Available online at www.sciencedirect.com

ScienceDirect

Discrete Applied Mathematics 155 (2007) 654–661

DISCRETE APPLIED MATHEMATICS

www.elsevier.com/locate/dam

Note

Resistance distance and the normalized Laplacian spectrum☆

Haiyan Chen[a], Fuji Zhang[b]

[a] *School of Sciences, Jimei University, Xiamen 361021, China*
[b] *Institute of Mathematics, Xiamen University, Xiamen 361005, China*

Received 7 June 2005; received in revised form 23 June 2006; accepted 6 September 2006
Available online 30 October 2006

Abstract

It is well known that the resistance distance between two arbitrary vertices in an electrical network can be obtained in terms of the eigenvalues and eigenvectors of the combinatorial Laplacian matrix associated with the network. By studying this matrix, people have proved many properties of resistance distances. But in recent years, the other kind of matrix, named the normalized Laplacian, which is consistent with the matrix in spectral geometry and random walks [Chung, F.R.K., Spectral Graph Theory, American Mathematical Society: Providence, RI, 1997], has engendered people's attention. For many people think the quantities based on this matrix may more faithfully reflect the structure and properties of a graph. In this paper, we not only show the resistance distance can be naturally expressed in terms of the normalized Laplacian eigenvalues and eigenvectors of G, but also introduce a new index which is closely related to the spectrum of the normalized Laplacian. Finally we find a non-trivial relation between the well-known Kirchhoff index and the new index.

Keywords: Resistance distance; Normalized Laplacian matrix; Random walks

1. Introduction

The resistance distance is a novel distance function on a graph proposed by Klein and Randic [9]. The term resistance distance was used because of the physical interpretation: one imagines unit resistors on each edge of a graph G and takes the resistance distance between vertices i and j of G to be the effective resistance between vertices i and j, denoted by r_{ij}. This resistance distance is in fact intrinsic to the graph, with some nice purely mathematical interpretations and other interpretations [11,12]. On the other hand, there is the long recognized shortest path distance function which has been extensively studied and found many applications [5,14]. For these two distance functions, the shortest-path might be imagined to be more relevant when there is corpuscular communication (along edges) between two vertices, whereas the resistance distance might be imagined to be more relevant when the communication is wave-like. That the communication of many things is rather wave-like, such as, chemical communication in molecules and information communication in networks, suggests a substantial potential for applications, beyond the traditional electrical ones. So in recent years, the resistance distance was much studied, especially in the chemical literature [1,2,7–9,13,16,20–22], the method they used is the standard method within the theory of electrical networks, that is, computing the resistance distance is via the Moore-Penrose generalized inverse of the (combinatorial) Laplacian matrix $L = D - A$, where

☆ This work was supported by NSFC10501018 and z0511042.
E-mail address: chey6@sohu.com (H. Chen).

0166-218X/$ - see front matter © 2006 Elsevier B.V. All rights reserved.
doi:10.1016/j.dam.2006.09.008

A is the adjacency matrix of G and D is the diagonal matrix in which the ith diagonal entry is d_i (the degree of vertex i). Many results have been obtained by studying the combinatorial Laplacian, for example, the "Kirchhoff index" (a structure-descriptor)

$$Kf = \sum_{i<j} r_{ij} = n \sum_{k=2}^{n} \frac{1}{\mu_k},$$

where $0 = \mu_1 < \mu_2 \leqslant \cdots \leqslant \mu_n (n \geqslant 2)$ are the eigenvalues of L.

In this paper, we will use the intimate relations between random walks on graphs and electrical networks [6,18,3] to study the resistance distance. Along this line, so far there are relatively little work [17,10] had been done. Although that, those work had suggested that simple random walks based quantities should prove of further use, not yet fully recognized in many areas, for example, in chemical graph theory, the authors (including Klein, D.J.) of paper [10] said "Simple random walks with each step taken independently and randomly naturally are anticipated as a basis for novel chemical graph theory". Here we show the resistance distance r_{ij} can be naturally expressed in terms of the normalized Laplacian [4] eigenvalues and eigenvectors, which is consistent with the transition probability matrix of random walks and introduce a new index of a graph based on this matrix. Finally, we find an invertible matrix which is connected with the normalized Laplacian eigenvalues and eigenvectors. By studying this matrix, we verify some properties of the resistance matrix, and find a relation between the "Kirchhoff index" and the new index. To this end, in the following sections, we first present some definitions of random walks and relevant results, while at the same time, remind readers of a few results from the normalized Laplacian spectral theory.

2. The normalized Laplacian and a new index

Throughout this paper, the standard notation for a simple connected graph G is used. The vertex set is $V(G)$ and the edge is $E(G)$, and $n(\geqslant 2)$, m denote the vertex and edge number respectively.

On a graph $G = (V(G), E(G))$, we can define the *random walks* on G as the Markov chain $X_n, n \geqslant 0$, that from its current vertex i jumps to the neighboring vertex j with probability $p_{ij} = 1/d_i$, where d_i is the degree of the degree i. Apparently the transition probability matrix $P = (p_{ij}) = D^{-1}A$ is a stochastic matrix. The hitting time T_j of the vertex j is the number of jumps the walk needs to reach j. The expected value of T_j when the walk is started at the vertex i is denoted by $E_i T_j$. The expected commute time between vertices i and j is defined by $E_i T_j + E_j T_i$. Then there is an elegant relation between commute times and resistance distances [3,18]:

$$E_i T_j + E_j T_i = 2m r_{ij}. \tag{1}$$

The normalized Laplacian matrix of G defined to be

$$\mathscr{L} = I - D^{1/2} P D^{-1/2},$$

that is $\mathscr{L} = D^{-1/2} L D^{-1/2}$. For regular graphs (i.e., having all vertices of the same degree) L and $\mathscr{L}$ are basically the same (up to a scale factor), but for general graphs there is much difference between them. Evidently $\mathscr{L}$ is Hermitian and similar to $I - P$, so the eigenvalues of $\mathscr{L}$ are non-negative, we label them so that $0 = \lambda_1 < \lambda_2 \leqslant \cdots \leqslant \lambda_n$, and $v_1, \ldots, v_n$ are the corresponding mutually orthogonal eigenvectors of unit length. For clearness, let

$$v_i = (v_{i1}, v_{i2}, \ldots, v_{in})^{\mathrm{t}},$$

where t indicates transposition, $V = (v_1, v_2, \ldots, v_n)$. Then we have

(i)

$$V^{\mathrm{t}} \mathscr{L} V = diag[\lambda_1, \lambda_2, \ldots, \lambda_n], \tag{2}$$

and V is an orthogonal matrix, that is

$$\sum_{k=1}^{n} v_{ik} v_{jk} = \sum_{k=1}^{n} v_{ki} v_{kj} = \begin{cases} 1 & \text{if } i = j, \\ 0 & \text{otherwise.} \end{cases}$$

(ii)

$$\mathscr{L}_{ij} = \sum_{k=1}^{n} \lambda_k v_{ki} v_{kj} = \sum_{k=2}^{n} \lambda_k v_{ki} v_{kj}. \tag{3}$$

Let **1** and **0** be the n-dimensional column vectors whose components are equal to unity and zero, respectively. Then

$$(I - P)\mathbf{1} = \mathbf{0}.$$

This means the eigenvector v_1 is of the form

$$v_{1i} = \sqrt{d_i/2m}, \quad i = 1, \ldots, n.$$

For convenience, we present some fundamental results about the spectrum of $\mathscr{L}$, for more details see [4].

Theorem 2.1. *For a graph $G = (V(G), E(G))$, we have*

(i) *If G is a not a complete graph, then $1/2ml < \lambda_2 \leqslant 1$, where l is the diameter of G;*
(ii) *$n/(n-1) \leqslant \lambda_n \leqslant 2$ with $\lambda_n = 2$ if and only if G is bipartite;*
(iii) *$\prod_{i=1}^{n} d_i \prod_{k=2}^{n} \lambda_k = 2m\tau(G)$, where $\tau(G)$ is the number of spanning trees of G.*

For the notations as above, we have the following:

Theorem 2.2 (*Lovász [15]*). *For graph $G = (V(G), E(G))$, $\forall i, j \in V$,*

$$E_i T_j + E_j T_i = 2m \sum_{k=2}^{n} \frac{1}{\lambda_k} \left(\frac{v_{kj}}{\sqrt{d_j}} - \frac{v_{ki}}{\sqrt{d_i}} \right)^2.$$

So by Eq. (1), we naturally obtain that:

Theorem 2.3. *For graph $G = (V(G), E(G))$, $\forall i, j \in V$,*

$$r_{ij} = \sum_{k=2}^{n} \frac{1}{\lambda_k} \left(\frac{v_{kj}}{\sqrt{d_j}} - \frac{v_{ki}}{\sqrt{d_i}} \right)^2.$$

Using Theorem 2.1(i)(ii) along with the orthogonality of the matrix $V = (v_{ij})$, we get:

Corollary 2.4. *For graph $G = (V(G), E(G))$, $\forall i, j \in V (i \neq j)$*

$$\frac{1}{2}\left(\frac{1}{d_i} + \frac{1}{d_j}\right) \leqslant \frac{1}{\lambda_n}\left(\frac{1}{d_i} + \frac{1}{d_j}\right) \leqslant r_{ij} \leqslant \frac{1}{\lambda_2}\left(\frac{1}{d_i} + \frac{1}{d_j}\right) \leqslant 2ml\left(\frac{1}{d_i} + \frac{1}{d_j}\right).$$

As we pointed out in the introduction, the "Kirchhoff index" $Kf = \sum_{i<j} r_{ij}$ is closely related to the spectrum of L, that is $Kf = n\sum_{k=2}^{n}(1/\mu_k)$, this equality is first proved in [7,21], the authors presented the other proof. Here, we introduce a new graph index related to resistance distance, defined by

$$K'f = \sum_{i<j} d_i d_j r_{ij},$$

in the following, we prove this new index can be expressed by the spectrum of $\mathscr{L}$.

Theorem 2.5. *For graph $G = (V(G), E(G))$, $i, j \in V$*

$$K'f = \sum_{i<j} d_i d_j r_{ij} = 2m \sum_{k=2}^{n} \frac{1}{\lambda_k}.$$

Proof.

$$\begin{aligned}\sum_{i<j} d_i d_j r_{ij} &= \frac{1}{2}\sum_{i,j\in V} d_i d_j r_{ij}\\ &= \frac{1}{2}\sum_{i=1}^{n} d_i \sum_{k=2}^{n}\frac{1}{\lambda_k}\left(\sum_{j=1}^{n} v_{kj}^2 - 2\frac{v_{ki}}{\sqrt{d_i}}\sum_{j=1}^{n} v_{kj}\sqrt{d_j} + 2m\frac{v_{ki}^2}{d_i}\right)\\ &= \frac{1}{2}\sum_{i=1}^{n} d_i \sum_{k=2}^{n}\frac{1}{\lambda_k}\left(1 + 2m\frac{v_{ki}^2}{d_i}\right)\\ &= 2m\sum_{k=2}^{n}\frac{1}{\lambda_k}.\end{aligned}$$

Since the new index is related to the spectrum of $\mathscr{L}$, we naturally think the new index $K'f$ is worthy of studying. Here we only consider the relations between Kf and $K'f$. These two graph invariants are generally quite different, though by definitions, $Kf \leqslant K'f$, especially if a graph is d-regular, then $K'f = d^2 Kf$. In the next section, we will give a non-trivial relation between $K'f$ and Kf. □

3. A relation between $K'f$ and Kf

In this section, by studying an invertible matrix X, which is connected to the eigenvalues and eigenvectors of the normalized Laplacian matrix, we obtain some properties of the distance matrix. Then using those properties, we find a relation between $K'f$ and Kf.

Theorem 3.1. *For a graph $G = (V(G), E(G))$, let $X = (D - A + (1/2m)DJD)^{-1}$, where J denote the square matrix of order n with all entries equal to 1. Then for any $i, j \in V$*

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

Proof. By Eq. (2), we have

$$V^{\mathrm{t}} D^{1/2}(I-P)D^{-1/2}V = diag[\lambda_1, \lambda_2, \ldots, \lambda_n],$$

whence

$$V^{\mathrm{t}} D^{1/2}\frac{1}{2m} JDD^{-1/2}V = V^{\mathrm{t}} D^{1/2}\frac{1}{2m} JD^{1/2}V = diag[1, 0, \ldots, 0],$$

so

$$\left(I - P + \frac{1}{2m}JD\right)^{-1} = D^{-1/2}V diag\left[1, \frac{1}{\lambda_2}, \ldots, \frac{1}{\lambda_n}\right] V^{\mathrm{t}} D^{1/2},$$

$$\begin{aligned}X = \left(D - A + \frac{1}{2m}DJD\right)^{-1} &= \left(I - P + \frac{1}{2m}JD\right)^{-1} D^{-1}\\ &= D^{-1/2}V diag\left[1, \frac{1}{\lambda_2}, \ldots, \frac{1}{\lambda_n}\right] V^{\mathrm{t}} D^{-1/2}. \qquad (4)\end{aligned}$$

Then

$$x_{ij} = \frac{v_{1i}v_{1j}}{\sqrt{d_i d_j}} + \sum_{k=2}^{n} \frac{1}{\lambda_k} \frac{v_{ki}v_{kj}}{\sqrt{d_i d_j}}$$
$$= \frac{1}{2m} + \sum_{k=2}^{n} \frac{1}{\lambda_k} \frac{v_{ki}v_{kj}}{\sqrt{d_i d_j}}.$$

So by Theorem 2.3, we have

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

Now by studying the matrix X, we will determine some properties of the resistance matrix $R = (r_{ij})$, which is a symmetric matrix with zero diagonals. Firstly,

$$x_{ii} = \frac{1}{2m} + \sum_{k=2}^{n} \frac{1}{\lambda_k} \frac{v_{ki}^2}{d_i},$$

so

$$\sum_{i=1}^{n} d_i x_{ii} = 1 + \sum_{k=2}^{n} \frac{1}{\lambda_k}. \tag{5}$$

Secondly by the above theorem, R can be written as

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

So

$$V^{\mathrm{t}} D^{1/2} R D^{1/2} V = V^{\mathrm{t}} D^{1/2}\, diag[x_{11}, x_{22}, \ldots, x_{nn}] J D^{1/2} V$$
$$+ V^{\mathrm{t}} D^{1/2} J\, diag[x_{11}, x_{22}, \ldots, x_{nn}] D^{1/2} V - 2V^{\mathrm{t}} D^{1/2} X D^{1/2} V.$$

By Eq. (4), we have

$$V^{\mathrm{t}} D^{1/2} X D^{1/2} V = diag\left[1, \frac{1}{\lambda_2}, \ldots, \frac{1}{\lambda_n}\right].$$

whence

$$V^{\mathrm{t}} D^{1/2}\, diag[x_{11}, x_{22}, \ldots, x_{nn}] J D^{1/2} V = \begin{pmatrix} \sum_{i=1}^{n} d_i x_{ii} & 0 & \cdots & 0 \\ \sum_{i=1}^{n} \sqrt{2md_i}\, x_{ii} v_{2i} & 0 & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ \sum_{i=1}^{n} \sqrt{2md_i}\, x_{ii} v_{ni} & 0 & \cdots & 0 \end{pmatrix}$$

$$V^{\mathrm{t}} D^{1/2} J\, diag[x_{11}, x_{22}, \ldots, x_{nn}] D^{1/2} V$$
$$= \begin{pmatrix} \sum_{i=1}^{n} d_i x_{ii} & \sum_{i=1}^{n} \sqrt{2md_i}\, x_{ii} v_{2i} & \cdots & \sum_{i=1}^{n} \sqrt{2md_i}\, x_{ii} v_{ni} \\ 0 & 0 & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & 0 \end{pmatrix}$$

After this preparatory work, we can easily get the following:

Theorem 3.2. *For a graph $G = (V(G), E(G))$, the determinant of its resistance matrix*

$$\det R = \frac{(-2)^{n-1}}{2m\tau(G)} \left(S + 2\sum_{k=2}^{n} \frac{1}{\lambda_k} \right),$$

where $S = m(y_{11}, y_{22}, \ldots, y_{nn}) L (y_{11}, y_{22}, \ldots, y_{nn})^{\mathrm{t}}$ and $y_{ii} = \sum_{k=2}^{n} (1/\lambda_k) v_{ki}^2 / d_i$.

Proof. From above, we have

$$V^{\mathrm{t}}D^{1/2}RD^{1/2}V=\begin{pmatrix} 2\sum_{i=1}^{n}d_ix_{ii}-2 & \sum_{i=1}^{n}\sqrt{2md_i}x_{ii}v_{2i} & \cdots & \sum_{i=1}^{n}\sqrt{2md_i}x_{ii}v_{ni}\\ \sum_{i=1}^{n}\sqrt{2md_i}x_{ii}v_{2i} & -\dfrac{2}{\lambda_2} & \cdots & 0\\ \vdots & \vdots & \ddots & \vdots\\ \sum_{i=1}^{n}\sqrt{2md_i}x_{ii}v_{ni} & 0 & \cdots & -\dfrac{2}{\lambda_n}\end{pmatrix}$$

$$=\begin{pmatrix} 2\sum_{k=2}^{n}\dfrac{1}{\lambda_k}+m\sum_{k=2}^{n}\lambda_k\left(\sum_{i=1}^{n}\sqrt{d_i}x_{ii}v_{ki}\right)^2 & \sum_{i=1}^{n}\sqrt{2md_i}x_{ii}v_{2i} & \cdots & \sum_{i=1}^{n}\sqrt{2md_i}x_{ii}v_{ni}\\ 0 & -\dfrac{2}{\lambda_2} & \cdots & 0\\ \vdots & \vdots & \ddots & \vdots\\ 0 & 0 & \cdots & -\dfrac{2}{\lambda_n}\end{pmatrix},$$

where we use Eq. (5). Therefore

$$\det\ R=\frac{(-2)^{n-1}}{\prod_{i=1}^{n}d_i\prod_{k=2}^{n}\lambda_k}\left(2\sum_{k=2}^{n}\frac{1}{\lambda_k}+m\sum_{k=2}^{n}\lambda_k\left(\sum_{i=1}^{n}\sqrt{d_i}x_{ii}v_{ki}\right)^2\right).$$

Then by Theorem 2.1(iii), we get

$$\frac{(-2)^{n-1}}{2m\tau(G)}\left(2\sum_{k=2}^{n}\frac{1}{\lambda_k}+m\sum_{k=2}^{n}\lambda_k\left(\sum_{i=1}^{n}\sqrt{d_i}x_{ii}v_{ki}\right)^2\right).$$

Let $S=m\sum_{k=2}^{n}\lambda_k(\sum_{i=1}^{n}\sqrt{d_i}x_{ii}v_{ki})^2$, then by Eq. (3), we have

$$\begin{aligned} S&=m\sum_{k=2}^{n}\sum_{i=1}^{n}\sum_{j=1}^{n}\lambda_k(\sqrt{d_i}x_{ii}v_{ki})(\sqrt{d_j}x_{jj}v_{kj})\\ &=m\sum_{i=1}^{n}\sum_{j=1}^{n}x_{ii}x_{jj}\sqrt{d_i}\sqrt{d_j}\left(\sum_{k=2}^{n}\lambda_kv_{ki}v_{kj}\right)\\ &=m\sum_{i=1}^{n}\sum_{j=1}^{n}x_{ii}x_{jj}\sqrt{d_i}\sqrt{d_j}\mathscr{L}_{ij}=m\sum_{i=1}^{n}\sum_{j=1}^{n}x_{ii}x_{jj}L_{ij}\\ &=m(x_{11},x_{22},\ldots,x_{nn})L(x_{11},x_{22},\ldots,x_{nn})^{\mathrm{t}}.\end{aligned}$$

Thence $(x_{11},x_{22},\ldots,x_{nn})=(y_{11},y_{22},\ldots,y_{nn})+(1/2m,1/2m,\ldots,1/2m)$ So the result

$$S=m(y_{11},y_{22},\ldots,y_{nn})L(y_{11},y_{22},\ldots,y_{nn})^{\mathrm{t}}$$

is obtained. □

This theorem implies that det R is always different from zero, in other words the resistance matrix is nonsingular; and the sign of det R depends only on the parity of the number of vertices of G. Furthermore the resistance matrix has a single positive eigenvalue, and $n-1$ negative eigenvalues. This property was obtained earlier [21] by using the invertible matrix $(L+(1/n)J)^{-1}$.

So from a knowledge of linear algebra [19], if we introduce the inner product $(a,b)=aRb^{\mathrm{t}}$ in n-dimensional real vector space, then we obtain a Lorentz space L^n. In L^n a vector a is said to be positive if $(a,a)>0$, and for any two row vectors $a=(a_1,a_2,\ldots,a_n)$, $b=(b_1,b_2,\ldots,b_n)$, if one of them is positive vector, then

$$(aRb^{\mathrm{t}})^2 \geqslant (aRa^{\mathrm{t}})(bRb^{\mathrm{t}}), \tag{6}$$

with equality holding if and only if $b=\alpha a$, where α is a constant.

By this inequality, we can easily obtain the following:

Theorem 3.3. *For a graph $G=(V(G),E(G))$, Kf and $K'f$ satisfy*

$$Kf \leqslant \left(\frac{n}{4m}+\frac{1}{2\delta}\right)^2 K'f,$$

where δ is the minimum degree of G, the equality holds if and only if G is regular.

Proof. In Eq. (7), let $a=(d_1,d_2,\ldots,d_n)$, $b=(1,1,\ldots,1)$, then

$$aRa^{\mathrm{t}} = \sum_{i,j=1}^{n} d_i d_j r_{ij} = 2K'f, \quad bRb^{\mathrm{t}} = 2Kf;$$

and a is a positive vector, whence

$$\begin{aligned} aRb^{\mathrm{t}} &= \sum_{i=1}^{n}\sum_{j=1}^{n} d_i r_{ij} \\ &= \sum_{j=1}^{n}\sum_{k=2}^{n} \frac{1}{\lambda_k}\left(1+2m\frac{v_{kj}^2}{d_j}\right) \\ &\leqslant \left(n+\frac{2m}{\delta}\right)\sum_{k=2}^{n}\frac{1}{\lambda_k} = \left(\frac{n}{2m}+\frac{1}{\delta}\right)K'f. \end{aligned}$$

So

$$4K'fKf \leqslant \left(\frac{n}{2m}+\frac{1}{\delta}\right)^2 K'f^2,$$

that is

$$Kf \leqslant \left(\frac{n}{4m}+\frac{1}{2\delta}\right)^2 K'f,$$

and the equality holds if and only if $d_1=d_2=\cdots=d_n$, i.e., G is regular. □

References

[1] D. Babić, D.J. Klein, I. Lukovits, S. Nikolić, N. Trinajstić, Internat. J. Quantum Chem. 90 (2002) 161.
[2] D. Bonchey, A.T. Balaban, X. Liu, D.J. Klein, Int. J. Quantum Chem. 50 (1994) 1.
[3] A.K. Chandra, P. Raghavan, W.L. Ruzzo, R. Smolensky, P. Tiwari, in: Proceedings of the 21st Annual ACM Symposium on Theory of Computing, Seattle, Washington, 1989, pp. 574–586.
[4] F.R.K. Chung, Spectral Graph Theory, American Mathematical Society Providence, RI, 1997.
[5] A.A. Dobrynin, R. Entringer, I. Gutman, Acta. Appl. Math. 66 (2001) 211.
[6] P.G. Doyle, J.L. Snell, Random Walks and Electric Networks, MAA, 1984.
[7] I. Gutman, B. Mohar, J. Chem. Inform. Comput. Sci. 36 (1996) 982.
[8] D.J. Klein, M. Randić, J. Math. Chem. 12 (1993) 81–85.
[9] D.J. Klein, Commun. Math. Comput. Chem. (MATCH) 36 (1996) 7–27.
[10] D.J. Klein, H.Y. Zhu, J. Math. Chem. 23 (1998) 179–195.
[11] D.J. Klein, O. Ivanciuc, J. Math. Chem. (2001) 271.
[12] D.J. Klein, Croat. Chem. Acta. 75 (2002) 633.

[13] D.J. Klein, J.L. Palacios, M. Randić, N. Trinajstić, J. Chem. Inform. Comput. Sci. 44 (2004) 1521–1525.
[14] B. Lucić, I. Lukovits, S. Nikolić, N. Trinajstić, J. Chem. Inform. Comput. Sci. 41 (2001) 527.
[15] L. Lovász, Random walks on graphs: a survey, in combinatorics, Paul Erdos is Eighty, Bolyai Soc. Math. Stud. 2 (1) (1993) 1–46.
[16] I. Lukovits, S. Nikolić, N. Trinajstić, Internat. J. Quantum Chem. 71 (1999) 217.
[17] J.L. Palacios, Internat. J. Quantum Chem. 81, 29 and 135 (2001).
[18] P.J. Tetali, Theoret. Probab. 4 (1) (1991) 101–109.
[19] J.H. Van Lint, Linear Algebra Appl. 39 (1981) 1–8.
[20] W. Xiao, I. Gutman, MATCH, Commun. Math. Comput. Chem. 49 (2003) 67;
W. Xiao, I. Gutman, MATCH, Commun. Math. Comput. Chem. 51 (2004) 119
[21] W. Xiao, I. Gutman, Theoret. Chem. Acta. 110 (2003) 284–289.
[22] H.Y. Zhu, D.J. Klein, I. Lukovits, J. Chem. Inform. Comput. Sci. 36 (1996) 420.