

Some lower bounds on the Kirchhoff index

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Abstract: Let $G = (V, E)$, $V = \{v_1, v_2, \dots, v_n\}$, $E = \{e_1, e_2, \dots, e_m\}$, be a simple graph of order $n \geq 2$ and size m without isolated vertices. Denote with $\mu_1 \geq \mu_2 \geq \dots \geq \mu_{n-1} > \mu_n = 0$ the Laplacian eigenvalues of G . The Kirchhoff index of a graph G , defined in terms of Laplacian eigenvalues, is given as $Kf(G) = n \sum_{i=1}^{n-1} \frac{1}{\mu_i}$. Some new lower bounds on $Kf(G)$ are obtained.

Keywords: Topological indices, Laplacian eigenvalues, Kirchhoff index

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1. Introduction

Let $G = (V, E)$, $V = \{v_1, v_2, \dots, v_n\}$, $E = \{e_1, e_2, \dots, e_m\}$, be a simple graph of order $n \geq 2$ and size m without isolated vertices. Denote by $\Delta = d_1 \geq d_2 \geq \dots \geq d_n = \delta > 0$, $d_i = d(v_i)$, a sequence of vertex degrees given in nonincreasing order. If vertices v_i and v_j are adjacent in G , we denote it as $i \sim j$.

Let $N(i)$ be a set of all neighbours of the vertex v_i , i.e. $N(i) = \{v_j \mid v_j \in V, v_i \sim v_j\}$, and d_{ij} the distance between the vertices v_i and v_j . Denote by Γ_d a set of all d -regular graphs, $1 \leq d \leq n-1$, with diameter $D = 2$ and $|N(i) \cap N(j)| = d$, $i \not\sim j$, [15]. Denote by $A(G)$ and $D(G) = \text{diag}(d_1, d_2, \dots, d_n)$ the adjacency and the diagonal degree matrix of G , respectively. The Laplacian matrix of G is defined as $L(G) = D(G) - A(G)$. Eigenvalues of L , $\mu_1 \geq \mu_2 \geq \dots \geq \mu_{n-1} > \mu_n = 0$, form the Laplacian spectrum of G .

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The Wiener index, $W(G)$, originally termed as a “path index”, is a topological graph index defined as [17]

$$W(G) = \sum_{i < j} d_{ij},$$

where d_{ij} is the number of edges in the shortest path between the vertices v_i and v_j in graph G .

By analogy with Wiener index, in [8] the Kirchhoff index was introduced. It is defined as

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

where r_{ij} is the resistance distance between the vertices v_i and v_j of G , i.e. r_{ij} is equal to the resistance between two equivalent points on an associated electrical network, obtained by replacing each edge of G by a unit (1 ohm) resistor. In [6, 19] it was observed that the Kirchhoff index can be obtained from the non-zero eigenvalues of the Laplacian matrix, that is

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

If $G \in \Gamma_d$, then [15]

$$Kf(G) = \frac{n(n-1) - d}{d}.$$

The Kirchhoff index is investigated extensively in mathematical and chemical literatures [1, 3, 4, 9–13, 18] In the present paper we consider lower bounds on $Kf(G)$ as well as its relationship with some other topological indices.

2. Preliminaries

In this section we recall some analytical inequalities and lower bound on $Kf(G)$, reported in [18], that are of interest for the present paper.

Lemma 1. [14] *Let $p = (p_i)$, $i = 1, 2, \dots, n$, be a sequence of non-negative real numbers, and $a = (a_i)$, $i = 1, 2, \dots, n$, sequence of positive real numbers. Then, for any real r , $r \leq 0$ or $r \geq 1$, holds*

$$\left(\sum_{i=1}^n p_i \right)^{r-1} \sum_{i=1}^n p_i a_i^r \geq \left(\sum_{i=1}^n p_i a_i \right)^r. \quad (1)$$

If $0 \leq r \leq 1$, then the opposite inequality is valid. Equality holds if and only if either $r = 0$, or $r = 1$, or $a_1 = a_2 = \dots = a_n$, or $p_1 = \dots = p_t = 0$ and $a_{t+1} = \dots = a_n$, or $a_1 = \dots = a_t$ and $p_{t+1} = \dots = p_n = 0$, for some t , $1 \leq t \leq n-1$.

The inequality (1), originally proved in [7], is known as Jensen’s inequality.

Let $a = (a_i)$, $i = 1, 2, \dots, n$ be a sequence of non-negative real numbers, and $p = (p_i)$ a sequence of positive real numbers. Denote by $I = \{1, 2, \dots, n\}$ and $I_2 = \{1, n\}$ two index sets, and

$$M_1(a, p; I) = \frac{\sum_{i=1}^n p_i a_i}{\sum_{i=1}^n p_i}.$$

In [5] the following result was proven.

Lemma 2. [5] Let $a = (a_i)$ and $b = (b_i)$, $i = 1, 2, \dots, n$, be sequences of similar monotonicity of non-negative real numbers, and $p = (p_i)$, $i = 1, 2, \dots, n$, a sequence of positive real numbers. If the pairs $(M_1(a, p; I - I_2), M_1(a, p; I_2))$ and $(M_1(b, p; I - I_2), M_1(b, p; I_2))$ are similarly ordered, then

$$\sum_{i=1}^n p_i \sum_{i=1}^n p_i a_i b_i - \sum_{i=1}^n p_i a_i \sum_{i=1}^n p_i b_i \geq \frac{p_1 p_n (a_1 - a_n)(b_1 - b_n)}{p_1 + p_n} \sum_{i=1}^n p_i. \quad (2)$$

Equality holds if and only if $a_2 = a_3 = \dots = a_{n-1} = \frac{a_1 + a_n}{2}$, or $b_2 = b_3 = \dots = b_{n-1} = \frac{b_1 + b_n}{2}$. If the pairs $(M_1(a, p; I - I_2), M_1(a, p; I_2))$ and $(M_1(b, p; I - I_2), M_1(b, p; I_2))$ are oppositely ordered, then the sense of (2) reverses.

The inequality (2) is generalization of the inequality proven in [16]. On the other hand, it is a corollary of one more general result proven in [5].

Lemma 3. [2] Let $a_1 \geq a_2 \geq \dots \geq a_n > 0$ be real numbers. Then

$$\sum_{i=1}^n a_i \geq n \left(\prod_{i=1}^n a_i \right)^{1/n} + (\sqrt{a_1} - \sqrt{a_n})^2, \quad (3)$$

with equality if $a_2 = \dots = a_{n-1} = \sqrt{a_1 a_n}$.

A lower bound for $Kf(G)$ that depends on all vertex degrees of G was determined in [18].

Lemma 4. [18] Let G be a connected graph with $n \geq 2$ vertices. Then

$$Kf(G) \geq -1 + (n-1) \sum_{i=1}^n \frac{1}{d_i}. \quad (4)$$

Equality holds if and only if either $G \cong K_n$, or $G \cong K_{t, n-t}$, $1 \leq t \leq \lfloor \frac{n}{2} \rfloor$, or $G \in \Gamma_d$.

3. Main results

In the next theorem we determine a relationship between the Kirchhoff index and the first Zagreb index, $M_1(G)$.

Theorem 1. Let G be a connected graph of order $n \geq 4$ and size m with p , $0 \leq p \leq n-2$, pendant vertices. If G is a d -regular graph, $2 \leq d \leq n-1$, then

$$Kf(G) \geq \frac{n(n-1) - d}{d}, \quad (5)$$

with equality if and only if $G \cong K_n$, or $G \in \Gamma_d$. If $d_i \neq \Delta$ for at least one i , $2 \leq i \leq n-p$, then

$$Kf(G) \geq (n-1) \left(p - \frac{1}{n-1} + \frac{1}{\Delta} \left(n - p + \frac{(n\Delta - 2m - p(\Delta - 1))^2}{2m\Delta - M_1(G) - p(\Delta - 1)} \right) \right). \quad (6)$$

Equality holds if and only if $G \cong K_{t, n-t}$, $2 \leq t < \frac{n}{2}$.

Proof. Let $p, 0 \leq p \leq n - 2$, be an integer. Then, for any real $r, r \leq 0$ or $r \geq 1$, the inequality (1) can be observed in a following form

$$\left(\sum_{i=1}^{n-p} p_i \right)^{r-1} \sum_{i=1}^{n-p} p_i a_i^r \geq \left(\sum_{i=1}^{n-p} p_i a_i \right)^r. \quad (7)$$

For $r = 2, p = 0, p_i = \frac{1}{d_i}, a_i = d_i, i = 1, 2, \dots, n$, from (7), that is (1), we obtain

$$\sum_{i=1}^n \frac{1}{d_i} \geq \frac{n^2}{2m}.$$

Now, from the above and (4) we obtain that

$$Kf(G) \geq \frac{n^2(n-1) - 2m}{2m}. \quad (8)$$

If G is d -regular, $2 \leq d \leq n - 1$, from (8) and identity $2m = nd$, we arrive at (5). In [15] (see also [12]) it was proven that equality in (5) holds if and only if $G \cong K_n$, or $G \in \Gamma_d$.

For $r = 2, p_i = \frac{\Delta - d_i}{d_i}, a_i = d_i, i = 1, 2, \dots, n - p$, the inequality (7) becomes

$$\sum_{i=1}^{n-p} \frac{\Delta - d_i}{d_i} \sum_{i=1}^{n-p} (\Delta - d_i) d_i \geq \left(\sum_{i=1}^{n-p} (\Delta - d_i) \right)^2. \quad (9)$$

Since

$$\begin{aligned} \sum_{i=1}^{n-p} \frac{\Delta - d_i}{d_i} &= \Delta \sum_{i=1}^{n-p} \frac{1}{d_i} - n + p, \\ \sum_{i=1}^{n-p} (\Delta - d_i) d_i &= \Delta \sum_{i=1}^{n-p} d_i - \sum_{i=1}^{n-p} d_i^2 = 2m\Delta - M_1(G) - p(\Delta - 1), \\ \sum_{i=1}^{n-p} (\Delta - d_i) &= n\Delta - 2m - p(\Delta - 1), \end{aligned}$$

from the above identities and (9) we obtain

$$\left(\Delta \sum_{i=1}^{n-p} \frac{1}{d_i} - n + p \right) (2m\Delta - M_1(G) - p(\Delta - 1)) \geq (n\Delta - 2m - p(\Delta - 1))^2. \quad (10)$$

If $d_i = \Delta$, for every $i, i = 1, 2, \dots, n - p$, then in (10) equality occurs. Therefore, without affecting the generality, assume that $d_i \neq \Delta$ for at least one $i, 2 \leq i \leq n - p$. In that case

$$2m\Delta - M_1(G) - p(\Delta - 1) > 0,$$

and hence from (10) we get

$$\sum_{i=1}^{n-p} \frac{1}{d_i} \geq \frac{1}{\Delta} \left(n-p + \frac{(n\Delta - 2m - p(\Delta - 1))^2}{2m\Delta - M_1(G) - p(\Delta - 1)} \right). \quad (11)$$

On the other hand, if G has p , $0 \leq p \leq n - 2$, pendant vertices, the inequality (4) can be considered in the following way

$$Kf(G) \geq -1 + (n-1) \sum_{i=1}^n \frac{1}{d_i} = (n-1) \left(p - \frac{1}{n-1} + \sum_{i=1}^{n-p} \frac{1}{d_i} \right). \quad (12)$$

Now, from the above and inequality (11) we arrive at (6).

Equality in (12) holds if and only if either $G \cong K_n$, or $G \cong K_{t,n-t}$, $1 \leq t \leq \lfloor \frac{n}{2} \rfloor$, or $G \in \Gamma_d$. Since $d_i \neq \Delta$, for at least one i , $2 \leq i \leq n-p$ ($p \neq n-1$), equality in (11) holds if $G \cong K_{t,n-t}$, $2 \leq t < \frac{n}{2}$. This implies that equality in (6) holds if $G \cong K_{t,n-t}$, $2 \leq t < \frac{n}{2}$. \square

Remark 1. The inequality (5) was proven in [15], whereas (8) in [12]. If the condition for pendant vertices is omitted, then similarly as in Theorem 1, when $d_i \neq \Delta$, for at least one i , $2 \leq i \leq n$, it was proven that [9]

$$Kf(G) \geq \frac{n(n-1) - \Delta}{\Delta} + \frac{(n-1)(n\Delta - 2m)^2}{\Delta(2m\Delta - M_1(G))},$$

with equality if and only if $G \cong K_{t,n-t}$, $2 \leq t < \frac{n}{2}$.

Corollary 1. Let G be a connected graph of order $n \geq 3$ and size m , with p , $0 \leq p \leq n-1$, pendant vertices. Then

$$Kf(G) \geq (n-1)p + \frac{(n-1)(n-p)^2 - (2m-p)}{2m-p}. \quad (13)$$

Equality holds if and only if either $G \cong K_n$, or $G \cong K_{1,n-1}$, or $G \in \Gamma_d$.

Proof. For $r = 2$, $p_i = 1$, $a_i = d_i$, $i = 1, 2, \dots, n-p$, the inequality (7) becomes

$$\sum_{i=1}^{n-p} 1 \sum_{i=1}^{n-p} d_i^2 \geq \left(\sum_{i=1}^{n-p} d_i \right)^2,$$

That is

$$(n-p)(M_1(G) - p) \geq (2m-p)^2. \quad (14)$$

From the above and inequality (6) we obtain (13). \square

In the next theorem we determine a lower bound on $Kf(G)$ in terms of number of vertices, edges, pendant vertices, and vertex degrees $\Delta_2 = d_2$ and $\delta_p = d_{n-p}$.

Theorem 2. *Let G be a connected graph of order $n \geq 4$ and size m with p pendant vertices. If $p = n - 1$, then*

$$Kf(G) = (n - 1)^2.$$

If $0 \leq p \leq n - 2$, then

$$Kf(G) \geq (n - 1) \left(\frac{n - 1 - \Delta}{\Delta(n - 1)} + p + \frac{(n - p - 1)^2}{2m - \Delta - p} + \frac{(\Delta_2 - \delta_p)^2}{\Delta_2 \delta_p (\Delta_2 + \delta_p)} \right). \quad (15)$$

Equality holds if and only if $G \cong K_n$, or $G \in \Gamma_d$.

Proof. The inequality (2) can be considered as

$$\sum_{i=2}^{n-p} p_i \sum_{i=2}^{n-p} p_i a_i b_i - \sum_{i=2}^{n-p} p_i a_i \sum_{i=2}^{n-p} p_i b_i \geq \frac{p_2 p_{n-p} (a_2 - a_{n-p})(b_2 - b_{n-p})}{p_2 + p_{n-p}} \sum_{i=2}^{n-p} p_i,$$

where p is an integer such that $0 \leq p \leq n - 2$.

For $p_i = d_i$, $a_i = b_i = \frac{1}{d_i}$, $i = 2, 3, \dots, n - p$, the above inequality transforms into

$$\sum_{i=2}^{n-p} d_i \sum_{i=2}^{n-p} \frac{1}{d_i} - \left(\sum_{i=2}^{n-p} 1 \right)^2 \geq \frac{\Delta_2 \delta_p \left(\frac{1}{\delta_p} - \frac{1}{\Delta_2} \right)^2}{\Delta_2 + \delta_p} \sum_{i=2}^{n-p} d_i,$$

that is

$$(2m - \Delta - p) \sum_{i=2}^{n-p} \frac{1}{d_i} \geq (n - p - 1)^2 + \frac{(\Delta_2 - \delta_p)^2}{\Delta_2 \delta_p (\Delta_2 + \delta_p)} (2m - \Delta - p). \quad (16)$$

Since $m \geq n - 1$ and $0 \leq p \leq n - 2$, the following is valid

$$2m \geq 2(n - 1) = n - 1 + n - 1 > \Delta + n - 2 \geq \Delta + p,$$

that is

$$2m - \Delta - p > 0.$$

Now, from the above and inequality (16) we have that

$$\sum_{i=2}^{n-p} \frac{1}{d_i} \geq \frac{(n - p - 1)^2}{2m - \Delta - p} + \frac{(\Delta_2 - \delta_p)^2}{\Delta_2 \delta_p (\Delta_2 + \delta_p)}. \quad (17)$$

Since G has p pendant vertices, the inequality (4) can be considered as

$$\begin{aligned} Kf(G) &\geq -1 + (n - 1) \sum_{i=1}^n \frac{1}{d_i} = -1 + (n - 1) \left(\sum_{i=2}^{n-p} \frac{1}{d_i} + \frac{1}{\Delta} + p \right) = \\ &= (n - 1) \left(\frac{n - 1 - \Delta}{\Delta(n - 1)} + p + \sum_{i=2}^{n-p} \frac{1}{d_i} \right). \end{aligned} \quad (18)$$

From the above and inequality (17) we obtain (15).

Equality in (18) holds if and only if either $G \cong K_n$, or $G \cong K_{t, n-t}$, $1 \leq t \leq \lfloor \frac{n}{2} \rfloor$, or $G \in \Gamma_d$. Equality in (17) holds if and only if $\Delta_2 = d_2 = \dots = d_{n-p} = \delta_p$, or $\frac{1}{d_3} = \dots = \frac{1}{d_{n-p-1}} = \left(\frac{1}{\Delta_2} + \frac{1}{\delta_p} \right) / 2$, $0 \leq p \leq n - 2$. Since G is connected and $G \not\cong K_{1, n-1}$, $p \neq n - 1$, equality in (15) holds if and only if $G \cong K_n$ or $G \in \Gamma_d$. \square

Corollary 2. Let G be a connected graph of order $n \geq 4$ and size m with p pendant vertices. If $G \cong K_{1,n-1}$, then

$$Kf(G) = (n-1)^2.$$

If $0 \leq p \leq n-2$, then

$$Kf(G) \geq (n-1) \left(\frac{n-1-\Delta}{\Delta(n-1)} + p + \frac{(n-p-1)^2}{2m-\Delta-p} \right).$$

Equality holds if and only if $G \cong K_n$, or $G \in \Gamma_d$.

Remark 2. If the condition for pendant vertices is omitted, then similarly as in Theorem 2, the following results can be proven.

Let G be a connected graph with $n \geq 3$ vertices and m edges. Then

$$Kf(G) \geq \frac{n-1-\Delta}{\Delta} + \frac{(n-1)^3}{2m-\Delta} + \frac{(n-1)(\Delta_2-\delta)^2}{\Delta_2\delta(\Delta_2+\delta)}. \quad (19)$$

Equality holds if and only if either $G \cong K_n$, or $G \cong K_{1,n-1}$, or $G \in \Gamma_d$.
Let G be a connected graph with $n \geq 3$ vertices and m edges. Then

$$Kf(G) \geq \frac{n-1-\Delta}{\Delta} + \frac{(n-1)^3}{2m-\Delta}. \quad (20)$$

Equality holds if and only if either $G \cong K_n$, or $G \cong K_{1,n-1}$, or $G \in \Gamma_d$.
The inequality (20) was proven in [12].

Theorem 3. Let G be a connected graph of order $n \geq 4$ with p , $0 \leq p \leq n-2$, pendant vertices. Then

$$Kf(G) \geq (n-1) \left(\frac{n-1-\Delta}{\Delta(n-1)} + p + (n-p-1) \left(\frac{\Delta}{\det D} \right)^{\frac{1}{n-p-1}} + \frac{(\sqrt{\Delta_2} - \sqrt{\delta_p})^2}{\Delta_2\delta_p} \right). \quad (21)$$

Equality holds when $G \cong K_n$, or $G \in \Gamma_d$.

Proof. The inequality (3) can be considered as

$$\sum_{i=2}^{n-p} a_i \geq (n-p-1) \left(\prod_{i=2}^{n-p} a_i \right)^{\frac{1}{n-p-1}} + (\sqrt{a_2} - \sqrt{a_{n-p}})^2,$$

where p is an integer such that $0 \leq p \leq n-2$.

For $a_i = \frac{1}{d_i}$, $i = 2, 3, \dots, n-p$, the above inequality becomes

$$\sum_{i=2}^{n-p} \frac{1}{d_i} \geq (n-p-1) \left(\prod_{i=2}^{n-p} \frac{1}{d_i} \right)^{\frac{1}{n-p-1}} + \left(\frac{1}{\sqrt{\delta_p}} - \frac{1}{\sqrt{\Delta_2}} \right)^2,$$

that is

$$\sum_{i=2}^{n-p} \frac{1}{d_i} \geq (n-p-1) \left(\frac{\Delta}{\det D} \right)^{\frac{1}{n-p-1}} + \frac{(\sqrt{\Delta_2} - \sqrt{\delta_p})^2}{\Delta_2 \delta_p}. \tag{22}$$

From the above and inequality (18) we obtain (21).

Equality in (22) holds when $\Delta_2 = d_2 = \dots = d_{n-p} = \delta_p$, or $d_3 = \dots = d_{n-p-1} = \sqrt{\Delta_2 \delta_p}$. Equality in (18) holds if and only if either $G \cong K_n$, or $G \cong K_{t,n-t}$, $1 \leq t \leq \lfloor \frac{n}{2} \rfloor$, or $G \in \Gamma_d$. This implies that equality in (21) holds if $G \cong K_n$, or $G \in \Gamma_d$. \square

Corollary 3. *Let G be a connected graph of order $n \geq 3$ with p , $0 \leq p \leq n - 2$, pendant vertices. Then*

$$Kf(G) \geq (n-1) \left(\frac{n-1-\Delta}{\Delta(n-1)} + p + (n-p-1) \left(\frac{\Delta}{\det D} \right)^{\frac{1}{n-p-1}} \right).$$

Equality holds when $G \cong K_n$, or $G \in \Gamma_d$.

Remark 3. If the condition for pendant vertices is omitted, then similarly as in Theorem 3, the following results can be proven.

Let G be a connected graph with $n \geq 4$ vertices. Then

$$Kf(G) \geq \frac{n-1-\Delta}{\Delta} + (n-1)^2 \left(\frac{\Delta}{\det D} \right)^{\frac{1}{n-1}} + (n-1) \frac{(\sqrt{\Delta_2} - \sqrt{\delta})^2}{\Delta_2 \delta}. \tag{23}$$

Equality holds if either $G \cong K_n$, or $G \cong K_{1,n-1}$, or $G \in \Gamma_d$.

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

$$Kf(G) \geq \frac{n-1-\Delta}{\Delta} + (n-1)^2 \left(\frac{\Delta}{\det D} \right)^{\frac{1}{n-1}}. \tag{24}$$

Equality holds if and only if either $G \cong K_n$, or $G \cong K_{1,n-1}$, or $G \in \Gamma_d$.

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