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RELATIONS BETWEEN RESISTANCE AND LAPLACIAN MATRICES AND THEIR APPLICATIONS

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Abstract

The resistance distance r_{ij} between two vertices v_i and v_j of a (connected, molecular) graph G is equal to the resistance between the respective two nodes of an electric network, constructed so as to correspond to G, such that the resistance of any edge is unity. The matrix $R = ||r_{ij}||$ is the resistance matrix of G. Let L be the Laplacian matrix of G. In this work we obtain some new relations between R and L. Using these relations we give a new proof of the formula: $r_{ij} = \det L(i,j) / \det L[i,i]$ for $i \neq j$. Here $L[i,j]$ and $L(i,j)$ are the matrices obtained from L by deleting its i-th row and j-th column, and by deleting its i-th and j-th rows and columns, respectively.

INTRODUCTION

The ordinary distance between two vertices v_i and v_j of a (connected) graph G, denoted by d_{ij}, is defined as the length (= number of edges) of a shortest path that connects v_i and v_j [1]. The vertex–distance concept found numerous chemical applications; for details see the reviews [2, 3] and the recent papers [4–12]. In order to examine other possible metrics in (molecular) graphs the *resistance distance*, denoted by r_{ij}, has been put forward [13]. This distance is conceived as follows. To the graph G an electric network $\mathcal{N}(G)$ is associated, obtained so that each edge of G is replaced by a resistor of unit resistance. The nodes of $\mathcal{N}(G)$ correspond to the vertices of G. The resistance distance r_{ij} of the vertices v_i and v_j of G is then defined as the effective resistance between the respective two nodes of $\mathcal{N}(G)$. The quantities r_{ij} are computed by methods of the theory of resistive electric networks (based on Ohm's and Kirchhoff's laws). For acyclic graphs $r_{ij} = d_{ij}$ and therefore the resistance-distance-concept is primarily of interest in the case of cycle–containing (molecular) graphs.

The resistance–distance concept was much studied [13–28]. The matrix whose (i, j)-entry is r_{ij} is called the *resistance matrix* (of the respective graph G), and will be denoted by R. Evidently, R is symmetric, has a zero diagonal, and its order coincides with the number n of vertices of G.

Within the theory of electric networks the standard method to compute the resistance matrix [29–31] is via the so-called generalized inverse $L^\dagger$ of the Laplacian matrix of the underlying graph G:

$$r_{ij} = (L^\dagger)_{ii} + (L^\dagger)_{jj} - (L^\dagger)_{ij} - (L^\dagger)_{ji} \,. \tag{1}$$

Recall that the Laplacian matrix is singular and, therefore, has no usual inverse. More on the generalized inverse of a (singular) matrix can be found elsewhere [16,32–34].

Let G be a graph and let its vertices be labeled by $v_1, v_2, \ldots, v_n$. The Laplacian matrix of G, denoted by L is a square matrix of order n whose (i, j)-entry is defined by

$$L_{ij} = \begin{cases} -1 & \text{if } i \neq j \text{ and the vertices } v_i \text{ and } v_j \text{ are adjacent} \\ 0 & \text{if } i \neq j \text{ and the vertices } v_i \text{ and } v_j \text{ are not adjacent} \\ d_i & \text{if } i = j \end{cases}$$

where d_i is the degree (= number of first neighbors) of the vertex v_i.

By J we denote the square matrix of order n whose all elements are unity. Then for all connected graphs (with two or more vertices) the matrix $L + \frac{1}{n} J$ is non-singular, its inverse

$$X = ||x_{ij}|| = \left(L + \frac{1}{n} J\right)^{-1}$$

exists, and [24]

$$r_{ij} = x_{ii} + x_{jj} - 2\, x_{ij} \ .$$

Thus the matrix $R = ||r_{ij}||$ can be written as

$$R = diag[x_{11}, x_{22}, \ldots, x_{nn}]\, J + J\, diag[x_{11}, x_{22}, \ldots, x_{nn}] - 2\, X \ . \tag{2}$$

In this work we obtain some new relations, connecting the resistance and the Laplacian matrices. By means of these relations we give a new proof of a known formula [18, 28]:

$$r_{ij} = \frac{\det L(i,j)}{\det L[i,i]} \tag{3}$$

for $i \neq j$. Here $L[i,j]$ and $L(i,j)$ are the matrices obtained from the matrix L by deleting its i-th row and j-th column, and by deleting its i-th and j-th rows and columns, respectively.

NEW RELATIONS BETWEEN THE MATRICES R AND L

We first prove the following

Theorem 1. *If L and R are the Laplacian and resistance matrices, respectively, of a connected graph G, then*

$$L\, R\, L = -2\, L \ . \tag{4}$$

Proof. Since $X = ||x_{ij}|| = (L + \frac{1}{n} J)^{-1}$ and $L\, J = J\, L = 0$, it follows that $L\, X = X\, L = I - \frac{1}{n} J$, where I is the unit matrix of order n. Thus we have

$$L\, X\, L = \left(I - \frac{1}{n} J\right) L = L \ .$$

By Eq. (2) we further obtain

$$\begin{aligned} L\,R\,L &= L\,(diag[x_{11},x_{22},\ldots,x_{nn}]\,J + J\,diag[x_{11},x_{22},\ldots,x_{nn}] - 2\,X)L \\ &= -2\,L\,X\,L \\ &= -2\,L \quad \square \end{aligned}$$

Identity (4) is a useful and interesting result, in spite of the fact that its proof is simple. In what follows we outline some of its applications.

Let M be any matrix of order n, and let $Tr(M)$ denote its trace. In [15] it is proven (as Theorem B) that $Tr(L\,M\,L\,R) = -2\,Tr(M\,L)$.

We now offer a generalization of this result.

Corollary 1.1. *The matrices $L\,M\,L\,R$ and $-2\,M\,L$ have the same characteristic polynomial.*

Proof. It is sufficient to observe that the matrix $L\,M\,L\,R = L\,(M\,L\,R)$ has the same characteristic polynomial as $M\,L\,R\,L = (M\,L\,R)\,L$, and to apply Eq. (4). □

Corollary 1.2. *The matrices $L\,R$ and $diag[-2,\ldots,-2,0]$ are similar.*

Proof. We have $(L\,R)^2 = L\,R\,L\,R = -2\,L\,R$ and therefore the minimal polynomial of $L\,R$ is $\lambda^2 + 2\lambda$, which has no multiple roots. Therefore $L\,R$ is similar to a diagonal matrix whose diagonal elements are -2 and/or 0. Since R is non-singular [17], the rank of $L\,R$ is $n-1$. Thus $L\,R$ and $diag[-2,\ldots,-2,0]$ are similar. □

In what follows by δ_{ij} we denote the usual Kronecker delta, defined as

$$\delta_{ij} = \begin{cases} 1 & \text{if } i = j \\ 0 & \text{if } i \neq j\ . \end{cases}$$

Corollary 1.3. *Let for $i = 1,2,\ldots,n$,*

$$w_i = \frac{1}{2}\sum_{k=1}^{n} r_{1k}\,L_{1k} + \delta_{i1}\ .$$

Then

$$I + \frac{1}{2}\,R\,L = J\,diag[w_1,w_2,\ldots,w_n]\ .$$

Proof. By Corollary 1.1, the rank of the matrix $Q = I + \frac{1}{2} R\,L$ is 1. Hence any row of this matrix is a multiple of the first row. Since

$$\left(I + \frac{1}{2} R\,L\right) J = J$$

all rows of Q are the same. Therefore $Q = J\; diag[w_1, w_2, \ldots, w_n]$. □

PROOF OF FORMULA (3)

Bearing in mind Eq. (1), the fact that $L^\dagger$ is symmetric [34], and $J\,L = 0$ we have

$$\begin{aligned} R\,L &= \Big(diag[(L^\dagger)_{11}, (L^\dagger)_{22}, \ldots, (L^\dagger)_{nn}]\,J \\ &+ J\; diag[(L^\dagger)_{11}, (L^\dagger)_{22}, \ldots, (L^\dagger)_{nn}] - 2\,L^\dagger\Big)\; L \\ &= J\; diag[(L^\dagger)_{11}, (L^\dagger)_{22}, \ldots, (L^\dagger)_{nn}]\, L - 2\, L^\dagger\, L\,. \end{aligned}$$

Because of [34]

$$L^\dagger\, L = I - \frac{1}{n} J$$

we arrive at

$$R\,L = J\; diag[(L^\dagger)_{11}, (L^\dagger)_{22}, \ldots, (L^\dagger)_{nn}]\, L + \frac{2}{n} J - 2\,I\,.$$

This implies

$$\sum_{k=1}^{n} r_{ik}\, L_{kj} = \sum_{k=1}^{n} (L^\dagger)_{kk}\, L_{kj} + \frac{2}{n} - 2\,\delta_{ij} \tag{5}$$

which holds for $i, j = 1, 2, \ldots, n$. Setting in (5) $i = t$ we get

$$\sum_{k=1}^{n} r_{tk}\, L_{kj} = \sum_{k=1}^{n} (L^\dagger)_{kk}\, L_{kj} + \frac{2}{n} - 2\,\delta_{tj}$$

which subtracted from (5) yields

$$\sum_{k=1}^{n} (r_{ik} - r_{tk})\; L_{kj} = 2\,(\delta_{tj} - \delta_{ij})$$

and which holds for $i, j, t = 1, 2, \ldots, n$. For $i, t = 1, 2, \ldots, n$ we thus obtain

$$\begin{aligned} &(L[n,n])^t\; (r_{i1} - r_{t1}, r_{i2} - r_{t2}, \ldots, r_{i,n-1} - r_{t,n-1})^t \\ =\; & 2\; (\delta_{t1} - \delta_{i1}, \delta_{t2} - \delta_{i2}, \ldots, \delta_{t,n-1} - \delta_{i,n-1})^t \\ -\; & (r_{in} - r_{tn})\,(L_{n1}, L_{n2}, \ldots, L_{n,n-1})^t\,. \end{aligned} \tag{6}$$

Now, set $i = n, t = 1$ into (6) and assume that $n \neq 1$. Then

$$(r_{n1}, r_{n2} - r_{12}, \ldots, r_{n,n-1} - r_{1,n-1})^t$$

is the solution of the system (7) of linear equations in the variables $x_1, x_2, \ldots, x_{n-1}$:

$$(L[n,n])^t\ (x_1, x_2, \ldots, x_{n-1})^t = 2\,(1, 0, \ldots, 0)^t + r_{1n}\ (L_{n1}, L_{n2}, \ldots, L_{n,n-1})^t\ . \qquad (7)$$

In order to obtain r_{1n} we have by Cramer's rule

$$\begin{aligned} \det(L[n,n])^t\, r_{1n} &= 2\ \det L(1,n) + (-1)^n\ \det(L[n,1])^t\, r_{1n} \\ &= 2\ \det L(1,n) - \det(L[n,n])^t\, r_{1n}\ . \end{aligned}$$

Here we used the fact that

$$\det(L[n,1])^t = (-1)^{n-1}\ \det(L[n,n])^t$$

because

$$\sum_{k=1}^{n} L_{kj} = 0$$

for $j = 1, 2, \ldots, n$.

Since $\det(L[n,n])^t = \det L[n,n]$, we conclude that

$$r_{1n} = \det L(1,n) / \det L[n,n]\ . \qquad (8)$$

Because the labeling of vertices of the graph G was arbitrary, whichever result holds for the vertex pair v_1, v_n must hold for any other vertex pair v_i, v_j. Thus formula (8) implies the validity of the identity (3) for any i, j, $1 \leq i, j \leq n$, provided $i \neq j$. In other words, we proved the (earlier known [18])

Theorem 2. *Eq. (3) holds for any connected graph G of order $n > 1$.*

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References

[1] F. Buckley and F. Harary, *Distance in Graphs*, Addison-Wesley, Redwood, 1990.

[2] B. Lučić, I. Lukovits, S. Nikolić and N. Trinajstić, Distance-related indexes in the quantitative structure–property relationship modeling, *J. Chem. Inf. Comput. Sci.* **41** (2001) 527–535.

[3] A. A. Dobrynin, R. Entringer and I. Gutman, Wiener index of trees: theory and applications, *Acta Appl. Math.* **66** (2001) 211–249.

[4] M. V. Diudea, B. Pârv, P. E. John, O. Ursu and A. Graovac, Distance counting in tori, *MATCH Commun. Math. Comput. Chem.* **49** (2003) 23–36.

[5] A. A. Dobrynin, On the Wiener index decomposition for catacondensed benzenoid graphs, *Indian J. Chem.* **42A** (2003) 1270–1271.

[6] A. A. Dobrynin, Wiener index decomposition based on vertex degrees of catacondensed benzenoid graphs, *MATCH Commun. Math. Comput. Chem.* **49** (2003) 37–46.

[7] A. Graovac, M. Juvan, M. Petkovšek, A. Vesel and J. Žerovnik, The Szeged index of fasciagraphs, *MATCH Commun. Math. Comput. Chem.* **49** (2003) 47–66.

[8] A. A. Dobrynin and L. S. Mel'nikov, Trees and their quadratic line graphs having the same Wiener index, *MATCH Commun. Math. Comput. Chem.* **50** (2004) 146–164.

[9] M. Gorše and J. Žerovnik, A remark on modified Wiener indices, *MATCH Commun. Math. Comput. Chem.* **50** (2004) 109–116.

[10] M. Stefu and M. V. Diudea, Wiener index of C_4H_8 nanotubes, *MATCH Commun. Math. Comput. Chem.* **50** (2004) 133–144.

[11] D. Vukičević and A. Graovac, On modified Wiener indices of thorn graphs, *MATCH Commun. Math. Comput. Chem.* **50** (2004) 93–108.

[12] H. B. Walikar, V. S. Shigehalli and H. S. Ramane, *Bounds on the Wiener number of a graph*, *MATCH Commun. Math. Comput. Chem.* **50** (2004) 117–132.

[13] D. J. Klein and M. Randić, Resistance distance, *J. Math. Chem.* **12** (1993) 81–95.

[14] D. Bonchev, A. T. Balaban, X. Liu and D. J. Klein, Molecular cyclicity and centricity of polycyclic graphs. I. Cyclicity based on resistance distances or reciprocal distances, *Int. J. Quantum Chem.* **50** (1994) 1–20.

[15] H. Y. Zhu, D. J. Klein and I. Lukovits, Extensions of the Wiener number, *J. Chem. Inf. Comput. Sci.* **36** (1996) 420–428.

[16] I. Gutman and B. Mohar, The quasi–Wiener and the Kirchhoff indices coincide, *J. Chem. Inf. Comput. Sci.* **36** (1996) 982–985.

[17] D. J. Klein, Graph geometry, graph metrics, & Wiener, *MATCH – Commun. Math. Comput. Chem.* **35** (1997) 7–27.

[18] R. B. Bapat, Resistance distance in graphs, *Math. Student* **68** (1999) 87–98.

[19] I. Lukovits, S. Nikolić and N. Trinajstić, Resistance distance in regular graphs, *Int. J. Quantum Chem.* **71** (1999) 217–225.

[20] D. J. Klein and O. Ivanciuc, Graph cyclicity, excess conductance, and resistance deficit, *J. Math. Chem.* **30** (2001) 271–287.

[21] J. L. Palacios, Resistance distance in graphs and random walks, *Int. J. Quantum Chem.* **81** (2001) 29–33.

[22] J. L. Palacios, Closed–form formulas for Kirchhoff index, *Int. J. Quantum Chem.* **81** (2001) 135–140.

[23] D. J. Klein, Resistance–distance sum rules, *Croat. Chem. Acta* **75** (2002) 633–649.

[24] D. Babić, D. J. Klein, I. Lukovits, S. Nikolić and N. Trinajstić, Resistance–distance matrix. A computational algorithm and its application, *Int. J. Quantum Chem.* **90** (2002) 161–176.

[25] W. Xiao and I. Gutman, On resistance matrices, *MATCH – Commun. Math. Comput. Chem.* **49** (2003) 67–81.

[26] R. B. Bapat, I. Gutman and W. Xiao, A simple method for computing resistance distance, *Z. Naturforsch.* **58a** (2003) 494–498.

[27] I. Gutman, D. Vidović and B. Furtula, Chemical applications of the Laplacian spectrum. VII. Studies of the Wiener and Kirchhoff indices, *Indian J. Chem.* **42A** (2003) 1272–1278.

[28] W. Xiao and I. Gutman, Resistance distance and Laplacian spectrum, *Theor. Chem. Acc.* **110** (2003), in press.

[29] S. Seshu and M. B. Read, *Linear Graphs and Electrical Networks*, Addison–Wesley, Reading, 1961.

[30] J. A. Edminster, *Electric Circuits*, McGraw–Hill, New York, 1965.

[31] B. Bollobás, *Modern Graph Theory*, Springer–Verlag, New York, 1998, chapter 9.

[32] A. Ben–Israel and T. N. E. Greville, *Generalized Inverses - Theory and Applications*, Wiley, New York, 1974.

[33] S. L. Campbell and C. D. Meyer, *Generalized Inverses of Linear Transformations*, Pitman, London, 1979.

[34] I. Gutman and W. Xiao, Generalized inverse of the Laplacian matrix and some applications, *Bull. Acad. Serbe Sci. Arts (Cl. Math. Natur.)*, in press.