that this remarkable property is mainly a consequence of the possibility of isometric embedding of a finite metric space with a given distance matrix into the euclidean space.

*It means that the points $\vec{x}_j$ lie in the d-dimensional euclidean space or on a sphere.

We also note that if, instead of distance matrix (1), one considers new matrices

$$M_{ij}^{(\gamma)} = [\text{distance}(\vec{x}_i, \vec{x}_j)]^\gamma \ , \tag{8}$$

their eigenvalues also obey inequality (7) provided the exponent in the range $0 < \gamma \leq 2$ for the euclidean space and $0 < \gamma \leq 1$ for the spherical one.

The plan of this paper is the following. It is shown in Sect. 2 that if a finite metric space can be isometrically embedded into the euclidean space, then the matrix whose elements are the squares of distances between initial points is of negative type (cf. (20)–(21)). The inverse theorem is also true, namely, if a matrix N is of negative type, then the matrix with elements $\sqrt{N_{ij}}$ can be embedded into the euclidean space. A direct proof of the main theorem that matrices of negative type have all eigenvalues, except one, nonpositive, is presented in Sect. 3. In Section 4 it is shown that if a matrix N_{ij} is of negative type, a new matrix N_{ij}^γ with $0 < \gamma \leq 1$ will also be of negative type. The general form of such metric transforms is also shortly discussed in this section. The spherical spaces are discussed in Sect. 5 and in Sect. 6 a simple proof that geodesic distance matrices for the spherical spaces are of negative type is presented. A resumé of the results is given in Sect. 7. The derivation of the Cayley–Menger formula for the volume of multidimensional simplex is reproduced for completeness in the Appendix.

2. Isometric Embedding

Assume that we know a finite matrix M whose matrix elements M_{ij}, $i, j = 1, \ldots, N$, obey all properties of the distance (2)–(4). The isometric embedding into the euclidean space is to find points $\vec{x}_i$, if any, belonging to an euclidean space R^n such that the euclidean distance between each pair of points i, j coincides with M_{ij}

$$||\vec{x}_i - \vec{x}_j|| = M_{ij}, \tag{9}$$

for all i, $j = 1, \ldots, N$. Here $|| \ldots ||$ is the euclidean distance

$$D_{ij} \equiv ||\vec{x}_i - \vec{x}_j|| = \sqrt{\sum_{k=1}^{n} \left(x_i^{(k)} - x_j^{(k)} \right)^2} \tag{10}$$

and $x_i^{(k)}$ with $k = 1, \ldots, n$ are the euclidean coordinates of the n-dimensional point $\vec{x}_i$.

The necessary and sufficient conditions of the existence of solutions of (9) can be obtained from the following considerations [4] and [6, 7]. Choose a point, say $\vec{x}_N$, and consider the vectors $\vec{y}_i = \vec{x}_i - \vec{x}_N$ with $i = 1, \ldots, N-1$. They form a simplex in the n-dimensional space R^n. Construct the $(N-1) \times n$ matrix of coordinates of these vectors

$$V_{ik} = y_i^{(k)} \quad i = 1, \ldots, N-1, \quad k = 1, \ldots, n, \tag{11}$$

and multiply it by its transpose. The result is a $(N-1) \times (N-1)$ real symmetric matrix $C = V^T \cdot V$ of scalar products

$$C_{ij} = \vec{y}_i \cdot \vec{y}_j, \quad i, j = 1, \ldots, N-1 \ . \tag{12}$$

Because vectors $\vec{y}_j$ belong to the euclidean space, their scalar products can be expressed by the distances between points

$$\vec{y}_i \cdot \vec{y}_j = \frac{1}{2}(||\vec{y}_i||^2 + ||\vec{y}_j||^2 - ||\vec{y}_i - \vec{y}_j||^2). \tag{13}$$

Therefore the matrix C_{ij} can be found from the squares of matrix elements of the distance matrix

$$C_{ij} = \frac{1}{2}(M_{iN}^2 + M_{jN}^2 - M_{ij}^2). \tag{14}$$

If points $\vec{x}_j$ obeying (9) do exist, then by construction the matrix C_{ij} is such that the quadratic form

$$(\xi C \xi) = \sum_{i,j=1}^{N-1} C_{ij} \xi_i \xi_j \equiv \left(\sum_{i=1}^{N} \xi_i \vec{y}_i \right)^2 \tag{15}$$

is nonnegative (≥ 0) for any choice of real numbers $\xi_1, \xi_2, \ldots, \xi_{N-1}$. Inversely, if one has a symmetric positive matrix C, it can be written in the form

$$C = U^T U, \tag{16}$$

where matrix U can be chosen, e.g., in the lower triangular form (the Cholesky decomposition). Then the elements of $U = y_i^{(k)}$ give directly the coordinates $y_i^{(k)}$ of points obeying (14) which solve the problem of the isometric embedding.

The quadratic form (15) can be rewritten in a simpler form by introducing a new variable $\xi_N = -\sum_{j=1}^{N-1} \xi_j$. Then

$$(\xi C \xi) = -\frac{1}{2} \sum_{i,j=1}^{N} M_{ij}^2 \xi_i \xi_j. \tag{17}$$

Therefore the necessary and sufficient condition of the existence of isometric embedding of a finite metric space with the distance matrix M into the euclidean space is that a new matrix N whose matrix elements equal the square of matrix elements of the matrix M

$$N_{ij} = M_{ij}^2 \tag{18}$$

is such that the quadratic form associated with it,

$$(\xi N \xi) = \sum_{i,j=1}^{N} N_{ij}\xi_i\xi_j, \tag{19}$$

is nonpositive

$$\sum_{i,j=1}^{N} \xi_i N_{ij} \xi_j \leq 0 \tag{20}$$

for all choices of real numbers ξ_j, $j = 1, \ldots, N$, with zero sum

$$\sum_{j=1}^{N} \xi_j = 0. \tag{21}$$

In general, a real symmetric matrix obeying these conditions is called a matrix of negative type.

The Schoenberg theorem states that if a metric space with a distance matrix M_{ij} can be isometrically embedded into the euclidean space, the matrix M_{ij}^2 is of negative type and if a matrix N_{ij} is of negative type, the metric space with the distance matrix $\sqrt{N_{ij}}$ can be isometrically embedded into the euclidean space. The minimal dimension of the embedded euclidean space is the rank of the matrix C_{ij} in 14.

3. Eigenvalues of Negative Type Matrices

In this section we present, following [5], the direct proof that any matrix N_{ij} of the negative type has all eigenvalues except one nonpositive (≤ 0). An indirect proof of this statement can be found in [8].

The law of inertia (see e.g. [9, v. 1 p. 298]) states that if a real quadratic form

$$(xNx) = \sum_{i,j=1}^{N} N_{ij} x_i x_j \tag{22}$$

is transformed into a sum of squares of independent linear forms $X_i = \sum_{j=1}^{N} c_{ij} x_j$

$$(xNx) = \sum_{i=1}^{r} b_i X_i^2, \tag{23}$$

then the total number of positive and negative coefficients b_i is independent of the representation. In particular, in the eigenbasis of the real symmetric matrix

N_{ij}

$$(xNx) = \sum_{i=1}^{N} \Lambda_i u_i^2 \tag{24}$$

and the law of inertia permits to determine the number of positive and negative eigenvalues Λ_i.

According to the Jacobi theorem (see e.g. [9, v. 1 p. 305]), if the principal minors Δ_j of a matrix are nonzero, then the number of positive (resp. negative) terms in (23) coincides with the number of conservation (resp. alteration) of signs in the sequence

$$1, \Delta_1, \Delta_2, \ldots, \Delta_N \tag{25}$$

(we assume that the matrix a_{ij} is of full rank). Recall that the principal minor Δ_n of a matrix N is the determinant of the left-upper $n \times n$ submatrix

$$\Delta_n = \begin{vmatrix} N_{11} & N_{12} & N_{13} & \ldots & N_{1n} \\ N_{12} & N_{22} & N_{23} & \ldots & N_{2n} \\ \vdots & \vdots & \vdots & \vdots & \vdots \\ N_{1n} & N_{2n} & \ldots & N_{n-1\;n} & N_{nn} \end{vmatrix} . \tag{26}$$

For distance matrices $N_{ii} = 0$ and $\Delta_1 \equiv 0$ which prevents the direct application of the Jacobi theorem. This formal difficulty, for example, can be overcome as follows. It is clear that the eigenvalues and other principal minors of generic distance matrices are nonzero. Therefore if one adds to N a diagonal matrix $\epsilon\delta_{ij}$ with small ϵ the signs of eigenvalues will not change. But in such a case $\Delta_1 = \epsilon$ and the sequence (25) takes the form

$$1, \epsilon, \Delta_2, \Delta_3, \ldots, \Delta_N. \tag{27}$$

We shall prove below that principal minors Δ_n of distance matrices of negative type have alternating sign

$$\Delta_n = (-1)^{n-1} v_n^2, \;\; n = 2, 3, \ldots, N. \tag{28}$$

Irrespective of the sign of ϵ there is one conservation of sign and $N-1$ alterations of signs in the sequence (27). Therefore, according to the Jacobi theorem, distance matrices of negative type have one positive (the Perron–Frobenius) eigenvalue and all other eigenvalues are nonpositive.

Because the matrix N_{ij} is of negative type, the metric space with the distance $\sqrt{N_{ij}}$ can be embedded into the euclidean space. It means that there exist points $\vec{x}_j$ in the euclidean space such that the euclidean distances between any pairs of points equal

$$\tilde{D}_{ij} = \sqrt{N_{ij}} \; . \tag{29}$$

Let us consider one of these points as the origin (say $\vec{x}_1$). Points $\vec{x}_2, \ldots, \vec{x}_n$ can be viewed as vertices of a $(n-1)$-dimensional simplex. Denote $\tilde{D}_{1i} = r_i$. Then the distance between any pair of points can be expressed as follows

$$\tilde{D}_{ij} = \sqrt{r_i^2 + r_j^2 - 2r_i r_j \cos\varphi_{ij}}, \tag{30}$$

where φ_{ij} is the euclidean angle between vectors $\vec{x}_i - \vec{x}_1$ and $\vec{x}_j - \vec{x}_1$.

Let us perform an inversion $r_i \to 1/r_i$ for all $i = 2, \ldots, n$. Then instead of $n-1$ points $\vec{x}_2, \ldots, \vec{x}_n$ we get a new set of $n-1$ euclidean points $\tilde{\vec{x}}_2, \ldots, \tilde{\vec{x}}_n$ whose mutual distances D_{ij} can be expressed through the old distances as

$$D_{ij} = \sqrt{\frac{1}{r_i^2} + \frac{1}{r_j^2} - 2\frac{1}{r_i r_j}\cos\varphi_{ij}} = \frac{\tilde{D}_{ij}}{\tilde{D}_{1i}\tilde{D}_{1j}} \, . \tag{31}$$

Because the points $\vec{x}_j$ belong to the euclidean space the new points $\tilde{\vec{x}}_j$ with $j = 2, \ldots, N$ plus the point $\vec{x}_1$ form a $n-1$-dimensional euclidean simplex. The volume of this simplex can be computed by the Cayley–Menger determinantal formula (see e.g. [12, p. 124] and also [13] for an early reference) which expresses the volume $V(P_1, \ldots, P_n)$ of an n-dimensional euclidean simplex by the lengths of its sides

$$V^2(P_1, \ldots, P_n) = \frac{(-1)^n}{2^{n-1}[(n-1)!]^2} D(P_1, \ldots, P_n), \tag{32}$$

where the Cayley–Menger determinant is

$$D(P_1, \ldots, P_n) = \begin{vmatrix} 0 & 1 & 1 & \ldots & 1 \\ 1 & 0 & D_{12}^2 & \ldots & D_{1n}^2 \\ \vdots & \vdots & \vdots & \vdots & \vdots \\ 1 & D_{1n}^2 & D_{2n}^2 & \ldots & 0 \end{vmatrix}, \tag{33}$$

and D_{ij} are the distances between points i and j for $i, j = 1, \ldots, n$. For completeness we give a derivation of this formula in Appendix .

In our case the lengths of the transformed simplex are given by (31). As each $\tilde{D}_{ij} = \sqrt{N_{ij}}$, the squares of the lengths which enter the Cayley–Menger formula (33) are

$$D_{ij}^2 = \frac{N_{i,j}}{N_{1i}N_{1j}} \, . \tag{34}$$

Therefore for each $n = 2, \ldots, N$

$$D(\vec{y}_2, \ldots \vec{y}_n) \equiv \begin{vmatrix} 0 & 1 & 1 & \ldots & 1 \\ 1 & 0 & \frac{N_{23}}{N_{12}N_{13}} & \ldots & \frac{N_{2n}}{N_{12}N_{1n}} \\ 1 & \frac{N_{32}}{N_{13}N_{12}} & 0 & \ldots & \frac{N_{3n}}{N_{13}N_{1n}} \\ \vdots & \vdots & \vdots & \vdots & \vdots \\ 1 & \frac{N_{n2}}{N_{1n}N_{12}} & \frac{N_{n3}}{N_{1n}N_{1n}} & \ldots & 0 \end{vmatrix} \, . \tag{35}$$

As the determinant is a multilinear form of row and columns by multiplication of each row (ij) and each column (ji) by N_{ij} one gets

$$D(\vec{y}_2, \dots \vec{y}_n) = [N_{12}N_{13}\dots N_{1N}]^{-2} \begin{vmatrix} 0 & N_{12} & N_{13} & \dots & N_{1n} \\ N_{21} & 0 & N_{23} & \dots & N_{2n} \\ N_{31} & N_{32} & 0 & \dots & N_{3n} \\ \vdots & \vdots & \vdots & \vdots & \vdots \\ N_{n1} & N_{n2} & N_{n3} & \dots & 0 \end{vmatrix} . \quad (36)$$

But the determinant in this expression coincides with the principal minor of the initial distance matrix. Therefore

$$\Delta_n = (-1)^{n-1}[N_{12}N_{13}\dots N_{1N}]^2 2^{n-1}[(n-1)!]^2 V^2(\vec{y}_1, \dots, \vec{y}_n) , \quad (37)$$

which proves that the principal minors of matrices of negative type are of alternate signs. This relation, as explained above, implies that all eigenvalues of such matrices (except possibly one) are nonpositive.

4. Metric Transform

The problem of isometric embedding gives rise to different generalizations. One type of question is the following. Let the points $\vec{x}_j$ with $j = 1, \dots, N$ be the points of the euclidean space R^n. Find all functions $F(r)$ (called metric transforms) such that the finite metric space with the distance matrix

$$M_{ij} = F(||\vec{x}_i - \vec{x}_j||) \quad (38)$$

can be embedded into an euclidean space R^k with certain k. Here $||\vec{x}_i - \vec{x}_j||$ is the euclidean distance (10) between points $\vec{x}_i$ and $\vec{x}_j$.

In [5] it was proved that general metric transforms can be expressed via radial positive definite functions. A real function $f(r)$ is called radial positive definite provided

$$\sum_{i,j=1}^{N} f(||\vec{x}_i - \vec{x}_j||)\xi_i\xi_j \geq 0 \quad (39)$$

for all choices of points $\vec{x}_i \in R^n$ and of real numbers ξ.

An important example of this function is

$$f(r) = \exp(-\lambda^2 r^2) . \quad (40)$$

The positive definite property of the function is a direct consequence of the well-known formula

$$\exp(-\lambda^2||\vec{x}||^2) = \frac{1}{(4\pi)^{n/2}} \int\limits_{R^n} e^{i\lambda\vec{x}\cdot\vec{k}} \exp(-||\vec{k}||^2) d^n k , \quad (41)$$

from which it follows that

$$\sum_{i,j=1}^{N} \xi_i \xi_j e^{-\lambda^2 ||\vec{x}_i - \vec{x}_j||^2} = \frac{1}{(4\pi)^{n/2}} \int_{R^n} \left| \sum_{i=1}^{N} \xi_i e^{i\lambda \vec{x}_i \cdot \vec{k}} \right|^2 e^{-||\vec{k}||^2} d^n k \geq 0 \ . \tag{42}$$

The following theorem is easily proved [5]. The finite metric space with a distance matrix M_{ij} can be isometrically embedded into the euclidean space if and only if the quadratic form

$$\sum_{i,j=1}^{N} \exp(-\lambda^2 M_{ij}^2) \xi_i \xi_j \tag{43}$$

is nonnegative (≥ 0) for all choices of real numbers ξ_j and all $\lambda \to 0$.

The proof is as follows. If the space can be isometrically embedded into the euclidean space, then there exist points $\vec{x}_j \in R^n$ such that $M_{ij} = ||\vec{x}_i - \vec{x}_j||$. Because $\exp(-\lambda^2 r^2)$ is a radial positive definite function, the quadratic form (43) is nonnegative. Conversely, if the quadratic form is nonnegative for $\lambda \to 0$, then

$$\sum_{i.j=1}^{N} (1 - \lambda M_{ij}^2) \xi_i \xi_j \geq 0 \tag{44}$$

for all ξ_j. In view of the condition $\sum_{j=1}^{N} \xi_j = 0$, the first term vanishes and the above inequality reduces to (19), thus proving the existence of the embedding.

The fact that $\exp(-\lambda^2 r^2)$ is a radially positive definite function permits also to prove [5] that the metric space with the distance equal a power of the euclidean distance

$$M'_{ij} = ||\vec{x}_i - \vec{x}_j||^\gamma \quad i, j = 1, \ldots, N \ , \tag{45}$$

where $\vec{x}_i \in R^n$ and $0 < \gamma \leq 1$ can be embedded into the euclidean space. The proof follows from the identity valid for $0 < \gamma \leq 1$

$$|t|^{2\gamma} = c_\gamma \int_0^\infty (1 - \exp(-\lambda^2 t^2)) \frac{d\lambda}{\lambda^{1+2\gamma}} \ , \tag{46}$$

with

$$c_\gamma^{-1} = \int_0^\infty (1 - \exp(\lambda^2)) \frac{d\lambda}{\lambda^{1+2\gamma}} > 0 \ . \tag{47}$$

One has

$$\sum_{ij} ||\vec{x}_i - \vec{x}_j||^{2\gamma} \xi_i \xi_j = c_\gamma \sum_{ij} \xi_i \xi_j \int_0^\infty (1 - e^{-\lambda^2 ||\vec{x}_i - \vec{x}_j||^2}) \frac{d\lambda}{\lambda^{1+2\gamma}}$$

$$= c_\gamma \int_0^\infty \left[\left(\sum_i \xi_i \right)^2 - \left(\sum_{ij} e^{-\lambda^2 ||\vec{x}_i - \vec{x}_j||^2} \xi_i \xi_j \right) \right] \frac{d\lambda}{\lambda^{1+2\gamma}} \ . \quad (48)$$

If $\sum_i \xi_i = 0$, then the first term is zero and as $e^{-\lambda^2 r^2}$ is radial positive definite, the right-hand side is negative which proves that the matrix

$$||\vec{x}_i - \vec{x}_j||^{2\gamma} \quad (49)$$

with $0 < \gamma \leq 1$ is of negative type and the metric space with the distance (45) can be embedded into the euclidean space.

Combining together the above theorems, one concludes that if a matrix N_{ij} is of negative type, then the matrix N_{ij}^γ with $0 < \gamma \leq 1$ is also of negative type and all its eigenvalues, except at most one, are nonpositive.

General radial positive definite functions $f(r)$ have the form [5]

$$f(r) = \int_0^\infty \Omega_N(ru) d\mu(u) \ , \quad (50)$$

where the measure μ is nonnegative, $\mu(u) \geq 0$, and the function $\Omega_N(r)$ is the integral of $e^{i\vec{k}\cdot\vec{x}}$ with $||\vec{x}|| = r$ over the $(N-1)$-dimensional sphere

$$\Omega_N(r) = \frac{1}{\omega_{N-1}} \int_{S_{N-1}} e^{i\vec{x}\cdot\vec{k}} d\sigma_{N-1} = \Gamma\left(\frac{N}{2}\right) \left(\frac{2}{r}\right)^{(N-2)/2} J_{(N-2)/2}(r) \ . \quad (51)$$

Here $\omega_{N-1} = 2\pi^{N/2}/\Gamma(N/2)$ is the volume of the $(N-1)$-dimensional sphere, $\Gamma(x)$ is the Gamma function, and $J_n(x)$ is the Bessel function.

From the theorem (43) it follows [5] that the general form of a metric transform is

$$F(r) = \left\{ \int_0^\infty \frac{1 - \Omega_N(ru)}{u^2} d\nu(u) \right\}^{1/2} \quad (52)$$

with a positive measure $\nu(u)$ such that $\int_0^\infty d\nu(u)/u^2$ exists.

5. Spherical Spaces

Equation (52) gives the general form of the metric transforms which transform an euclidean space into another euclidean space. Similar questions can be asked about the unit radius spherical spaces* S_{d-1} which consist of points $\vec{x}_j \in R^d$ obeying

$$\vec{x}_1^2 + \vec{x}_2^2 + \ldots + \vec{x}_d^2 = 1. \tag{53}$$

The geodesic distance on the sphere is

$$d(\vec{x}, \vec{y}\,) = \arccos(\vec{x} \cdot \vec{y}\,). \tag{54}$$

The necessary and sufficient conditions that a metric space with the distance matrix M_{ij} can be embedded isometrically into the spherical space with the distance (54) coincide with the condition that N initial points plus one point at the origin can be embedded into the euclidean space. From (13) it follows that the later can be expressed as the nonnegativity condition of the quadratic form

$$\sum_{i,j=1}^{N} \cos(M_{ij})\xi_i\xi_j \geq 0 \tag{55}$$

for all choices of real numbers ξ_j.

Similarly as for the euclidean spaces one can find all positive definite functions on the spherical spaces. In [10] it was proved that these functions have the form

$$g(t) = \sum_{l=0}^{\infty} a_l C_l^{p/2}(\cos t), \tag{56}$$

where all coefficients a_l are nonnegative $a_l \geq 0$. Here $p = d - 2$ and $C_l^k(\cos t)$ are the Gegenbauer polynomials.

This condition can easily be understood from the expression of the Gegenbauer polynomial through the orthogonal set of the hyperspherical harmonics $Y_l^{(k)}(\vec{x}\,)$ (see e.g. [11, 11.4.2])

$$\frac{C_l^{p/2}(\vec{x} \cdot \vec{y}\,)}{C_l^{p/2}(1)} = \frac{\omega_{d-1}}{h(p,l)} \sum_{k=1}^{h(p,l)} Y_l^{(k)}(\vec{x}\,)Y_l^{(k)}(\vec{y}\,), \tag{57}$$

where $h(p,l)$ is the dimension of the irreducible representations of the $d-1$ dimensional rotation group

$$h(p,l) = (2l+p)\frac{(l+p-1)!}{p!\ l!}. \tag{58}$$

*Modifications for spherical spaces of radius R are evident.

If (56) is valid, one has

$$\sum_{i,j=1}^{N} g(d(\vec{x}_i,\vec{x}_j))\xi_i\xi_j = \omega_{d-1}\sum_{l=0}^{\infty}\frac{a_l}{h(p,l)}\sum_{k=1}^{h(p,l)}\left|\sum_{j=1}^{N} Y_l^{(k)}(\vec{x}_j)\xi_j\right|^2 , \qquad (59)$$

which is evidently nonnegative (≥ 0).

6. Embedding of the Spherical Space into the Euclidean Space

In this section we show that distance matrices resulting from spherical geodesic distances are of negative type and, consequently, the metric space with the distance equal the square root of spherical distances can be embedded into the euclidean space.

The proof is based on the following lemma: the spherical geodesic distance (54) has the expansion

$$d(\vec{x},\vec{y}) \equiv \arccos(\vec{x}\cdot\vec{y}\,) = \lambda_0 + \sum_{l=\mathrm{odd}} \lambda_l C_l^{p/2}(\vec{x}\cdot\vec{y}) \ , \qquad (60)$$

where all λ_l with odd l are negative but λ_0 is positive.

Equation (60) is the expansion of $\arccos(t)$ over d-dimensional spherical harmonics. The coefficients λ_l of this series are

$$\lambda_l = \frac{1}{h_l(p)}\int_0^{\pi} \theta C_l^{p/2}(\cos\theta)\sin^p\theta d\theta \ , \qquad (61)$$

where $h_l(p)$ is the normalization integral of the Gegenbauer polynomials

$$h_l(p) = \int_0^{\pi} [C_l^{p/2}(\cos\theta)]^2 \sin^p\theta d\theta \qquad (62)$$

whose explicit expression is (see e.g. [11, 10.9.7])

$$h_l(p) = \frac{\sqrt{\pi}(l+p-1)!\Gamma((p+1)/2)}{(l+p/2)l!(p-1)!\Gamma(p/2)}. \qquad (63)$$

As $C_0^{\lambda} = 1$, one gets

$$\lambda_0 = \frac{\pi}{2} \ . \qquad (64)$$

To compute λ_l with $l \neq 0$ it is convenient to use the Gegenbauer integral (see e.g. [11, 10.9.38])

$$n!\int_0^{\pi} e^{iz\cos\theta} C_n^{\lambda}(\cos\theta)\sin^{2\lambda}\theta d\theta = 2^{\lambda}\sqrt{\pi}\Gamma(\lambda+1/2)\frac{\Gamma(n+2\lambda)}{\Gamma(2\lambda)} i^n z^{-\lambda} J_{n+\lambda}(z), \quad (65)$$

from which one obtains (cf. [11, 11.4])

$$\lambda_l = i^l 2^{p/2}(l+p/2)\Gamma(p/2) \int_{-\infty}^{\infty} t^{-p/2} J_{l+p/2}(t) \hat{f}(t) dt, \tag{66}$$

where $\hat{f}(t)$ is the Fourier transform of the initial function

$$\hat{f}(t) = \frac{1}{2\pi} \int_0^{\pi} \theta \sin\theta e^{-it\cos\theta} d\theta = \frac{1}{2it}(e^{it} - J_0(t)). \tag{67}$$

To the two terms in $\hat{f}(t)$ there are two corresponding terms in λ_l. The integral including e^{it} is zero for all $l \neq 0$ and the integral with $J_0(t)$ is zero for even l. For odd l

$$\lambda_l = -i^{l-1} 2^{p/2}(l+p/2)\Gamma(p/2) \int_0^{\infty} t^{-1-p/2} J_{l+p/2}(t) J_0(t) dt \ . \tag{68}$$

The last integral can be computed using the integral ([11, 7.7.4.30])

$$\int_0^{\infty} t^{-\rho} J_\mu(t) J_\nu(t) dt = \tag{69}$$

$$\frac{\Gamma(\rho)\Gamma((1+\nu+\mu-\rho)/2)}{2^\rho \Gamma((1+\nu-\mu+\rho)/2)\Gamma((1+\nu+\mu+\rho)/2)\Gamma((1+\mu-\nu+\rho)/2)} \ .$$

The final result is

$$\lambda_l = -\frac{p(p+2l)}{8\pi} \left[\frac{\Gamma(p/2)\Gamma(l/2)}{\Gamma(1+(l+p)/2)} \right]^2 . \tag{70}$$

This expression is negative which proves the lemma.

Using this lemma and (57), one concludes that

$$\sum_{i,j=1}^{N} d(\vec{x}_i, \vec{x}_j) \xi_i \xi_j = \lambda_0 (\sum_{i=1}^{N} \xi_i)^2 + \sum_{l=\text{odd}} \frac{\lambda_l}{h(p,l)} \sum_{k=1}^{h(p,l)} \left| \sum_{j=1}^{N} \xi_j Y_l^{(k)}(\vec{x}_j)) \right|^2 . \tag{71}$$

As all λ_l with $l \geq 1$ are negative, this expression is negative for all choices of ξ_j such that $\sum_{j=1}^N \xi_j = 0$, i.e., the spherical geodesic distance matrices are of negative type.

From the theorem of the preceding sections it follows that a new metric space with the distance

$$d^{(\gamma)}(\vec{x}, \vec{y}) = [\arccos(\vec{x} \cdot \vec{y}\ )]^\gamma \tag{72}$$

is also of negative type when $0 < \gamma \leq 1$ and the space with the distance

$$[\arccos(\vec{x}\cdot\vec{y}\,)]^{\gamma/2} \tag{73}$$

can be isometrically embedded into the euclidean space.

7. Conclusion

The distance matrices for points in the euclidean and spherical spaces are of negative type and, consequently, they have all eigenvalues, except one, nonpositive.

More generally, if points $\vec{x}_j$ belong to the euclidean space, the above statement is true for the matrices

$$||\vec{x}_i - \vec{x}_j||^{2\gamma} \tag{74}$$

with $0 < \gamma \leq 1$.

If points $\vec{x}_j$ belong to the spherical space with the distance $d(\vec{x}_i, \vec{x}_j)$ given by (54), then the matrix

$$d^{\gamma}(\vec{x}_i, \vec{x}_j) \tag{75}$$

with $0 < \gamma \leq 1$ is of negative type and has all eigenvalues, except one, nonnegative.

The following theorems are also of interest.

The matrices with elements

$$\exp(-\lambda^2||\vec{x}_i - \vec{x}_j||^{2\gamma}) \tag{76}$$

with $0 < \gamma \leq 1$ are positive definite and have all eigenvalues positive for all $\lambda \to 0$. For $\gamma = 1$ this fact was mentioned in [14].

The similar theorem for the spherical space states that matrices

$$\exp(-\lambda^2 d^{\gamma}(\vec{x}_i, \vec{x}_j)) \tag{77}$$

with $0 < \gamma \leq 1$ are positive definite for all λ.

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Appendix

The purpose of this Appendix is to give, following [12], a proof of the Cayley–Menger determinantal formula (32).

The volume V_n of the n-dimensional Euclidean simplex with one vertex on a point $\vec{x}_{n+1}$ and n vertices on points $\vec{x}_j$ with $j = 1, \ldots, n$ is proportional to the determinant of components of the n vectors $\vec{x}_j - \vec{x}_{n+1}$

$$V_n = \frac{1}{n!} \begin{vmatrix} x_1^{(1)} - x_{n+1}^{(1)} & x_1^{(2)} - x_{n+1}^{(2)} & \ldots & x_1^{(n)} - x_{n+1}^{(n)} \\ x_2^{(1)} - x_{n+1}^{(1)} & x_2^{(2)} - x_{n+1}^{(2)} & \ldots & x_2^{(n)} - x_{n+1}^{(n)} \\ \vdots & \vdots & \vdots & \vdots \\ x_n^{(1)} - x_{n+1}^{(1)} & x_n^{(2)} - x_{n+1}^{(2)} & \ldots & x_n^{(n)} - x_{n+1}^{(n)} \end{vmatrix} . \tag{78}$$

As above the subscripts denote the points and the superscripts denote their coordinates. This expression can be rewritten in a more symmetric form through the determinant of the $(n+1) \times (n+1)$ matrix

$$V_n = \frac{1}{n!} \begin{vmatrix} x_1^{(1)} & x_1^{(2)} & \ldots & x_1^{(n)} & 1 \\ x_2^{(1)} & x_2^{(2)} & \ldots & x_2^{(n)} & 1 \\ \vdots & \vdots & \vdots & \vdots & \vdots \\ x_n^{(1)} & x_n^{(2)} & \ldots & x_n^{(n)} & 1 \\ x_{n+1}^{(1)} & x_{n+1}^{(2)} & \ldots & x_{n+1}^{(n)} & 1 \end{vmatrix} . \tag{79}$$

Simple manipulations show that it can be transformed in two different ways

$$V_n = \frac{(-1)^n}{2^n n!} \det A_n = -\frac{1}{n!} \det B_n, \tag{80}$$

where the $(n+2) \times (n+2)$ matrices A_n and B_n have the following forms:

$$A_n = \begin{pmatrix} 1 & 0 & \ldots & 0 & 0 \\ (\vec{x}_1)^2 & -2x_1^{(1)} & \ldots & -2x_1^{(n)} & 1 \\ (\vec{x}_2)^2 & -2x_2^{(1)} & \ldots & -2x_2^{(n)} & 1 \\ \vdots & \vdots & \vdots & \vdots & \vdots \\ (\vec{x}_n)^2 & -2x_n^{(1)} & \ldots & -2x_n^{(n)} & 1 \\ (\vec{x}_{n+1})^2 & -2x_{n+1}^{(1)} & \ldots & -2x_{n+1}^{(n)} & 1 \end{pmatrix}, \tag{81}$$

and

$$B_n = \begin{pmatrix} 0 & 0 & \dots & 0 & 1 \\ 1 & x_1^{(1)} & \dots & x_1^{(n)} & (\vec{x}_1)^2 \\ 1 & x_2^{(1)} & \dots & x_2^{(n)} & (\vec{x}_2)^2 \\ \vdots & \vdots & \vdots & \vdots & \vdots \\ 1 & x_n^{(1)} & \dots & x_n^{(n)} & (\vec{x}_n)^2 \\ 1 & x_{n+1}^{(1)} & \dots & x_{n+1}^{(n)} & (\vec{x}_{n+1})^2 \end{pmatrix}. \tag{82}$$

Notice the position of the column of 1 in B_n. Therefore

$$V_n^2 = \frac{(-1)^{n+1}}{2^n (n!)^2} \det C_n, \tag{83}$$

where $C_n = A_n \cdot B_n^T$.

Direct calculations give the Cayler–Menger formula

$$V_n^2 = \frac{(-1)^{n+1}}{2^n (n!)^2} \begin{pmatrix} 0 & 1 & 1 & \dots & 1 \\ 1 & 0 & D_{12}^2 & \dots & D_{1\ n+1}^2 \\ 1 & D_{12}^2 & 0 & \dots & D_{2\ n+1}^2 \\ \vdots & \vdots & \vdots & \vdots & \vdots \\ 1 & D_{1\ n}^2 & \dots & 0 & D_{n\ n+1}^2 \\ 1 & D_{1\ n+1}^2 & \dots & D_{n\ n+1}^2 & 0 \end{pmatrix}, \tag{84}$$

where $D_{ij} = ||\vec{x}_i - \vec{x}_j||$ is the length of the edge (i, j) of the n-dimensional simplex.

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