

On Some Spectral, Vertex and Edge Degree-Based Graph Invariants

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Abstract

Let G be a simple graph of order $n \geq 2$, with m edges and with no isolated vertices. Denote by d_i vertex degree, by $d(e_i)$ edge degree, by λ_i ordinary eigenvalues, by μ_i the Laplacian eigenvalues and by ρ_i the normalized Laplacian eigenvalues of the graph G . The sums $Q_\alpha = \sum_{i=1}^n d_i^\alpha$, $EQ_\alpha = \sum_{i=1}^m d(e_i)^\alpha$, $R_\alpha = \sum_{i \sim j} (d_i d_j)^\alpha$, $E_\alpha = \sum_{i=1}^n |\lambda_i|^\alpha$, $S_\alpha = \sum_{i=1}^{n-1} \mu_i^\alpha$ and $S_\alpha^* = \sum_{i=1}^{n-1} \rho_i^\alpha$ are special cases of the sum $A_\alpha = \sum_{i=1}^t a_i^\alpha$, where $t \in \mathbb{N}$, $\alpha \in \mathbb{R}$ and a_i are real numbers with the property $0 < r \leq a_i \leq R < +\infty$. We first prove new inequalities for A_α . Then some special cases are illustrated.

1 Introduction

Let $G = (V, E)$, $V = \{1, 2, \dots, n\}$, $E = \{e_1, e_2, \dots, e_m\}$ be a simple graph, without isolated vertices, of order n and size m . Denote by $d_1 \geq d_2 \geq \dots \geq d_n > 0$, $d_i = d(i)$, $i = 1, 2, \dots, n$, and $d(e_1) \geq d(e_2) \geq \dots \geq d(e_m) > 0$ a sequence of vertex and edge degrees, respectively. The degree of an edge $e = \{i, j\}$ is defined as $d(e) = d_i + d_j - 2$. If i -th and j -th vertices (edges) of graph G are adjacent, we denote it as $i \sim j$ ($e_i \sim e_j$).

In the text that follows we give definitions of some degree-based topological indices that are of interest for our work.

The first general Zagreb index (or general zeroth-order Randić index [26]), Q_α , is defined as

$$Q_\alpha = Q_\alpha(G) = \sum_{i=1}^n d_i^\alpha = \sum_{i \sim j} (d_i^{\alpha-1} + d_j^{\alpha-1}),$$

where α is an arbitrary real number (see [24, 25]). Particular interesting for us are the first Zagreb index $M_1 = Q_2$,

$$M_1 = M_1(G) = Q_2 = \sum_{i=1}^n d_i^2 = \sum_{i \sim j} (d_i + d_j)$$

and so called forgotten topological index, $F_1 = Q_3$,

$$F_1 = F_1(G) = Q_3 = \sum_{i=1}^n d_i^3 = \sum_{i \sim j} (d_i^2 + d_j^2),$$

defined in [17] (see also [11, 14]).

The generalized Randić index (or connectivity index [22]), R_α , is defined as

$$R_\alpha = R_\alpha(G) = \sum_{i \sim j} (d_i d_j)^\alpha,$$

where α is an arbitrary real number defined in [3] (see also [10, 27, 29]). Especially interesting are the ordinary Randić index, $R_{-1/2}$ [35], the general Randić index, R_{-1} [5, 42], and the second Zagreb index $M_2 = R_1$ [17]

$$M_2 = M_2(G) = R_1 = \sum_{i \sim j} d_i d_j.$$

The first reformulated general Zagreb index is defined as [41]

$$EQ_\alpha = EQ_\alpha(G) = \sum_{i=1}^m d(e_i)^\alpha.$$

Here we are interested in the reformulated first Zagreb index $EM_1 = EM_1(G) = EQ_2(G)$ (see [30]) and reformulated forgotten topological index, $EF_1 = EF_1(G) = EQ_3$ (see for example [11]).

Let $L(G)$ be a line-graph of the underlining graph G . Then in accordance with the definition of a line-graph (see [7]) we have that

$$EQ_\alpha(G) = Q_\alpha(L(G)). \tag{1}$$

In the text that follows we recall some graph invariants that are of interest for the subsequent considerations.

Denote by \mathbf{A} the adjacency matrix of G . The eigenvalues of adjacency matrix \mathbf{A} , $\lambda_1 \geq \lambda_2 \geq \dots \geq \lambda_n$, represent ordinary eigenvalues of the graph G . Some well known properties of graph eigenvalues are [1]:

$$\sum_{i=1}^n \lambda_i = 0 \quad \text{and} \quad \sum_{i=1}^n \lambda_i^2 = \sum_{i=1}^n d_i = 2m.$$

Denote by $|\lambda_1^*| \geq |\lambda_2^*| \geq \dots \geq |\lambda_n^*|$, $\lambda_1 = |\lambda_1^*|$, a non increasing sequence of absolute values of the eigenvalues of G . The graph invariant called energy, $E(G)$, of G is defined to be the sum of the absolute values of the eigenvalues of G [15] (see also [23]), i.e.

$$E(G) = \sum_{i=1}^n |\lambda_i| = \sum_{i=1}^n |\lambda_i^*|.$$

Denote by

$$E_\alpha = E_\alpha(G) = \sum_{i=1}^n |\lambda_i^*|^\alpha$$

sum of degrees of non-zero ordinary eigenvalues of G , where α is an arbitrary real number.

Let G be a simple connected graph with the Laplacian eigenvalues $\mu_1 \geq \mu_2 \dots \geq \mu_{n-1} > \mu_n = 0$. Some well known properties of the Laplacian eigenvalues are (see [7])

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

The sum of degrees of Laplacian eigenvalues of the graph G is denoted with (see [40])

$$S_\alpha = S_\alpha(G) = \sum_{i=1}^{n-1} \mu_i^\alpha,$$

where α is an arbitrary real number.

The Kirchhoff index [16] is a graph invariant defined in terms of Laplacian eigenvalues as

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

The normalized Laplacian eigenvalues, $\rho_1 \geq \rho_2 \geq \dots \geq \rho_{n-1} > \rho_n = 0$, of graph G have the following properties [42]

$$\sum_{i=1}^{n-1} \rho_i = n \quad \text{and} \quad \sum_{i=1}^{n-1} \rho_i^2 = n + 2R_{-1}.$$

The sum of degrees of normalized Laplacian eigenvalues [2] of the graph G is denoted by

$$S_\alpha^* = S_\alpha^*(G) = \sum_{i=1}^{n-1} \rho_i^\alpha,$$

where α is an arbitrary real number. The degree Kirchhoff index [6] is defined in terms of the normalized Laplacian eigenvalues as

$$DKf(G) = 2m \sum_{i=1}^{n-1} \frac{1}{\rho_i}.$$

Instead of considering sums $Q_\alpha, EQ_\alpha, R_\alpha, E_\alpha, S_\alpha$ and S_α^* , it is enough to consider the sum

$$A_\alpha = A_\alpha(a) = \sum_{i=1}^t a_i^\alpha, \quad A_0 = t, \quad (2)$$

where $t \in \mathbb{N}$, while $a_i, i = 1, 2, \dots, t$, are positive real numbers with the properties

$$0 < r \leq a_i \leq R < +\infty, \quad 1 \leq i \leq t$$

or

$$0 < r_1 \leq a_i \leq R_1 < +\infty, \quad 2 \leq i \leq t,$$

and α is an arbitrary real number. Namely, by the appropriate choice of parameter t and real numbers a_i , each of the above mentioned sums can be obtained. Therefore in the text that follows we will prove new inequalities that are valid for the sum (2). Then, for the sake of illustration we will point out to some special cases.

2 Main result

Theorem 1 *Let $a_1 \geq a_2 \geq \dots \geq a_t > 0$ be real numbers with the property $0 < r \leq a_i \leq R < +\infty$. Then for each real α the following inequality is valid*

$$A_{\alpha+1} \leq (r + R)A_\alpha - rRA_{\alpha-1} \quad (3)$$

with equality if and only if for some $v, 1 \leq v \leq t$, hold $R = a_1 = \dots = a_v$ and $a_{v+1} = \dots = a_t = r$.

Proof. For the positive real numbers p_1, p_2, \dots, p_t and x_1, x_2, \dots, x_t with the properties

$$\sum_{i=1}^t p_i = 1 \quad \text{and} \quad 0 < X \leq x_i \leq Y < +\infty, \quad i = 1, 2, \dots, t$$

in [36] the following inequality was proved

$$\sum_{i=1}^t p_i x_i + XY \sum_{i=1}^t \frac{p_i}{x_i} \leq X + Y. \quad (4)$$

For $p_i = \frac{a_i^\alpha}{A_\alpha}$, $x_i = a_i, i = 1, 2, \dots, t$, $X = r$ and $Y = R$, where α is an arbitrary real number, the inequality (4) transforms into

$$\frac{1}{A_\alpha} \sum_{i=1}^t a_i^{\alpha+1} + \frac{rR}{A_\alpha} \sum_{i=1}^t a_i^{\alpha-1} \leq r + R,$$

i.e.

$$A_{\alpha+1} + rRA_{\alpha-1} \leq (r + R)A_{\alpha}, \tag{5}$$

wherefrom we obtain (3).

Equality in (4) holds if and only if for some $v, 1 \leq v \leq t$, hold $Y = x_1 = \dots = x_v$ and $x_{v+1} = \dots = x_t = X$, hence the equalities in (3) hold if and only if for some $v, 1 \leq v \leq t$, hold $R = a_1 = \dots = a_v$ and $a_{v+1} = \dots = a_t = r$. ■

Corollary 1 *Let $a_1 \geq a_2 \geq \dots \geq a_t > 0$ are real numbers with the property $0 < r \leq a_i \leq R < +\infty$. Then, for every real α*

$$A_{\alpha+1} \leq \frac{1}{4} \left(\sqrt{\frac{R}{r}} + \sqrt{\frac{r}{R}} \right)^2 \frac{A_{\alpha}^2}{A_{\alpha-1}}. \tag{6}$$

Equality holds if and only if $r = a_1 = \dots = a_t = R$.

Proof. According to AG (arithmetic-geometric mean) inequality (see for example [34]) and (5) we have

$$2\sqrt{rRA_{\alpha+1}A_{\alpha-1}} \leq A_{\alpha+1} + rRA_{\alpha-1} \leq (r + R)A_{\alpha},$$

wherefrom we obtain (6). ■

Let $(W_i), W_0 = 0$, be a sequence of real numbers defined as

$$W_i = \begin{cases} \frac{R^i - r^i}{R - r}, & \text{if } r \neq R \\ iR^{i-1}, & \text{if } r = R, \end{cases}$$

for every $i, i \geq 1$.

Using the sequence $(W_i), i \in N_0$, and the sum A_{α} we prove the following result.

Theorem 2 *Let $a_1 \geq a_2 \geq \dots \geq a_t > 0$ be real numbers with the property $0 < r \leq a_i \leq R < +\infty$. Then for each nonnegative integer $k \geq 0$, the following inequalities are valid*

$$A_{k+1} \leq W_{k+1}A_1 - trRW_k, \tag{7}$$

and

$$A_{k+1} \leq W_kA_2 - rRW_{k-1}A_1. \tag{8}$$

Equalities hold if and only if $R = a_1 = \dots = a_v$ and $a_{v+1} = \dots = a_t = r$, for some $v, 1 \leq v \leq t$. In addition, the equality in (7) holds if $k = 0$ and in (8) if $k = 1$.

Proof. According to (5), for each $i \geq 1$ the following is valid

$$A_{i+1} - (r + R)A_i + rRA_{i-1} \leq 0.$$

After multiplying the above inequality by W_{k-i+1} and summing up over i , $i = 1, 2, \dots, k$, we get

$$\begin{aligned} 0 \geq & \sum_{i=1}^k (A_{i+1} - (r + R)A_i + rRA_{i-1})W_{k-i+1} = W_1A_{k+1} + (W_2 - (r + R)W_1)A_k + \\ & (rRW_{k-1} - (r + R)W_k)A_1 + rRW_kA_0 + \sum_{i=1}^{k-2} (W_{k-i+1} - (r + R)W_{k-i} + rRW_{k-i-1})A_{i+1}. \end{aligned}$$

Since for each $i \geq 1$ we have

$$W_{i+1} - (r + R)W_i + rRW_{i-1} = 0,$$

from the above inequality we get

$$0 \geq A_{k+1} - W_{k+1}A_1 + trRW_k,$$

wherefrom we obtain (7). ■

Remark 1 *If for some fixed i , $1 \leq i \leq k-1$, values A_i and A_{i-1} are known, then instead of the inequality (7) (i.e. (8)), the inequality*

$$A_{k+1} \leq W_{k-i+2}A_i - rRW_{k-i+1}A_{i-1}$$

should be used. This inequality can be proved similarly as (7). It becomes stronger as i increases.

Remark 2 *If a_1 is known or can be easily assessed, and for $a_2 \geq a_3 \geq \dots \geq a_t > 0$ holds $0 < r_1 \leq a_i \leq R_1 < +\infty$, then the following inequalities*

$$A_{\alpha+1} \leq a_1^{\alpha+1} + (r_1 + R_1)(A_\alpha - a_1^\alpha) - r_1R_1(A_{\alpha-1} - a_1^{\alpha-1}), \quad (9)$$

$$A_{\alpha+1} \leq a_1^{\alpha+1} + \frac{1}{4} \left(\sqrt{\frac{R_1}{r_1}} + \sqrt{\frac{r_1}{R_1}} \right)^2 \frac{(A_\alpha - a_1^\alpha)^2}{A_{\alpha-1} - a_1^{\alpha-1}}, \quad (10)$$

$$A_{k+1} \leq a_1^{k+1} + \bar{W}_{k+1}(A_1 - a_1) - (t-1)r_1R_1\bar{W}_k, \quad (11)$$

$$A_{k+1} \leq a_1^{k+1} + \bar{W}_k(A_2 - a_1^2) - r_1R_1\bar{W}_{k-1}(A_1 - a_1), \quad (12)$$

where

$$\bar{W}_i = \begin{cases} \frac{R_1^i - r_1^i}{R_1 - r_1}, & \text{if } R_1 \neq r_1 \\ iR_1^{i-1}, & \text{if } R_1 = r_1 \end{cases}$$

should be considered. Equalities in (9), (11) and (12) hold if and only if $R_1 = a_2 = \dots = a_v$ and $a_{v+1} = \dots = a_t = r_1$ for some v , $2 \leq v \leq t$, whereas equality in (10) hold if and only if $R_1 = a_2 = \dots = a_t = r_1$. In addition, equality in (11) holds if $k = 0$, and in (12) if $k = 1$.

Now we will illustrate obtained results on some examples.

For $t = n$, $a_i = d_i$, $i = 1, 2, \dots, n$, $r = d_n$ and $R = d_1$, the following corollaries of the obtained results are valid.

Corollary 2 *Let G be a simple graph of order $n \geq 3$, with m edges and without isolated vertices. Then*

$$Q_{\alpha+1} \leq (d_1 + d_n)Q_\alpha - d_1 d_n Q_{\alpha-1}, \tag{13}$$

$$Q_{\alpha+1} \leq \frac{1}{4} \left(\sqrt{\frac{d_1}{d_n}} + \sqrt{\frac{d_n}{d_1}} \right)^2 \frac{Q_\alpha^2}{Q_{\alpha-1}}, \tag{14}$$

$$Q_{k+1} = \sum_{i=1}^n d_i^{k+1} \leq 2m \frac{d_1^{k+1} - d_n^{k+1}}{d_1 - d_n} - nd_1 d_n \frac{d_1^k - d_n^k}{d_1 - d_n}, \tag{15}$$

$$Q_{k+1} = \sum_{i=1}^n d_i^{k+1} \leq M_1 \frac{d_1^k - d_n^k}{d_1 - d_n} - 2md_1 d_n \frac{d_1^{k-1} - d_n^{k-1}}{d_1 - d_n}. \tag{16}$$

Equalities in (13), (15) and (16) hold if and only if G is regular or bidegreed graph. Equality in (14) holds if and only if G is regular. In addition, equality in (15) holds if $k = 0$, and in (16) if $k = 1$.

Remark 3 *For $\alpha = 1$ from (13) (i.e. $k = 1$ in (15)) we get*

$$M_1 \leq 2m(d_1 + d_n) - nd_1 d_n.$$

This inequality was proved in [9] (see also [18, 19, 21, 24]).

For $\alpha = 2$ from (13) and $k = 2$ in (15) we get

$$F_1 \leq M_1(d_1 + d_n) - 2md_1 d_n \tag{17}$$

and

$$F_1 \leq 2m(d_1^2 + d_1 d_n + d_n^2) - nd_1 d_n (d_1 + d_n).$$

The inequality (17) was proved in [41] (see also [20]).

Since $2M_2 \leq F_1$ and $2R_{-1} \leq \sum_{i=1}^n \frac{1}{d_i}$, the following inequalities

$$\begin{aligned} M_2 &\leq \frac{1}{2}(M_1(d_1 + d_n) - 2md_1d_n) \leq d_1M_1 - md_1d_n, \\ M_2 &\leq (2m(d_1^2 + d_1d_n + d_n^2) - nd_1d_n(d_1 + d_n)) \end{aligned} \quad (18)$$

and

$$R_{-1} \leq \frac{2m(d_1 + d_n) - M_1}{2d_1d_n}$$

are also valid. The second inequality in (18) was proved in [37].

Remark 4 For $\alpha = 1$ and $\alpha = 2$ from (14) follows

$$M_1 \leq \frac{m^2}{n} \left(\sqrt{\frac{d_1}{d_n}} + \sqrt{\frac{d_n}{d_1}} \right)^2, \quad (19)$$

and

$$F_1 \leq \frac{M_1^2}{8m} \left(\sqrt{\frac{d_1}{d_n}} + \sqrt{\frac{d_n}{d_1}} \right)^2,$$

i.e.

$$M_2 \leq \frac{M_1^2}{16m} \left(\sqrt{\frac{d_1}{d_n}} + \sqrt{\frac{d_n}{d_1}} \right)^2.$$

The inequality (19) was proved in [28] (see also [12, 19, 38]). Additionally, for $\alpha = 0$ from (14) we get

$$R_{-1} \leq \frac{n^2}{16m} \left(\sqrt{\frac{d_1}{d_n}} + \sqrt{\frac{d_n}{d_1}} \right)^2.$$

Let us note that one generalization of inequality (19) was proved in [33].

Remark 5 In [8] the following inequality was proved

$$Q_{\alpha+1} \leq \frac{2m}{n}Q_\alpha + \frac{2m(n-1)}{n}(d_1^\alpha - d_n^\alpha) - \frac{2m}{n}Q_2(d_1^\alpha - d_n^\alpha).$$

The inequality (13) is stronger than the above one when $G \cong P_n$, $G \cong K_{\frac{n}{2}, \frac{n}{2}}$ (n is even), $G \cong K_{1, n-1}$ and when G is bidegreed graph.

Remark 6 Let $t = n$, $a_i = |\lambda_i^*|$, $i = 1, 2, \dots, n$, $r = |\lambda_n^*|$, $R = |\lambda_1^*|$ and $\alpha = 1$. According to (3) and (6) we get

$$E \geq \frac{2m + n|\lambda_1^*||\lambda_n^*|}{|\lambda_1^*| + |\lambda_n^*|}, \quad (20)$$

and

$$E \geq \frac{2\sqrt{2mn}|\lambda_1^*||\lambda_n^*|}{|\lambda_1^*| + |\lambda_n^*|}. \quad (21)$$

The inequality (20) was proved in [32], and (21) in [13].

Remark 7 For $t = n - 1$, $a_i = \mu_i$, $i = 1, 2, \dots, n - 1$, $r = \mu_{n-1}$, $R = \mu_1$ and $\alpha = 0$, according to (3) and (6) we get

$$Kf(G) \leq \frac{n((n-1)(\mu_1 + \mu_{n-1}) - 2m)}{\mu_1 \mu_{n-1}},$$

and

$$Kf(G) \leq \frac{n(n-1)^2}{8m} \left(\sqrt{\frac{\mu_1}{\mu_{n-1}}} + \sqrt{\frac{\mu_{n-1}}{\mu_1}} \right)^2.$$

The first inequality was proved in [31] whereas the second one in [12].

Remark 8 For $t = n - 1$, $a_i = \rho_i$, $i = 1, 2, \dots, n - 1$, $r = \rho_{n-1}$, $R = \rho_1$ and $\alpha = 0$, according to (3) and (6) we get

$$DKf(G) \leq \frac{2m((n-1)(\rho_1 + \rho_{n-1}) - n)}{\rho_1 \rho_{n-1}},$$

and

$$DKf(G) \leq \frac{m(n-1)^2}{n} \left(\sqrt{\frac{\rho_1}{\rho_{n-1}}} + \sqrt{\frac{\rho_{n-1}}{\rho_1}} \right)^2.$$

The above inequalities were proved in [31].

Remark 9 For $t = n - 1$, $a_i = \rho_i$, $i = 1, 2, \dots, n - 1$, $r = \rho_{n-1}$, $R = \rho_1$ and $\alpha = 1$, according to (3) and (6) we have that

$$R_{-1} \leq \frac{1}{2} ((\rho_1 + \rho_{n-1} - 1)n + (n-1)\rho_1 \rho_{n-1})$$

and

$$\sqrt{\frac{\rho_1}{\rho_{n-1}}} + \sqrt{\frac{\rho_{n-1}}{\rho_1}} \geq \frac{2}{n} \sqrt{(n-1)(n + 2R_{-1})}.$$

The second inequality was proved in [4].

Remark 10 For $t = 2m$, $a_i = d_i d_j$, $i \sim j$, $R = p = \max_{i \sim j} \{d_i d_j\}$, $r = q = \min_{i \sim j} \{d_i d_j\}$ and $\alpha = 0$, from (3) and (6) we get

$$M_2 \leq 2m(p + q) - pqR_{-1} \tag{22}$$

and

$$M_2 \leq \frac{m^2}{R_{-1}} \left(\sqrt{\frac{p}{q}} + \sqrt{\frac{q}{p}} \right)^2. \tag{23}$$

Equality in (22) holds if and only if G is regular or complete bipartite graph. Equality in (23) holds if and only if G is a regular graph.

Remark 11 For $t = n - 1$, $a_i = \mu_i$, $i = 1, 2, \dots, n - 1$, $r = \mu_{n-1}$, $R = \mu_1$ and $\alpha = 1$, from (3) and (6) we get

$$M_1 \leq 2m(\mu_1 + \mu_{n-1} - 1) - (n - 1)\mu_1\mu_{n-1}$$

and

$$M_1 \leq \frac{m^2}{n - 1} \left(\sqrt{\frac{\mu_1}{\mu_{n-1}}} + \sqrt{\frac{\mu_{n-1}}{\mu_1}} \right)^2 - 2m.$$

The second inequality was proved in [13] and [39].

Remark 12 For $t = m$, $a_i = d(e_i)$, $i = 1, 2, \dots, m$, $r = 2(d_n - 1)$, $R = 2(d_1 - 1)$ and $\alpha = 1$, from (3) and (6) we get

$$EM_1 \leq 2(d_1 + d_n - 2)M_1 - 4m(d_1d_n - 1),$$

and

$$EM_1 \leq \frac{(d_1 + d_n - 2)^2}{4m(d_1 - 1)(d_n - 1)}(M_1 - 2m)^2.$$

The above inequalities were proved in [10].

Remark 13 For $t = n$, $a_i = d_i$, $i = 1, 2, \dots, n$, $r_1 = d_n$, $R_1 = d_2$ and $\alpha = 1$, from (9) and (10) we get

$$M_1 \leq d_1^2 + (d_2 + d_n)(2m - d_1) - d_2d_n(n - 1), \tag{24}$$

and

$$M_1 \leq d_1^2 + \left(\sqrt{\frac{d_2}{d_n}} + \sqrt{\frac{d_n}{d_2}} \right)^2 \frac{(2m - d_1)^2}{4}. \tag{25}$$

Equality in (24) holds if and only if $d_2 = \dots = d_v$ and $d_{v+1} = \dots = d_n$, for some v , $2 \leq v \leq n$, and in (25) if and only if $d_2 = d_3 = \dots = d_n$. The inequality (24) was proved in [19].

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