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# The Distance Matrix for a Simplex

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In this paper we consider some geometric questions relating to a higher dimensional analogon of a triangle, called simplex. In particular, we shall be concerned with the distance matrix of its vertices. We shall also majorize the volume of a simplex in terms of the distances between vertices. As consequences, we shall derive some inequalities for determinants and, in particular, an improvement of the well-known Hadamard's inequality. We shall also point to some possible applications to the chemical graph theory.

## INTRODUCTION

In the first part of this paper, we consider the problem of the existence of a simplex (a higher dimensional analogon of a triangle or a tetrahedron) with prescribed edge lengths and a similar problem involving prescribed dihedral angles. We shall also give some connections between these two approaches. Similar problems in non-Euclidean spaces are also of interest and we shall address them as well. The basic tool in these considerations will be the so called (geometric) distance matrix of an appropriate set of points.

In the second part, we consider the problem of majorizing the volume of a simplex in terms of the edge lengths, *i.e.* elements of its distance matrix. The main ingredients here are some geometric facts, like the so called sine law and others.

In the third part, we give some consequences of the results from the first two parts. There are some geometric as well as some purely algebraic consequences. In fact, these consequences are mainly some inequalities involving volumes of some polytopes or inequalities (rather upper bounds) of some determinants in terms of their entries. Among others, one of the obtained inequalities improves substantially the well-known Hadamard's inequality (often used not only in mathematics but also in mathematical physics and mathematical chemistry).

In the final part, we describe some possible applications of the previous material to mathematical chemistry, in particular to the chemical graph theory which, in turn, applies to various problems in chemistry. For example, some inequalities involving the eigenvalues of the associated matrix, which is related to the bound of certain chemical indices (*e.g.* Wiener index).

## *Simplex and its Distance Matrix*

As we all know from our high-school days, the three edge lengths of a triangle determine it up to congruence, provided they satisfy the triangle inequality: $a+b>c$, $b+c>a$, $c+a>b$ (Figure 1).

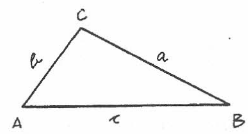



Figure 1.

A natural question arises for a tetrahedron. Namely, is it true that all the required triangle inequalities guarantee the existence of a tetrahedron? In other words, suppose six positive numbers $a$, $b$, $c$, $d$, $e$, $f$ are given. What is the necessary and sufficient condition for the existence of a tetrahedron with these (prescribed) edge lengths? See Figure 2.

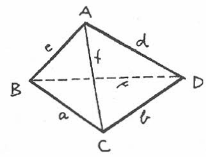



Figure 2.

It turns out that all the required triangle inequalities (*i.e.* $a + b > c$, $b + c > a$, ..., $b + f > d$, ...) are not sufficient for the existence of a tetrahedron. For example (see Figure 3), three segments of length $a$ and three segments of length $b$ can form an »$a$-tripoid« on a »$b$-triangle« or a »$b$-tripoid« on an »$a$-triangle« or in a third »zig-zag« way.

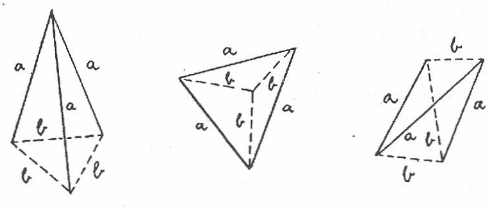


Figure 3.

If $a$ is much larger than $b$, it is plausible (and, in fact, true) that only the first construction can be realized, but if $a$ is only slightly larger than $b$, it is plausible (and, indeed, true) that all three possibilities can occur. The condition $b < a \leq 2b$ is not sufficient for the existence of a »$b$-tripoid« on an »$a$-triangle« and, hence, the figures that satisfy the triangle inequality in all the required ways are not necessarily realizable.

So, what is a »triangle-inequality« for a tetrahedron? The answer to this question is given by the following theorem, rediscovered by many authors in the long history of this natural question. For a proof, see *e.g.* Ref. 15.

**Theorem 1**. Let $a$, $b$, $c$, $d$, $e$, $f$ be given positive numbers. The inequalities

$$a+b>c, \quad b+c>a, \quad c+a>b,$$

and

$$\begin{vmatrix} 0 & c^2 & b^2 & d^2 & 1 \\ c^2 & 0 & a^2 & e^2 & 1 \\ b^2 & a^2 & 0 & f^2 & 1 \\ d^2 & e^2 & f^2 & 0 & 1 \\ 1 & 1 & 1 & 1 & 0 \end{vmatrix} > 0$$

are necessary and sufficient conditions for the existence of a tetrahedron $S$ = ABCD with edge lengths $a$ = |BC|, $b$ = |CA|, $c$ = |AB|, $d$ = |AD|, $e$ = |BD|, $f$ = |CD|.

Now, let's go a step further, and consider the same question for a simplex. An $n$-dimensional **simplex** $S = \langle A_o, A_1, \ldots A_n \rangle$ is the smallest convex set (*i.e.* the convex hull) that contains $n+1$ points $A_o, A_1, \ldots, A_n$ in $n$-dimensional space $\boldsymbol{R}^n$ which are in the general position (*i.e.* the vectors $\overrightarrow{\boldsymbol{A}_0\boldsymbol{A}_1}$ form a basis in $\boldsymbol{R}^n$) and these points are called its **vertices**. 1-dimensional simplex is usually called a **segment**, 2-dimensional simplex is a triangle, and 3-dimensional a tetrahedron. An $n$-dimensional simplex (shortly $n$-simplex) can be thought of as a complete graph $K_{n+1}$ on $n$ + 1 vertices, but »embedded« in $\boldsymbol{R}^n$ so that there are no crossings of its edges. *E.g.* 4-dimensional simplex can be represented by $K_5$ (Figure 4).

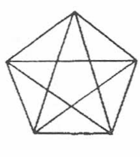


Figure 4.

(For basic graph-theoretical concepts and results, the reader may consult Ref. 6 – in Croatian, or *e.g.* Ref. 7 – in English).

For vertices $A_i$, $A_j$ of the simplex $S = \langle A_o, A_1, \ldots, A_n \rangle$, let $d_{ij} = |A_iA_j|$ be the distance between them, *i.e.* the length of the edge $A_iA_j$. We form the **distance matrix**.

$$D = (d_{ij}).$$

Denote by $D^{(2)} = (d_{ij}^2)$ the matrix of the squares of distances, and let $M = (m_{ij})$, where $m_{ij} = d_{i0}^2 + d_{j0}^2 - d_{ij}^2$. Then, as it is easy to show

$$\det\begin{pmatrix} & & & & 1 \\ & & & & 1 \\ & D^{(2)} & & & \vdots \\ & & & & 1 \\ & & & & 1 \\ 1 & 1 & \dots & 1 & 1 & 0 \end{pmatrix} = (-1)^{n+1}\det M.$$

Any determinant of the form

$$\det\begin{pmatrix} & & & & 1 \\ & & & & 1 \\ & d_{ij}^2 & & & \vdots \\ & & & & 1 \\ & & & & 1 \\ 1 & 1 & \dots & 1 & 1 & 0 \end{pmatrix},$$

where $i, j \in I$ and $I \subseteq \{0, 1, \dots, n\}$ is called a **Cayley-Menger determinant**. $D^{(2)}$ itself is often called the distance matrix.

Now, what is a »triangle-inequality« for a simplex? In geometry and physics, one often considers not only the ordinary Euclidean (»flat«) space $\boldsymbol{R}^n$ but also the »curved« spaces of constant curvature $\kappa$. If this constant curvature $\kappa$ is positive (it can be taken to be equal +1), then we can assume that this space is an $n$-dimensional (unit) sphere $S^n$, and if the space has a negative constant curvature $\kappa$ (it can be taken to be equal $-1$), then it is the hyperbolic $n$-dimensional space $H^n$. In all three of these types of spaces it makes sense to consider simplices (flat or curved »triangles«); see Figure 5.

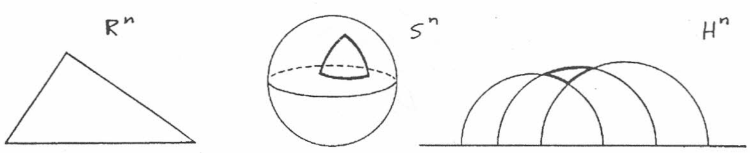



Figure 5.

The appropriate notion of distances in all three geometries can also be defined and, hence, one can ask for the »triangle inequality« for simplices in all three geometries. The answer is given by the following theorem.

**Theorem 2** (Dekster-Wilker, 1991[1]). Let $\boldsymbol{D} = (d_{ij})$ be an $(n+1) \times (n+1)$ real matrix with $d_{ii} = 0$, $d_{ij} = d_{ji} \geq 0$, $i, j = 0, 1, ..., n$, $n \geq 2$, and let its entries be used to form the $n \times n$ matrix $\boldsymbol{M} = \boldsymbol{M}(D) = (m_{ij})$, where

$$m_{ij} = \begin{cases} \cosh d_{i0} \cosh d_{j0} - \cosh d_{ij}, & \text{in the hyperbolic case} \\ d_{i0}^2 + d_{j0}^2 - d_{ij}^2, & \text{in the Euclidean case} \\ \cos d_{ij} - \cos d_{i0} \cos d_{j0}, & \text{in the spherical case.} \end{cases}$$

Then, an $n$-dimensional simplex $S = \langle A_o, A_1, ..., A_n \rangle$ exists in the $n$-space under consideration such that the entries of $\boldsymbol{D}$ occur as the distance between the $A_i$'s, *i.e.* $d_{ij} = |A_iA_j|$, if and only if the eigenvalues of $\boldsymbol{M}$ are all real and non-negative.

Such a matrix $\boldsymbol{D}$ is then called **realizable** and any such simplex is called a **realization** of $\boldsymbol{D}$ and $\boldsymbol{D}$ is called the **distance matrix** of its realization.

Furthermore, if $\boldsymbol{D}$ is realizable, then the dimension of the convex hull of each realization of $\boldsymbol{D}$ is equal to the rank of $\boldsymbol{M}$.

For the Euclidean case, see also Ref. 12.

Besides the lengths of edges of a simplex, one can also measure the dihedral angles, *i.e.* the angles between the (hyper-) planes of the simplex. Let again $S = \langle A_o, A_1, ..., A_n \rangle$ be an $n$-simplex and let $\alpha_{ij}$ be its dihedral angle along the edge $A_iA_j$, *i.e.* the angle between the hyperplanes $A_oA_1 \ldots \hat{A}_i \ldots A_n$ and $A_oA_1 \ldots \hat{A}_j \ldots A_n$ (the symbol ^ means »omitted«). We now define another matrix $\boldsymbol{C} = (c_{ij})$, where $c_{ii} = 1$ and $c_{ij} = -\cos \alpha_{ij}$ for $i \neq j$, and $0 \leq i, j \leq n$. Let $C_{ij}$ be the cofactor of the entry $c_{ij}$ of $\boldsymbol{C}$. Then, the following theorem holds.

**Theorem 3** (Yang-Zhang, 1983[10]). The necessary and sufficient conditions for the existence of an $n$-simplex in $\boldsymbol{R}^n$ with prescribed dihedral angles $\alpha_{ij}$ $(i,j = 0, 1, ..., n)$ are

$$\det \boldsymbol{C} = 0 \text{ and } C_{ij} > 0 \text{ for all } i, j.$$

The determinant det $\boldsymbol{C}$ is known as the **Schläfli determinant**.

In fact, in spaces of constant curvature, this result was extended in the following way.

**Theorem 4** (Böhm, 1986[11]). In the spaces of constant curvature $\kappa$ we have the existence of an $n$-simplex with prescribed dihedral angles $\alpha_{ij}$ if an only if all $C_{ij} > 0$ and in the cases

$$\begin{aligned} \kappa &= 1 \text{ (spherical)} \Leftrightarrow \det \boldsymbol{C} > 0 \\ \kappa &= 0 \text{ (Euclidean)} \Leftrightarrow \det \boldsymbol{C} = 0 \\ \kappa &= -1 \text{ (hyperbolic)} \Leftrightarrow \det \boldsymbol{C} < 0. \end{aligned}$$

A relation between matrices $\boldsymbol{C}$ and $\boldsymbol{D}$ (at least in the Euclidean case) is as follows. Let

$$\boldsymbol{D}^{(2)} = \boldsymbol{D}^{(2)}(A_0, A_1, \ldots, A_n) = \det \begin{pmatrix} & & & & 1 \\ & & & & 1 \\ & & d_{ij}^2 & & \vdots \\ & & & & 1 \\ & & & & 1 \\ 1 & 1 & \ldots & 1 \; 1 & 0 \end{pmatrix},$$

and let $D_{ij}^{(2)} = D_{ij}^{(2)}(A_0, A_1, \ldots, A_n)$ be the cofactor of the $(i,j)$-th entry $d_{ij}^2$ of $\boldsymbol{D}^{(2)}$, $0 \le i,\ j \le n,\ i < j$. Then, the following holds.

**Theorem 5** (Yang-Zhang, 1989[10]). With the above notations

$$-c_{ij} = \cos\alpha_{ij} = \frac{D_{ij}^{(2)}(A_0, A_1, \ldots A_n)}{\sqrt{\boldsymbol{D}^{(2)}(A_0, \ldots, \hat{A}_i, \ldots, A_n) \cdot \boldsymbol{D}^{(2)}(A_0, \ldots, \hat{A}_j, \ldots, A_n)}}.$$

In particular,

$$[D_{ij}(A_0, A_1, \ldots, A_n)]^2 \le \boldsymbol{D}^{(2)}(A_0, \ldots, \hat{A}_i, \ldots, A_n) \cdot \boldsymbol{D}^{(2)}(A_0, \ldots, \hat{A}_j, \ldots, A_n).$$

*Volume and the Sine Law for Simplices*

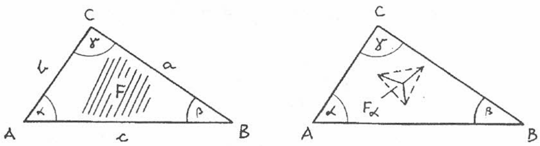
In the first section, we have seen how some basic laws (existence) of a simplex depend on determinants, mainly of its distance matrix. In this section, we continue in the same spirit.

Another important gadget of a simplex is its volume. Again, from high-school days we recall the famous Heron's formula for the area of a triangle in terms of its sides (or edge lengths). Volume $V$ of an $n$-simplex $S = \langle A_o, A_1, \ldots, A_n \rangle$ with $d_{ij} = |A_iA_j|$ is given by the following Heron's formula for a simplex (*e.g.* see Ref. 12):

$$2^n (n!)^2 V^2 = \left| \det \begin{pmatrix} & & & & 1 \\ & & & & 1 \\ & & d_{ij}^2 & & \vdots \\ & & & & 1 \\ & & & & 1 \\ 1 & 1 & \ldots & 1 \; 1 & 0 \end{pmatrix} \right|.$$

Although this is an exact formula, it is rather impractical, since in order to compute an $n \times n$ determinant, at least $n!$ computations are required in general. Therefore, very sharp estimates and actually very sharp upper bounds for the volume of a simplex are of great interest. For this purpose, recall again your nice high-school days and one of the basic triangle laws, the sine law. It simply says that for the area $F$ of a triangle, such as in Figure 6a, we have

$$bc \sin\alpha = ca \sin\beta = ab \sin\gamma (= 2F), \text{ or } \frac{\sin\alpha}{a} = \frac{\sin\beta}{b} = \frac{\sin\gamma}{c} \left( = \frac{2F}{abc} \right).$$




6a 6b

Figure 6.

But, one can look at this in the following way. Pick a point within the triangle and draw from it unit outward normals to the sides. Then, this gives rise to three new little triangles with areas $F_\alpha$, $F_\beta$, $F_\gamma$ (see Figure 6b). The sine law can than be interpreted as follows:

$$bcF_\alpha = caF_\beta = abF_\gamma \; .$$

Generalizing this idea to simplices, we have the following basic rule.

**Theorem 6** (The sine law for simplices, Ref. 2). Let $S = \langle A_o, A_1, \ldots, A_n \rangle$ be an $n$-simplex in $\boldsymbol{R}^n$, $V = \text{vol}\, S$ (volume of $S$), $S_i = \langle A_0, \ldots, \hat{A}_i, \ldots, A_n \rangle$ its side opposite to the vertex $A_i$, $\pi_i$ the hyperplane of $S_i$, $V_i = \text{vol}_{n-1} S_i$ (*i.e.* the »surface area« of $S_i$). Let O be any internal point in $S$, $\vec{e}_i = \overrightarrow{\boldsymbol{OB}}_i$, the unit »outward« normal to $\pi_i$ and $E_i = \langle O, B_0, \ldots, \hat{B}_i, \ldots, B_n \rangle$ associated »unit« $n$-simplex and $W_i = \text{vol}\, E_i$ its volume. Then

$$V_0 \cdots V_{i-1} W_i V_{i+1} \cdots V_n = \frac{(nV)^{n-1}}{n!\,(n-1)!}, \qquad i = 0, 1, \ldots, n.$$

From this basic law it is not hard to derive the basic upper bound for the volume of a simplex in terms of its facets. Namely, the following inequality holds.

**Theorem 7** (Main inequality[2]). With the same notations as in the previous theorem we have

$$V^{n-1} \le n! \sqrt{\frac{(n+1)^{n-1}}{n^{3n}}} \left( \prod_{i=0}^{n} V_i \right)^{\frac{n}{n+1}},$$

with equality if and only if the simplex is regular.

From this by falling induction, the promised sharp upper bound of volume by the edge-lengths is given in the following way.

**Theorem 8** (Ref. 2). With the same notation as above, $d_{ij} = |A_i A_j|$, we have

$$V \le \frac{1}{n!} \sqrt{\frac{n+1}{2^n}} \left( \prod_{0 \le i < j \le n} d_{ij} \right)^{\frac{2}{n+1}},$$

with equality if and only if the simplex is regular.

So, for example, for a tetrahedron with edges $a, b, c, d, e, f$, we have

$$V \leq \frac{\sqrt{2}}{12} \sqrt{abcdef},$$

with equality if and only if $a = b = c = d = e = f$.

*Some Geometric and Algebraic Consequences*

The above results have some nice geometric and algebraic consequences. We shall present here some of them. Firstly, some geometric corollaries are as follows.

**Theorem 9** (Isoperimetric inequality for a simplex). With the same notations as in Theorem 6, let $F = \Sigma_{i=0}^{n} V_i$ be the »total area« of the simplex $S$. Then

$$\frac{F^n}{V^{n-1}} \geq \frac{1}{n!} \sqrt{n^{3n} (n+1)^{n+1}} \ ,$$

with equality if and only if $S$ is regular.

In other words, among all $n$-simplices with a given »total area«, the regular simplex has the largest volume.

**Theorem 10**. Let P be an $n$-dimensional polyhedron in $\boldsymbol{R}^n$ consisting of $p$ simplices $S_i$ of dimension $n$, such that they satisfy the codimension 2 intersection property, *i.e.* for $i \neq j$, $\dim(S_i \cap S_j) \leq n - 2$. Let $V_i = \text{vol } S_i$, $F_i$ = »total area« of $S_i$, $V = \text{vol P} = \Sigma V_i$ the volume of P and $F = \Sigma F_i$ = »total area« of P. Then, the following inequalities hold:

$$V \leq \left( \frac{n!}{\sqrt{n^{3n} (n+1)^{n-1}}} \right)^{\frac{1}{n-1}} \left( \frac{1}{1+n} \right)^{\frac{n}{n-1}} \sum_{i=1}^{p} F_i^{\frac{n}{n-1}},$$

and

$$\prod_{i=1}^{p} V_i^{n-1} \leq \left[ \frac{n!}{\sqrt{n^{3n} (n+1)^{n+1}}} \left( \frac{F}{p} \right)^n \right]^p .$$

Next, we give an upper bound for the volume of a convex simplicial polytope. A **simplical polytope** is a polytope all of whose faces are simplices.

**Theorem 11**. Let P be an $n$-dimensional convex simplicial polytope (*i.e.* all top-dimensional faces – called facets – are $(n-1)$-simplices). Let the $i$-th of these $(n-1)$-simplices have the edges of lengths $d_{pq}^{(i)}$, $p, q = 1, 2, \ldots, n$, $i = 1, 2, \ldots, f$. Let O be any internal point of P and let $h_i$ be the distance from O to the $i$-th facet. Then, the volume $V$(P) can be majorized as follows

$$V(\mathrm{P}) \leq \frac{1}{n!} \sqrt{\frac{n}{2^{n-1}}} \sum_{i=1}^{f} h_i \left( \prod_{1 \leq p < q \leq n} d_{pq}^{(i)} \right)^{\frac{2}{n}} \leq \frac{1}{n!} \sqrt{\frac{n}{2^{n-1}}} (\mathrm{diam\ P}) d_{\max}^{n-1} f \ ,$$

where $d_{\max} = \max_{i,p,q} d_{pq}^{(i)}$ is the largest edge of P, and $\mathrm{diam\ P} = \max_{X,Y \in \mathrm{P}} d(X,Y)$ the diameter of P (*i.e.* the largest distance between two points of P).

There are many more interesting geometric consequences of the main inequality. Let us mention just one more. Let $S = \langle A_o, A_1, ..., A_n\rangle$ be an $n$-simplex with volume $V$ and $O \in S$ any point in that simplex. If $h_i$ is the distance from O to the facet opposite to the vertex $A_i$, $i = 0, 1, ..., n$, then

$$\left(\prod_{i=1}^{n} h_i\right)^n \le \left[\frac{(n-1)!}{\sqrt{(n+1)^{n+1}}} V\right]^{n+1},$$

with equality if and only if $h_0V_0 = h_1V_1 = ... = h_nV_n = (nV)/(n+1)$; in particular, the equality holds if $S$ is regular and O is its centre.

Now, we turn to some algebraic consequences. In fact, we shall give some (sharp) upper bounds for determinants.

Let again $S = \langle A_0, A_1, ..., A_n\rangle$ be an $n$-simplex of volume $V$, and let $S$ be embedded in $\boldsymbol{R}^n$ and let $A_i = (a_1^{(i)}, a_2^{(i)}, ..., a_n^{(i)})$ be coordinates of the vertex $A_i$, $i = 0, 1, ..., n$. Denote by $\boldsymbol{P}$ the (extended) matrix of coordinates

$$\boldsymbol{P} = \begin{pmatrix} a_1^{(0)} & a_2^{(0)} & \dots & a_n^{(0)} & 1 \\ \vdots & & & & \vdots \\ a_1^{(n)} & a_2^{(n)} & \dots & a_n^{(n)} & 1 \end{pmatrix}.$$

Then, $V = |\det \boldsymbol{P}|/n!$. Let $a^{(i)}$ be the $i$-th row of $\boldsymbol{P}$ and

$$d_{ij} = \| a^{(i)} - a^{(j)}\| = \left[\sum_{k=1}^{n} \left(a_k^{(i)} - a_k^{(j)}\right)^2\right]^{1/2}.$$

Now, recall that the well known Hadamard's inequality reads as follows (see Ref. 13):

$$|\det \boldsymbol{P}| = n!V \le \left(\prod_{i<j} d_{ij}\right)^{\frac{2}{n+1}} = \left(\prod_{0\le i<j\le n} \| a^{(i)} - a^{(j)}\|\right)^{\frac{2}{n+1}}$$

But, from Theorem 8 it follows that we have an improvement of this inequality by factor $\sqrt{(n+1)/2^n}$. In other words, we have.

**Theorem 12**. For any matrix $\boldsymbol{P}$ as above,

$$|\det \boldsymbol{P}| \le \sqrt{\frac{n+1}{2^n}} \left(\prod_{0\le i<j\le n} \| a^{(i)} - a^{(j)}\|\right)^{\frac{2}{n+1}},$$

with equality if and only if all $\| a^{(i)} - a^{(j)}\|$ are mutually equal.

From Heron's formula, we also get the following.

**Theorem 13**. For any realizable $(n + 1) \times (n + 1)$ distance matrix $\boldsymbol{D} = (d_{ij})$,

$$\left|\det\begin{pmatrix} & & 1 \\ & & 1 \\ & d_{ij}^2 & \vdots \\ & & 1 \\ & & 1 \\ 1\ 1 & \dots\ 1\ 1 & 0 \end{pmatrix}\right| \le (n+1)\left(\prod_{i<j} d_{ij}\right)^{\frac{4}{n+1}},$$

with equality if and only if $d_{ij}$'s are mutually equal.

Now, for an $n$-dimensional $S = \langle A_0, A_1, \dots, A_n\rangle$, think of vectors $\vec{\boldsymbol{a}}_i = \overrightarrow{\boldsymbol{A}_0\boldsymbol{A}_i}$, $i = 1, 2, \dots, n$ as a basis of $\boldsymbol{R}^n$. Then, from the fact that the volume $V = \mathrm{vol}\, S$ is given by $(n!V)^2 = \det(a_{ij})$, where $a_{ij} = \vec{\boldsymbol{a}}_i \cdot \vec{\boldsymbol{a}}_j$ (scalar product), and from Theorem 8, the following can be deduced for the determinant of the Gram matrix.

**Theorem 14**. Let $\vec{\boldsymbol{a}}_1, \vec{\boldsymbol{a}}_2, \dots, \vec{\boldsymbol{a}}_n$ be any basis of $\boldsymbol{R}^n$ and $a_{ij} = \vec{\boldsymbol{a}}_i \cdot \vec{\boldsymbol{a}}_j$. Then,

$$\det(a_{ij}) \le \frac{n+1}{2^n}\left[\left(\prod_{i=1}^{n} a_{ii}\right)\left(\prod_{1\le i<j\le n}(a_{ii} + a_{jj} - 2a_{ij})\right)\right]^{\frac{2}{n+1}},$$

with equality if and only if $a_{11} = \dots = a_{nn} = a^2$ and $a_{ij} = a^2/2$ for $i \ne j$.

As a final inequality in this series, we mention the following fact.

**Theorem 15**. Like in the previous theorem, let $\boldsymbol{M}_i = \det(a_{kl})_{k,\, l\ne i}$, $i = 1, 2, \dots, n$ be principal minors. Then,

$$[\det(a_{ij})]^{n-1} \le \frac{(n+1)^{n-1}}{n^n}[M_1M_2\dots M_n \det(a_{11} + a_{kl} - a_{1k} - a_{1l})]^{\frac{n}{n+1}}$$

with equality if and only if $a_{ii} = a^2$ and $a_{ij} = a^2/2$, $i \ne j$.

The above bounds hold for any real $n \times n$ symmetric, positive definite matrix. A bit stronger results can be obtained by improving Theorem 8 as in Ref. 8. and, hence, all its consequences can be slightly improved.

All these results came out from geometric considerations in Euclidean space and, in particular, from the sine law for simplices. Let us say that very little is known about simplices in non-Euclidean spaces, particularly in hyperbolic space. The problem of computing the volume of such a simplex seems to be an extremely difficult task, although many efforts in this direction have been made through history, starting with Gauss, Riemann and others. Therefore, it would be of great interest to have analogous bounds for the volume of simplices in hyperbolic space, spherical space, Minkowski space *etc.*, which are also often encountered by physicists.

As we have so far seen in this survey, the basic laws have a decisive role, like the sine law. So, it would be of great importance to have on disposal the sine law for hyperbolic and other geometries. There have been, in principle, some results in this direction (*e.g.* by Hsiang), but not an explicit and useful result like the one presented here (except for a triangle which was known long ago). However, in terms of the above results, we have some results in this direction. For example, if $\boldsymbol{D} = (d_{ij})$ is an $(n + 1) \times (n + 1)$ realizable matrix in the hyperbolic space, then the corresponding (symmetric) matrix $\boldsymbol{M} = (m_{ij})$ is a positive definite $(n + 1) \times (n + 1)$ matrix and by the inequality in Theorem 14 we have (seemingly not a very remarkable result, but still):

$$\det \boldsymbol{M} = \det(\cosh d_{i0} \cosh d_{j0} - \cosh d_{ij}) \le$$

$$\le \frac{n+1}{2^n} \left[ \left( \prod_{i=1}^{n} \sinh^2 d_{i0} \right) \prod_{i<j} (\sinh^2 d_{i0} + \sinh^2 d_{j0} + 2 \cosh d_{i0} \cosh d_{j0} - 2 \cosh d_{ij}) \right]^{\frac{2}{n+1}} .$$

A similar result can be obtained for the spherical case.

## *Applications to the Chemical Graph Theory*

So far, we have considered the so called geometric distance matrix. In graph-theoretical applications to chemistry (or, rather, in the chemical graph theory, as it is called in the last decade or so, see Ref. 13), one usually considers a graph G on its vertices $v_1, v_2, \ldots, v_n$ and then its $n \times n$ **distance matrix** $\Delta(\mathrm{G}) = (d(v_i, v_j))$, where $d(v_i, v_j)$ is the number of edges in the shortest path from $v_i$ to $v_j$, if it exists; if not, we put $d(v_i, v_j) = \infty$ (see Refs. 3, 5). This is a source of very useful tools in chemistry, used to predict certain properties of chemical substances even before they have been synthesized by organic chemists. Among the most useful of such tools are various »topological indices« arising from the underlying graph of a chemical compound; for example, the **Wiener index**, introduced by Harry Wiener from Brooklyn College in 1947, has been used in a variety of ways, from predicting antibacterial activity in drugs to correlating thermodynamic parameters in physical chemistry and modeling all kinds of solid state phenomena (see *e.g.* Ref. 16 as one of the latest papers on this much explored topic). The Wiener index $W(\mathrm{G})$ of a graph G is simply defined as the sum of all the entries of $\Delta(\mathrm{G})$ in the upper triangular part, *i.e.*

$$W(\mathrm{G}) = \sum_{i<j} d(v_i, v_j).$$

The distance matrix was first used in chemistry by Hosoya (see Ref. 17)and since it has become a standard tool used in the variety of applications, from considering evolutionary distances in DNA sequences to predicting carcinogenecity in arene systems.[4,5] In doing so, it seems that the (ordinary) distance matrix $\Delta(\mathrm{G})$ has a close relation to the **Laplacian matrix** $\boldsymbol{L}(\mathrm{G})$ of a graph G (see the excellent survey[8]). The Laplacian $\boldsymbol{L}(\mathrm{G})$ of a graph G is defined by

$$\boldsymbol{L}(\mathrm{G}) = \boldsymbol{D}(\mathrm{G}) - \boldsymbol{A}(\mathrm{G}).$$

where $\boldsymbol{D}(\mathrm{G})$ is the diagonal matrix consisting of vertex degrees, while $\boldsymbol{A}(\mathrm{G})$ is the common adjacency matrix of G. This assertion can be supported by the following »interlacing theorem« about the eigenvalues of $\Delta(\mathrm{T})$ and $\boldsymbol{L}(\mathrm{T})$ of a tree T, as well as some other facts about $\Delta(\mathrm{T})$ and $\boldsymbol{L}(\mathrm{T})$.

**Theorem 16**. Let T be a tree on $n$ vertices. The first (»interlacing«) fact is this. Let $\delta_1 > 0 > \delta_2 \geq \dots \geq \delta_n$ be the eigenvalues of $\Delta(\mathrm{T})$ and $\lambda_1 \geq \lambda_2 \geq \dots \geq \lambda_{n-1} > 0 = \lambda_n$ the eigenvalues of $\boldsymbol{L}(\mathrm{T})$. Then,

$$0 > \frac{-2}{\lambda_1} \geq \delta_2 \geq \frac{-2}{\lambda_2} \geq \delta_3 \geq \dots \geq \frac{-2}{\lambda_{n-1}} \geq \delta_n .$$

As the second fact, the Wiener index $W(\mathrm{T})$ is given by

$$W(\mathrm{T}) = n \sum_{i=1}^{n-1} \frac{1}{\lambda_i} .$$

The third fact is that $\det \Delta(\mathrm{T}) = (-1)^{n-1}(n-1)2^{n-2}$, *i.e.* $\det \Delta(\mathrm{T})$ depends only on $n$ and not at all on the structure of T.

To relate our research to the Laplacian and (ordinary) distance matrix of a graph, let us recall *M*. Fiedler's geometric approach as described in Ref. 8. Namely, the Laplacian $\boldsymbol{L}(\mathrm{G})$ of a graph G on $n$ vertices can be viewed as a Gram matrix based on certain $n$ vectors, $x_1, x_2, \dots, x_n$ in $\boldsymbol{R}^{n-1}$. Taking the tangent plane $\mathrm{P}_i$ to the standard sphere $S^{n-2}$ in $\boldsymbol{R}^{n-1}$ at the intersection of the ray generated by $x_i$ and this sphere, and then taking the half-space defined by $\mathrm{P}_i$ containing the origin, as the intersection of these half-spaces, we get an $(n-1)$-simplex $S = \langle \mathrm{A}_1, \mathrm{A}_2, \dots, \mathrm{A}_n \rangle$. Let $d_{ij} = |\mathrm{A}_i\mathrm{A}_j|$ be the distance between vertices $\mathrm{A}_i$ and $\mathrm{A}_j$ and let $\boldsymbol{D}^{(2)}(\mathrm{G}) = (d_{ij}^{\,2})$be the **Cayley-Menger matrix** of a graph G.

In the case of a tree, the Cayley-Menger and the distance matrix agree, *i.e.* if T is a tree, then $\boldsymbol{D}^{(2)}(\mathrm{T}) = \Delta(\mathrm{T})$; in words, the distance matrix of a tree is the Cayley-Menger matrix arising from its Laplacian matrix.

In a general case, we can apply our results of Theorems 13 and 14 to get new information about $\boldsymbol{L}(\mathrm{G})$ and then, in turn, on G. On the other hand, we can also apply our geometric results (notably Theorems 7 and 8) and obtain geometric information about the resulting simplex $S = S(\mathrm{G})$. Of course, another possibility is to start with a weighted graph. One can also consider the weighted strong directed digraph. A nice result in this direction is a theorem proved by Graham, Hoffmann and Hosoya saying that for the distance matrix $\boldsymbol{D}(\mathrm{W})$ of such a digraph W with blocks $\mathrm{G}_1, \mathrm{G}_2, \dots, \mathrm{G}_n$ the following formula holds

$$\det \boldsymbol{D}(\mathrm{W}) = \sum_{i=1}^{n} [\det \boldsymbol{D}(\mathrm{G}_i) \prod_{j \neq i} \operatorname{cof} \boldsymbol{D}(\mathrm{G}_j)],$$

where $\operatorname{cof}(M)$ denotes the sum of the cofactors of $M$, see Ref. 3.

The **permanent** of an $n \times n$ matrix $\boldsymbol{A} = (a_{ij})$ is defined by

$$\operatorname{per} \boldsymbol{A} = \sum_{\sigma \in S_n} \prod_{i=1}^{n} a_{i\sigma(i)} ,$$

where $S_n$ is the symmetric group of all permutations of $\{1, 2, \ldots, n\}$. In chemistry, permanents are important because they are used to count the »Kekule's structures« (or perfect matchings) of a graph. Per $\boldsymbol{L}(\mathrm{G}) \geq 2(n-1)$ for every connected graph G on $n$ vertices was the first important result in this direction. Determinants and permanents are connected (or »homotopic«) *via* so called **immanents**. Namely, for any irreducible character $\chi$ of $S_n$, the corresponding immanent $d_\chi$ of an $n \times n$ matrix $\boldsymbol{A} = (a_{ij})$ is defined by

$$d_\chi (\boldsymbol{A}) = \sum_{\sigma \in S_n} \chi(\sigma) \prod_{i=1}^{n} a_{i\sigma(i)} .$$

For $\chi = \varepsilon$ (the signum character), $d_\chi = \det$, while for $\chi = 1$, $d_\chi = \operatorname{per}$. Immanents are important in counting the Hamiltonian cycles of a graph, and they are, perhaps, another instance where we can extend our results. However, we shall not consider the above mentioned possible projects in this paper.

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## SAŽETAK

### Matrica udaljenosti simpleksa

*Darko Veljan*

U radu se razmatraju neka geometrijska pitanja o simpleksu, višedimenzionalnom analogonu trokuta, pri čemu je posebna pozornost obraćena matrici udaljenosti za vrhove simpleksa. Također je provedena majorizacija volumena simpleksa i izražena s pomoću udaljenosti među njegovim vrhovima. Kao rezultat slijedi izvod nekih nejednakosti za determinante, a posebice jedno poboljšanje dobro poznate Hadamardove nejednakosti. U radu su istaknute neke moguće primjene u kemijskoj teoriji grafova.