Distance Matrices Yielding Angles between Arcs of the Graphs

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If distances d_{ij} in distance matrices **D** express consequently, with the topological distance matrices, squares of Euclidean distances of corresponding vertices, then the difference scheme $\mathbf{SDS}^T$, where $\mathbf{S}^T$ is the transposed incidence matrix of the graph, gives the correct angles between the arcs. The straight chain lowest eigenvalue is its Wiener number.

1. INTRODUCTION

Topological distance matrices, where the distance d_{ij} measures the number of arcs (edges) between vertices i and j in the graph, were used to characterize graphs in graph theory.[1,2] Recently distance matrices measuring the Euclidean geometrical distances of corresponding vertices were introduced[3–7] as well as matrices with reciprocal distance values.[8]

In my previous paper,[9] I interpreted the difference scheme $\mathbf{SDS}^T = -2\mathbf{I}$, true for trees (Rutherford[10]), as a symptom of orthogonality of arcs in trees. $\mathbf{S}^T$ is the transposed incidence matrix **S**; $s_{ij} = -1$, when the arc i goes from the vertex j, $s_{ij} = 1$, when the arc i goes to the vertex j, and $s_{ij} = 0$ otherwise. I also noted that a straight chain can remain straight in spaces of all dimensions. Nevertheless, I was not able to formulate distance matrices of straight chains. Their form is surprising because of its simplicity.

2. SQUARED CARTESIAN DISTANCES

If two consecutive orthogonal displacements lead to the distance 2, the square of the diagonal, than two consecutive straight displacements must lead to the distance 4, the square of the straight Cartesian (Euclidean) distance. The distances should be expressed as the Hilbert distances.

For straight linear chains, the following matrix product is obtained. **2** is the squared length of a difference vector (..., −1, 1, ...).

$$\mathbf{S}_L \mathbf{D}_L \mathbf{S}_L^T = 2\mathbf{JJ}^T - 4\mathbf{I}$$

$$\begin{Vmatrix} -1 & 1 & 0 & 0 \\ 0 & -1 & 1 & 0 \\ 0 & 0 & -1 & 1 \end{Vmatrix} \begin{Vmatrix} 0 & 1 & 4 & 9 \\ 1 & 0 & 1 & 4 \\ 4 & 1 & 0 & 1 \\ 9 & 4 & 1 & 0 \end{Vmatrix} \begin{Vmatrix} -1 & 0 & 0 \\ 1 & -1 & 0 \\ 0 & 1 & -1 \\ 0 & 0 & 1 \end{Vmatrix} = \begin{Vmatrix} -2 & -2 & -2 \\ -2 & -2 & -2 \\ -2 & -2 & -2 \end{Vmatrix}$$

The other three distances between the vertices, to which no arcs correspond, are obtained similarly. On the diagonal their squared lengths appear as follows:

$$\begin{Vmatrix} -1 & 0 & 1 & 0 \\ -1 & 0 & 0 & 1 \\ 0 & -1 & 0 & 1 \end{Vmatrix} \begin{Vmatrix} 0 & 1 & 4 & 9 \\ 1 & 0 & 1 & 4 \\ 4 & 1 & 0 & 1 \\ 9 & 4 & 1 & 0 \end{Vmatrix} \begin{Vmatrix} -1 & -1 & 0 \\ 0 & 0 & -1 \\ 1 & 0 & 0 \\ 0 & 1 & 1 \end{Vmatrix} = \begin{Vmatrix} -8 & -12 & -8 \\ -12 & -18 & -12 \\ -8 & -12 & -8 \end{Vmatrix}$$

After normalization, we get again collinear distances. The usual topological distance matrix, where Cartesian distances seem to be, gives for missing arcs squared diagonal distances (two squares and one cube).

The difference scheme $\mathbf{SDS}^T$ of symmetrical square matrices must be interpreted as the quadratic form; the scalar product $\mathbf{DS}^T$ is projected onto the matrix vector **S**. This gives angles between the consecutive differences.

If these differences are orthogonal, then the off-diagonal elements are 0; if the off-diagonal elements are −2, then the differences are collinear. The second difference of the symmetrical square matrix is equal to its scalar product onto the difference matrix, except the negative signs and the dimensionality. The second difference of n is $d^2n = 0$; the second difference of n^2 is $d^2n^2 = 2$.

If arcs do not have the unit length, then they must be normalized; e.g. for a right triangle we have consecutively

$$\begin{Vmatrix} 0 & 4 & 1 \\ 4 & 0 & 3 \\ 1 & 3 & 0 \end{Vmatrix} \rightarrow \begin{Vmatrix} -8 & 6 & 2 \\ 6 & -6 & 0 \\ 2 & 0 & -2 \end{Vmatrix} \rightarrow \begin{Vmatrix} -2 & 1.73 & 1 \\ 1.73 & -2 & 0 \\ 1 & 0 & -2 \end{Vmatrix}$$

where we obtain angles 30°, 60°, and 90° as required.

The analysis of the difference scheme shows that from four distances one is always zero (the distance of the vertex to itself). The off-diagonal elements are therefore always cosines of the corresponding angles in triangles

$$\cos A = (b^2 + c^2 - a^2)/2bc$$

If we interpret distances through the arcs as the squared Euclidean geometrical distances, then we can study configurations of graphs embedded into the graph space. The trees were already mentioned; all their arcs are orthogonal.

Conformations of cycles with an even number of vertices are interesting. The C_4 forms a square; each arc is orthogonal with both its neighbors and collinear with the fourth arc

$$\begin{Vmatrix} 0 & 1 & 2 & 1 \\ 1 & 0 & 1 & 2 \\ 2 & 1 & 0 & 1 \\ 1 & 2 & 1 & 0 \end{Vmatrix} \rightarrow \begin{Vmatrix} -2 & 0 & 2 & 0 \\ 0 & -2 & 0 & 2 \\ 2 & 0 & -2 & 0 \\ 0 & 2 & 0 & -2 \end{Vmatrix}$$

C_4 bent on the regular tetrahedron with the distance matrix corresponding to the distance matrix of the complete graph K_4 gives other matrix angles. Neighbor arcs form angles of 60°, and each arc is orthogonal with its opposite

$$\begin{Vmatrix} 0 & 1 & 1 & 1 \\ 1 & 0 & 1 & 1 \\ 1 & 1 & 0 & 1 \\ 1 & 1 & 1 & 0 \end{Vmatrix} \rightarrow \begin{Vmatrix} -2 & 1 & 0 & 1 \\ 1 & -2 & 1 & 0 \\ 0 & 1 & -2 & 1 \\ 1 & 0 & 1 & -2 \end{Vmatrix}$$

There exist three embeddings of the cycle C_6 onto vertices of the cube. The first one is identical with the usual distance

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matrix and leads to three collinear pairs of orthogonal arcs

$$\begin{Vmatrix} 0 & 1 & 2 & 3 & 2 & 1 \\ 1 & 0 & 1 & 2 & 3 & 2 \\ 2 & 1 & 0 & 1 & 2 & 3 \\ 3 & 2 & 1 & 0 & 1 & 2 \\ 2 & 3 & 2 & 1 & 0 & 1 \\ 1 & 2 & 3 & 2 & 1 & 0 \end{Vmatrix} \rightarrow \begin{Vmatrix} -2 & 0 & 0 & 2 & 0 & 0 \\ 0 & -2 & 0 & 0 & 2 & 0 \\ 0 & 0 & -2 & 0 & 0 & 2 \\ 2 & 0 & 0 & -2 & 0 & 0 \\ 0 & 2 & 0 & 0 & -2 & 0 \\ 0 & 0 & 2 & 0 & 0 & -2 \end{Vmatrix}$$

The two other forms have some shorter distances and lead to another arrangement of collinear arcs.

$$\begin{Vmatrix} 0 & 1 & 2 & 3 & 2 & 1 \\ 1 & 0 & 1 & 2 & 3 & 2 \\ 2 & 1 & 0 & 1 & 2 & 1 \\ 3 & 2 & 1 & 0 & 1 & 2 \\ 2 & 3 & 2 & 1 & 0 & 1 \\ 1 & 2 & 1 & 2 & 1 & 0 \end{Vmatrix} \rightarrow \begin{Vmatrix} -2 & 0 & 0 & 2 & 0 & 0 \\ 0 & -2 & 0 & 0 & 0 & 2 \\ 0 & 0 & -2 & 0 & 2 & 0 \\ 2 & 0 & 0 & -2 & 0 & 0 \\ 0 & 0 & 2 & 0 & -2 & 0 \\ 0 & 2 & 0 & 0 & 0 & -2 \end{Vmatrix}$$

The collinear arcs in the third conformation are (1–5), (2–4), and (3–6), respectively.

The planar conformation of C_6 has the following matrix and resulting matrix of angles between bonds

$$\begin{Vmatrix} 0 & 1 & 3 & 4 & 3 & 1 \\ 1 & 0 & 1 & 3 & 4 & 3 \\ 3 & 1 & 0 & 1 & 3 & 4 \\ 4 & 3 & 1 & 0 & 1 & 3 \\ 3 & 4 & 3 & 1 & 0 & 1 \\ 1 & 3 & 4 & 3 & 1 & 0 \end{Vmatrix} \rightarrow \begin{Vmatrix} -2 & -1 & 1 & 2 & 1 & -1 \\ -1 & -2 & -1 & 1 & 2 & 1 \\ 1 & -1 & -2 & -1 & 1 & 2 \\ 2 & 1 & -1 & -2 & -1 & 1 \\ 1 & 2 & 1 & -1 & -2 & -1 \\ -1 & 1 & 2 & 1 & -1 & -2 \end{Vmatrix}$$

where angles are 120°, 60°, 180°, 300°, and 240°, respectively.

The uneven cycles each have arcs orthogonal with its neighbors on both sides, but the pair of its opposites forms angles 60° to it. This conformation is obtained by a rotation of two consecutive right angles for 60° through the given arc. The result appears at arcs closing the cycle.

$$\begin{Vmatrix} 0 & 1 & 2 & 3 & 3 & 2 & 1 \\ 1 & 0 & 1 & 2 & 3 & 3 & 2 \\ 2 & 1 & 0 & 1 & 2 & 3 & 3 \\ 3 & 2 & 1 & 0 & 1 & 2 & 3 \\ 3 & 3 & 2 & 1 & 0 & 1 & 2 \\ 2 & 3 & 3 & 2 & 1 & 0 & 1 \\ 1 & 2 & 3 & 3 & 2 & 1 & 0 \end{Vmatrix} \rightarrow \begin{Vmatrix} -2 & 0 & 0 & 1 & 1 & 0 & 0 \\ 0 & -2 & 0 & 0 & 1 & 1 & 0 \\ 0 & 0 & -2 & 0 & 0 & 1 & 1 \\ 1 & 0 & 0 & -2 & 0 & 0 & 1 \\ 1 & 1 & 0 & 0 & -2 & 0 & 0 \\ 0 & 1 & 1 & 0 & 0 & -2 & 0 \\ 0 & 0 & 1 & 1 & 0 & 0 & -2 \end{Vmatrix}$$

The distance matrices of complete graphs K_n can be expressed as $\mathbf{D}_k = \mathbf{JJ}^T - \mathbf{I}$, where $\mathbf{J}$ is the unit vector column and $\mathbf{I}$ is the unit diagonal vector. The product $\mathbf{SJJ}^T\mathbf{S}^T = \mathbf{0}$, where $\mathbf{0}$ is the zero matrix. Therefore, $\mathbf{SD}_k\mathbf{S}^T = -\mathbf{SS}^T$. The outer product of the incidence matrix of a graph with simple arcs has on the diagonal 2. The off-diagonal elements are either 0, if the arcs do not have any common vertex, or 1, if two arcs meet in a vertex. The cosine 60° is 0.5; therefore equilateral structures appear in complete graphs. K_3 is the equilateral triangle, and K_4, the equilateral tetrahedron. Six edges of the equilateral tetrahedron form three pairs of orthogonal arcs.

The quadratic form of complete graphs can be formulated in block form consecutively using the $(n-1)$ complete graphs and unit vectors

$$\begin{array}{cc|c|cc} & & & \mathbf{S}^T & -\mathbf{I} \\ & & & & \mathbf{J}^T \\ \hline \mathbf{S} & & & \mathbf{SS}^T & -\mathbf{S} \\ -\mathbf{I} & \mathbf{J}^T & & -\mathbf{S}^T & \mathbf{I}+\mathbf{JJ}^T \end{array}$$

Increasing the dimension of the complete graph, there will appear $(n-3)$ orthogonal arcs to each parent arc.

Inserting the distance matrix of the star rooted in the nth vertex into $\mathbf{SS}^T$ of the complete graph, we get for the star graph the product

$$\mathbf{SD_S S}^T = \begin{array}{c|c} 2\mathbf{SS}^T & -2\mathbf{S} \\ \hline -2\mathbf{S}^T & -2\mathbf{I} \end{array}$$

The arcs of the star are orthogonal. The arcs connecting its loose vertices have the double length (on the diagonal, 4 appears). These are diagonals of corresponding squares, as can be checked by the calculation of cosines: $2/8^{1/2}$ is cos 45°. The direct verification is possible only for S_4, with three orthogonal axes.

3. EIGENVALUES AND EIGENVECTORS

Distance matrices of straight chains have three nonzero eigenvalues: $W+a$, $-a$, and $-W$, where W is the topological Wiener number and a has the following values

n	a	n	a
2	0	6	5.7272
3	0.4495	7	9.0405
4	1.4031	8	13.7494
5	3.0384		

The eigenvector of the smallest eigenvalue W has elements $v_j = -1 + 2(j-1)/(n-1)$, which weight n consecutive squared numbers k from $-(n-1)$ to $(n-1)$. It leads to the combinatorial identity

$$\sum_{k=0}^{n/2} [1 - 2k/(n-1)][(n-1-k-x)^2 - (k-x)^2] = [1 - 2x/(n-1)]\binom{n+1}{3}$$

where x ranges from 0 to $(n-1)$. If chain increments are two vertices, then the change between consecutive counts gives a possibility of using the full induction

	$7/7 \times (25-4) = 21$
$5/5 \times (16-1) = 75/5$	$5/7 \times (16-1) = 75/7$
$3/5 \times (9-0) = 27/5$	$3/7 \times (9-0) = 27/7$
$1/5 \times (4-1) = 3/5$	$1/7 \times (4-1) = 3/7$
$105/5$	$21 + 105/7$

as

$$[1 - 2x/(n+1)]\binom{n-1}{3} + (n-1-x)^2 - x^2 = [1 - 2x/(n-1)]\binom{n+1}{3}$$

which is verified by direct calculation. For $x = 0$, the identity simplifies to

$$(n-1-2k)^2 = \binom{n+1}{3}$$

We can compare three nonzero eigenvalues of straight linear chains with three distinct eigenvalues of topological distance matrices of stars. The positive eigenvalue is the sum of all negative eigenvalues, as observed by Trinajstić et al.[2] There are $(n-2)$ eigenvalues of -2 and a special eigenvalue $-a = (n-2)/2 + [n^2 - 3n + 3]^{1/2}$.

Corresponding eigenvectors for stars rooted in v_1 are

a	1	1	1	...
0	1	$-1/(n-2)$	$-1/(n-2)$	...
1	$-a/(n-1)$	$-a/(n-1)$	$-a/(n-1)$	...

Due to the monotony of the distance matrices, all products can be easily found. The eigenvalue a is obtained as a solution of the quadratic equation

$$a^2 + 2(n-2)a - (n-1) = 0$$

The planar conformation of C_6 has following eigenvalues 12, 0, 0, 0, −6, and −6, compared with two conformations of C_6 embedded onto the cube 9, 0, 0, −1, −4, −4 and 8.4244, 0, 0, −1.4244, −3, −4 (two permutations with lesser distances).

The maximal eigenvalue of even planar cycles on the circle with unit radius is $2n$, and its eigenvector is the unit vector (this corresponds to $n^2/4$ for topological distance matrices). The even distances on the circle form right triangles over the diameter as the hypotenuse, and their pairs sum to 4.

4. DISCUSSION

The given examples show a consistent picture. The elements of topological distance matrices are the Mahalanobis distances, squares of the unit Cartesian (Euclidean) distances in multidimensional space. Squared geometrical Euclidean distances give correct angles between arcs of graphs in three-dimensional space, too. This consistency is a sole argument for their support against matrices with straight distances.

The question, if they will have some practical value for chemistry as a source of topological indices, remains open. The variation in linear normal alkanes with the Wiener number was already interpreted as the change of the shape of molecules from stiff rods to bent chains.[11]

Note Added in Proof. The eigenvalue a at straight chains is produced by the reflection plane (elements of the eigenvector are symmetrical to the center of the chain) and it is a rotation tensor $\mathbf{b} = (a + W/2) = [\sum d^4 - 3/4W^2]^{1/2}$.

The proof is simple. The sum of squared eigenvalues must be equal to the trace of the squared matrix, it means to the double sum of d_{ij}^4

$$({}^1/_2W + a)^2 + W^2 + (a - {}^1/_2W)^2 = 2\sum d_{ij}^4$$

Solving the quadratic equation gives the result. Four eigenvalues (including zero) can be expressed as $W/2 \pm (b$ or $W/2)$.

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