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A note on the Kirchhoff index of graphs

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Abstract: Let G be a simple connected graph with n vertices, m edges, and a sequence of vertex degrees $\Delta = d_1 \geq d_2 \geq \cdots \geq d_n = \delta > 0$. Denote by $\mu_1 \geq \mu_2 \geq \cdots \geq \mu_{n-1} > \mu_n = 0$ the Laplacian eigenvalues of G. The Kirchhoff index of G is defined as $Kf(G) = n\sum_{i=1}^{n-1}\frac{1}{\mu_i}$. A couple of new lower bounds for $Kf(G)$ that depend on n, m, Δ and some other graph invariants are obtained.

Keywords: Kirchhoff index, Zagreb indices, forgotten index.

MSC: 05C50, 15A18.

1. Introduction

Let $G = (V, E)$, $V = \{v_1, v_2, \ldots, v_n\}$, be a simple connected graph with n vertices, m edges and let $\Delta = d_1 \geq d_2 \geq \cdots \geq d_n = \delta > 0$, $d_i = d(v_i)$, be a sequence of vertex degrees of G. If vertices v_i and v_j are adjacent we write $v_i \sim v_j$ or, for brevity, $i \sim j$.

In graph theory, an invariant is a property of graphs that depends only on their abstract structure, not on the labeling of vertices or edges. Such quantities are also referred to as topological indices. The topological indices are an important class of molecular structure descriptors used for quantifying information on molecules. Many of them are defined as simple functions of the degrees of the vertices of (molecular) graph (see e.g. [1–3]). Historically, the first vertex-degree-based (VDB) structure descriptors were the graph invariants that are nowadays called Zagreb indices. The first and the second Zagreb index, M_1 and M_2, are defined as

$$M_1(G) = \sum_{i=1}^{n} d_i^2 \,,$$

and

$$M_2(G) = \sum_{i\sim j} d_i d_j \,.$$

The quantity M_1 was first time considered in 1972 [4], whereas M_2 in 1975 [5]. These were named Zagreb group indices [6] (in view of the fact that the authors of [4,5] were members of the "Rudjer Bošković" Institute in Zagreb, Croatia). Eventually, the name was shortened into first Zagreb index and second Zagreb index [7].

In [4] another topological index defined as sum of cubes of vertex degrees, that is

$$F(G) = \sum_{i=1}^{n} d_i^3 \,,$$

was encountered. However, for the unknown reasons, it did not attracted any attention until 2015 when it was reinvented in [8] and named the *forgotten topological index*. Details of the theory and applications of these topological indices can be found, for example, in [9,10].

In [11] Fajtlowicz defined a topological index called the inverse degree, $ID(G)$, as

$$ID(G) = \sum_{i=1}^{n} \frac{1}{d_i}.$$

Here we are interested in a graph invariant called the Kirchhoff index, which was introduced by Klein and Randić in [12]. 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, i.e. r_{ij} is equal to the resistance between equivalent points on an associated electrical network obtained by replacing each edge of G by a unit (1 ohm) resistor. The Kirchhoff index has a very nice purely mathematical interpretation. Namely, in [13] and [14] it was demonstrated that the Kirchhoff index of a connected graph can also be represented 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.

In this paper we obtain new lower bounds for $Kf(G)$ which depend on some of the graph structural parameters and above mentioned topological indices.

Before we proceed, let us define one special class of d-regular graphs Γ_d [15]. Let $N(i)$ be a set of all neighbors of vertex i, i.e. $N(i) = \{k \,|\, k \in V,\, k \sim i\}$, and $d(i,j)$ the distance between vertices i and j. Denote by Γ_d a set of all d-regular graphs, $1 \leq d \leq n-1$, with diameter $D = 2$ and $|N(i) \cap N(j)| = d$ for $i \nsim j$.

2. Preliminaries

In this section we recall some results from the literature which are needed for the subsequent considerations.

Lemma 1. *[16] Let $p = (p_i)$, $i = 1, 2, \ldots, n$, be a nonnegative real number sequence and $a = (a_i)$, $i = 1, 2, \ldots, n$, a positive real number sequence. Then for any real r, such that $r \geq 1$ or $r \leq 0$, holds*

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

If $0 \leq r \leq 1$, then the sense of (1) reverses. Equality holds if and only if either $r = 0$, or $r = 1$, or $a_1 = a_2 = \cdots = a_n$, or $p_1 = p_2 = \cdots = p_t = 0$ and $a_{t+1} = a_{t+2} = \cdots = a_n$, for some t, $1 \leq t \leq n-1$.

Lemma 2. *[17] Let G be a simple connected graph with $n \geq 2$ vertices. Then*

$$Kf(G) \geq -1 + (n-1) ID(G). \tag{2}$$

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 new lower bound for $Kf(G)$ in terms of the invariant $M_1(G)$ and graph parameters n, m and Δ.

Theorem 3. *Let G be a simple connected graph with $n \geq 2$ vertices and m edges. If G is d-regular graph, $1 \leq d \leq n-1$, then*

$$Kf(G) \geq \frac{n(n-1) - d}{d}. \tag{3}$$

Otherwise

$$Kf(G) \geq \frac{n(n-1) - \Delta}{\Delta} + \frac{(n-1)(n\Delta - 2m)^2}{\Delta(2m\Delta - M_1(G))}. \tag{4}$$

Equality in (3) holds if and only if $G \cong K_n$, or $G \in \Gamma_d$. Equality in (4) holds if and only if $G \cong K_{\Delta,n-\Delta}$.

Proof. If G is d-regular graph, $1 \le d \le n-1$, then

$$ID(G) = \frac{n}{d}.$$

From the above and (2) we arrive at (3).

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

$$\sum_{i=1}^{n} \left(\frac{\Delta}{d_i} - 1 \right) \sum_{i=1}^{n} (\Delta - d_i) d_i \ge \left(\sum_{i=1}^{n} (\Delta - d_i) \right)^2,$$

that is

$$(\Delta ID(G) - n)(2m\Delta - M_1(G)) \ge (n\Delta - 2m)^2. \tag{5}$$

If G is d-regular graph, $1 \le d \le n-1$, then $2m\Delta - M_1(G) = 0$. Therefore, we assume that G is not d-regular graph, $1 \le d \le n-1$. Then, according to (5) we have

$$ID(G) \ge \frac{n}{\Delta} + \frac{(n\Delta - 2m)^2}{\Delta(2m\Delta - M_1(G))}.$$

The inequality (4) is obtained from the above and (2).

The inequality (3) was proven in [18] with equality holding if and only if $G \cong K_n$ or $G \in \Gamma_d$.

Since G is not d-regular graph, $1 \le d \le n-1$, then equality in (5) is attained if and only if $\Delta = d_1 = d_2 = \cdots = d_t > d_{t+1} = \cdots = d_n$, for some t, $2 \le t \le n-1$, which implies that equality in (4) holds if and only if $G \cong K_{\Delta, n-\Delta}$. □

Remark 1. According to (4) follows

$$Kf(G) \ge \frac{n(n-1) - \Delta}{\Delta},$$

which was proven in [15].

Corollary 4. *Let G be a simple connected graph with $n \ge 2$ vertices and m edges. If $G \cong K_n$, then*

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

Otherwise

$$Kf(G) \ge n - 1 + \frac{(n(n-1) - 2m)^2}{2m(n-1) - M_1(G)}. \tag{6}$$

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

Proof. For $r = 2$, $p_i := \frac{n-1}{d_i} - 1$, $a_i := d_i$, $i = 1, 2, \ldots, n$, the inequality (1) transforms into

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

that is

$$((n-1)ID(G) - n)(2m(n-1) - M_1(G)) \ge (n(n-1) - 2m)^2. \tag{7}$$

If $G \cong K_n$, then $Kf(G) = n - 1$ and $2m(n-1) - M_1(G) = 0$. If $G \ncong K_n$, from (7) we obtain

$$(n-1)ID(G) \ge n + \frac{(n(n-1) - 2m)^2}{2m(n-1) - M_1(G)}.$$

The inequality (6) follows from the above and (2).

Equality in (7), $G \ncong K_n$, is attained if and only if $\Delta = d_1 = d_2 = \cdots = d_n \neq n-1$, or $n-1 = \Delta = d_1 = d_2 = \cdots = d_t > d_{t+1} = \cdots = d_n$, for some t, $1 \leq t \leq n-1$. This implies that equality in (6) holds if and only if $G \cong K_{1,n-1}$, or $G \in \Gamma_d$. □

Remark 2. In [19] the following was proven

$$Kf(G) \geq \frac{2mn(n-1)(n-2)}{4m^2 - M_1(G) - 2m}, \tag{8}$$

with equality holding if and only if $G \cong K_n$. We have performed testing on a large number of connected graphs, but could not find any graph for which the inequality (8) is stronger than (6).

Corollary 5. *Let G be a simple connected graph with $n \geq 2$ vertices and m edges. Then*

$$Kf(G) \geq \frac{n^2(n-1) - 2m}{2m}. \tag{9}$$

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

Proof. The inequality (9) is obtained according to (6) and inequality

$$M_1(G) \geq \frac{4m^2}{n},$$

which was proven in [20] (see also [21,22]). The inequality (9) was proven in [23] (see also [18]). □

The proof of the next theorem is fully analogous to that of the Theorem 3, hence omitted.

Theorem 6. *Let G be a simple connected graph with $n \geq 2$ vertices and m edges. If G is d-regular graph, $1 \leq d \leq n-1$, then the inequality (3) holds. Otherwise*

$$Kf(G) \geq \frac{n(n-1) - \Delta}{\Delta} + \frac{(n-1)(n\Delta - 2m)^{3/2}}{\Delta(\Delta M_1(G) - F(G))^{1/2}}. \tag{10}$$

Equality in (10) holds if and only if $G \cong K_{\Delta,n-\Delta}$.

Corollary 7. *Let G be a simple connected graph with $n \geq 2$ vertices and m edges. If $G \cong K_n$, then*

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

If $G \ncong K_n$, then

$$Kf(G) \geq n - 1 + \frac{(n(n-1) - 2m)^{3/2}}{((n-1)M_1(G) - F(G))^{1/2}}. \tag{11}$$

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

Corollary 8. *Let G be a simple connected graph with $n \geq 2$ vertices and m edges. If $G \cong K_n$, then*

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

If $G \ncong K_n$, then

$$Kf(G) \geq n - 1 + \frac{(n(n-1) - 2m)^{3/2}}{((n-1)M_1(G) - 2M_2(G))^{1/2}}. \tag{12}$$

Equality holds if and only if $G \in \Gamma_d$.

Proof. The inequality (12) is obtained from (11) and inequality $F(G) \geq 2M_2(G)$. □

Remark 3. In [24] a vertex–degree–based topological index called the Lanzhou index, $Lz(G)$, is defined as

$$Lz(G) = \sum_{i=1}^{n} (n-1-d_i)d_i^2.$$

According to (11) the following relation between topological indices $Kf(G)$ and $Lz(G)$ follows

$$(Kf(G) - n + 1)Lz(G)^{1/2} \geq (n(n-1) - 2m)^{3/2},$$

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

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