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Bounds for Resistance–Distance Spectral Radius

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Abstract

Lower and upper bounds as well as Nordhauss-Gaddum-type results for the resistance–distance spectral radius are obtained.

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1. Introduction and preliminaries

The resistance distance is a metric function on a graph, proposed by Klein and Randić [18]. The resistance distance R_{ij} between the vertices v_i and v_j of a connected graph G is defined to be equal to the resistance between the respective two nodes of an electrical network, corresponding to G, in which the resistance between any two adjacent nodes is 1 Ohm. It is known that the resistance distance satisfies the mathematical requirements for a distance ([2, 3, 17]).

It is known that the resistance distance can be expressed in terms of the eigenvalues and eigenvectors of the Laplacian matrix and normalized Laplacian matrix associated with the network; for details on this matter see [8, 14, 15, 21, 22, 23, 24]. We also refer to [4] for a new method for computing the resistance distances.

In [18] a molecular structure descriptor was introduced, equal to the sum of resistance distances of all pairs of vertices of a molecular graph:

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

Eventually, it has been named the "*Kirchhoff index*" ([6]).

The Kirchhoff index was much studied in mathematical chemistry. Details on its theory can be found in the recent papers [5, 9, 12, 25, 27, 28, 32] and the references cited therein.

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The Laplacian matrix of the graph G, denoted by $L = ||L_{ij}||$, 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 of the vertex v_i. Further, J is the square matrix of order n whose all elements are unity. Then for all connected graphs (with two or more vertices) the matrix $L + \dfrac{1}{n} J$ is non-singular, its inverse

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

does exist and, by [22], $R_{ij} = x_{ii} + x_{jj} - 2x_{ij}$. The resistance–distance matrix is an $n \times n$ matrix $\mathbf{R} = \mathbf{R}(G) = \|R_{ij}\|$. Note that the diagonal elements of $\mathbf{R}$ are equal to zero.

Since $\mathbf{R}$ is a real symmetric matrix, all its eigenvalues are real numbers. Let $\lambda_1(G)$ be the maximum eigenvalue (i.e., the *spectral radius*) of $\mathbf{R}$. Balaban et al. ([1]) proposed to use the maximum eigenvalues of distance–based matrices as structural descriptors in chemical researches. For more work along these line see [13, 16, 29, 31].

In this paper we present our results for the maximum eigenvalue of the resistance–distance matrix. We also provide some lower and upper bounds for $\lambda_1(G)$ for molecular graphs and a few Nordhaus–Gaddum–type results [20]. (Recall that in [20] the bounds have been obtained for the sum of chromatic numbers of a graph and its complement. Eventually, such Nordhaus–Gaddum–type results were elaborated also for other graph invariants.)

The following lemma is one of the key point in our considerations.

1.1. Lemma. [29, 30] Let $\mathbf{B} = (\mathbf{B}_{ij})$ be an $n \times n$ nonnegative, irreducible, symmetric matrix ($n \geq 2$) with row sums $B_1, B_2, \ldots, B_n$. If $\lambda_1(\mathbf{B})$ is the maximum eigenvalue of $\mathbf{B}$, then

$$\sqrt{\frac{\sum_{i=1}^n B_i^2}{n}} \leq \lambda_1(\mathbf{B}) \leq \max_{1 \leq j \leq n} \sum_{i=1}^n \mathbf{B}_{ij} \sqrt{\frac{B_j}{B_i}}$$

with equality holding if and only if $B_1 = B_2 = \cdots = B_n$ or if there is a permutation matrix $\mathbf{Q}$ such that

$$\mathbf{Q}^T \mathbf{B} \mathbf{Q} = \begin{pmatrix} \mathbf{0} & \mathbf{C} \\ \mathbf{C}^T & \mathbf{0} \end{pmatrix},$$

where all the row sums of $\mathbf{C}$ are equal.

2. Bounds for λ_1

2.1. Theorem. *Let G be a connected graph with $n \geq 2$ vertices. Then*

$$\sqrt{\frac{\sum_{i=1}^n R_i^2}{n}} \leq \lambda_1(G) \leq \max_{1 \leq j \leq n} \sum_{i=1}^n R_{ij} \sqrt{\frac{R_j}{R_i}} \tag{2.1}$$

where R_i is the sum of i-th row of the matrix $\mathbf{R}$. Moreover equality holds in (2.1) *if and only if $R_1 = R_2 = \cdots = R_n$.*

Proof. It is clear that the matrix $\mathbf{R}$ is irreducible for $n \geq 2$, and then, by Lemma 1.1, we obtain the inequality in (2.1). By definition, we know that $R_{ij} \neq 0$ for $i \neq j$ and $R_{ij} = 0$ otherwise. We note that for $n \geq 3$, there is no permutation matrix $\mathbf{Q}$ such that

$$\mathbf{Q}^T \mathbf{R}\, \mathbf{Q} = \begin{pmatrix} \mathbf{0} & \mathbf{C} \\ \mathbf{C}^T & \mathbf{0} \end{pmatrix}$$

where all the row sums of $\mathbf{C}$ are equal. By Lemma 1.1, the equality in (2.1) holds if and only if $R_1 = R_2 = \cdots = R_n$. □

2.2. Corollary. *Let G be a connected graph with $n \geq 2$ vertices. Then*

$$\lambda_1(G) \geq \frac{2\,Kf}{n} \tag{2.2}$$

with equality holding if and only if $R_1 = R_2 = \cdots = R_n$ or $G \cong K_n$.

Proof. By the left part of the inequality given in (2.1) and in view of the Cauchy–Schwarz inequality, we obtain

$$\lambda_1(G) \geq \sqrt{\frac{\sum_{i=1}^n R_i^2}{n}} \geq \frac{\sum_{i=1}^n R_i}{n} = \frac{2\,Kf}{n}$$

and equality holds if and only if $R_1 = R_2 = \cdots = R_n$ or $G \cong K_n$. □

Note that $trace[\mathbf{R}] = 0$ and denote by $S = S(G)$ the trace of $\mathbf{R}^2$. Therefore, the eigenvalues $\lambda_i(G)$, $i = 1, 2, \ldots, n$, of $\mathbf{R}$ satisfy the relations

$$\sum_{i=1}^{n} \lambda_i(G) = 0 \tag{2.3}$$

and

$$\sum_{i=1}^{n} \lambda_i^2(G) = S(G) . \tag{2.4}$$

It can be shown that $S(G)$ is maximum for $G \cong P_n$ (where P_n is the n-vertex path), and $S(G)$ is minimum for $G \cong K_n$.

We first recall the long–time known fact ([19, 26]) that if G is a connected graph and G' is the graph obtained from G by adding to it a new edge, then $Kf(G) > Kf(G')$. This result is, of course, equivalent to the claim that if G is a connected graph and e is its edge, and if $G - e$ is also connected, then $Kf(G) < Kf(G - e)$.

From this result it immediately follows that among connected n-vertex graphs, the complete graph has minimum Kirchhoff index.

It also follows that the (connected) graph with maximum Kirchhoff index must be a tree. Because in the case of trees, the Kirchhoff and Wiener indices coincide, and because we know that among n-vertex trees, the path is the tree with maximum Wiener index ([11, 10]), it follows that the path is also the n-vertex connected graph with maximum Kirchhoff index.

Let $\mathcal{G}$ be the class of connected graphs whose resistance–distance matrices have exactly one positive eigenvalue. In the following, we give upper and lower bounds for $\lambda_1(G)$ of graphs in the class $\mathcal{G}$ in terms of number of vertices and $S(G)$. Before that we state a lemma that will be needed for determining the equality cases in the bounds given in the following.

2.3. Lemma. [7] Let $\mathbf{B}$ be a nonnegative, irreducible, symmetric matrix with exactly two distinct eigenvalues. Then $\mathbf{B} = uu^T + r\,\mathbf{I}$ for some positive column vector u and some r.

2.4. Theorem. *Let $G \in \mathcal{G}$ with $n \geq 2$ vertices. Then*

$$\lambda_1(G) \leq \sqrt{\frac{n-1}{n}\,S(G)} \tag{2.5}$$

with equality holding if and only if $G \cong K_n$.

Proof. By (2.3), we have $\lambda_1(G) = -\sum_{i=2}^{n} \lambda_i(G)$. Further, by the Cauchy–Schwarz inequality and using (2.4),

$$\lambda_1^2(G) = \left[\sum_{i=2}^{n} \lambda_i(G)\right]^2 \leq (n-1)\sum_{i=2}^{n} n\,\lambda_i^2(G)$$

$$= (n-1)\left[S(G) - \lambda_1^2(G)\right]$$

with equality if and only if $\lambda_2(G) = \cdots = \lambda_n(G)$. We thus have

$$n\,\lambda_1^2(G) \leq (n-1)\,S(G)$$

as required in (2.5).

Suppose now that equality holds in (2.5). Then $\lambda_2(G) = \cdots = \lambda_n(G)$, and so the matrix $\mathbf{R}$ has exactly two distinct eigenvalues. Now we prove that the diameter of G is one, i. e., G does not contain an induced shortest path P_m, $m \geq 3$.

Assume that G contains an induced shortest path P_m, $m \geq 3$. Let $\mathbf{M}$ be the principal submatrix of $\mathbf{R}$ indexed by the vertices in P_m. For an arbitrary matrix $\mathbf{A}$, let $\theta_i(\mathbf{A})$ denote its i-th eigenvalue. Then, by the interlacing theorem,

$$\theta_i(\mathbf{R}) \geq \theta_i(\mathbf{M}) \geq \theta_{n-m+i}(\mathbf{R}), \qquad i = 1, 2, \ldots, m$$

or, in other words,

$$\theta_2(\mathbf{R}) \geq \theta_2(\mathbf{M}) \geq \theta_3(\mathbf{M}) \geq \cdots \geq \theta_m(\mathbf{M}) \geq \theta_n(\mathbf{R})\,.$$

This then shows that P_m has at most two distinct $\mathbf{R}$-eigenvalues for $m \geq 3$, which is impossible. Therefore G does not contain any two vertices at distance two or more, and hence it is complete. The other way around is quite obvious, i.e., if $G \cong K_n$, then the equality holds in (2.5). □

2.5. Remark. By considering Lemma *2.3*, the equality part of *(2.5)* in Theorem *2.4* can be obtained quite similarly as in the proof of Theorem 3 of the paper [31].

The next result provides a lower bound for $\lambda_1(G)$ in terms of $S(G)$. Recall that $\mathcal{G}$ is the class of connected graphs whose resistance–distance matrices have exactly one positive eigenvalue.

2.6. Theorem. *Let $G \in \mathcal{G}$ with $n \geq 2$. Then*

$$\lambda_1(G) \geq \sqrt{\frac{S(G)}{2}}\,. \tag{2.6}$$

Equality holds in (2.6) *if and only if $G \cong K_2$.*

Proof. We first note that $\lambda_1(G) > 0$ and $\lambda_2(G) \leq 0$. Then by (2.3),

$$2\,\lambda_1(G) = \sum_{i=1}^{n} |\lambda_i(G)|\,.$$

From (2.3) and (2.4) we also have

$$\sum_{1\le i<j\le n} |\lambda_i(G)\,\lambda_j(G)| \ge \left|\sum_{1\le i<j\le n} \lambda_i(G)\,\lambda_j(G)\right| = \frac{S(G)}{2}$$

and so

$$\begin{aligned} 4\,\lambda_1^2(G) &= \left[\sum_{i=2}^{n} |\lambda_i(G)|\right]^2 \\ &= \sum_{i=1}^{n} \lambda_i^2(G) + 2\sum_{i<j} |\lambda_i(G)\,\lambda_j(G)| \ge 2\,S(G) \end{aligned}$$

from which (2.6) follows.

If we take $n = 2$, then (2.6) is actually an equality. For the case $n \ge 3$, in order to see that (2.6) is not an equality, the same approach can be applied as in [31, Theorem 4]. Hence the result. □

3. Nordhaus-Gaddum-type bounds for λ_1

In this section we consider general graphs, not only those from the class $\mathcal{G}$. We establish some more bounds involving the Kirchhoff index Kf as well as Nordhaus–Gaddum–type bounds for $\lambda_1(G)$.

Before that, consider some fundamental structural parameters of a connected (molecular) graph G and its complement $\overline{G}$. Let G be a connected (molecular) graph on $n > 2$ vertices, m edges, maximum degree Δ, second maximum degree Δ_2, minimum degree δ, and second minimum degree δ_2. Further, assume that G has a connected complement $\overline{G}$ with $\overline{m}$ edges and related parameters $\overline{\Delta}$, $\overline{\Delta_2}$, $\overline{\delta}$, and $\overline{\delta_2}$. As one can easily prove, the following equalities exist between these parameters:

$$\left.\begin{aligned} 2(m+\overline{m}) &= n(n-1) \\ \Delta &= n-1-\overline{\delta} \\ \delta &= n-1-\overline{\Delta} \\ \Delta_2 &= n-1-\overline{\delta_2} \\ \delta_2 &= n-1-\overline{\Delta_2} \end{aligned}\right\} . \tag{3.1}$$

The following two lemmas have been recently proven in [9]. We nevertheless state them here (without proof), since these are used for obtaining lower bounds for $\lambda_1(G)$ involving Kf (cf. Theorem 3.3 below).

3.1. Lemma. [9] Let G be a connected graph on $n > 2$ vertices and m edges with parameters Δ, Δ_2, and δ as defined in (3.1). Then

$$Kf(G) \ge \frac{n}{\Delta+1} + \frac{n}{2m-\Delta-1}\left[(n-2)^2 + \frac{(\Delta_2-\delta)^2}{\Delta_2\,\delta}\right] \tag{3.2}$$

with equality holding if and only if $G \cong K_{1,n-1}$ or $G \cong K_n$.

3.2. Lemma. [9] Let G be a connected graph (not equal to K_n) on $n > 2$ vertices and m edges with parameters Δ, Δ_2 and δ as given in (3.1). Then

$$Kf(G) \ge 1 + \frac{n}{\delta} + \frac{n(n-3)^2}{2m-\Delta-\delta-1} \tag{3.3}$$

with equality holding if and only if $G \cong K_{1,n-1}$.

After that we have the following lower bounds for $\lambda_1(G)$. Their proofs are immediate, by considering inequalities in (2.2), (3.2), and (3.3).

3.3. Theorem. *Let G be a connected graph on $n > 2$ vertices and m edges with parameters Δ, Δ_2 and δ as given in* (3.1). *Then*

$$\lambda_1(G) \geq 2\left\{\frac{1}{\Delta+1} + \frac{1}{2m-\Delta-1}\left[(n-2)^2 + \frac{(\Delta_2-\delta)^2}{\Delta_2\,\delta}\right]\right\} \tag{3.4}$$

and

$$\lambda_1(G) \geq 2\left\{\frac{1}{n} + \frac{n}{\delta} + \frac{n(n-3)^2}{2m-\Delta-\delta-1}\right\}\,. \tag{3.5}$$

Our next three theorems deal with Nordhaus-Gaddum type results for $\lambda_1(G)$.

3.4. Theorem. *Let G be a connected graph on $n > 2$ vertices and m edges, such that its complement $\overline{G}$ is also connected. Then with the parameters given in* (3.1),

$$\begin{aligned} \lambda_1(G) + \lambda_1(\overline{G}) \quad &\geq \quad 2\left\{\frac{1}{\Delta+1} + \frac{1}{n-\delta} + (n-2)^2\left[\frac{1}{2m-\Delta-1} + \right.\right. \\ &+ \quad \left.\frac{1}{n(n-2)-2m+1+\delta}\right] + \left(\frac{1}{2m-\Delta-1}\right)\left(\frac{(\Delta_2-\delta)^2}{\Delta_2\,\delta}\right) + \\ &+ \quad \left.\left(\frac{1}{n(n-2)-2m+1+\delta}\right)\left(\frac{(\Delta-\delta_2)^2}{(n-1-\delta_2)(n-1-\Delta)}\right)\right\} \end{aligned} \tag{3.6}$$

with equality holding if and only if $G \cong K_n$.

Proof. Using the inequality (3.4) from Theorem 3.3, we arrive at

$$\begin{aligned} \lambda_1(G) + \lambda_1(\overline{G}) &\geq 2\left\{\frac{1}{\Delta+1} + \frac{1}{2m-\Delta-1}\left[(n-2)^2 + \frac{(\Delta_2-\delta)^2}{\Delta_2\,\delta}\right]\right\} \\ &+ 2\left\{\frac{1}{\overline{\Delta}+1} + \frac{1}{2\overline{m}-\overline{\Delta}-1}\left[(n-2)^2 + \frac{(\overline{\Delta_2}-\overline{\delta})^2}{\overline{\Delta_2}\,\overline{\delta}}\right]\right\} \\ &= 2\left\{\frac{1}{\Delta+1} + \frac{1}{2m-\Delta-1}\left[(n-2)^2 + \frac{(\Delta_2-\delta)^2}{\Delta_2\,\delta}\right]\right\} \\ &+ 2\left\{\frac{1}{n-\delta} + \frac{1}{n(n-2)-2m+1+\delta}\left[(n-2)^2 + \frac{(\Delta-\delta_2)^2}{(n-1-\delta_2)(n-1-\Delta)}\right]\right\} \end{aligned}$$

and, by rearranging the terms in this final inequality, we obtain (3.6).

By using Corollary 2.2 and Lemma 3.1, one can easily see that the equality in (3.6) holds if and only if $G \cong K_n$. Hence the result. $\square$

3.5. Theorem. *Let G be a connected graph on $n > 2$ vertices and m edges, such that its complement $\overline{G}$ is also connected. Then with the parameters given in* (3.1),

$$\begin{aligned} \lambda_1(G) + \lambda_1(\overline{G}) \geq \frac{4}{n} + 2\left\{\left(\frac{1}{\delta} + \frac{1}{(n-1-\Delta)}\right)\right. \\ \left. + (n-3)^2\left[\frac{1}{2m-\Delta-\delta-1} + \frac{1}{n(n-3)-2m+1+\Delta+\delta}\right]\right\}\,. \end{aligned}$$

Proof. Using the inequality (3.5) from Theorem 3.3 and applying similar arguments as in the proof of Theorem 3.4, we get the result. □

In view of the equality $S(\overline{G}) = n^3 + S(G)$ and by using Theorem 2.4, we arrive at the following result, which we present without proof.

3.6. Theorem. *Let $G \in \mathcal{G}$ with $n > 2$ vertices, and let $\overline{G}$ be connected. Then,*

$$\lambda_1(G) + \lambda_1(\overline{G}) \leq \sqrt{\frac{n-1}{n}} \left[\sqrt{S(G)} + \sqrt{n^3 + S(G)} \right]$$

with equality holding if and only if $G \cong K_n$.

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