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ORIGINAL PAPER

On resistance-distance and Kirchhoff index

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Abstract We provide some properties of the resistance-distance and the Kirchhoff index of a connected (molecular) graph, especially those related to its normalized Laplacian eigenvalues.

Keywords Kirchhoff index · Laplacian eigenvalues · Laplacian matrix · Resistance-distance

1 Introduction

Klein and Randić [1] introduced in 1993 the resistance-distance as a novel graphical distance. They used concepts from the theory of resistive electrical networks (the Ohm and Kirchhoff laws) [2,3] and the theory of graphs [4]. A merging of concepts from these two theories [5] was achieved by viewing an electrical network as a connected graph, such that vertices of the graph correspond to junctions in the electrical network and the edges of the graph to unit resistors of one ohm. Then the resistance-distance defined as the effective resistance between pairs of vertices is a graphical distance. The concept of the effective resistance has been discussed already in 1949 for another purpose by Foster [6] as recently (2004) pointed out by Palacios [7].

Let G be a simple connected (molecular) graph with the vertex set $V(G) = \{v_1, v_2, \ldots, v_n\}$. Let r_{ij} be the resistance-distance between vertices v_i and v_j in G. The Kirchhoff index of the graph G is defined as [1,8]

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$$\mathrm{Kf}(G) = \sum_{i<j} r_{ij}.$$

Mathematical, computational properties and the range of applicability of the Kirchhoff index are discussed by a number of authors [1,8–17].

Let G be a connected graph with $n \geq 2$ vertices. For $v_i \in V(G)$, $\Gamma(v_i)$ denotes the set of its (first) neighbors in G and the degree of v_i is $d_i = |\Gamma(v_i)|$. Let $\mathbf{D}(G) = \mathrm{diag}(d_1, d_2, \ldots, d_n)$. The adjacency matrix $\mathbf{A}(G)$ of G is an $n \times n$ matrix (a_{ij}) such that $a_{ij} = 1$ if the vertices v_i and v_j are adjacent and 0 otherwise [18]. The ordinary (combinatorial) Laplacian matrix of G is $\mathbf{L}(G) = \mathbf{D}(G) - \mathbf{A}(G)$ [18–20]. The normalized Laplacian matrix of G is $\mathsf{L}(G) = \mathbf{D}^{-1/2}\mathbf{L}(G)\mathbf{D}^{-1/2}$, where $\mathbf{D}^s = \mathrm{diag}\left(d_1^s, d_2^s, \ldots, d_n^s\right)$, $\mathbf{D} = \mathbf{D}(G)$ [21]. The ordinary and normalized Laplacian eigenvalues of G are the eigenvalues of $\mathbf{L}(G)$ and $\mathsf{L}(G)$, respectively.

Let $\lambda_1, \lambda_2, \ldots, \lambda_n$ be the ordinary Laplacian eigenvalues and $\mu_1, \mu_2, \ldots, \mu_n$ the normalized Laplacian eigenvalues of G, arranged in a non-increasing order. Then $\lambda_{n-1} > \lambda_n = 0$ and $\mu_{n-1} > \mu_n = 0$. Zhu et al. [10], Gutman and Mohar [11] and Mohar et al. [22] proved that

$$\mathrm{Kf}(G) = n \sum_{k=1}^{n-1} \frac{1}{\lambda_k},$$

and discussed the relationship between the Wiener index and the Kirchhhof index. Recently, Chen and Zhang [16] introduced a quantity $\mathrm{Kf}^*(G)$, which is defined as:

$$\mathrm{Kf}^*(G) = \sum_{i<j} d_i r_{ij} d_j,$$

and showed that

$$\mathrm{Kf}^*(G) = 2m \sum_{k=1}^{n-1} \frac{1}{\mu_k},$$

where m is the number of edges of G.

We present in this report several properties of the resistance-distance and the Kirchhoff index of a connected (molecular) graph, especially those related to its *normalized* Laplacian eigenvalues.

2 Properties of the resistance-distance and the Kirchhoff index

Let $\mathbf{C}^T$ denotes the transpose of the vector or matrix $\mathbf{C}$. Let $\mathbf{I}$ be the identity matrix of appropriate dimension. Let $\mathbf{z}_1, \mathbf{z}_2, \ldots, \mathbf{z}_n$ be the orthonormal eigenvectors of $\mathsf{L}(G)$ corresponding to $\mu_1, \mu_2, \ldots, \mu_n$, respectively. Let $\mathbf{Z} = (\mathbf{z}_1, \mathbf{z}_2, \ldots, \mathbf{z}_n)$.

Lemma 1 [9,16] *Let G be a connected (molecular) graph with $n \geq 2$ vertices. Then*

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

where $\mathbf{z}_i = (z_{i1}, z_{i2}, \ldots, z_{in})^T$ for $i = 1, 2, \ldots, n$.

Proposition 2 *Let G be a connected (molecular) graph with $n \geq 2$ vertices, maximal vertex degree Δ and minimal vertex degree δ, and let α be any real number. Then*

$$\sum_{i<j} d_i^\alpha r_{ij} d_j^\alpha \leq \begin{cases} \Delta^{\alpha-1} \sum_{i=1}^{n} d_i^\alpha \sum_{k=1}^{n-1} \frac{1}{\mu_k} & \text{if } \alpha \geq 1 \\ \delta^{\alpha-1} \sum_{i=1}^{n} d_i^\alpha \sum_{k=1}^{n-1} \frac{1}{\mu_k} & \text{if } \alpha < 1 \end{cases} \tag{1}$$

with equality if and only if $\alpha = 1$ or G is regular.

Proof By Lemma 1, $r_{ij} = \sum_{k=1}^{n-1} \frac{1}{\mu_k} \left(\frac{z_{ki}}{\sqrt{d_i}} - \frac{z_{kj}}{\sqrt{d_j}} \right)^2$ and then

$$\begin{aligned}
\sum_{i<j} d_i^\alpha r_{ij} d_j^\alpha &= \frac{1}{2} \sum_{i=1}^{n} \sum_{j=1}^{n} d_i^\alpha r_{ij} d_j^\alpha = \frac{1}{2} \sum_{i=1}^{n} \sum_{j=1}^{n} \left[d_i^\alpha \sum_{k=1}^{n-1} \frac{1}{\mu_k} \left(\frac{z_{ki}}{\sqrt{d_i}} - \frac{z_{kj}}{\sqrt{d_j}} \right)^2 d_j^\alpha \right] \\
&= \frac{1}{2} \sum_{k=1}^{n-1} \frac{1}{\mu_k} \\
&\quad \times \sum_{i=1}^{n} \sum_{j=1}^{n} \left(d_i^{\alpha-1} z_{ki}^2 d_j^\alpha + d_i^\alpha z_{kj}^2 d_j^{\alpha-1} - 2 \cdot d_i^{\alpha-\frac{1}{2}} z_{ki} \cdot d_j^{\alpha-\frac{1}{2}} z_{kj} \right) \\
&= \frac{1}{2} \sum_{k=1}^{n-1} \frac{1}{\mu_k} \left[\sum_{j=1}^{n} d_j^\alpha \sum_{i=1}^{n} d_i^{\alpha-1} z_{ki}^2 + \sum_{i=1}^{n} d_i^\alpha \sum_{j=1}^{n} d_j^{\alpha-1} z_{kj}^2 \right. \\
&\qquad \left. -2 \left(\sum_{i=1}^{n} d_i^{\alpha-\frac{1}{2}} z_{ki} \right) \left(\sum_{j=1}^{n} d_j^{\alpha-\frac{1}{2}} z_{kj} \right) \right] \\
&= \sum_{k=1}^{n-1} \frac{1}{\mu_k} \left[\sum_{i=1}^{n} d_i^\alpha \sum_{j=1}^{n} d_j^{\alpha-1} z_{kj}^2 - \left(\sum_{i=1}^{n} d_i^{\alpha-\frac{1}{2}} z_{ki} \right)^2 \right] \\
&\leq \sum_{k=1}^{n-1} \frac{1}{\mu_k} \sum_{i=1}^{n} d_i^\alpha \sum_{j=1}^{n} d_j^{\alpha-1} z_{kj}^2 .
\end{aligned}$$

Note that $\sum_{i=1}^{n} z_{ki}^2 = 1$. Thus $\sum_{i<j} d_i^\alpha r_{ij} d_j^\alpha \leq \Delta^{\alpha-1} \sum_{k=1}^{n-1} \frac{1}{\mu_k} \sum_{i=1}^{n} d_i^\alpha \sum_{j=1}^{n} z_{kj}^2 = \Delta^{\alpha-1} \sum_{i=1}^{n} d_i^\alpha \sum_{k=1}^{n-1} \frac{1}{\mu_k}$ if $\alpha \geq 1$, and similarly, $\sum_{i<j} d_i^\alpha r_{ij} d_j^\alpha \leq$

$\delta^{\alpha-1}\sum_{k=1}^{n-1}\frac{1}{\mu_k}\sum_{i=1}^{n}d_i^{\alpha}\sum_{j=1}^{n}z_{kj}^2 = \delta^{\alpha-1}\sum_{i=1}^{n}d_i^{\alpha}\sum_{k=1}^{n-1}\frac{1}{\mu_k}$ if $\alpha < 1$. This proves (1). Suppose that equality holds in (1). Then $\sum_{i=1}^{n}d_i^{\alpha-\frac{1}{2}}z_{ki} = 0$ for $k = 1, 2, \ldots, n-1$, i.e., $\mathbf{Z}^T\left(d_1^{\alpha-\frac{1}{2}}, d_2^{\alpha-\frac{1}{2}}, \ldots, d_n^{\alpha-\frac{1}{2}}\right)^T = 0$. Since $\mathbf{Z}$ is an orthogonal matrix, then $\left(d_1^{\alpha-\frac{1}{2}}, d_2^{\alpha-\frac{1}{2}}, \ldots, d_n^{\alpha-\frac{1}{2}}\right)$ is a multiple of $z_n^T = \left(\frac{d_1^{1/2}}{(2m)^{1/2}}, \frac{d_2^{1/2}}{(2m)^{1/2}}, \ldots, \frac{d_n^{1/2}}{(2m)^{1/2}}\right)$, where m is the number of edges of G. Thus $d_1^{\alpha-1} = d_2^{\alpha-1} = \cdots = d_n^{\alpha-1}$, which is obviously equivalent to $\alpha = 1$or G is regular. Conversely, (1) is an equality if $\alpha = 1$or G is regular. □

Setting $\alpha = 0$ in Proposition 2, we have $\mathrm{Kf}(G) = \sum_{i<j} r_{ij} \leq \frac{n}{\delta}\sum_{k=1}^{n-1}\frac{1}{\mu_k}$ with equality if and only if G is regular. This may also be deduced by a connection between the ordinary Laplacian and normalized Laplacian eigenvalues, which, from the matrix theory point of view, seems to be known, however, we give a proof here. We need a result from [23]: $\rho_k = \min\limits_{\substack{\mathbf{x}\perp\mathbf{w}_{k+1},\ldots,\mathbf{w}_n\\ \mathbf{x}\neq\mathbf{0}}}\frac{\mathbf{x}^T\mathbf{M}\mathbf{x}}{\mathbf{x}^T\mathbf{x}}$ and $\rho_k = \max\limits_{\substack{\mathbf{x}\perp\mathbf{w}_1,\ldots,\mathbf{w}_{k-1}\\ \mathbf{x}\neq\mathbf{0}}}\frac{\mathbf{x}^T\mathbf{M}\mathbf{x}}{\mathbf{x}^T\mathbf{x}}$, where $\rho_1, \rho_2, \ldots, \rho_n$ are the eigenvalues of the $n \times n$ symmetric real matrix $\mathbf{M}$ arranged in non-increasing order, $\mathbf{w}_1, \mathbf{w}_2, \ldots, \mathbf{w}_n$ are the orthonormal eigenvectors of $\mathbf{M}$ corresponding to $\rho_1, \rho_2, \ldots, \rho_n$, respectively, $\mathbf{x}\perp\mathbf{w}$ means $\mathbf{x}^T\mathbf{w} = 0$ for vectors $\mathbf{x}$ and $\mathbf{w}$, and $\mathbf{x}$ may be any nonzero real vector if $k = 1$ in the second equation. Let $\mathrm{tr}(\mathbf{B})$ be the trace of the square matrix $\mathbf{B}$.

Lemma 3 *Let G be a connected (molecular) graph with $n \geq 2$ vertices, maximal vertex degree Δ and minimal vertex degree δ. Then for $k = 1, 2, \ldots, n-1$, we have $\frac{\lambda_k}{\Delta} \leq \mu_k \leq \frac{\lambda_k}{\delta}$ with left (right) equalities for all $k = 1, 2, \ldots, n-1$ if and only if G is regular.*

Proof Let $\mathbf{y}_1, \mathbf{y}_2, \ldots, \mathbf{y}_n$ be the orthonormal eigenvectors of $\mathbf{L}(G)$ corresponding to $\lambda_1, \lambda_2, \ldots, \lambda_n$, respectively. Obviously, $\mathbf{y}_1, \mathbf{y}_2, \ldots, \mathbf{y}_k, \mathbf{D}^{-1/2}\mathbf{z}_k, \mathbf{D}^{-1/2}\mathbf{z}_{k+1}, \ldots, \mathbf{D}^{-1/2}\mathbf{z}_n$ are linearly dependent and then there are real numbers $a_1, a_2, \ldots, a_k, b_k, b_{k+1}, \ldots, b_n$, not all zero, such that $\sum_{i=1}^{k}a_i\mathbf{y}_i + \sum_{j=k}^{n}\left(-b_j\right)\left(\mathbf{D}^{-1/2}\mathbf{z}_j\right) = \mathbf{0}$, and then $\tilde{\mathbf{x}} = \sum_{i=1}^{k}a_i\mathbf{y}_i = \mathbf{D}^{-1/2}\sum_{j=k}^{n}b_j\mathbf{z}_j \neq \mathbf{0}$, $\mathbf{D}^{1/2}\tilde{\mathbf{x}} \neq \mathbf{0}$, $\tilde{\mathbf{x}}\perp\mathbf{y}_{k+1}, \mathbf{y}_{k+2}, \ldots, \mathbf{y}_n$ and $\mathbf{D}^{1/2}\tilde{\mathbf{x}}\perp\mathbf{z}_1, \mathbf{z}_2, \ldots, \mathbf{z}_{k-1}$. Thus

$$\mu_k = \max_{\substack{\mathbf{x}\perp\mathbf{z}_1,\ldots,\mathbf{z}_{k-1}\\ \mathbf{x}\neq\mathbf{0}}}\frac{\mathbf{x}^T\mathbf{L}(G)\mathbf{x}}{\mathbf{x}^T\mathbf{x}} \geq \frac{\left(\mathbf{D}^{1/2}\tilde{\mathbf{x}}\right)^T\mathbf{L}(G)(\mathbf{D}^{1/2}\tilde{\mathbf{x}})}{\left(\mathbf{D}^{1/2}\tilde{\mathbf{x}}\right)^T(\mathbf{D}^{1/2}\tilde{\mathbf{x}})} = \frac{\tilde{\mathbf{x}}^T\left[\mathbf{D}^{1/2}\mathbf{L}(G)\mathbf{D}^{1/2}\right]\tilde{\mathbf{x}}}{\tilde{\mathbf{x}}^T\left(\mathbf{D}^{1/2}\mathbf{D}^{1/2}\right)\tilde{\mathbf{x}}}$$

$$= \frac{\tilde{\mathbf{x}}^T\mathbf{L}(G)\tilde{\mathbf{x}}}{\tilde{\mathbf{x}}^T\mathbf{D}\tilde{\mathbf{x}}} \geq \frac{\tilde{\mathbf{x}}^T\mathbf{L}(G)\tilde{\mathbf{x}}}{\Delta\tilde{\mathbf{x}}^T\tilde{\mathbf{x}}} \geq \frac{1}{\Delta}\min_{\substack{\mathbf{x}\perp\mathbf{y}_{k+1},\ldots,\mathbf{y}_n\\ \mathbf{x}\neq\mathbf{0}}}\frac{\mathbf{x}^T\mathbf{L}(G)\mathbf{x}}{\mathbf{x}^T\mathbf{x}} = \frac{\lambda_k}{\Delta}.$$

Similarly, since $\mathbf{y}_k, \mathbf{y}_{k+1}, \ldots, \mathbf{y}_n, \mathbf{D}^{-1/2}\mathbf{z}_1, \mathbf{D}^{-1/2}\mathbf{z}_2, \ldots, \mathbf{D}^{-1/2}\mathbf{z}_k$ are linearly dependent, there are real numbers $c_k, c_{k+1}, \ldots, c_n, l_1, l_2, \ldots, l_k$, not all zero, such that

$\hat{\mathbf{x}} = \sum_{i=k}^{n} c_i \mathbf{y}_i = \mathbf{D}^{-1/2} \sum_{j=1}^{k} l_j \mathbf{z}_j \neq \mathbf{0}$, $\mathbf{D}^{1/2}\hat{\mathbf{x}} \neq \mathbf{0}$, $\hat{\mathbf{x}} \perp \mathbf{y}_1, \mathbf{y}_2, \ldots, \mathbf{y}_{k-1}$, $\mathbf{D}^{1/2}\hat{\mathbf{x}} \perp \mathbf{z}_{k+1}, \mathbf{z}_{k+2}, \ldots, \mathbf{z}_n$, and then

$$\mu_k = \min_{\substack{\mathbf{x}\perp\mathbf{z}_{k+1},\ldots,\mathbf{z}_n \\ \mathbf{x}\neq\mathbf{0}}} \frac{\mathbf{x}^T \mathsf{L}(G)\mathbf{x}}{\mathbf{x}^T\mathbf{x}} \leq \frac{(\mathbf{D}^{1/2}\hat{\mathbf{x}})^T \mathsf{L}(G)(\mathbf{D}^{1/2}\hat{\mathbf{x}})}{(\mathbf{D}^{1/2}\hat{\mathbf{x}})^T(\mathbf{D}^{1/2}\hat{\mathbf{x}})}$$
$$= \frac{\hat{\mathbf{x}}^T \mathbf{L}(G)\hat{\mathbf{x}}}{\hat{\mathbf{x}}^T\mathbf{D}\hat{\mathbf{x}}} \leq \frac{\hat{\mathbf{x}}^T \mathbf{L}(G)\hat{\mathbf{x}}}{\delta\hat{\mathbf{x}}^T\hat{\mathbf{x}}} \leq \frac{1}{\delta} \max_{\substack{\mathbf{x}\perp\mathbf{y}_1,\ldots,\mathbf{y}_{k-1} \\ \mathbf{x}\neq\mathbf{0}}} \frac{\mathbf{x}^T \mathbf{L}(G)\mathbf{x}}{\mathbf{x}^T\mathbf{x}} = \frac{\lambda_k}{\delta}.$$

If G is regular then $\frac{\lambda_k}{\Delta} = \mu_k = \frac{\lambda_k}{\delta}$ for any k. Suppose that $\mu_k = \frac{\lambda_k}{\Delta}$ for all $k = 1, 2, \ldots, n-1$. Then for $\mathbf{Y} = (\mathbf{y}_1, \mathbf{y}_2, \ldots, \mathbf{y}_n)$,we have $\mathbf{Y}^T\mathbf{L}(G)\mathbf{Y} = \mathrm{diag}(\lambda_1, \lambda_2, \ldots, \lambda_n) = \Delta\mathrm{diag}(\mu_1, \mu_2, \ldots, \mu_n) = \Delta\mathbf{Z}^T\mathsf{L}(G)\mathbf{Z}$ and thus $\mathbf{L}(G) = \Delta\mathbf{Y}\mathbf{Z}^T\mathsf{L}(G)\mathbf{Z}\mathbf{Y}^T$, from which we have $\sum_{i=1}^{n} d_i = \mathrm{tr}\,(\mathbf{L}(G)) = \Delta\mathrm{tr}\left(\mathbf{Y}\mathbf{Z}^T\mathsf{L}(G)\mathbf{Z}\mathbf{Y}^T\right) = \Delta\mathrm{tr}\left(\mathsf{L}(G)\mathbf{Z}\mathbf{Y}^T\mathbf{Y}\mathbf{Z}^T\right) = \Delta \cdot \mathrm{tr}\,(\mathsf{L}(G)) = n\Delta$, implying that G is regular of degree Δ. Similarly, if $\mu_k = \frac{\lambda_k}{\delta}$ for all $k = 1, 2, \ldots, n-1$, then G is regular of degree δ. □

Proposition 4 *Let G be a connected (molecular) graph with $n \geq 2$ vertices, maximal vertex degree Δ and minimal vertex degree δ. Then*

$$\frac{n}{\Delta} \sum_{k=1}^{n-1} \frac{1}{\mu_k} \leq Kf(G) \leq \frac{n}{\delta} \sum_{k=1}^{n-1} \frac{1}{\mu_k} \tag{2}$$

with either equality if and only if G is regular.

Proof By Lemma 3, $\frac{1}{\Delta}\sum_{k=1}^{n-1}\frac{1}{\mu_k} \leq \sum_{k=1}^{n-1}\frac{1}{\lambda_k} \leq \frac{1}{\delta}\sum_{k=1}^{n-1}\frac{1}{\mu_k}$, with either equality if and only if G is regular. Thus (2) follows and either equality in (2) holds if and only if G is regular. □

Evidently, (2) may be written as $\frac{n}{2m\Delta}\mathrm{Kf}^*(G) \leq \mathrm{Kf}(G) \leq \frac{n}{2m\delta}\mathrm{Kf}^*(G)$, where m is the number of edges of G. Since $\frac{n}{2m\delta} \leq \left(\frac{n}{4m} + \frac{1}{2\delta}\right)^2$, we have the upper bound in [16]: $\mathrm{Kf}(G) \leq \left(\frac{n}{4m} + \frac{1}{2\delta}\right)^2 \mathrm{Kf}^*(G)$.

The diameter of a connected graph G, $\mathrm{diam}(G)$, is the maximum distance between any two vertices of G. For a connected graph G with $n \geq 2$ vertices, since $\mathsf{L}(G) = \mathbf{I} - \mathbf{D}^{-1/2}\mathbf{A}(G)\mathbf{D}^{-1/2}$, the number of distinct normalized Laplacian eigenvalues is equal to the number of distinct eigenvalues of the matrix $\mathbf{D}^{-1/2}\mathbf{A}(G)\mathbf{D}^{-1/2}$, which is at least diam(G) + 1 by straightforward modification of the adjacent argument (Theorem 3.13 in Ref. [24]). Let $K_{a,b}$ be the complete bipartite graph with two partite sets having a and b vertices, respectively.

Proposition 5 *Let G be a connected (molecular) bipartite graph with $n \geq 2$ vertices and m edges. Then*

$$Kf^*(G) \geq (2n-3)m \tag{3}$$

with equality if and only if $G = K_{r,n-r}$ for $1 \leq r \leq \left\lfloor \frac{n}{2} \right\rfloor$.

Proof It is true for $n = 2$. Suppose that $n \geq 3$. Since G is bipartite, we have $\mu_1 = 2$ (see p. 7, [21]). Recall that $\sum_{i=1}^{n-1} \mu_i = n$. By the Cauchy-Schwarz inequality,

$$\sum_{i=2}^{n-1} \frac{1}{\mu_i} \geq \frac{(n-2)^2}{\sum_{i=2}^{n-1} \mu_i} = \frac{(n-2)^2}{n-\mu_1} = n-2$$

and then

$$\mathrm{Kf}^*(G) = 2m\left(\frac{1}{\mu_1} + \sum_{i=2}^{n-1} \frac{1}{\mu_i}\right) \geq (2n-3)m$$

with equality if and only if $\mu_2 = \cdots = \mu_{n-1} = 1$. Thus equality holds in (3) if and only if $2 < \mathrm{diam(G)} + 1 \leq 3$, i.e., $\mathrm{diam(G)} = 2$. So the result follows. □

By Propositions 4 and 5, we have:

Proposition 6 *Let G be a connected (molecular) bipartite graph with $n \geq 2$ vertices and maximum vertex degree Δ. Then*

$$Kf(G) \geq \frac{n(2n-3)}{2\Delta}$$

with equality if and only if $G = K_{\frac{n}{2},\frac{n}{2}}$.

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