Communications in Combinatorics and Optimization
Vol. 5 No. 1, 2020 pp.1-8
DOI: 10.22049/CCO.2019.26270.1088

On relation between the Kirchhoff index and number of spanning trees of graphs

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Received: 4 June 2018; Accepted: 23 May 2019
Published Online: 25 May 2019

Abstract: Let G be a simple connected graph with degree sequence $(d_1, d_2, \ldots, d_n)$ where $\Delta = d_1 \geq d_2 \geq \cdots \geq d_n = \delta > 0$ and let $\mu_1 \geq \mu_2 \geq \cdots \geq \mu_{n-1} > \mu_n = 0$ be the Laplacian eigenvalues of G. Let $Kf(G) = n\sum_{i=1}^{n-1} \frac{1}{\mu_i}$ and $\tau(G) = \frac{1}{n}\prod_{i=1}^{n-1} \mu_i$ denote the Kirchhoff index and the number of spanning trees of G, respectively. In this paper we establish several lower bounds for $Kf(G)$ in terms of $\tau(G)$, the order, the size and maximum degree of G.

Keywords: Topological indices, Kirchhoff index, spanning tree

AMS Subject classification: 05C12, 05C50

1. Introduction

Let $G = (V, E)$ be a simple connected graph (no loops or multiple edges) with vertex set $V(G) = \{v_1, \ldots, v_n\}$ and edge set $E(G)$. Denote by $d(v_i)$ or $d_G(v_i)$ the degree of vertex v_i. If $\mathbf{D} = \mathrm{diag}(d_1, d_2, \ldots, d_n)$ is the diagonal matrix of vertex degrees of G and $\mathbf{A}$ is the (0, 1) adjacency matrix of G, then the matrix $\mathbf{L} = \mathbf{D} - \mathbf{A}$ is called the Laplacian matrix of a graph G. It is obvious that $\mathbf{L}$ is positive semidefinite matrix. Thus the all eigenvalues of $\mathbf{L}$ are called the Laplacian eigenvalues (or sometimes just eigenvalues) of G and arranged in nonincreasing order:

$$\mu_1 \geq \mu_2 \geq \cdots \geq \mu_{n-1} > \mu_n = 0.$$

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The set of the μ_i's is usually called the spectrum of $\mathbf{L}$ (or the spectrum of the associated graph G). The Laplacian eigenvalues of the complete graph K_n are $n^{(n-1)}$ and 0, and the Laplacian eigenvalues of the complete bipartite graph $K_{m,n}$ are $n+m$, $n^{(m-1)}$, $m^{(n-1)}$ and 0.
The Wiener index, $W(G)$, originally termed as a "path number", is a topological graph index defined for a graph on n vertices by

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

where d_{ij} is the number of edges in a shortest path between vertices v_i and v_j in G. The first investigations into the Wiener index were made by Harold Wiener in 1947 [17] 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.
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, 8, 18]). Gutman and Mohar [6] (see also [21]) proved that the Kirchhoff index can be obtained from the non-zero eigenvalues of Laplacian matrix, that is

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

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

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

spanning trees.
In this paper we present lower bounds for the Kirchhoff index of a connected graph G in terms of the number of spanning trees, the order, the size and the maximum degree of G. For similar results one can refer to [4, 20].

2. Preliminaries

In this section we recall some analytical inequalities for sequences of real numbers that will be used in the sequel.
Let $p = (p_i)$ and $a = (a_i)$, $i = 1, 2, \dots, n$, be two sequences of positive real numbers. Then for any real number r with $r \geq 1$ or $r \leq 0$, the following inequality 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 sign of (1) will be reversed. This inequality is known as Jensen's inequality (see for example [15]).
Let $a = (a_i)$, $i = 1, 2, \dots, n$, be a sequence of non-negative real numbers. In [19] (see also [10]) the following inequalities are proved.

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

Let $p = (p_i)$ and $a = (a_i)$, $i = 1, 2, \dots, n$, be two sequences of positive real numbers such that $p_1 + p_2 + \cdots + p_n = 1$ and $0 < r \leq a_i \leq R < +\infty$. The following inequality is proved in [13] (see also [7]).

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

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

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

3. Main results

In this section we present some lower bounds on the Kirchhoff index of a graph. First we provide a lower bound for Kirchhoff index of a graph G in terms of number of spanning trees t, the order, the size and the maximum degree.

Theorem 1. *Let G be a simple connected graph with $n \geq 3$ vertices and m edges. Then*

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

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

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

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.

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

From (6) and (7) we get

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

Since $1 + \Delta \leq \mu_1 \leq n$ (see [12, 14]), according to the above we get

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

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. □

Next results are immediate consequences of Theorem 1.

Corollary 1. *If G be a simple connected graph with $n \geq 3$ vertices, then*

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

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

Corollary 2. *Let T be a tree with $n \geq 2$ 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 $T \cong K_{1,n-1}$.

Remark 1. Laplacian-energy-like invariant, LEL, was defined in [11] by

$$LEL = LEL(G) = \sum_{i=1}^{n-1} \sqrt{\mu_i}\,.$$

According to (6) the following inequality, firstly proved in [4], follows.

$$\left(LEL(G) - \sqrt{1+\Delta}\right)^2 (Kf(G) - 1) \geq n(n-2)^3\,.$$

Likewise as Theorem 1, the following result can be proved.

Theorem 2. *Let G be a simple connected graph with $n \geq 3$ vertices and m edges. Then*

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

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

Theorem 3. *Let G be a simple connected graph with $n \geq 2$ vertices and m edges. Then*

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

with equality 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.

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

Equality in (10) is attained if G is a complete graph. Suppose that G is not a complete graph. Then $\mu_{n-1} \leq \delta$ by Theorem 4.1 in [5].
Based on the above and inequality $\mu_1 \geq 1 + \Delta > \Delta$, inequality (10) leads to the desired bound. □

Next we establish a lower bound for $Kf(G)$ in terms of $\tau(G)$, the order and an arbitrary real number k with $\mu_{n-1} \geq k > 0$.

Theorem 4. *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

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

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 [16]) we have that

$$\sum_{i=1}^{n-1}\frac{1}{\mu_i^2}\ge(n-1)\left(\prod_{i=1}^{n-1}\frac{1}{\mu_i^2}\right)^{\frac{1}{n-1}}=(n-1)(n\tau(G))^{-\frac{2}{n-1}}\,. \tag{13}$$

Using inequalities (12) and (13) we get

$$\frac{4n^2(n-1)^2}{(n\tau(G))^{\frac{2}{n-1}}}\le\left(\sqrt{\frac{\mu_1}{\mu_{n-1}}}+\sqrt{\frac{\mu_{n-1}}{\mu_1}}\right)^2 Kf(G)^2\,. \tag{14}$$

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 (14) we obtain

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

wherefrom we arrive at (11). □

Acknowledgement

This paper was supported by the Serbian Ministry of Education, Science and Technological development, grants TR32009 and TR32012.

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