Communications in Combinatorics and Optimization
Vol. 8, No. 1 (2023), pp. 243-251
DOI: 10.22049/CCO.2022.27492.1275

CCO
Commun. Comb. Optim.

Research Article

Improved bounds for Kirchhoff index of graphs

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Received: 1 November 2021; Accepted: 12 January 2022
Published Online: 15 January 2022

Abstract: Let G be a simple connected graph with n vertices. The Kirchhoff index of G is defined as $Kf(G) = n\sum_{i=1}^{n-1}\frac{1}{\mu_i}$, where $\mu_1 \geq \mu_2 \geq \cdots \geq \mu_{n-1} > \mu_n = 0$ are the Laplacian eigenvalues of G. Some bounds on $Kf(G)$ in terms of graph parameters such as the number of vertices, the number of edges, first Zagreb index, forgotten topological index, etc., are presented. These bounds improve some previously known bounds in the literature.

Keywords: Laplacian eigenvalues (of graph), topological indices, Kirchhoff index.

AMS Subject classification: 05C12, 05C50

1. Introduction

Let $G = (V, E)$, $V = \{v_1, v_2, \ldots, v_n\}$, be a simple connected graph with n vertices and m edges. The degree of the vertex v_i of G will be denoted by d_i, where $i = 1, 2, \ldots, n$. Denote by $A(G)$ and $D(G)$ the adjacency matrix and the diagonal degree matrix of G, respectively. The matrix $L(G) = D(G) - A(G)$ is the Laplacian matrix of G with the eigenvalues $\mu_1 \geq \mu_2 \geq \cdots \geq \mu_{n-1} > \mu_n = 0$ [7]. The eigenvalues of $L(G)$ represent the Laplacian eigenvalues of G. Some well known properties for Laplacian eigenvalues are [12, 30]

$$\sum_{i=1}^{n-1}\mu_i = \sum_{i=1}^{n} d_i = 2m, \quad \sum_{i=1}^{n-1}\mu_i^2 = \sum_{i=1}^{n} d_i^2 + \sum_{i=1}^{n} d_i = M_1(G) + 2m, \tag{1}$$

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and

$$\sum_{i=1}^{n-1} \mu_i^3 = \sum_{i=1}^{n} d_i^3 + 3\sum_{i=1}^{n} d_i^2 - 6T = F(G) + 3M_1(G) - 6T \tag{2}$$

where $M_1(G)$ is the first Zagreb index [9], $F(G)$ is the forgotten topological index [6] and T is the number of triangles of G. Also, by the matrix-tree theorem from [19]

$$\prod_{i=1}^{n-1} \mu_i = nt$$

where t is the number of spanning trees of G.
The Kirchhoff index of a connected graph G was defined as [10]

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

where r_{ij} is the effective resistance distance between the vertices v_i and v_j of G. Independently, in [8] and [28], it was shown that the Kirchhoff index can be also expressed in terms of Laplacian eigenvalues as:

$$Kf(G) = n\sum_{i=1}^{n-1} \frac{1}{\mu_i}. \tag{3}$$

After this, the Kirchhoff index has attracted great attention in spectral/chemical graph theory. For more details, see [1, 4, 5, 13–17, 20, 21, 25–27, 29].
In this paper, we obtain some bounds on Kirchhoff index in terms of graph parameters such as the number of vertices, the number of edges, first Zagreb index, forgotten topological index, etc. Our bounds improve some results obtained in [4, 14].

2. Lemmas

In this section, we recall some known results over spectral graph theory and analytical inequalities that will be needed in the subsequent section.

Lemma 1. *[11] Let G be a connected graph of order n. Then, $\mu_1 \leq n$ with equality holding if and only if G^c is disconnected, where G^c is the complement of G.*

Lemma 2. *[3] Let G be a connected graph with n vertices. Then $\mu_1 = \mu_2 = \cdots = \mu_{n-1}$ if and only if $G \cong K_n$.*

Lemma 3. *[3] Let G be a connected graph of order n. Then $\mu_2 = \mu_3 = \cdots = \mu_{n-1}$ if and only if $G \cong K_n$ or $G \cong K_{1,n-1}$ or $G \cong K_{\frac{n}{2},\frac{n}{2}}$.*

Lemma 4. *[18, 22] Let $p_1, p_2, \ldots, p_n$ be non-negative real numbers such that $\sum_{i=1}^{n} p_i = 1$. Further, let $a_1, a_2, \ldots, a_n$ be real numbers for which there exist real constants r and R so that for each i,$i = 1, 2, \ldots, n$, the inequalities $0 < r \le a_i \le R < +\infty$ hold. Then*

$$\sum_{i=1}^{n} p_i a_i + rR \sum_{i=1}^{n} \frac{p_i}{a_i} \le r + R.$$

The equality holds if and only if $a_1 = a_2 = \cdots = a_k = R$ and $a_{k+1} = a_{k+2} = \cdots = a_n = r$ for some k, $1 \le k \le n$.

Let $x_1, x_2, \ldots, x_r$ be positive real numbers. Denote by S_k the average of all products of k of the x_i's, i.e.,

$$\begin{aligned} S_1 &= \frac{x_{1+}x_2 + \ldots + x_r}{r} \\ S_2 &= \frac{x_1x_2 + x_1x_3 + \cdots + x_1x_r + x_2x_3 + \cdots + x_{r-1}x_r}{\frac{1}{2}r\left(r-1\right)} \\ &\vdots \\ S_{r-1} &= \frac{x_1x_2 \ldots x_{r-1} + x_1x_2 \ldots x_{r-2}x_r + \cdots + x_2x_3 \ldots x_{r-1}x_r}{r} \\ S_r &= x_1x_2 \ldots x_r. \end{aligned}$$

Notice that S_1 is the arithmetic mean and $S_r^{1/r}$ is the geometric mean of the positive real numbers $x_1, x_2, \ldots, x_r$ [4].

Lemma 5. *(Maclaurin's symmetric mean inequality)[2] For positive real numbers $x_1, x_2, \ldots, x_r$,*

$$S_1 \ge S_2^{1/2} \ge S_3^{1/3} \ge \cdots \ge S_r^{1/r}.$$

The equality holds if and only if $x_1 = x_2 = \cdots = x_r$.

Lemma 6. *(Newton's inequality) [24] Let $x_1, x_2, \ldots, x_r$ be positive real numbers and let S_k, $k = 1, 2, \ldots, r$, be given as in Lemma 5. Then*

$$S_{k-1}S_{k+1} \le S_k^2$$

where $k = 1, 2, \ldots, r-1$ and $S_0 = 1$. Moreover, the equality holds if and only if $x_1 = \cdots = x_r$.

Lemma 5 is corollary of Lemma 6.

3. Main Results

Theorem 1. *Let G be a connected graph with $n \geq 3$ vertices. Then for any real α such that $\mu_1 \leq \alpha \leq n$,*

$$Kf(G) \leq \frac{n}{\alpha} + n\frac{(\mu_2 + \mu_{n-1})(n-2) - (2m - \alpha)}{\mu_2 \mu_{n-1}}. \tag{4}$$

If $\alpha = n$, the equality holds if and only if $G \cong K_n$ or $G \cong K_{1,n-1}$.

Proof. Taking $p_i = \frac{1}{n-2}$, $a_i = \mu_i$ for $i = 2, 3, \ldots, n-1$, $R = \mu_2$ and $r = \mu_{n-1}$ in Lemma 4 and considering Eq. (1), we obtain

$$\sum_{i=1}^{n-1} \frac{1}{\mu_i} \leq \frac{1}{\mu_1} + \frac{(\mu_2 + \mu_{n-1})(n-2)}{\mu_2 \mu_{n-1}} - \frac{2m - \mu_1}{\mu_2 \mu_{n-1}}, \tag{5}$$

(see, [14, Theorem 3.7]).
Let us consider the function $f(x)$ defined as

$$f(x) = \frac{1}{x} - \frac{2m - x}{\mu_2 \mu_{n-1}}.$$

It is easy to see that f is increasing with respect to the x. Then for any real α, $\mu_1 \leq \alpha \leq n$,

$$f(\mu_1) \leq f(\alpha) = \frac{1}{\alpha} - \frac{2m - \alpha}{\mu_2 \mu_{n-1}}.$$

From the above and Eqs. (3) and (5), we obtain that

$$Kf(G) \leq \frac{n}{\alpha} + n\frac{(\mu_2 + \mu_{n-1})(n-2) - (2m - \alpha)}{\mu_2 \mu_{n-1}}.$$

Hence the upper bound (4) holds. The equality in (4) holds if and only if

$$\mu_1 = \alpha \text{ and } \mu_2 = \mu_3 = \cdots = \mu_{n-1}.$$

If $\alpha = n$, by Lemmas 1 and 3, one can readily see that the equality in (4) holds if and only if $G \cong K_n$ or $G \cong K_{1,n-1}$. □

By Theorem 1 and Lemma 1, we have the following upper bound on $Kf(G)$.

Corollary 1. *Let G be a connected graph with $n \geq 3$ vertices. Then*

$$Kf(G) \leq 1 + n\frac{(\mu_2 + \mu_{n-1})(n-2) - (2m - n)}{\mu_2 \mu_{n-1}}. \tag{6}$$

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

Remark 1. Since $\Delta \le n-1$, we have

$$\begin{aligned} Kf\left(G\right) &\le 1+n\frac{\left(\mu_2+\mu_{n-1}\right)\left(n-2\right)-\left(2m-n\right)}{\mu_2\mu_{n-1}} \\ &\le \frac{n}{1+\Delta}+n\frac{\left(\mu_2+\mu_{n-1}\right)\left(n-2\right)-\left(2m-n\right)}{\mu_2\mu_{n-1}}. \end{aligned}$$

This implies that the upper bound (6) is stronger than upper bound in [14, Theorem 3.7].

Remark 2. In [14], it was pointed out that the upper bound in [14, Theorem 3.7] is stronger than the upper bound in [14, Corollary 3.4]. Therefore, by Remark 1, the upper bound (6) is also stronger than the upper bound in [14, Corollary 3.4].

Remark 3. For a graph G of order n, in [23] Rojo et al. obtained the following nontrivial upper bound for the largest Laplacian eigenvalue

$$\mu_1 \le \max\left\{d_i+d_j-\left|N_i\cap N_j\right| : 1\le i<j\le n\right\}$$

where $\left|N_i\cap N_j\right|$ is the number of common neighbours of the vertices v_i and v_j of G. We should note that it is possible to improve the upper bound (6) applying $\alpha = \max\left\{d_i+d_j-\left|N_i\cap N_j\right| : 1\le i\le j\le n\right\}$ in Theorem 1.

Theorem 2. *Let G be a connected graph with n vertices, m edges and the number of spanning trees t. Then*

$$Kf\left(G\right) \le \frac{\left(n-1\right)}{t}\left[\frac{2F\left(G\right)-6\left(m-1\right)M_1\left(G\right)+4m^2\left(2m-3\right)-12T}{\left(n-1\right)\left(n-2\right)\left(n-3\right)}\right]^{(n-2)/3}. \qquad (7)$$

The equality holds if and only if $G\cong K_n$.

Proof. Substituting $r=n-1$ and $x_i=\mu_i$, $i=1,2,\ldots,n-1$ in Lemma 5, we have

$$S_3^{1/3} \ge S_{n-2}^{1/(n-2)}.$$

Observe that

$$\begin{aligned} S_3 &= \frac{6\sum\limits_{i<j<k}\mu_i\mu_j\mu_k}{\left(n-1\right)\left(n-2\right)\left(n-3\right)} \\ &= \frac{2\sum_{i=1}^{n-1}\mu_i^3+\left(\sum_{i=1}^{n-1}\mu_i\right)^3-3\sum_{i=1}^{n-1}\mu_i\sum_{i=1}^{n-1}\mu_i^2}{\left(n-1\right)\left(n-2\right)\left(n-3\right)} \\ &= \frac{2\left(F\left(G\right)+3M_1\left(G\right)-6T\right)+8m^3-6m\left(M_1\left(G\right)+2m\right)}{\left(n-1\right)\left(n-2\right)\left(n-3\right)}, \text{ by Eqs. (1) and (2)} \\ &= \frac{2F\left(G\right)-6\left(m-1\right)M_1\left(G\right)+4m^2\left(2m-3\right)-12T}{\left(n-1\right)\left(n-2\right)\left(n-3\right)}. \end{aligned}$$

In [4, Theorem 1], it was obtained that

$$S_{n-2}=\frac{\prod_{i=1}^{n-1}\mu_i}{n-1}.\sum_{i=1}^{n-1}\frac{1}{\mu_i}=\frac{nt}{n-1}.\frac{Kf\left(G\right)}{n}=\frac{t}{n-1}Kf\left(G\right).$$

Then, from the above results we arrive at

$$\frac{t}{\left(n-1\right)}Kf\left(G\right)\leq\left[\frac{2F\left(G\right)-6\left(m-1\right)M_1\left(G\right)+4m^2\left(2m-3\right)-12T}{\left(n-1\right)\left(n-2\right)\left(n-3\right)}\right]^{(n-2)/3},$$

wherefrom the upper bound (7) follows. According to Lemma 5, the equality holds in (7) if and only if

$$\mu_1=\mu_2=\cdots=\mu_{n-1}.$$

Then, by Lemma 2, we conclude that $G\cong K_n$. □

Remark 4. For a connected graph G with n vertices and m edges, in [4, Theorem 1], it was proven that

$$Kf\left(G\right)\leq\frac{\left(n-1\right)}{t}\left[\frac{4m^2-M_1\left(G\right)-2m}{\left(n-1\right)\left(n-2\right)}\right]^{(n-2)/2},\tag{8}$$

with equality holding if and only if $G\cong K_n$. Since $S_2^{1/2}\geq S_3^{1/3}$, the upper bound (7) is stronger than the upper bound (8).

Theorem 3. *Let G be a connected graph with n vertices and m edges. Then*

$$Kf\left(G\right)\geq\frac{n\left(n-1\right)\left(n-3\right)\left(4m^2-M_1\left(G\right)-2m\right)}{2F\left(G\right)-6\left(m-1\right)M_1\left(G\right)+4m^2\left(2m-3\right)-12T}.\tag{9}$$

The equality holds if and only if $G\cong K_n$.

Proof. From Newton's inequality given in Lemma 6, it was observed that [4]

$$\frac{S_1}{S_2}\leq\frac{S_2}{S_3}\leq\cdots\leq\frac{S_{r-1}}{S_r}.$$

By the above result, we have

$$S_2S_r\leq S_{r-1}S_3,\ r\geq3.\tag{10}$$

Let us take $r=n-1$ and $x_i=\mu_i,\ \ i=1,2,\ldots,n-1$ in Eq. (10). In [4, Theorem 3] it was obtained that

$$S_2=\frac{4m^2-M_1\left(G\right)-2m}{\left(n-1\right)\left(n-2\right)}$$

$$S_{n-2} = \frac{t}{n-1} Kf(G)$$

and

$$S_{n-1} = \prod_{i=1}^{n-1} \mu_i = nt.$$

Recall from Theorem 2 that

$$S_3 = \frac{2F(G) - 6(m-1) M_1(G) + 4m^2(2m-3) - 12T}{(n-1)(n-2)(n-3)}.$$

Considering these results with Eq. (10), we get that

$$\frac{4m^2 - M_1(G) - 2m}{(n-1)(n-2)} nt \leq \frac{2F(G) - 6(m-1) M_1(G) + 4m^2(2m-3) - 12T}{(n-1)(n-2)(n-3)} \frac{t}{n-1} Kf(G)$$

i.e.,

$$Kf(G) \geq \frac{n(n-1)(n-3)\left(4m^2 - M_1(G) - 2m\right)}{2F(G) - 6(m-1) M_1(G) + 4m^2(2m-3) - 12T}$$

which is the lower bound (9). From Lemma 6, the equality holds in (9) if and only if

$$\mu_1 = \mu_2 = \cdots = \mu_{n-1}.$$

Thus, in view of Lemma 2, we get that $G \cong K_n$. □

Remark 5. For a connected graph G with n vertices and m edges, in [4, Theorem 3], Das established the following lower bound for Kirchhoff index

$$Kf(G) \geq \frac{2mn(n-1)(n-2)}{4m^2 - M_1(G) - 2m} \tag{11}$$

where the equality holds if and only if $G \cong K_n$. Since $\frac{S_1}{S_2} \leq \frac{S_2}{S_3}$, it is easy to conclude that the lower bound (9) is stronger than the lower bound (11).

References

[1] M. Bianchi, A. Cornaro, J.L. Palacios, and A. Torriero, *Bounds for the Kirchhoff index via majorization techniques*, J. Math. Chem. **51** (2013), no. 2, 569–587.

[2] P. Biler and A. Witkowski, *Problems in Mathematical Analysis*, CRC Press, New York, 2017.

[3] K.C. Das, *A sharp upper bound for the number of spanning trees of a graph*, Graphs Combin. **23** (2007), no. 6, 625–632.

[4] ______, *On the Kirchhoff index of graphs*, Z. Naturforschung **68a** (2013), no. 8-9, 531–538.

[5] K.C. Das and K. Xu, *On relation between Kirchhoff index, Laplacian-energy-like invariant and Laplacian energy of graphs*, Bull. Malays. Math. Sci. Soc. **39** (2016), no. 1, 59–75.

[6] B. Furtula and I. Gutman, *A forgotten topological index*, J. Math. Chem. **53** (2015), no. 4, 1184–1190.

[7] R. Grone and R. Merris, *The Laplacian spectrum of a graph ii*, SIAM J. Discrete Math. **7** (1994), no. 2, 221–229.

[8] I. Gutman and B. Mohar, *The quasi-Wiener and the Kirchhoff indices coincide*, J. Chem. Inf. Comput. Sci. **36** (1996), no. 5, 982–985.

[9] I. Gutman and N. Trinajstić, *Graph theory and molecular orbitals. Total φ-electron energy of alternant hydrocarbons*, Chem. Phys. Lett. **17** (1972), no. 4, 535–538.

[10] D.J. Klein and M. Randić, *Resistance distance*, J. Math. Chem. **12** (1993), no. 1, 81–95.

[11] J. Li, W.C. Shiu, and W.H. Chan, *The Laplacian spectral radius of some graphs*, Linear Algebra Appl. **431** (2009), no. 1-2, 99–103.

[12] R. Merris, *Laplacian matrices of graphs: A survey*, Linear Algebra Appl. **197& 198** (1994), 143–176.

[13] I. Milovanović, E. Glogic, M. Matejić, and E. Milovanović, *On relation between the Kirchhoff index and number of spanning trees of graph*, Commun. Comb. Optim. **5** (2020), no. 1, 1–8.

[14] I. Milovanović, I. Gutman, and E. Milovanović, *On Kirchhoff and degree Kirchhoff indices*, Filomat **29** (2015), no. 8, 1869–1877.

[15] I. Milovanović and E. Milovanović, *Bounds of Kirchhoff and degree Kirchhoff indices*, Bounds in Chemical Graph Theory – Mainstreams (I. Gutman, B. Furtula, K.C. Das, E. Milovanović, and I. Milovanović, eds.), Univ. Kragujevac, Kragujevac, 2017, pp. 93–119.

[16] ______, *On some lower bounds of the Kirchhoff index*, MATCH Commun. Math. Comput. Chem. **78** (2017), 169–180.

[17] I. Milovanović, E. Milovanović, E. Glogić, and M. Matejić, *On Kirchhoff index, Laplacian energy and their relations*, MATCH Commun. Math. Comput. Chem. **81** (2019), no. 2, 405–418.

[18] D.S. Mitrinović and P.M. Vasić, *Analytic inequalities*, Springer, Berlin, 1970.

[19] B. Mohar, *The Laplacian spectrum of graphs*, Graph Theory, Combinatorics, and Applications (G. Alavi, O.R. Chartrand, and A.J.S. Oellermann, eds.), Wiley, New York, 1991, pp. 871–898.

[20] J.L. Palacios, *Some additional bounds for the Kirchhoff index*, MATCH Commun. Math. Comput. Chem. **75** (2016), no. 2, 365–372.

[21] S. Pirzada, H.A. Ganie, and I. Gutman, *On Laplacian-energy-like invariant and Kirchhoff index*, MATCH Commun. Math. Comput. Chem. **73** (2015), no. 1, 41–59.

[22] B.C. Rennie, *On a class of inequalities*, J. Austral. Math. Soc. **3** (1963), no. 4,

442–448.

[23] O. Rojo, R. Soto, and H. Rojo, *An always nontrivial upper bound for Laplacian graph eigenvalues*, Linear Algebra Appl. **312** (2000), no. 1-3, 155–159.

[24] S. Rosset, *Normalized symmetric functions, Newton's inequalities, and a new set of stronger inequalities*, Amer. Math. Soc. **96** (1989), no. 9, 815–819.

[25] Y. Yang, H. Zhang, and D.J. Klein, *New Nordhaus-Gaddum-type results for the Kirchhoff index*, J. Math. Chem. **49** (2011), no. 8, 1587–1598.

[26] B. Zhou and N. Trinajstić, *A note on Kirchhoff index*, Chem. Phys. Lett. **455** (2008), no. 1-3, 120–123.

[27] ———, *On resistance-distance and Kirchhoff index.*, J. Math. Chem. **46** (2009), no. 1, 283–289.

[28] H.-Y. Zhu, D.J. Klein, and I. Lukovits, *Extensions of the Wiener number*, J. Chem. Inf. Comput. Sci. **36** (1996), no. 3, 420–428.

[29] E. Zogic and E. Glogic, *A note on the Laplacian resolvent energy, Kirchhoff index and their relations*, Discrete Math. Lett. **2** (2019), no. 1, 32–37.

[30] P. Zumstein, *Comparison of spectral methods through the adjacency matrix and the Laplacian of a graph*, Th Diploma, ETH Zürich, 2005.