A MÖBIUS INVERSION OF THE ULAM SUBGRAPHS CONJECTURE

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Abstract

The generalized Eichinger matrices are defined as $\mathbf{E} = \sum_{j=1}^{n}(\delta_j \mathbf{S}^{\mathrm{T}}\mathbf{S})^{-1}$, where $\delta_j \mathbf{M}$ denotes the matrix $\mathbf{M}$ with jth row and column deleted. S is the incidence matrix and $\mathbf{M}^{\mathrm{T}}$ is the transposed matrix. The conjecture $\mathbf{S}^{\mathrm{T}}\mathbf{S}\mathbf{E} = \mathbf{S}_K^{\mathrm{T}}\mathbf{S}_K$, where $\mathbf{S}_K$ is the incidence matrix of the complete graph, is proven for trees, simple cycles and complete graphs. The consequence of the conjecture is $\mathbf{S}_G^{\mathrm{T}}\mathbf{S}_G(\mathbf{E}_G - \mathbf{I}) = \mathbf{S}_{\overline{G}}^{\mathrm{T}}\mathbf{S}_{\overline{G}}$, where $\overline{G}$ is the complementary graph of G. It leads to graphs with imaginary arcs as the complements of graphs with multiple arcs.

1. Introduction

The Ulam conjecture, which states that the knowledge of n subgraphs obtained by the excision of each vertex v_j and all edges incident upon v_j is sufficient for reconstruction of the parent graph, brought important results for the theory of characteristic polynomials [1,2] but its direct proof has not yet been given [3].

Graphs are usually mapped on the vector space by matrices:

(a) The incidence matrix S at oriented trees, $s_{ij} = -1$ if the arc i goes from the vertex j, $s_{ij} = 1$ if the arc i goes into the vertex j, $s_{ij} = 0$ otherwise.

(b) The incidence matrix G at unoriented trees, $g_{ij} = 1$ if the edge i is incident with the vertex j, $g_{ij} = 0$ otherwise.

(c) The Kirchhoff matrix $\mathbf{S}^{\mathrm{T}}\mathbf{S}$.

(d) The adjacency matrix $\mathbf{A}: \mathbf{A} = 1/2(\mathbf{G}^{\mathrm{T}}\mathbf{G} - \mathbf{S}^{\mathrm{T}}\mathbf{S})$. $a_{ij} = 1$ if the vertex i is connected to the vertex j by an arc or an edge, $a_{ij} = 0$ otherwise.

(e) The distance matrix $\mathbf{D}$, d_{ij} = the length of the shortest walk or path between the vertices i and j.

The Ulam subgraphs correspond to the adjacency matrix difference $\delta_j \mathbf{A}$ with the jth row and column deleted. If vertices are labeled, then it is no problem to reconstruct the graph from only three Ulam submatrices. The sum of these adjacency matrices contains once mutual adjacencies of three deleted vertices, twice their

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adjacencies with other $(n-3)$ vertices and three times the unperturbed part of the adjacency matrix.

In connection with the work on inverses of graph matrices [4,5], another problem emerged: Can a graph be reconstructed from its inverse matrices? This problem is ill-defined for the adjacency matrices, where the simplest cases, namely the linear chains L, do not always have inverses, because in the spectra of linear chains with uneven vertices one zero appears [1].

However, it is well known that the Kirchhoff matrix $\mathbf{S}^{\mathrm{T}}\mathbf{S}$ of a connected graph has only one zero eigenvalue and that inverses of all its submatrices $\delta_j\mathbf{S}^{\mathrm{T}}\mathbf{S}$ exist. Thus, it was possible to find an analogue of the Ulam subgraphs conjecture in the form

$$\mathrm{S}_G^{\mathrm{T}}\mathrm{S}_G\left[\sum_{j=1}^{n}\left(\delta_j \mathrm{S}_G^T \mathrm{S}_G\right)^{-1}\right] = \mathrm{S}_K^{\mathrm{T}}\mathrm{S}_K\,, \tag{1}$$

The product of the Kirchhoff matrix of a connected graph without loops and the sum of the inverse of its Kirchhoff submatrices is the Kirchhoff matrix of the complete graph K.

We propose to name this sum the Eichinger matrix $\mathbf{E}$, because Eichinger was the first to use these matrices of linear chains [6]. He defined the generalized unit matrix $\mathbf{U} = (1/n)\mathrm{S}_K^{\mathrm{T}}\mathrm{S}_K$, too.

2. The inverse matrices of trees

The oriented trees with n vertices have only $(n-1)$ arcs and if their Kirchhoff matrix $\mathbf{S}^{\mathrm{T}}\mathbf{S}$ has only one zero eigenvalue, the other quadratic form of the incidence matrix $\mathbf{S}\mathbf{S}^{\mathrm{T}}$ has none and has its true inverse $\mathbf{W}^{\mathrm{T}}\mathbf{W}$ [4]. Recently, it was found that there are many formally equivalent inverses [5],

$$(\mathbf{S}\mathbf{S}^{\mathrm{T}})^{-1} = (1/n)\mathbf{W}^{\mathrm{T}}\mathbf{W} = -(1/2)\mathbf{S}\mathbf{D}\mathbf{S}^{-1} = (1/n)\mathbf{S}\mathbf{E}\mathbf{S}^{-1}. \tag{2}$$

The elements of the quadratical forms $\mathbf{W}^{\mathrm{T}}\mathbf{W}$ of the walk matrix $\mathbf{W}$ are incidencies of arcs in all $\binom{n}{2}$ walks between vertices of a tree, the elements on the diagonal show how many times each arc is used in all walks, the off-diagonal elements show how many times the arcs i and j meet together in the walks [4]. The elements of the distance matrices $\mathbf{D}$ are distances, i.e. the number of arcs between two vertices and the elements of the Eichinger matrices of trees are sums of distances, too (see appendix B).

The distances are eliminated if multiplied with their incidence matrices

$$\mathbf{S}\mathbf{D}\mathbf{S}^{\mathrm{T}} = -2\,\mathbf{I}_{n-1}, \quad \mathbf{S}\mathbf{E}\mathbf{S}^{\mathrm{T}} = n\,\mathbf{I}_{n-1}, \quad \mathbf{W}^{\mathrm{T}}\mathbf{W}\mathbf{S}\mathbf{S}^{\mathrm{T}} = n\,\mathbf{I}_{n-1},$$

where $\mathbf{I}_{n-1}$ is the unit diagonal matrix with dimension $(n-1)$. The multiplications with the formal inverses $\mathrm{S}^{-\mathrm{T}}$ and S^{-1} show the equivalence.

The conjecture holds for small graphs and trees [5] (see appendices B and C); in this paper, it will be proven for complete graphs and simple cycles C.

3. The complete graphs

The conjecture proceeds from the definition of the generalized inverse $\mathbf{U}$ by Eichinger [6], $\mathbf{U}^2 = \mathbf{U}$, but it is necessary to show that $n\mathbf{U}$ is the sum of $(\delta_j \mathbf{S}_K^{\mathrm{T}} \mathbf{S}_K)^{-1}$. The Kirchhoff matrix of the complete graph $\mathbf{S}_K^{\mathrm{T}} \mathbf{S}_K$ has as diagonal elements $(n-1)$ and as off-diagonal elements (-1). Simple calculations show that the inverse of its difference is

$$\left(\delta_j \mathbf{S}_K^{\mathrm{T}} \mathbf{S}_K\right)^{-1} = (1/n)\left(\mathbf{I} + \mathbf{J}\mathbf{J}^{\mathrm{T}}\right)_{n-1},$$

where $\mathbf{J}$ is the unit column vector.

The diagonal elements which appear $(n-1)$ times give sums $e_{ii} = 2(n-1)$, the off-diagonal elements which appear in the Eichinger matrix $(n-2)$ times give sums $e_{ij} = (n-2)$. After rearrangement into the sum of two matrices, the Eichinger matrix of the complete graph is $\mathbf{E}_K = \mathbf{I} + [(n-2)/n]\mathbf{J}\mathbf{J}^{\mathrm{T}}$. It gives the product $\mathbf{S}_K^{\mathrm{T}} \mathbf{S}_K \mathbf{E}_K = \mathbf{S}_K^{\mathrm{T}} \mathbf{S}_K + [(n-2)/n]\mathbf{S}_K^{\mathrm{T}} \mathbf{S}_K \mathbf{J}\mathbf{J}^{\mathrm{T}}$. Because $\mathbf{S}_K^{\mathrm{T}} \mathbf{S}_K \mathbf{J}\mathbf{J}^{\mathrm{T}} = \mathbf{0}$, we obtain the identity. □

4. Simple circles

The difference matrix $\delta_j \mathbf{S}_C^{\mathrm{T}} \mathbf{S}_C$ of a simple cycle is identical to the matrix $\mathbf{S}_L \mathbf{S}_L^{\mathrm{T}}$ of a linear chain with n vertices and $(n-1)$ arcs. It means that the inverse of this difference is $(\delta_j \mathbf{S}_C^{\mathrm{T}} \mathbf{S}_C)^{-1} = (1/n)\mathbf{W}_L^{\mathrm{T}} \mathbf{W}_L$ and $\mathbf{E} = \Sigma(1/n)\mathbf{W}_L^{\mathrm{T}} \mathbf{W}_L$.

The summation is somewhat tricky due to the fact that the matrices $\mathbf{W}_L^{\mathrm{T}} \mathbf{W}_L$ are split by the deleted row and column. The elements of the Eichinger matrix are traces of all diagonals of the inverse matrix $\mathbf{W}_L^{\mathrm{T}} \mathbf{W}_L$. The trace of the main diagonal $\mathbf{W}_L^{\mathrm{T}} \mathbf{W}_L$ is the Wiener number of the linear chain $W(n) = \binom{n+1}{n-2}$, the traces of the side diagonals are the Wiener numbers of the shorter chains, as the analysis of the recurrence shows. There appear always the sums of two diagonals; thus, $e_{i,i \pm k} = (1/n)[W(n-k) + W(k)]$, e.g. for $n = 6$, $k = (j-1)$, we obtain

$W(n-k)$	35	20	10	4	1	0
$W(k)$		0	1	4	10	20
e_{1j}	35	20	11	8	11	20

The diagonal elements of the product $\mathbf{S}_C^{\mathrm{T}} \mathbf{S}_C \mathbf{E}_C$ are

$$(1/n)[2W(n) - 2W(n-1)] = (n-1),$$

and the off-diagonal elements are

$$(1/n)(2[W(n-k) + W(k)] - W(n-k+1)$$
$$- W(k-1) - W(n-k-1) - W(k+1)) = -1.$$

□

5. The Eichinger matrices of the complementary graphs

To each graph G its complementary graph $\overline{G}$ is defined by the formal sum $G + \overline{G} = K$; the complementary graph contains arcs from the complete graph which are not in the graph G. It is equivalent to the matrix sums

$$\mathbf{A}_G + \mathbf{A}_{\overline{G}} = \mathbf{A}_K \quad \text{and} \quad \mathbf{S}_G^{\mathrm{T}}\mathbf{S}_G + \mathbf{S}_{\overline{G}}^{\mathrm{T}}\mathbf{S}_{\overline{G}} = \mathbf{S}_K^{\mathrm{T}}\mathbf{S}_K .$$

Applying this in (1), we straightforwardly obtain

$$\mathbf{E}_{\overline{G}} = (\mathbf{E}_G - \mathbf{I}).$$

Simple examples support this consequence. It can be proven for stars which complementary graph is the complete graph K_{n-1}.

The Eichinger matrix of the star rooted in v_1 is

$$\mathbf{E}_S = \begin{Vmatrix} (n-1) & (n-2) & (n-2) \\ (n-2) & [2(n-2)+1] & (n-3) \\ (n-2) & (n-3) & [2(n-2)+1] \end{Vmatrix}.$$

Then,

$$(\mathbf{E}_S - \mathbf{I}) = \begin{Vmatrix} (n-2) & (n-2) & (n-2) \\ (n-2) & [2(n-2)] & (n-3) \\ (n-2) & (n-3) & [2(n-2)] \end{Vmatrix}.$$

This gives with

$$\mathbf{S}_S^{\mathrm{T}}\mathbf{S}_S = \begin{Vmatrix} (n-1) & -1 & -1 \\ -1 & 1 & 0 \\ -1 & 0 & 1 \end{Vmatrix},$$

the demanded result. If we return to the proof of the conjecture for the complete graphs, we can say that $[(n-2)/n]\mathbf{J}\mathbf{J}^{\mathrm{T}}$ is just the Eichinger matrix of the complementary graph to the complete graph, the empty graph.

However, for the graphs with multiple arcs the consequence gives rather surprising results. For example,

$$\begin{array}{cccc} \mathbf{S}^{\mathrm{T}}\mathbf{S} & \mathbf{E} & (\mathbf{E}-\mathbf{I}) & \mathbf{S}_G^{\mathrm{T}}\mathbf{S}_G \\ \begin{Vmatrix} 2 & -2 & 0 \\ -2 & 3 & -1 \\ 0 & -1 & 1 \end{Vmatrix} & \begin{Vmatrix} 2 & 1 & 0 \\ 1 & 3/2 & 1/2 \\ 0 & 1/2 & 5/2 \end{Vmatrix} & \begin{Vmatrix} 1 & 1 & 0 \\ 1 & 1/2 & 1/2 \\ 0 & 1/2 & 3/2 \end{Vmatrix} & \begin{Vmatrix} 0 & 1 & -1 \\ 1 & -1 & 0 \\ -1 & 0 & 1 \end{Vmatrix}. \end{array}$$

The Kirchhoff matrix $\mathbf{S}^{\mathrm{T}}\mathbf{S}$ is the quadratical form of the incidence matrix $\mathbf{S}$. On its diagonal are squares of the elements of the matrix $\mathbf{S}$. If negative values appear on the diagonal $\mathbf{S}^{\mathrm{T}}\mathbf{S}$, it suggests the existence of imaginary units i in the incidence matrix $\mathbf{S}$ and the existence of graphs with imaginary arcs. In the given example, the matrix $\mathbf{S}_G$ is, e.g.,

$$\begin{Vmatrix} -\mathrm{i} & \mathrm{i} & \\ -1 & & 1 \end{Vmatrix}.$$

6. Conclusions

The conjecture about the existence of generalized inverse Eichinger matrices is valid only at oriented connected graphs without loops. It does not hold for unoriented graphs, as some counterexamples show.

The calculation at L_4 shows that there appears the matrix $\mathbf{J}\mathbf{J}^{\mathrm{T}}$ with alternating signs $(-1)^{i+j}$. Similar results are obtained at simple cycles but at the complete unoriented graphs the procedure is not applicable. They have non-singular $\mathbf{G}^{\mathrm{T}}\mathbf{G}$ matrices with the spectrum $(2n-2)(n-2)^{n-1}$ and their true inverse $(\mathbf{G}^{\mathrm{T}}\mathbf{G})^{-1}$. The necessary condition for the existence of Eichinger matrices is $\mathbf{J}^{\mathrm{T}}\mathbf{S}^{\mathrm{T}}\mathbf{S} = \mathbf{S}^{\mathrm{T}}\mathbf{S}\mathbf{J} = \mathbf{0}$, the oriented graph vector must form a closed path.

The conjecture has an interesting consequence: The Kirchhoff matrices of graphs with loops should be nonsingular, because they correspond to $\delta_{n+1}\mathbf{S}^{\mathrm{T}}\mathbf{S}$ of graphs with $(n+1)$ vertices, the $(n+1)$th vertex being connected to vertices with loops.

The proposed conjecture differs from the Ulam subgraphs conjecture in one important point. The adjacency matrices of the Ulam subgraphs do not contain any trace of the deleted vertex and its arcs on their diagonals, but the Kirchhoff submatrices do, provided that loops are not allowed. The sums of matrix elements in rows and columns are unbalanced and it is always possible to reconstruct the original matrix from one $\delta_j\mathbf{S}^{\mathrm{T}}\mathbf{S}$.

There seems to be no direct proof of the Ulam subgraphs conjecture, except a somewhat cumbersome method, to compare the set of n Ulam subgraphs with the sets of Ulam subgraphs of all graphs with n vertices, to find which of them coincides.

The proof of the Ulam conjecture was given by using characteristic polynomials and their integration.

On the contrary, the inverse problem can be proven in simple cases by combinatorial techniques at trees by comparing distances passed in different walks, at simple cycles and complete graphs by direct countings of the matrix elements.

However, this difference is circumstantial only; the characteristic polynomials are obtained by combinatorial means, too, by counting the characteristic figures [1].

Möbius bands were defined on graphs before. The proposed conjecture is an example of the Möbius inversion used extensively in combinatorics [8].

It is questionable if the Eichinger matrices will have some practical importance for chemistry as other graph matrices have. However, they give us a deeper insight into how the matrix space is built. It can be hoped that the study of their characteristic polynomials can contribute to spectral theory of graphs.

Appendix A [5]

The distance matrix $\mathbf{D}$ of an oriented tree is the multiple of the inner inverse of the quadratical form $\mathbf{SS}^{\mathrm{T}}$ of its incidence matrix $\mathbf{S}$:

$$\mathbf{SDS}^{\mathrm{T}} = -2\mathbf{I}_{n-1}.$$

Proof

In trees, there are no circuits. If in a row or a column of the distance matrix $\mathbf{D}$ there are some equal distances, then there are no arcs incident with both equidistant vertices. It means that in the product matrix $\mathbf{DS}^{\mathrm{T}}$ can appear only elements ± 1, corresponding to the differences of distances between vertices. The difference is positive if the distance is counted in the same direction as the arc was oriented, and negative if the distance is counted in the opposite direction. Otherwise, the elements of $\mathbf{DS}^{\mathrm{T}}$ are differences $(d_{ik} - d_{il})$. The second multiplication $\mathbf{SDS}^{\mathrm{T}}$ gives the differences $(d_{jk} - d_{jl}) - (d_{ik} - d_{il})$. If $k = j$ and $l = i$, then $d_{jj} = d_{ii} = 0$ and the result is $(d_{ji} - d_{ij}) = -2$, which appears on the diagonal. The off-diagonal elements are 0, because $(d_{jk} - d_{jl}) = (d_{ik} - d_{il})$. The distances forming both differences lie on the same side of the considered arc and they have the same sign. □

Appendix B [5]

The elements of the Eichinger matrix $\mathbf{E}$ of a tree are sums of distances of the vertex j to all other vertices $e_{jj} = \sum_{i=1}^{n} d_{ij}$, or sums of all $n-1$ walks to the other $(n-1)$ vertices $e_{jj} = \sum_{i=1}^{n} w_{ij}$. The off-diagonal elements are these sums e_{jj} diminished by parts of walks passing the walk ij.

THE CONJECTURE

The Eichinger matrix $\mathbf{E}$ of a tree is the sum of the inverses of the differences of its Kirchhoff matrix $\delta_j \mathbf{S}_{\mathrm{T}}^{\mathrm{T}} \mathbf{S}_{\mathrm{T}}$:

$$\mathbf{E} = \sum_{j=1}^{n} \left(\delta_j \mathbf{S}_{\mathrm{T}}^{\mathrm{T}} \mathbf{S}_{\mathrm{T}} \right)^{-1}.$$

Proof for stars

The Kirchhoff matrices of stars rooted in v_1 all have the same form

$$\begin{Vmatrix} (n-1) & -1 & -1 \\ -1 & 1 & \\ -1 & & 1 \end{Vmatrix}.$$

The $\delta_1 \mathbf{S}_S^{\mathrm{T}} \mathbf{S}_S$ is $\mathbf{I}$, similarly $(\delta_1 \mathbf{S}_S^{\mathrm{T}} \mathbf{S}_S)^{-1}$. The other $(\delta_j \mathbf{S}_S^{\mathrm{T}} \mathbf{S}_S)^{-1}$ have the form

$$\begin{Vmatrix} 1 & 1 & 1 \\ 1 & 2 & 1 \\ 1 & 1 & 2 \end{Vmatrix},$$

with different rows and columns deleted.

The resulting sum is always

$$\mathbf{E}_S = \begin{Vmatrix} (n-1) & (n-2 & (n-2) \\ (n-2 & [2[n-2)+1] & (n-3) \\ (n-2) & (n-3) & [2(n-2)+1] \end{Vmatrix}.$$

The root sum is given by $(n-1)$ arcs to $(n-1)$ leaves, from them $(n-2)$ are unpassed by the walk $1j$, other diagonal elements are given by $(n-2)$ walks of length 2 to other leaves and one arc to the root, in one walk to another leaf $(n-3)$ arcs from the root to remaining leaves are left unpassed.

The matrix product $\mathbf{E}\mathbf{S}_S^{\mathrm{T}}$ has the form

$$\begin{Vmatrix} -1 & -1 & -1 \\ (n-1) & 0 & 0 \\ -1 & (n-1) & 0 \\ -1 & 0 & (n-1) \end{Vmatrix}$$

and $\mathbf{S}_S \mathbf{E} \mathbf{S}_S^{\mathrm{T}} = n\, \mathbf{I}_{n-1}$.

Proof for linear chains

Here we obtain $\mathbf{E}$ as the sum

$$\begin{Vmatrix} & & & \\ & 1 & 1 & 1 \\ & 1 & 2 & 2 \\ & 1 & 2 & 3 \end{Vmatrix} + \begin{Vmatrix} 1 & & & \\ & & & \\ & & 1 & 1 \\ & & 1 & 2 \end{Vmatrix} + \begin{Vmatrix} 2 & 1 & & \\ 1 & 1 & & \\ & & & \\ & & & 1 \end{Vmatrix} + \begin{Vmatrix} 3 & 2 & 1 & \\ 2 & 2 & 1 & \\ 1 & 1 & 1 & \\ & & & \end{Vmatrix} = \begin{Vmatrix} 6 & 3 & 1 & 0 \\ 3 & 4 & 2 & 1 \\ 1 & 2 & 4 & 3 \\ 0 & 1 & 3 & 6 \end{Vmatrix}.$$

The elements of the inverse differences $(\delta_j \mathbf{S}_L^{\mathrm{T}} \mathbf{S}_L)^{-1}$ are parts of walks from the vertex j to other vertices passed in common to the vertex i. Thus, the elements of the Eichinger matrices $\mathbf{E}_L$ are sums of distances.

At longer chains, the first $(n-1)$ rows and columns of $(\delta_j \mathbf{S}_L^{\mathrm{T}} \mathbf{S}_L)^{-1}$ remain unchanged and to the unchanged part of the matrix $\mathbf{E}_L$ the inversion $(\delta_n \mathbf{S}_L^{\mathrm{T}} \mathbf{S}_L)^{-1}$ is added.

This inversion can be defined as the quadratical form $\mathbf{TT}^{\mathrm{T}}$ of the matrix $\mathbf{T}$, which is the inverse from the right of the incidence matrix $\mathbf{S}_L$ of the linear chain. The elements of the matrix $\mathbf{T}$ are $t_{ij} = -1$, if $(j-i) \geq 0$ and $t_{ij} = 0$ otherwise. The transposed matrix $\mathbf{T}^{\mathrm{T}}$ is the left inverse of $\mathbf{S}^{\mathrm{T}}$ and $\mathbf{TT}^{\mathrm{T}}$ is the inner inverse of $\mathbf{SS}^{\mathrm{T}}$. We have the sum of two inner inverses and we can apply the full induction. If the conjecture is correct for the sum $\mathbf{E}_{n-1}$ and $\mathbf{TT}^{\mathrm{T}}$, it leaves unsolved the last row and column. However, due to the symmetry of the linear chain, the last row and column repeat the elements of the first row and column in reversed order and the difference of the last and last but one elements is the same as the difference of the first and second elements, only the sign is opposite.

The direct matrix multiplication gives:

$$\mathbf{S}(\mathbf{E}_{n-1} + \mathbf{TT}^{\mathrm{T}})\mathbf{S}^{\mathrm{T}} = \mathbf{SE}_{n-1}\mathbf{S}^{\mathrm{T}} + \mathbf{STT}^{\mathrm{T}}\mathbf{S}^{\mathrm{T}} = (n-1)\mathbf{I}_{n-2} + \mathbf{I}_{n-2} = n\,\mathbf{I}_{n-2},$$

which together with the last row and column completes the proof. □

Elements of the matrices $(\delta_j \mathbf{S}^{\mathrm{T}}\mathbf{S})^{-1}$ are in both cases distances inside the tree from the vertex j, taken as the root to all other vertices. We can generalize the result for all trees. Let us suppose that the assumption is true for all trees with n vertices. When we add the $(n+1)$th vertex rooted in the nth vertex, the difference of the matrix $\mathbf{E}_n$ is $(\delta_{n+1}\mathbf{S}^{\mathrm{T}}\mathbf{S})^{-1}$, this is equal to $[(\delta_n \mathbf{S}^{\mathrm{T}}\mathbf{S})^{-1} + \mathbf{JJ}^{\mathrm{T}})$, each distance from the vertex n is increased by one arc. However, $\mathbf{SJJ}^{\mathrm{T}}\mathbf{S}^{\mathrm{T}} = \mathbf{0}$. Because each tree has at least two leaves, we can repeat the procedure for the last and last but one column and row with the second leaf. We have thus proven the theorem: The Eichinger matrix of a tree is the inner inverse of $\mathbf{SS}^{\mathrm{T}}$. □

Appendix C [5]

The Eichinger matrix of a tree multiplied by the Kirchhoff matrix of the tree gives the Kirchhoff matrix of the complete graph:

$$\mathbf{E}\,\mathbf{S}_{\mathrm{T}}^{\mathrm{T}}\mathbf{S}_{\mathrm{T}} = \mathbf{S}_{\mathrm{T}}^{\mathrm{T}}\mathbf{S}_{\mathrm{T}}\,\mathbf{E} = \mathbf{S}_K^{\mathrm{T}}\mathbf{S}_K\,.$$

Proof

Both matrices are symmetrical and it is sufficient to show just one product. In appendix B, it was shown that the elements of the matrix $\mathbf{E}$ are sums of distances from the diagonal vertices to all $(n-1)$ other vertices, the off-diagonal elements are decreased by walks passed between vertices ij. Because there are no cycles, the elements e_{ij} in a row are different only if vertices lie on the same walks.

When both matrices are multiplied, we obtain for the same rows and columns the sums $(v_{jj}\, e_{jj} - \sum e_{ij})$. The number of elements in the summation is equal to the number of vertices incident to the vertex j, but the sum of e_{ij} is less than the product $v_{jj}\, e_{jj}$ by $(n-1)$ walks passed through the incident arcs to $n-1$ other vertices. On the product diagonal, $(n-1)$ appears. If unequal rows and columns are multiplied, the products are $(v_{jj}\, e_{ij} - \sum e_{ik})$, where the index k is used for v_{jj} vertices incident with the vertex j. The elements e_{ik} are smaller or greater than e_{ij}, but their sum differs from the product $v_{jj}\, e_{ij}$ by just one arc ij, which is taken with the negative sign. The off-diagonal elements are -1 and the product matrix is $\mathbf{S}_K^{\mathrm{T}}\mathbf{S}_K$. □

References

[1] D.M. Cvetković, M. Doob and H. Sachs, *Spectra of Graphs* (Deutsche Verlag der Wissenschaften, Berlin, 1980).

[2] N. Trinajstić, J. Math. Chem. 2(1988)197.

[3] P. Křivka, R.B. Mallion and N. Trinajstić, J. Mol. Struct. (THEOCHEM) 164(1988)363.

[4] M. Kunz, Coll. Czech. Chem. Commun. 54(1989)2148.

[5] M. Kunz, in: *Proc. Chemometrics II*, ed. J. Havel and M. Holík, Masaryk University of Brno (1990), p. 142.

[6] E.B. Eichinger, J. Polymer Sci. Polymer Symp. 54(1976)127.

[7] A.C. Day, R.B. Mallion and M.J. Rigby, in: *Chemical Applications of Topology and Graph Theory*, ed. R.B. King (Elsevier, Amsterdam, 1983).

[8] G.C. Rota, Z. Wahrscheinlichkeitstheorie 2(1964)340.