Bulletin T.CXXIX de l'Académie serbe des sciences et des arts - 2004
Classe des sciences mathématiques et naturelles
sciences mathématiques, № 29

GENERALIZED INVERSE OF THE LAPLACIAN MATRIX AND SOME APPLICATIONS

I. GUTMAN, W. XIAO

(Presented at the 9th Meeting, held on December 26, 2003)

A b s t r a c t. The generalized inverse $L^\dagger$ of the Laplacian matrix of a connected graph is examined and some of its properties are established. In some physical and chemical considerations the quantity $r_{ij} = (L^\dagger)_{ii} + (L^\dagger)_{jj} - (L^\dagger)_{ij} - (L^\dagger)_{ji}$ is encountered; it is called resistance distance. Based on the results obtained for $L^\dagger$ we prove some previously known and deduce some new properties of the resistance distance.

AMS Mathematics Subject Classification (2000): 05C50
Key Words: Laplacian matrix, Laplacian eigenvector (of graph), Laplacian eigenvalue (of graph), resistance distance

1. *Introduction*

In this work we are concerned with simple graphs, i.e., graphs without multiple or directed edges, and without loops. Let G be such a graph and let n be the number of its vertices, $n \geq 2$. Denote the vertices of G by $v_1, v_2, \ldots, v_n$. Throughout this paper it is assumed that G is connected.

The degree d_i of the vertex v_i is the number of first neighbors of this vertex. Then the Laplacian matrix $L = L(G) = ||L_{ij}||$ of the graph G is defined as a square matrix of order n whose (i,j)-entry is given by

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

Consequently, the Laplacian matrix is real and symmetric. Because the sum of each row and of each column is zero, this matrix is singular.

In what follows all matrices encountered are supposed to be square, of order n. If M is such a matrix, then M^t denotes its transpose and M^{-1} its inverse (provided it exists). By I is denoted the unit matrix, whereas by J and O the matrices whose all elements are, respectively, equal to unity and to zero.

The eigenvectors and eigenvalues of $L(G)$ are said to be the Laplacian eigenvectors and Laplacian eigenvalues of the graph G. The Laplacian eigenvalues of the graph G will be denoted by μ_k and the corresponding eigenvectors by u_k , $k = 1, 2, \ldots, n$, so that the equality

$$L(G)\, u_k = \mu_k\, u_k$$

holds for $k = 1, 2, \ldots, n$. In addition, $u_k = (u_{1k}, u_{2k}, \ldots, u_{nk})^t$ for $k = 1, 2, \ldots, n$.

As usual, the Laplacian eigenvalues are labeled so that $\mu_1 \geq \mu_2 \geq \cdots \geq \mu_n$.

For details of Laplacian graph spectral theory see the surveys [1–7] and the recent paper [8]. Of the known results in this field we need the following.

It is always possible to choose the Laplacian eigenvectors to be real, normalized and mutually orthogonal. Throughout this paper we assume that this is the case.

Then $U = (u_1, u_2, \ldots, u_n) = ||u_{ij}||$ is an orthogonal matrix, i.e., $U\,U^t = U^t\,U = I$, implying

$$\sum_{k=1}^{n} u_{ki}\, u_{kj} = \sum_{k=1}^{n} u_{ik}\, u_{jk} = \delta_{ij} \tag{2}$$

where, as usual, $\delta_{ij} = 1$ for $i = j$ and $\delta_{ij} = 0$ for $i \neq i$.

Because of $U^t\, L(G)\, U = \text{diag}\,(\mu_1, \mu_2, \ldots, \mu_n)$, we further have

$$L_{ij} = \sum_{k=1}^{n} \mu_k\, u_{ik}\, u_{jk} \ . \tag{3}$$

For all graphs, $\mu_n = 0$. For all connected graphs, $\mu_{n-1} > 0$. The eigenvector corresponding to μ_n is of the form $u_n = \frac{1}{\sqrt{n}}(1,1,\ldots,1)^t$. Because the eigenvectors u_k, $k = 1,2,\ldots,n-1$, are orthogonal to u_n, the relations

$$\sum_{j=1}^{n} u_{jk} = 0 \tag{4}$$

are obeyed for $k = 1,2,\ldots,n-1$.

Let $M = ||M_{ij}||$ be a square matrix, $\lambda_1, \lambda_2, \ldots, \lambda_n$ its eigenvalues and $c_k = (c_{1k}, c_{2k}, \ldots, c_{nk})^t$ its eigenvector, corresponding to λ_k, $k = 1,2,\ldots,n$. Let the eigenvectors of M be real, normalized and mutually orthogonal. Then,

$$M_{ij} = \sum_{k=1}^{n} \lambda_k \, c_{ik} \, c_{jk}$$

and if $f(\lambda_k)$ exists for all values of k, then the matrix $f(M) = ||(f(M))_{ij}||$ is defined as

$$(f(M))_{ij} = \sum_{k=1}^{n} f(\lambda_k) \, c_{ik} \, c_{jk} \ .$$

In particular, if no eigenvalue of M is equal to zero,

$$(M^{-1})_{ij} = \sum_{k=1}^{n} \frac{1}{\lambda_k} \, c_{ik} \, c_{jk} \ .$$

If the matrix M is singular (i.e., some of its eigenvalues are equal to zero) then it has no inverse. For such matrices one defines the so-called *generalized inverse* [9,10] $M^\dagger = ||(M^\dagger)_{ij}||$, as

$$(M^\dagger)_{ij} = \sum_{k=1}^{n} g(\lambda_k) \, c_{ik} \, c_{jk}$$

where

$$g(\lambda_k) = \begin{cases} 1/\lambda_k & \text{if } \lambda_k \neq 0 \\ 0 & \text{if } \lambda_k = 0 \ . \end{cases}$$

In the special case of the Laplacian matrix of a connected graph, the generalized inverse $L^\dagger = L^\dagger(G) = ||(L^\dagger)_{ij}||$ is defined via

$$(L^\dagger)_{ij} = \sum_{k=1}^{n-1} \frac{1}{\mu_k} \, u_{ik} \, u_{jk} \ . \tag{5}$$

Formula (5) is equivalent to $U^t L^\dagger(G)\, U = \mathrm{diag}\ (1/\mu_1, 1/\mu_2, \ldots, 1/\mu_{n-1}, 0)$, and implies that $u_1, u_2, \ldots, u_{n-1}, u_n$ are the eigenvectors of $L^\dagger$ with eigenvalues $1/\mu_1, 1/\mu_2, \ldots, 1/\mu_{n-1}, 0$, respectively.

2. *Elementary Results*

From (5) it immediately follows:

Lemma 1. *The generalized inverse $L^\dagger$ of the Laplacian matrix of a connected graph is a real and symmetric matrix.*

Lemma 2. *The Laplacian matrix and its generalized inverse satisfy the relations*

$$L\,J = J\,L = O \qquad ; \qquad L^\dagger J = J\,L^\dagger = O\ .$$

P r o o f. The relations stated in Lemma 2 are direct consequences of the fact that the sum of each row and each column of both L and $L^\dagger$ is equal to zero. For the Laplacian matrix this is evident from its definition, Eq. (1). For the sum of the elements in a row of $L^\dagger$ we get

$$\sum_{j=1}^{n} (L^\dagger)_{ij} = \sum_{j=1}^{n} \sum_{k=1}^{n-1} \frac{1}{\mu_k}\, u_{ik}\, u_{jk} = \left(\sum_{k=1}^{n-1} \frac{1}{\mu_k}\, u_{ik} \right) \left(\sum_{j=1}^{n} u_{jk} \right)$$

which is equal to zero because of relations (4). □

Lemma 3. *If L and $L^\dagger$ pertain to a connected graph on n vertices, then*

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

P r o o f. In view of Eqs. (3) and (5), and taking into account (2),

$$\begin{aligned}
(L\,L^\dagger)_{ij} &= \sum_{h=1}^{n} L_{ih}\, (L^\dagger)_{hj} = \sum_{h=1}^{n} \left(\sum_{k=1}^{n} \mu_k\, u_{ik}\, u_{hk} \right) \left(\sum_{\ell=1}^{n-1} \frac{1}{\mu_\ell}\, u_{h\ell}\, u_{j\ell} \right) \\
&= \sum_{k=1}^{n} \sum_{\ell=1}^{n-1} \frac{\mu_k}{\mu_\ell}\, u_{ik}\, u_{j\ell} \left(\sum_{h=1}^{n} u_{hk}\, u_{h\ell} \right) = \sum_{k=1}^{n} \sum_{\ell=1}^{n-1} \frac{\mu_k}{\mu_\ell}\, u_{ik}\, u_{j\ell}\, \delta_{k\ell} \\
&= \sum_{\ell=1}^{n-1} u_{i\ell}\, u_{j\ell} = \sum_{\ell=1}^{n} u_{i\ell}\, u_{j\ell} - u_{in}\, u_{jn} = \delta_{ij} - \frac{1}{n}
\end{aligned}$$

because of $u_{in} = u_{jn} = \frac{1}{\sqrt{n}}$. □

3. *An Auxiliary Matrix*

Whereas the Laplacian matrix L of a connected graph is singular, the matrix $L + \frac{1}{n} J$ is non-singular.

Theorem 4. *Let G be a connected graph, with Laplacian eigenvectors $u_1, u_2, \ldots, u_n$ and Laplacian eigenvalues $\mu_1, \mu_2, \ldots, \mu_{n-1}, \mu_n = 0$. Then $u_1, u_2, \ldots, u_n$ are also the eigenvectors of the matrix $L(G) + \frac{1}{n} J$ with eigenvalues $\mu_1, \mu_2, \ldots, \mu_{n-1}, 1$.*

P r o o f. Let $k < n$. Then

$$\left(L + \frac{1}{n} J\right) u_k = L\, u_k + \frac{1}{n} J\, u_k = \mu_k\, u_k$$

because, as a consequence of (4), $J\, u_k = (0, 0, \ldots, 0)^t$.

Let $k = n$. Then $L\, u_n = (0, 0, \ldots, 0)^t$ whereas $J\, u_n = n\, u_n$ because of $u_n = \frac{1}{\sqrt{n}}(1, 1, \ldots, 1)^t$. Therefore,

$$\left(L + \frac{1}{n} J\right) u_n = \frac{1}{n} J\, u_n = u_n$$

and thus the eigenvalue of the matrix $L + \frac{1}{n} J$, corresponding to the eigenvector u_n, is equal to 1. □

Theorem 5. *If G is a connected graph, then the inverse of the matrix $L(G) + \frac{1}{n} J$ exists and is equal to $L^\dagger(G) + \frac{1}{n} J$.*

P r o o f. The existence of $(L(G) + \frac{1}{n} J)^{-1}$ is guaranteed by Theorem 4. Using Lemmas 2 and 3, and the fact that $J^2 = n\, J$, we have

$$\begin{aligned} \left(L + \frac{1}{n} J\right)\left(L^\dagger + \frac{1}{n} J\right) &= L\, L^\dagger + \frac{1}{n} J\, L^\dagger + \frac{1}{n} L\, J + \frac{1}{n^2} J^2 \\ &= \left(I - \frac{1}{n} J\right) + O + O + \frac{1}{n} J = I\,. \end{aligned}$$ □

In what follows we denote the matrix $(L(G) + \frac{1}{n} J)^{-1}$ by X. This matrix was studied in an earlier work [11] where also Theorem 4 was proven. According to Theorem 5 we now have

$$X = L^\dagger + \frac{1}{n} J\,. \tag{6}$$

4. *A Connection to Physics and Chemistry*

In theoretical chemistry the notion of *resistance distance* was recently introduced [12]. This quantity is conceived in the following manner. To a connected graph G an electric network $\mathcal{N}(G)$ is associated, so that each edge of G is replaced by a resistor of unit resistance. Then the resistance distance between two distinct vertices v_i and v_j of the graph G, denoted by r_{ij}, is the effective electrical resistance between the corresponding two nodes of the network $\mathcal{N}(G)$. By standard methods of the theory of electrical networks (using the Ohm and Kirchhoff laws) is can be shown that [13–15]

$$r_{ij} = (L^{\dagger})_{ii} + (L^{\dagger})_{jj} - (L^{\dagger})_{ij} - (L^{\dagger})_{ji} \tag{7}$$

which holds for $i \neq j$. If, in addition we set $r_{ii} = 0$ for all $i = 1, 2, \ldots, n$, then (7) formally holds also in this case, and we may define the *resistance matrix* as $R = R(G) = ||r_{ij}||$.

The resistance distance and the resistance matrix were much studied in the recent mathematico–chemical literature; for details see [11,16–20] and the references cited therein. Using the results from the preceding sections, we can now easily deduce some previously known and some hitherto not communicated relations for the resistance distance.

First of all, because of the symmetry of the generalized inverse (Lemma 1), formula (7) is simplified as

$$r_{ij} = (L^{\dagger})_{ii} + (L^{\dagger})_{jj} - 2\,(L^{\dagger})_{ij}\ . \tag{8}$$

Combining (8) with (5) we obtain

$$r_{ij} = \sum_{k=1}^{n-1} \frac{1}{\mu_k}\,(u_{ik}\,u_{ik} + u_{jk}\,u_{jk} - 2\,u_{ik}\,u_{jk}) = \sum_{k=1}^{n-1} \frac{1}{\mu_k}\,(u_{ik} - u_{jk})^2\,,$$

a formula earlier deduced in [19], but in a completely different (and more complicated) manner. Combining (8) with (6) we obtain

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

also a formula earlier deduced in [11], again in a completely different and more complicated manner.

Theorem 6. *If the matrices L, $L^{\dagger}$, and R pertain to a connected graph, then*

$$L\,R\,L = -2\,L \tag{9}$$

and

$$L^\dagger \, R \, L^\dagger = -2 \, (L^\dagger)^3 \ . \tag{10}$$

P r o o f. We first deduce the identity (10).

$$\begin{aligned}
(L^\dagger \, R \, L^\dagger)_{ij} &= \sum_{k=1}^{n} \sum_{\ell=1}^{n} (L^\dagger)_{ik} \, r_{k\ell} \, (L^\dagger)_{\ell j} \\
&= \sum_{k=1}^{n} \sum_{\ell=1}^{n} (L^\dagger)_{ik} \left[(L^\dagger)_{kk} + (L^\dagger)_{\ell\ell} - 2 \, (L^\dagger)_{k\ell} \right] (L^\dagger)_{\ell j} \\
&= \sum_{k=1}^{n} (L^\dagger)_{ik} \, (L^\dagger)_{kk} \left(\sum_{\ell=1}^{n} (L^\dagger)_{\ell j} \right) + \sum_{\ell=1}^{n} (L^\dagger)_{\ell j} \, (L^\dagger)_{\ell\ell} \left(\sum_{k=1}^{n} (L^\dagger)_{ik} \right) \\
&- 2 \sum_{k=1}^{n} \sum_{\ell=1}^{n} (L^\dagger)_{ik} \, (L^\dagger)_{k\ell} \, (L^\dagger)_{\ell j} \ .
\end{aligned}$$

By Lemma 2,

$$\sum_{\ell=1}^{n} (L^\dagger)_{\ell j} = 0 \quad \text{and} \quad \sum_{k=1}^{n} (L^\dagger)_{ik} = 0$$

and therefore,

$$(L^\dagger \, R \, L^\dagger)_{ij} = -2 \sum_{k=1}^{n} \sum_{\ell=1}^{n} (L^\dagger)_{ik} \, (L^\dagger)_{k\ell} \, (L^\dagger)_{\ell j} = -2 \, [(L^\dagger)^3]_{ij}$$

which is tantamount to Eq. (10).

Now, multiplying (10) by L^2 from both left and right we get

$$L^2 \, L^\dagger \, R \, L^\dagger \, L^2 = -2 \, L^2 (L^\dagger)^3 \, L^2 \ .$$

By Lemmas 2 and 3,

$$\begin{aligned}
L^2 \, L^\dagger &= L \, (L \, L^\dagger) = L \left(I - \frac{1}{n} \, J \right) = L \\
L^\dagger \, L^2 &= (L^\dagger \, L) \, L = \left(I - \frac{1}{n} \, J \right) L = L \ .
\end{aligned}$$

Therefore

$$L^2 \, L^\dagger \, R \, L^\dagger \, L^2 = L \, R \, L$$

and

$$L^2 (L^\dagger)^3 \, L^2 = L \, L^\dagger \, L = \left(I - \frac{1}{n} \, J \right) \, L = L \; .$$

Formula (9) follows. □

Theorem 7. *In the case of connected graphs, the generalized inverse of the Laplacian matrix can be expressed in terms of the resistance matrix:*

$$L^\dagger = -\frac{1}{2} \left[R - \frac{1}{n} \, (R \, J + J \, R) + \frac{1}{n^2} \, J \, R \, J \right] \; .$$

P r o o f. Multiply (10) by L from both left and right, and use the same way of reasoning as in the proof of Theorem 6. □

REFERENCES

[1] R. B. B a p a t, The Laplacian matrix of a graph, Math. Student 65 (1996) 214–223.

[2] R. G r o n e, R. M e r r i s, *The Laplacian spectrum of a graph II*, SIAM J. Discr. Math. 7 (1994), 221–229.

[3] R. G r o n e, R. M e r r i s, V. S. S u n d e r, *The Laplacian spectrum of a graph*, SIAM J. Matrix Anal. Appl. 11 (1990), 218–238.

[4] R. M e r r i s, *Laplacian matrices of graphs: A survey*, Lin. Algebra Appl. 197–198 (1994), 143–176.

[5] R. M e r r i s, *A survey of graph Laplacians*, Lin. Multilin. Algebra 39 (1995), 19–31.

[6] R. M e r r i s, *Laplacian graph eigenvectors*, Lin. Algebra Appl. 278 (1988), 221–236.

[7] B. M o h a r, *The Laplacian spectrum of graphs*, in: Y. Alavi, G. Chartrand, O. R. Ollermann, A. J. Schwenk (Eds.), *Graph theory, combinatorics, and applications*, Wiley, New York, 1991, pp. 871–898.

[8] I. G u t m a n, *Some properties of Laplacian eigenvectors*, Bull. Acad. Serbe Sci. Arts (Cl. Math. Natur.) 127 (2003) 1–6.

[9] A. B e n – I s r a e l, T. N. E. G r e v i l l e, *Generalized Inverses – Theory and Applications*, Wiley, New York, 1974.

[10] S. L. C a m p b e l l, C. D. M e y e r, *Generalized Inverses of Linear Transformations*, Pitman, London, 1979.

[11] W. X i a o, I. G u t m a n, *On resistance matrices*, MATCH Commun. Math. Comput. Chem. 49 (2003), 67–81.

[12] D. J. K l e i n, M. R a n d i ć, *Resistance distance*, J. Math. Chem. 12 (1993), 81–95.

[13] S. S e s h u, M. B. R e a d, *Linear Graphs and Electrical Networks*, Addison–Wesley, Reading, 1961.

[14] J. A. E d m i n s t e r, *Electric Circuits*, McGraw–Hill, New York, 1965.

[15] B. B o l l o b á s, *Modern Graph Theory*, Springer–Verlag, New York, 1998, chapter 9.

[16] R. B. B a p a t, *Resistance distance in graphs*, Math. Student 68 (1999), 87–98.

[17] J. L. P a l a c i o s, *Resistance distance in graphs and random walks*, Int. J. Quantum Chem. 81 (2001), 29–33.

[18] D. J. K l e i n, *Resistance–distance sum rules*, Croat. Chem. Acta 75 (2002), 633–649.

[19] W. X i a o, I. G u t m a n, *Resistance distance and Laplacian spectrum*, Theor. Chem. Acc. 110 (2003) 284–289.

[20] R. B. B a p a t, I. G u t m a n, W. X i a o, *A simple method for computing resistance distance*, Z. Naturforsch. 58a (2003) 494–498.

Faculty of Science
University of Kragujevac
P. O. Box 60
34000 Kragujevac
Serbia and Montenegro

Department of Computer Science
South China University of Technology
Guangzhou 510641
P. R. China, and
Xiamen University
P. O. Box 1003
Xiamen 361005
P. R. China