SCIENTIFIC PUBLICATIONS OF THE STATE UNIVERSITY OF NOVI PAZAR
SER. A: APPL. MATH. INFORM. AND MECH. vol. 10, 2 (2018), 107-114.

On some lower bounds for the Kirchhoff index

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Abstract: Let $G=(V,E)$, $V=\{1,2,\ldots,n\}$, be a simple connected graph of order n and size m, with sequence of vertex degrees $\Delta = d_1 \geq d_2 \geq \cdots \geq d_n = \delta > 0$, $d_i = d(i)$. Denote by $\mu_1 \geq \mu_2 \geq \cdots \geq \mu_{n-1} > \mu_n = 0$ the Laplacian eigenvalues of G. Further, denote with $Kf(G) = n\sum_{i=1}^{n-1}\frac{1}{\mu_i}$ and $t = t(G) = \frac{1}{n}\prod_{i=1}^{n-1}\mu_i$, the Kirchhoff index and the number of spanning trees of G, respectively. In this paper we determine several lower bounds for $Kf(G)$ depending on $t(G)$ and some of the graph parameters n, m or Δ.

Keywords: Topological indices, vertex degree, Kirchhoff index.

1 Introduction

Let $G=(V,E)$, $V=\{1,2,\ldots,n\}$, be a simple connected graph with n vertices and m edges. Denote with $\Delta = d_1 \geq d_2 \geq \cdots \geq d_n = \delta > 0$, a sequence of vertex degrees of G, $\mathbf{A}$ the adjacency matrix of graph, and by $\mathbf{D} = \mathrm{diag}(d_1, d_2, \ldots, d_n)$ the diagonal matrix of its vertex degrees. Matrix $\mathbf{L} = \mathbf{D} - \mathbf{A}$ is the Laplacian matrix of G. Eigenvalues of $\mathbf{L}$, $\mu_1 \geq \mu_2 \geq \cdots \geq \mu_{n-1} > \mu_n = 0$, form the so-called Lapacian spectrum of graph G.

The Wiener index, $W(G)$, originally termed as a "path number", is a topological graph index defined for a graph on n nodes by

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

where d_{ij} is the number of edges in the shortest path between vertices i and j in graph G. The first investigations into the Wiener index were made by Harold Wiener in 1947 [22] who realized that there are correlations between the boiling points of paraffin and the structure of the molecules. Since then it has become one of the most frequently used topological indices in chemistry, as molecules are usually modeled as undirected graphs. Based on its success, many other topological indices of chemical graphs have been developed.

Manuscript received May 13, 2018; accepted October 30, 2018.
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In analogy to the Wiener index, Klein and Randić [9] defined the Kirchhoff index, $Kf(G)$, as

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

where r_{ij} is the resistance-distance between the vertices i and j of a simple connected graph 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. There are several equivalent ways to define the resistance distance (see for example [1, 10, 23]). Gutman and Mohar [7] (see also [26]) proved that the Kirchhoff index can be obtained from the non-zero eigenvalues of Laplacian matrix:

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

It is well known that a connected graph G of order n has

$$t = t(G) = \frac{1}{n}\prod_{i=1}^{n-1} \mu_i$$

spanning trees.

In this paper we report lower bounds for the Kirchhoff index of a connected graph in terms of number of spanning trees, and some of its structural parameters such as the number of vertices, the number of edges and maximum vertex degree. For similar results one can refer to [4, 25].

2 Preliminaries

In this section we recall some analytical inequalities for the real number sequences that will be used in the subsequent considerations.

Let $p = (p_i)$ and $a = (a_i)$, $i = 1, 2, \ldots, n$, be positive real number sequences. Then for any real number r, $r \geq 1$ 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. This inequality is known as Jensen's inequality (see for example [20]).

Let $a=(a_i)$, $i=1,2,\ldots,n$, be a sequence of non-negative real numbers. In [24] (see also [11]) the following was proven:

$$
\begin{aligned}
n\left(\frac{1}{n}\sum_{i=1}^{n}a_i-\left(\prod_{i=1}^{n}a_i\right)^{\frac{1}{n}}\right) &\le n\sum_{i=1}^{n}a_i-\left(\sum_{i=1}^{n}\sqrt{a_i}\right)^2 \le \\
&\le n(n-1)\left(\frac{1}{n}\sum_{i=1}^{n}a_i-\left(\prod_{i=1}^{n}a_i\right)^{\frac{1}{n}}\right).
\end{aligned} \tag{2}
$$

Let $p=(p_i)$ and $a=(a_i)$, $i=1,2,\ldots,n$, be positive real number sequences with the properties $p_1+p_2+\cdots+p_n=1$ and $0<r\le a_i\le R<+\infty$. The following inequality was proven in [14] (see also [8]):

$$
\sum_{i=1}^{n}p_ia_i\sum_{i=1}^{n}\frac{p_i}{a_i}\le\frac{1}{4}\left(\sqrt{\frac{R}{r}}+\sqrt{\frac{r}{R}}\right)^2. \tag{3}
$$

Let $a_1\ge a_2\ge\cdots\ge a_n>0$ be a sequence of real numbers. In [2] the following was proved:

$$
\sum_{i=1}^{n}a_i-n\left(\prod_{i=1}^{n}a_i\right)^{\frac{1}{n}}\ge\left(\sqrt{a_1}-\sqrt{a_n}\right)^2. \tag{4}
$$

3 Main results

In the next theorem we establish lower bound for $Kf(G)$ in terms of number of spanning trees t, and parameters n, m and Δ.

Theorem 3.1. *Let G be a simple connected graph with $n\ge 2$ vertices and m edges. Then*

$$
Kf(G)\ge 1+\frac{n(n-2)^3}{(n-3)(2m-\Delta-1)+(n-2)\left(\frac{nt}{1+\Delta}\right)^{\frac{1}{n-2}}}, \tag{5}
$$

with equality if and only if $G\cong K_n$, or $G\cong K_{1,n-1}$, or $G\cong K_{\frac{n}{2},\frac{n}{2}}$ for even n.

Proof. For $r=3$ we rewrite inequality (1) as

$$
\left(\sum_{i=2}^{n-1}p_i\right)^2\sum_{i=2}^{n-1}p_ia_i^3\ge\left(\sum_{i=2}^{n-1}p_ia_i\right)^3.
$$

For $p_i = \sqrt{\mu_i}$ and $a_i = \frac{1}{\sqrt{\mu_i}}$, $i = 2, 3, \ldots, n-1$, the above inequality becomes

$$\left(\sum_{i=2}^{n-1} \sqrt{\mu_i} \right)^2 \left(\sum_{i=2}^{n-1} \frac{1}{\mu_i} \right) \geq (n-2)^3 . \tag{6}$$

Similarly, we can rewrite left-hand side of inequality (2) as

$$\left(\sum_{i=2}^{n-1} \sqrt{a_i} \right)^2 \leq (n-3) \sum_{i=2}^{n-1} a_i + (n-2) \left(\prod_{i=2}^{n-1} a_i \right)^{\frac{1}{n-2}} .$$

For $a_i = \mu_i$, $i = 2, 3, \ldots, n-1$, the above inequality transforms into

$$\left(\sum_{i=2}^{n-1} \sqrt{\mu_i} \right)^2 \leq (n-3) \sum_{i=2}^{n-1} \mu_i + (n-2) \left(\prod_{i=2}^{n-1} \mu_i \right)^{\frac{1}{n-2}} ,$$

i.e.

$$\left(\sum_{i=2}^{n-1} \sqrt{\mu_i} \right)^2 \leq (n-3)(2m - \mu_1) + (n-2) \left(\frac{nt}{\mu_1} \right)^{\frac{1}{n-2}} . \tag{7}$$

From (6) and (7) we get

$$\left((n-3)(2m - \mu_1) + (n-2) \left(\frac{nt}{\mu_1} \right)^{\frac{1}{n-2}} \right) \frac{1}{n} \left(Kf(G) - \frac{n}{\mu_1} \right) \geq (n-2)^3 .$$

Since [15, 12]

$$1 + \Delta \leq \mu_1 \leq n ,$$

according to the above we get

$$\left((n-3)(2m - \Delta - 1) + (n-2) \left(\frac{nt}{1+\Delta} \right)^{\frac{1}{n-2}} \right) (Kf(G) - 1) \geq n(n-2)^3 , \tag{8}$$

wherefrom we arrive at (5).

Equalities in (6) and (7) hold if and only if $\mu_2 = \mu_3 = \cdots = \mu_{n-1}$. Equality in (8) holds if and only if $\mu_1 = 1 + \Delta = n$ and $\mu_2 = \mu_3 = \cdots = \mu_{n-1}$. Therefore (see [3]) equality in (5) holds if and only if $G \cong K_n$, or $G \cong K_{1,n-1}$, or $G \cong K_{\frac{n}{2},\frac{n}{2}}$ for even n. □

Corollary 3.2. *Let G be a simple connected graph with $n \geq 3$ vertices. Then*

$$Kf(G) \geq 1 + \frac{n(n-2)^3}{(n-3)(n\Delta - \Delta - 1) + (n-2) \left(\frac{nt}{1+\delta} \right)^{\frac{1}{n-2}}} ,$$

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

Corollary 3.3. *Let T be a tree with $n \geq 3$ vertices. Then*

$$Kf(T) \geq 1 + \frac{n(n-2)^3}{(n-3)(2n-\Delta-3) + (n-2)\left(\frac{n}{1+\Delta}\right)^{\frac{1}{n-2}}},$$

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

Theorem 3.4. *Let G be a simple connected graph with $n \geq 2$ vertices and m edges. Then*

$$Kf(G) \geq \frac{n(n-1)}{(nt)^{\frac{1}{n-1}}} + n\frac{\left(\sqrt{\Delta+1}-\sqrt{\delta}\right)^2}{\delta(\Delta+1)}, \tag{9}$$

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

Proof. For $a_i = \dfrac{1}{\mu_{n-i}}$, $i = 1,2,\ldots,n-1$, the inequality (4) transforms into

$$\sum_{i=1}^{n-1} \frac{1}{\mu_i} \geq (n-1)\left(\prod_{i=1}^{n-1} \frac{1}{\mu_i}\right)^{\frac{1}{n-1}} + \left(\frac{1}{\sqrt{\mu_{n-1}}} - \frac{1}{\sqrt{\mu_1}}\right)^2,$$

i.e.

$$Kf(G) \geq \frac{n(n-1)}{(nt)^{\frac{1}{n-1}}} + n\left(\frac{1}{\sqrt{\mu_{n-1}}} - \frac{1}{\sqrt{\mu_1}}\right)^2. \tag{10}$$

Equality in (10) is attained if G is a complete graph. Suppose that G is not a complete graph. Then [6]

$$\mu_{n-1} \leq \delta.$$

Based on the above and inequality $\mu_1 \geq 1+\Delta$, from (10) the inequality (9) is obtained.

Equality in (10) holds if and only if $\mu_2 = \mu_3 = \cdots = \mu_{n-2} = \sqrt{\mu_1\mu_{n-1}}$. □

In the next theorem we determine lower bound for $Kf(G)$ in terms of $t = t(G)$, n and k, where k is arbitrary real number such that $\mu_{n-1} \geq k > 0$.

Theorem 3.5. *Let G be a simple connected graph with $n \geq 2$ vertices. Then, for any real k with the property $\mu_{n-1} \geq k > 0$,*

$$Kf(G) \geq \frac{2n(n-1)\sqrt{nk}}{(n+k)(nt)^{\frac{1}{n-1}}}. \tag{11}$$

Equality holds if and only if $k = n$ and $G \cong K_n$.

Proof. For $p_i = \dfrac{\mu_i^{-1}}{\sum_{i=1}^{n-1} \frac{1}{\mu_i}}$, $a_i = \mu_i$, $R = \mu_1$, $r = \mu_{n-1}$, $i = 1, 2, \ldots, n-1$, the inequality (3) becomes

$$\frac{(n-1)\sum_{i=1}^{n-1} \mu_i^{-2}}{\left(\sum_{i=1}^{n-1} \frac{1}{\mu_i}\right)^2} \le \frac{1}{4}\left(\sqrt{\frac{\mu_1}{\mu_{n-1}}} + \sqrt{\frac{\mu_{n-1}}{\mu_1}}\right)^2,$$

i.e.

$$(n-1)\sum_{i=1}^{n-1} \frac{1}{\mu_i^2} \le \frac{1}{4n^2}\left(\sqrt{\frac{\mu_1}{\mu_{n-1}}} + \sqrt{\frac{\mu_{n-1}}{\mu_1}}\right)^2 Kf(G)^2. \tag{12}$$

Based on the AG (arithmetic–geometric mean) inequality for real numbers (see for example [19]) we have that

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

From the above and inequality (12) we get

$$\frac{4n^2(n-1)^2}{(nt)^{\frac{2}{n-1}}} \le \left(\sqrt{\frac{\mu_1}{\mu_{n-1}}} + \sqrt{\frac{\mu_{n-1}}{\mu_1}}\right)^2 Kf(G)^2. \tag{13}$$

Since $\mu_1 \le n$ and $\mu_{n-1} \ge k > 0$ we have

$$\left(\sqrt{\frac{\mu_1}{\mu_{n-1}}} + \sqrt{\frac{\mu_{n-1}}{\mu_1}}\right)^2 \le \left(\sqrt{\frac{n}{k}} + \sqrt{\frac{k}{n}}\right)^2 = \frac{(n+k)^2}{nk}.$$

From this and (13) we obtain

$$Kf(G)^2 \ge \frac{4n^2(n-1)^2 nk}{(n+k)^2(nt)^{\frac{2}{n-1}}},$$

wherefrom we arrive at (11). □

Acknowledgement

This paper was supported by the Serbian Ministry of Education, Science and Technological development.

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