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On upper bounds for VDB topological indices of graphs

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Abstract. Let $G = (V, E)$, $V = \{1, 2, \dots, n\}$, be a simple graph of order n and size m, without isolated vertices. Denote by $d_1 \geq d_2 \geq \cdots \geq d_n$, $d_i = (d_i)$, a sequence of its vertex degrees in nondecreasing order. If vertices i and j are adjacent, we write $i \sim j$. Denote with $TI = TI(G) = \sum_{i\sim j} F(d_i, d_j)$ a class of vertex-degree-based invariants, where $F(x, y)$ may be any function satisfying the condition $F(x, y) = F(y, x)$. We define three new adjacency matrices for G which are joined to TI, and then determine upper bounds for TI.

1. Introduction

Let $G = (V, E)$, $V = \{1, 2, \dots, n\}$, be a simple graph of order n and size m, without isolated vertices. Denote by $d_1 \geq d_2 \geq \cdots \geq d_n$, $d_i = d(i)$, the sequence of its vertex degree. If vertices i and j are adjacent, we write $i \sim j$.

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. Topological indices might be classified into several distinct groups. One of the most investigated and widely used is a group of so-called vertex–degree–based indices (VDB), whose general formula is

$$TI = TI(G) = \sum_{i\sim j} F(d_i, d_j),$$

where $F(x, y)$ may be any real function satisfying the condition $F(x, y) = F(y, x)$.

In what follows we list some particular VDB indices of this kind that are of interest for our work.

- For $F(d_i, d_j) = d_i + d_j$ we obtain the oldest VDB topological index, named the first Zagreb index, M_1, [11].
- For $F(d_i, d_j) = d_i d_j$ we get the second Zagreb index [12].
- For $F(d_i, d_j) = d_i^2 + d_j^2$, a so-called Forgotten topological index, F, is obtained [11] (see also [9, 15]).

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- For $F(d_i, d_j) = \frac{1}{\sqrt{d_i d_j}}$, the classical Randić (or connectivity index), R, is obtained [20]
- For $F(d_i, d_j) = \frac{1}{d_i d_j}$, another version of Randić index,called general Randić index, R_{-1} is obtained [20].
- For $F(d_i, d_j) = \frac{2}{d_i + d_j}$, we get the harmonic index, H [7]
- For $F(d_i, d_j) = \frac{1}{\sqrt{d_i + d_j}}$, the sum-connectivity index, SCI, introduced in [25] is obtained.
- For $F(d_i, d_j) = \frac{d_i d_j}{d_i + d_j}$, we have the inverse sum indeg index, ISI, defined in [23].
- For $F(d_i, d_j) = \frac{d_i}{d_j} + \frac{d_j}{d_i}$, we get symmetric division deg index, SDD [24].
- For $F(d_i, d_j) = |d_i - d_j|$, the Albertson index, Alb, [1] (see also [13]) is obtained.

To each topological index, TI, we can associate general extended adjacency matrix $\mathcal{A} = (a_{ij})$, Randić vertex–degree adjacency matrix $\mathcal{B} = (b_{ij})$ and sum-connectivity vertex–degree adjacency matrix $C = (c_{ij})$, which are, respectively, defined as:

$$a_{ij} = \begin{cases} F(d_i, d_j), & \text{if } i \sim j, \\ 0, & \text{otherwise,} \end{cases} \tag{1}$$

$$b_{ij} = \begin{cases} \frac{F(d_i, d_j)}{\sqrt{d_i d_j}}, & \text{if } i \sim j, \\ 0, & \text{otherwise,} \end{cases} \tag{2}$$

$$c_{ij} = \begin{cases} \frac{F(d_i, d_j)}{\sqrt{d_i + d_j}}, & \text{if } i \sim j, \\ 0, & \text{otherwise.} \end{cases} \tag{3}$$

For some particular values of $F(d_i, d_j)$ the corresponding adjacency matrices were considered in [2–4, 6, 14, 18, 21, 26].

Let $f_1 \geq f_2 \geq \cdots \geq f_n$, $\gamma_1 \geq \gamma_2 \geq \cdots \geq \gamma_n$, and $\delta_1 \geq \delta_2 \geq \cdots \geq \delta_n$, be eigenvalues of matrices $\mathcal{A}$, $\mathcal{B}$ and C, respectively. Since these matrices are real and symmetric, corresponding eigenvalues are real. It can be easily proved that for the traces of these matrices, tr, as well as their squares the following results hold.

Lemma 1. *Let G be a simple (n, m) graph without isolated vertices. Then*

$$tr(\mathcal{A}) = f_1 + f_2 + \cdots + f_n = 0,$$
$$tr(\mathcal{B}) = \gamma_1 + \gamma_2 + \cdots + \gamma_n = 0,$$
$$tr(C) = \delta_1 + \delta_2 + \cdots + \delta_n = 0,$$
$$tr(\mathcal{A}^2) = f_1^2 + f_2^2 + \cdots + f_n^2 = 2 \sum_{i \sim j} F(d_i, d_j)^2,$$
$$tr(\mathcal{B}^2) = \gamma_1^2 + \gamma_2^2 + \cdots + \gamma_n^2 = 2 \sum_{i \sim j} \frac{F(d_i, d_j)^2}{d_i d_j},$$
$$tr(C^2) = \delta_1^2 + \delta_2^2 + \cdots + \delta_n^2 = 2 \sum_{i \sim j} \frac{F(d_i, d_j)^2}{d_i + d_j}.$$

In this paper we determine upper bounds for the index TI depending on the traces of $\mathcal{A}^2$, $\mathcal{B}^2$ and C^2. Also, we give some corollaries of these inequalities for some particular TI, some of which are new, and some already reported in the literature.

2. Main results

In the following theorem we prove inequality that establishes the relation between TI and traces of the corresponding matrices $\mathcal{A}^2$, $\mathcal{B}^2$ and C^2.

Theorem 1. *Let G be a simple graph of size m, without isolated vertices. Then*

$$TI \le \sqrt{\frac{m\, tr(\mathcal{A}^2)}{2}}, \tag{4}$$

$$TI \le \sqrt{\frac{M_2\, tr(\mathcal{B}^2)}{2}}, \tag{5}$$

$$TI \le \sqrt{\frac{M_1\, tr(C^2)}{2}}. \tag{6}$$

Equalities in (4)–(6), respectively, hold if $F(d_i, d_j) = c$, $F(d_i, d_j) = d_i d_j$ and $F(d_i, d_j) = d_i + d_j$.

Proof. Let $a = (a_i)$, $i = 1, 2, \dots, m$, be a positive real number sequence. Then for any r, $r \le 0$, or $r \ge 1$, Jensen's inequality holds (see e.g. [17])

$$m^{r-1} \sum_{i=1}^{m} a_i^r \ge \left(\sum_{i=1}^{m} a_i \right)^r . \tag{7}$$

If $0 < r < 1$, then the sense of (7) reverses.

For $r = 2$, $a_i := F(d_i, d_j)$, where summation goes over all edges in G, the inequality (7) becomes

$$m \sum_{i\sim j} F(d_i, d_j)^2 \ge \left(\sum_{i\sim j} F(d_i, d_j) \right)^2 ,$$

i.e.

$$\frac{1}{2} m\, tr(\mathcal{A}^2) \ge TI^2,$$

wherefrom we get the inequality (4).

Let $x = (x_i)$ and $a = (a_i)$, $i = 1, 2, \dots, m$, be positive real number sequences. In [19] it was proven that for any $r \ge 0$ holds

$$\sum_{i=1}^{m} \frac{x_i^{r+1}}{a_i^r} \ge \frac{\left(\sum_{i=1}^{m} x_i \right)^{r+1}}{\left(\sum_{i=1}^{m} a_i \right)^{r}}. \tag{8}$$

For $r = 1$, $a_i := d_i d_j$, $x_i := F(d_i, d_j)$, where summing goes over all adjacent vertices in graph G, the inequality (8) transforms into

$$\sum_{i\sim j} \frac{F(d_i, d_j)^2}{d_i d_j} \ge \frac{\left(\sum_{i\sim j} F(d_i, d_j) \right)^2}{\sum_{i\sim j} d_i d_j},$$

that is

$$\frac{1}{2}tr(\mathcal{B}^2) \geq \frac{TI^2}{M_2},$$

wherefrom we arrive at (5).

For $r = 1$, $a_i := d_i + d_j$, $x_i := F(d_i, d_j)$, where summations goes over all adjacent vertices in graph G, the inequality (8) becomes

$$\sum_{i\sim j} \frac{F(d_i, d_j)^2}{d_i + d_j} \geq \frac{\left(\sum_{i\sim j} F(d_i, d_j)\right)^2}{\sum_{i\sim j}(d_i + d_j)},$$

that is

$$\frac{1}{2}tr(C^2) \geq \frac{TI^2}{M_1},$$

wherefrom we obtain (6). □

The inequalities (4)–(6) enable us to determine a number of relations, either new or known, between many topological indices. We illustrate this in the following corollaries of Theorem 1.

Corollary 1. *Let G be a simple graph of size m, without isolated vertices. Then*

$$M_2 R_{-1} \geq m^2 \tag{9}$$

and

$$M_1 H \geq 2m^2. \tag{10}$$

Proof. The inequalities (9) and (10) are obtained for $F(d_i, d_j) = 1$ from inequalities (5) and (6), respectively. □

Corollary 2. *Let G be a simple graph of size m, without isolated vertices. Then*

$$F \geq \frac{M_1^2}{m} - 2M_2 \tag{11}$$

and

$$SDD \geq \frac{M_1^2}{M_2} - m. \tag{12}$$

Proof. The inequalities (11) and (12) are obtained for $F(d_i, d_j) = d_i + d_j$ from (4) and (5), respectively. □

The inequality (11) was proven in [9] (see also [8]).

Corollary 3. *Let G be a simple graph of size m, without isolated vertices. Then*

$$M_2 \geq \frac{m^3}{R^2} \tag{13}$$

and

$$ISI \geq \frac{m^4}{M_1 R^2}. \tag{14}$$

Proof. For $F(d_i, d_j) = \sqrt{d_i d_j}$, the inequality (4) becomes

$$m \sum_{i\sim j} d_i d_j \geq \left(\sum_{i\sim j} \sqrt{d_i d_j} \right)^2 ,$$

that is

$$mM_2 \geq \left(\sum_{i\sim j} \sqrt{d_i d_j} \right)^2 . \tag{15}$$

By arithmetic-harmonic mean inequality for real numbers (see e.g. [16]), we have

$$\left(\sum_{i\sim j} \sqrt{d_i d_j} \right)^2 \left(\sum_{i\sim j} \frac{1}{\sqrt{d_i d_j}} \right)^2 \geq m^4,$$

i.e.

$$\left(\sum_{i\sim j} \sqrt{d_i d_j} \right)^2 \geq \frac{m^4}{R^2}. \tag{16}$$

In view of the above and inequality (15) we obtain (13).

For $F(d_i, d_j) = \sqrt{d_i d_j}$ the inequality (6) becomes

$$\sum_{i\sim j} \frac{d_i d_j}{d_i + d_j} \geq \frac{\left(\sum_{i\sim j} \sqrt{d_i d_j} \right)^2}{\sum_{i\sim j} (d_i + d_j)},$$

that is

$$M_1 ISI \geq \left(\sum_{i\sim j} \sqrt{d_i d_j} \right)^2 .$$

From the above and inequality (16) we obtain (14). □

Corollary 4. *Let G be a simple graph of order n and size m, without isolated vertices. Then*

$$SCI \geq \sqrt{\frac{m^3}{M_1}} \tag{17}$$

and

$$SCI \geq \frac{m^2}{\sqrt{nM_2}}. \tag{18}$$

Proof. For $F(d_i, d_j) = \sqrt{d_i + d_j}$ the inequality (4) becomes

$$m \sum_{i\sim j} (d_i + d_j) \geq \left(\sum_{i\sim j} \sqrt{d_i + d_j} \right)^2 ,$$

i.e.

$$mM_1 \geq \left(\sum_{i \sim j} \sqrt{d_i + d_j} \right)^2 . \tag{19}$$

By applying the arithmetic-harmonic mean inequality for real numbers (see e.g. [16]), we get

$$\left(\sum_{i \sim j} \sqrt{d_i + d_j} \right)^2 \left(\sum_{i \sim j} \frac{1}{\sqrt{d_i + d_j}} \right)^2 \geq m^4,$$

i.e.

$$\left(\sum_{i \sim j} \sqrt{d_i + d_j} \right)^2 \geq \frac{m^4}{(SCI)^2}. \tag{20}$$

From (19) and (20) we arrive at (17).

For $F(d_i, d_j) = \sqrt{d_i + d_j}$ the inequality (5) transforms into

$$\sum_{i \sim j} \frac{d_i + d_j}{d_i d_j} \geq \frac{\left(\sum_{i \sim j} \sqrt{d_i + d_j} \right)^2}{\sum_{i \sim j} d_i d_j},$$

that is

$$nM_2 \geq \left(\sum_{i \sim j} \sqrt{d_i + d_j} \right)^2 .$$

From this and inequality (20) we obtain (18). □

The inequality (17) was proven in [25].

Corollary 5. *Let G be a simple graph of size m, without isolated vertices. Then*

$$SCI \leq \sqrt{\frac{mH}{2}}. \tag{21}$$

Proof. For $F(d_i, d_j) = \frac{1}{\sqrt{d_i + d_j}}$ the inequality (4) becomes

$$m \sum_{i \sim j} \frac{1}{d_i + d_j} \geq \left(\sum_{i \sim j} \frac{1}{\sqrt{d_i + d_j}} \right)^2,$$

i.e.

$$\frac{1}{2} mH \geq (SCI)^2 ,$$

which completes the proof. □

Corollary 6. *Let G be a simple graph of size m, without isolated vertices. Then*

$$Alb \leq \sqrt{m(F - 2M_2)}. \tag{22}$$

Proof. For $F(d_i, d_j) = |d_i - d_j|$ the inequality (4) becomes

$$m \sum_{i \sim j} |d_i - d_j|^2 \geq \left(\sum_{i \sim j} |d_i - d_j| \right)^2 ,$$

i.e.

$$m(F - 2M_2) \geq (Alb)^2,$$

wherefrom we obtain (22). □

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