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On the Relationship between the Kirchhoff and the Narumi-Katayama Indices

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Abstract. Let G be a simple connected graph with n vertices and m edges, sequence of vertex degrees $\Delta = d_1 \geq d_2 \geq \cdots \geq d_n = \delta > 0$ and diagonal matrix $D = \mathrm{diag}(d_1, d_2, \ldots, d_n)$ of its vertex degrees. Denote by $Kf(G) = n\sum_{i=1}^{n-1} \frac{1}{\mu_i}$, where μ_i are the Laplacian eigenvalues of graph G, the Kirchhoff index of G, and by $NK = \prod_{i=1}^{n} d_i$ the Narumi-Katayama index. In this paper we prove some inequalities that exhibit relationship between the Kirchhoff and Narumi-Katayama indices.

1. Introduction

Let $G = (V, E)$, $V = \{1, 2, \ldots, n\}$, be a simple connected graph with n vertices and m edges and let $\Delta = d_1 \geq d_2 \geq \cdots \geq d_n = \delta > 0$, $d_i = d(i)$, be its vertex degree sequence. Further, let **D** be the diagonal matrix of order n, whose diagonal elements are $d_1, d_2, \ldots, d_n$. Vertex–degree–based topological index, $NK = NK(G)$, known as the Narumi–Katayama index, is defined as [26]

$$NK = NK(G) = \det D = \prod_{i=1}^{n} d_i.$$

This topological index was introduced in [26] and referred to as "simple topological index". For a long period of time it was not in the spotlight. The situation has changed significantly when Todeschini and Consonni [31] proposed a descriptor named multiplicative Zagreb index, defined as

$$\Pi_1(G) = \prod_{i=1}^{n} d_i^2.$$

One can easily observe that $\Pi_1(G) = (NK(G))^2$. Current name, i.e. the Narumi-Katayama index, was proposed in [9]. Details on this topological index can be found in [8–10, 18, 34, 35].

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Denote by $\mathbf{A}$ the adjacency matrix of G. Then the Laplacian matrix of G is defined as $\mathbf{L} = \mathbf{D} - \mathbf{A}$. Eigenvalues of matrix $\mathbf{L}$, $\mu_1 \geq \mu_2 \geq \cdots \geq \mu_{n-1} > \mu_n = 0$, form the so-called Laplacian spectrum of graph. These eigenvalues have the following properties (see for example [5])

$$\sum_{i=1}^{n-1} \mu_i = \sum_{i=1}^{n} d_i = 2m \quad \text{and} \quad \sum_{i=1}^{n-1} \mu_i^2 = \sum_{i=1}^{n} d_i^2 + \sum_{i=1}^{n} d_i = M_1 + 2m,$$

where $M_1 = M_1(G) = \sum_{i=1}^{n} d_i^2$ is the first Zagreb index [11]. More about this topological index one can find in [2, 3, 12].

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 [32] who realized that there are correlations between the boiling points of paraffin and the structure of the molecules. Namely, he observed that the boiling point T_B can be well approximated by the formula

$$T_B = aW + bP + c\,,$$

where W is the Wiener index, P the polarity number and a, b and c are constants for a given isomeric group. 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 [17] 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. They proved that $Kf(G) \leq W(G)$, with equality if and only if G is a tree, $G \cong T$. There are several equivalent ways to define the resistance distance (see for example [1, 16, 33]). Gutman and Mohar [13] (see also [37]) proved that the Kirchhoff index can be obtained from the non-zero eigenvalues of Laplacian matrix:

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

More on the Kirchhoff index, as well as its applications in various areas, such as in spectral graph theory, molecular chemistry, computer science, etc. can be found, for example, in [6, 7, 13, 14, 17, 20–23, 27, 32, 35, 37].

In this paper we prove some inequalities that exhibit relationship between the Kirchhoff and Narumi-Katayama indices.

2. Preliminaries

In this section we recall some lower bounds for $Kf(G)$ reported in the literature and some analytic inequalities for real number sequences needed for our work.

Let us first define one special class of d-regular graphs Γ_d (see [27]). Let $N(i)$ be a set of all neighbors of the 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 2 such that for $i \nsim j$ holds $|N(i) \cap N(j)| = d$.

In [35] a lower bound for $Kf(G)$ depending on parameters n, $d_1, d_2, \dots, d_n$ was established, i.e. the following was proven

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

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

For the Narumi-Katayama index, $NK = NK(G)$, in [29] the following inequalities were proven

$$NK(G) \leq (n-1)^n, \tag{2}$$

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

$$NK(G) \leq \left(\frac{2m}{n}\right)^n, \tag{3}$$

with equality if and only if G is regular, and

$$NK(G) \leq \left(\frac{M_1}{n}\right)^{\frac{n}{2}}, \tag{4}$$

with equality if and only if G is regular.

Let $p = (p_i)$, and $a = (a_i)$, $i = 1, 2, \dots, n$, be two positive real number sequences such that $p_1 + p_2 + \cdots + p_n = 1$ and $0 < r \leq a_i \leq R < +\infty$. In [28] (see also [24]) it was proven

$$\sum_{i=1}^{n} p_i a_i + rR \sum_{i=1}^{n} \frac{p_i}{a_i} \leq r + R, \tag{5}$$

with equality if and only if $R = a_1 = \cdots = a_n = r$, or for arbitrary k $(1 \leq k \leq n-1)$ holds $R = a_1 = \cdots = a_k \geq a_{k+1} = \cdots = a_n = r$.

Let $a = (a_i)$, $i = 1, 2, \dots, n$, be a positive real number sequence such that $0 < r \leq a_i \leq R < +\infty$. In [30] the following inequality was proven

$$n\sum_{i=1}^{n} a_i^2 - \left(\sum_{i=1}^{n} a_i\right)^2 \geq \frac{n}{2}(R-r)^2, \tag{6}$$

with equality if and only if $a_1 = R$, $a_n = r$, and $a_2 = \cdots = a_{n-1} = \frac{r+R}{2}$.

Let $a_1, a_2, \dots, a_n$, be a non-negative real number sequence. In [36] (see also [19]) it was proven that

$$\begin{aligned} n\left[\frac{1}{n}\sum_{i=1}^{n} a_i - \left(\prod_{i=1}^{n} a_i\right)^{\frac{1}{n}}\right] &\leq n\sum_{i=1}^{n} a_i - \left(\sum_{i=1}^{n} \sqrt{a_i}\right)^2 \\ &\leq n(n-1)\left[\frac{1}{n}\sum_{i=1}^{n} a_i - \left(\prod_{i=1}^{n} a_i\right)^{\frac{1}{n}}\right], \end{aligned} \tag{7}$$

with equality holding if and only if $a_1 = a_2 = \cdots = a_n$.

Let $p = (p_i)$, $i = 1, 2, \dots, n$, be a positive real number sequence and let $a = (a_i)$, $b = (b_i), \dots, c = (c_i)$, $i = 1, 2, \dots, n$, be r sequences of non-negative real numbers of similar monotonicity. In [15] (see also [25]) the following inequality was proven

$$\left(\sum_{i=1}^{n} p_i\right)^{r-1} \sum_{i=1}^{n} p_i a_i b_i \cdots c_i \geq \sum_{i=1}^{n} p_i a_i \sum_{i=1}^{n} p_i b_i \cdots \sum_{i=1}^{n} p_i c_i, \tag{8}$$

with equality if and only if $r-1$ sequences are constant.

Let $a_1 \geq a_2 \geq \cdots \geq a_n > 0$ be a positive real number sequence. The following inequality holds [4]:

$$\sum_{i=1}^{n} a_i - n\left(\prod_{i=1}^{n} a_i\right)^{\frac{1}{n}} \geq \left(\sqrt{a_1} - \sqrt{a_n}\right)^2 , \tag{9}$$

with equality if and only if $a_2 = a_3 = \cdots = a_{n-1} = \sqrt{a_1 a_n}$.

3. On interplay between the Kirchhoff and the Narumi-Katayama indices

In this section we consider relations between the Kirchhoff index, $Kf(G)$, and the Narumi-Katayama index, $NK(G)$.

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

$$Kf(G) \geq \frac{n(n-1) - (\Delta + \delta)}{\Delta + \delta} + \frac{n(n-1)\Delta\delta}{(\Delta + \delta)(NK)^{\frac{2}{n}}} + \frac{(n-1)(\Delta - \delta)^2}{(\Delta + \delta)\Delta\delta}, \tag{10}$$

with equality if and only if either $G \cong K_n$, or $G \in \Gamma_d$.

Proof. For $p_i = \dfrac{\frac{1}{d_i}}{\sum_{i=1}^{n} \frac{1}{d_i}}$, $a_i = d_i$, $i = 1, 2, \ldots, n$, $R = d_1 = \Delta$, $r = d_n = \delta$, the inequality (5) becomes

$$\frac{n}{\sum_{i=1}^{n} \frac{1}{d_i}} + \Delta\delta \frac{\sum_{i=1}^{n} \frac{1}{d_i^2}}{\sum_{i=1}^{n} \frac{1}{d_i}} \leq \Delta + \delta ,$$

i.e.

$$\sum_{i=1}^{n} \frac{1}{d_i} \geq \frac{n + \Delta\delta \sum_{i=1}^{n} \frac{1}{d_i^2}}{\Delta + \delta} \tag{11}$$

For $a_i = \frac{1}{d_{n-i+1}^2}$, $i = 1, 2, \ldots, n$, the inequality (9) transforms into

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

that is

$$\sum_{i=1}^{n} \frac{1}{d_i^2} \geq \frac{n}{(NK)^{\frac{2}{n}}} + \frac{(\Delta - \delta)^2}{(\delta\Delta)^2} . \tag{12}$$

Now from (11), (12) and (1) we obtain (10).

Equality in (11) holds if and only if $\Delta = d_1 = d_2 = \cdots = d_n = \delta$, or if for some k, $1 \leq k \leq n-1$, holds $\Delta = d_1 = \cdots = d_k \geq d_{k+1} = \cdots = d_n = \delta$. Equality in (12) is attained if and only if $d_2 = \cdots = d_{n-1} = \sqrt{d_1 d_n}$. This means that equalities in both (11) and (12) are attained if and only if $\Delta = d_1 = d_2 = \cdots = d_n = \delta$. In that case (10) becomes

$$Kf(G) \geq \frac{n(n-1) - d}{d} . \tag{13}$$

This inequality was proven in [27]. Equality in (13), and consequently in (10), holds if and only if $G \cong K_n$, or $G \in \Gamma_d$. $\square$

In the following theorem we determine lower bound for $Kf(G)$ in terms of the parameters n, m, and invariant $NK(G)$.

Theorem 3.2. *Let G be a simple connected graph with $n \geq 2$ vertices and m edges. Then*

$$Kf(G) \geq -1 + \frac{n^3(n-1)}{2m(n-1) + n(NK(G))^{\frac{1}{n}}}, \tag{14}$$

with equality if and only if $G \cong K_n$, or $G \in \Gamma_d$.

Proof. For $r = 3$, $p_i = \sqrt{d_i}$, $a_i = b_i = c_i = \frac{1}{\sqrt{d_i}}$, $i = 1, 2, \ldots, n$, the inequality (8) becomes

$$\left(\sum_{i=1}^{n} \sqrt{d_i}\right)^2 \sum_{i=1}^{n} \frac{1}{d_i} \geq n^3. \tag{15}$$

From the left-hand side of (7), for $a_i = d_i$, $i = 1, 2, \ldots, n$, we obtain inequality

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

i.e.

$$\left(\sum_{i=1}^{n} \sqrt{d_i}\right)^2 \leq 2m(n-1) + n(NK(G))^{\frac{1}{n}}. \tag{16}$$

From (15) and (16) follows

$$\sum_{i=1}^{n} \frac{1}{d_i} \geq \frac{n^3}{2m(n-1) + n(NK(G))^{\frac{1}{n}}}. \tag{17}$$

Now, the inequality (14) is a direct consequence of (1) and (17).

Equalities in (15) and (16) hold if and only if $d_1 = d_2 = \cdots = d_n$, i.e. if and only if G is regular. Equality in (1) is attained if and only if $G \cong K_n$, or $G \cong K_{1,n-1}$, or $G \in \Gamma_d$, therefore equality in (14) holds if and only if $G \cong K_n$, or $G \in \Gamma_d$. □

Since $2m \leq n\Delta$ and $NK(G) \leq \Delta^n$, according to (3) we have the following corollary of Theorem 3.2.

Corollary 3.3. *Let G be a simple connected graph with $n \geq 2$ vertices and m edges. Then*

$$Kf(G) \geq \frac{n(n-1) - \Delta}{\Delta}, \tag{18}$$

and

$$Kf(G) \geq \frac{n^2(n-1) - 2m}{2m}, \tag{19}$$

with equality if and only if $G \cong K_n$, or $G \in \Gamma_d$.

Inequalities (18) and (19) were proven in [22] (see also [23]).

By a similar argument as in case of Theorem 3.2, the following results can be proved.

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

$$Kf(G) \geq \frac{n-1-\Delta}{\Delta} + \frac{(n-1)^4}{(n-2)(2m-\Delta) + (n-1)(NK(G))^{\frac{1}{n-1}}\Delta^{-\frac{1}{n-1}}},$$

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

Theorem 3.5. *Let G be a simple connected graph with $n \geq 2$ vertices and m edges. Then*

$$Kf(G) \geq \frac{n-1-\delta}{\delta} + \frac{(n-1)^4}{(n-2)(2m-\delta) + (n-1)(NK(G))^{\frac{1}{n-1}}\delta^{-\frac{1}{n-1}}},$$

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

Theorem 3.6. *Let G be a simple connected graph with $n \geq 3$ vertices and m edges. Then*

$$\begin{aligned} Kf(G) &\geq \frac{(n-1)(\Delta+\delta) - \Delta\delta}{\Delta\delta} \\ &+ \frac{(n-1)(n-2)^3}{(n-3)(2m-\Delta-\delta) + (n-2)(NK(G))^{\frac{1}{n-2}}\Delta^{-\frac{1}{n-2}}\delta^{-\frac{1}{n-2}}}, \end{aligned}$$

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

In the next theorem we determine lower bound for $Kf(G)$ in terms of parameters n, Δ, δ, and invariant $NK(G)$.

Theorem 3.7. *Let G be a simple connected graph with $n \geq 2$ vertices. Then*

$$Kf(G) \geq -1 + \frac{n(n-1)}{(NK(G))^{\frac{1}{n}}} + \frac{n\left(\sqrt{\Delta} - \sqrt{\delta}\right)^2}{2\Delta\delta}, \tag{20}$$

with equality if and only if $G \cong K_n$, or $G \in \Gamma_d$.

Proof. For $a_i = \frac{1}{\sqrt{d_i}}$, $i = 1, 2, \ldots, n$, $R = \frac{1}{\sqrt{d_n}} = \frac{1}{\sqrt{\delta}}$, and $r = \frac{1}{\sqrt{d_1}} = \frac{1}{\sqrt{\Delta}}$, the inequality (6) becomes

$$n\sum_{i=1}^{n}\frac{1}{d_i} \geq \left(\sum_{i=1}^{n}\frac{1}{\sqrt{d_i}}\right)^2 + \frac{n}{2}\left(\frac{1}{\sqrt{\delta}} - \frac{1}{\sqrt{\Delta}}\right)^2. \tag{21}$$

From the right-hand side of inequality (7), for $a_i = \frac{1}{d_i}$, $i = 1, 2, \ldots, n$, we get

$$\left(\sum_{i=1}^{n}\frac{1}{\sqrt{d_i}}\right)^2 \geq \sum_{i=1}^{n}\frac{1}{d_i} + n(n-1)\left(\prod_{i=1}^{n}\frac{1}{d_i}\right)^{\frac{1}{n}}. \tag{22}$$

According to (21) and (22) we have that

$$(n-1)\sum_{i=1}^{n}\frac{1}{d_i} \geq \frac{n(n-1)}{(NK(G))^{\frac{1}{n}}} + \frac{n\left(\sqrt{\Delta} - \sqrt{\delta}\right)^2}{2\Delta\delta}. \tag{23}$$

Finally, from (1) and (23) we obtain (20).

Equality in (22) holds if and only if $d_1 = d_2 = \cdots = d_n$, that is if and only if graph G is regular. Equality in (1) is attained if and only if $G \cong K_n$, or $G \cong K_{1,n-1}$, or $G \in \Gamma_d$, therefore equality in (20) holds if and only if $G \cong K_n$, or $G \in \Gamma_d$. $\square$

From (20), (2), (3) and (4) we have the following corollary of Theorem 3.7.

Corollary 3.8. *Let G be a simple connected graph with $n \geq 2$ vertices. Then*

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

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

$$Kf(G) \geq \frac{n\sqrt{n}(n-1) - \sqrt{M_1}}{\sqrt{M_1}} + \frac{n\left(\sqrt{\Delta} - \sqrt{\delta}\right)^2}{2\Delta\delta},$$

with equality if and only if $G \cong K_n$, or $G \in \Gamma_d$,

$$Kf(G) \geq \frac{n^2(n-1) - 2m}{2m} + \frac{n\left(\sqrt{\Delta} - \sqrt{\delta}\right)^2}{2\Delta\delta}, \tag{24}$$

with equality if and only if $G \cong K_n$, or $G \in \Gamma_d$.

Remark 3.9. *The inequality* (24) *is stronger than* (19). *Since* $2m \leq n\Delta$, *from* (24) *we get*

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

which is stronger than (18).

In a similar way as in Theorem 3.7, the following results can be proved.

Theorem 3.10. *Let G be a simple connected graph with $n \geq 3$ vertices. Then*

$$Kf(G) \geq \frac{n-1-\Delta}{\Delta} + (n-1)^2\left(\left(\frac{\Delta}{NK(G)}\right)^{\frac{1}{n}} + \frac{\left(\sqrt{\Delta_2} - \sqrt{\delta}\right)^2}{2(n-2)\Delta_2\delta}\right),$$

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

Corollary 3.11. *Let G be a simple connected graph with $n \geq 3$ vertices. Then*

$$Kf(G) \geq \frac{n(n-1) - \Delta}{\Delta} + \frac{(n-1)^2\left(\sqrt{\Delta_2} - \sqrt{\delta}\right)^2}{2(n-2)\Delta_2\delta},$$

with equality if and only if $G \cong K_n$, or $G \in \Gamma_d$.

Theorem 3.12. *Let G be a simple connected graph with $n \geq 4$ vertices. Then*

$$\begin{aligned} Kf(G) \quad &\geq \quad \frac{(n-1)(\Delta+\delta) - \Delta\delta}{\Delta\delta} \\ &+ \quad (n-1)(n-2)\left(\left(\frac{\Delta\delta}{NK(G)}\right)^{\frac{1}{n-2}} + \frac{\left(\sqrt{\Delta_2} - \sqrt{\delta_2}\right)^2}{2(n-3)\Delta_2\delta_2}\right), \end{aligned}$$

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

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