SCIENTIFIC PUBLICATIONS OF THE STATE UNIVERSITY OF NOVI PAZAR
SER. A: APPL. MATH. INFORM. AND MECH. vol. 10, 1 (2018), 33-40.

On bounds of eigenvalues of Randić vertex–degree–based adjacency matrix

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Abstract: Let $G = (V,E)$, $V = \{1,2,\ldots,n\}$, be a simple graph of order n and size m, without isolated vertices. Denote by $d_1 \geq d_2 \geq \cdots \geq d_n > 0$, $d_i = d(i)$, a sequence of its vertex degrees. If vertices i and j are adjacent, we write $i \sim j$. With TI we denote a topological index that can be represented as $TI = TI(G) = \sum_{i\sim j} F(d_i,d_j)$, where F is an appropriately chosen function with the property $F(x,y) = F(y,x)$. Randić vertex–degree–based adjacency matrix $RA = (r_{ij})$ is defined as $r_{ij} = \frac{F(d_i,d_j)}{\sqrt{d_i d_j}}$, if $i \sim j$, and 0 otherwise. Denote by $f_1 \geq f_2 \geq \cdots \geq f_n$ the eigenvalues of RA. Upper and lower bounds for f_i, $i = 1,2,\ldots,n$ are obtained.

Keywords: Topological indices, adjacency matrices, bounds of eigenvalues.

1 Introduction

Let $G = (V,E)$, $V = \{1,2,\ldots,n\}$, be a simple connected graph of order n and size m, with the sequence of vertex degrees $d_1 \geq d_2 \geq \cdots \geq d_n > 0$, $d_i = d(i)$. If vertices i and j are adjacent, we write $i \sim j$. Let $F(x,y)$ be a real symmetric function, that is $F(x,y) = F(y,x)$. With

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

we denote a class of vertex–degree-based (VDB) topological indices (see [9]). To each such index we can join Randić VDB adjacency matrix $RA = (r_{ij})$, of order $n \times n$, defined as

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

Manuscript received December 2 2017; accepted May 12, 2018.

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As matrix RA is real and symmetric, its eigenvalues $f_1 \geq f_2 \geq \cdots \geq f_n$ are real also. It is easily to observe that

$$\operatorname{tr}(RA) = \sum_{i=1}^{n} f_i = 0\,, \tag{1}$$

and

$$\operatorname{tr}(RA^2) = \sum_{i=1}^{n} f_i^2 = 2\sum_{i\sim j} \frac{F(d_i,d_j)^2}{d_i d_j}\,, \tag{2}$$

where $\operatorname{tr}(RA)$ and $\operatorname{tr}(RA^2)$ are traces of matrices RA and RA^2, respectively.

In this paper we are interested in bounds for f_i, $i = 1,2,\ldots,n$.

2 Preliminaries

In this section we recall definitions of some VDB indices that are of interest for our work.

Among the oldest VDB indices are the first and the second Zagreb index, M_1 and M_2, defined as [10, 11]:

$$M_1 = M_1(G) = \sum_{i=1}^{n} d_i^2 \quad \text{and} \quad M_2 = M_2(G) = \sum_{i\sim j} d_i d_j.$$

In [17] it was observed that

$$M_1 = \sum_{i\sim j} (d_i + d_j)\,. \tag{3}$$

Denote with $e = ij$ an arbitrary edge of graph G. Then the edge degree is defined as $d(e) = d_i + d_j - 2$. Since from (3) we have that

$$M_1 = \sum_{i=1}^{m} (d(e_i) + 2)\,,$$

the index M_1 can be considered as edge–degree-based topological index as well. Details of the theory and applications of the two Zagreb indices can be found in surveys [1, 3, 4, 12, 17] and in the references quoted therein.

Generalization of the second Zagreb index, reported in [21], known as general Randić index, 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. For $\alpha = -\frac{1}{2}$, the connectivity or Randić index, $R = R(G)$, [19] is obtained. For $\alpha = -1$, general Randić R_{-1} index is obtained (see [7]), also met under the name *modified second Zagreb index*, see for example [17]. For $\alpha = \frac{1}{2}$, the reciprocal Randić index, RR, defined in [13] is obtained.

The symmetric division deg index, *SDD*, was introduced in [20] and defined as

$$SDD = SDD(G) = \sum_{i\sim j} \frac{d_i^2 + d_j^2}{d_i d_j}\,.$$

As the quantitative topological characterization of irregularity of graphs, Albertson [2] proposed a measure defined as

$$Alb = Alb(G) = \sum_{i\sim j} |d_i - d_j|,$$

which is usually referred to as the Albertson index [13], although the name ”third Zagreb index” has also been proposed [22].

3 Main result

In the next theorem we determine bounds for eigenvalues $f_1 \geq f_2 \geq \cdots \geq f_n$ of matrix RA.

Theorem 3.1. *The following inequalities are valid for the eigenvalues* $f_1 \geq f_2 \geq \cdots \geq f_n$ *of matrix RA*

$$\begin{aligned}
\sqrt{\frac{\mathrm{tr}(RA^2)}{n(n-1)}} &\leq f_1 \leq \sqrt{\frac{(n-1)\mathrm{tr}(RA^2)}{n}}\,,\\
-\sqrt{\frac{(i-1)\mathrm{tr}(RA^2)}{n(n-i+1)}} &\leq f_i \leq \sqrt{\frac{(n-i)\mathrm{tr}(RA^2)}{in}}, \quad i = 2,3,\ldots,n-1\,, \\
-\sqrt{\frac{(n-1)\mathrm{tr}(RA^2)}{n}} &\leq f_n \leq -\sqrt{\frac{\mathrm{tr}(RA^2)}{n(n-1)}}\,.
\end{aligned} \tag{4}$$

Proof. Let $P_n(a_1,a_2)$ be a class of real polynomials, with real roots, of the form

$$P_n(x) = x^n + a_1 x^{n-1} + a_2 x^{n-2} + b_3 x^{n-3} + \cdots + b_n\,,$$

where the coefficients a_1 and a_2 are fixed. In [14] it was proven that for the roots of this polynomial, $x_1 \geq x_2 \geq \cdots \geq x_n$, hold

$$\begin{aligned}
\bar{x} + \frac{1}{n}\sqrt{\frac{\Delta}{n-1}} &\leq x_1 \leq \bar{x} + \frac{1}{n}\sqrt{(n-1)\Delta},\\
\bar{x} - \frac{1}{n}\sqrt{\frac{(i-1)\Delta}{n-i+1}} &\leq x_i \leq \bar{x} + \frac{1}{n}\sqrt{\frac{(n-i)\Delta}{i}}, \quad i = 2,3,\ldots,n-1\,, \\
\bar{x} - \frac{1}{n}\sqrt{(n-1)\Delta} &\leq x_n \leq \bar{x} - \frac{1}{n}\sqrt{\frac{\Delta}{n-1}}\,,
\end{aligned} \tag{5}$$

where

$$\bar{x} = \frac{1}{n}\sum_{i=1}^{n} x_i \qquad \text{and} \qquad \Delta = n\sum_{i=1}^{n} x_i^2 - \left(\sum_{i=1}^{n} x_i\right)^2 . \tag{6}$$

Now consider the polynomial

$$P_n(x) = \prod_{i=1}^{n}(x - f_i) = x^n + a_1 x^{n-1} + a_2 x^{n-2} + b_3 x^{n-3} + \cdots + b_n . \tag{7}$$

Since by Vieta's formulas we have

$$a_1 = \sum_{i=1}^{n} f_i = 0 \qquad \text{and} \qquad a_2 = \frac{1}{2}\left(\left(\sum_{i=1}^{n} f_i\right)^2 - \sum_{i=1}^{n} f_i^2\right) = -\frac{1}{2}\mathrm{tr}(RA^2)$$

the polynomial (7) belongs $P_n(0, -\frac{1}{2}\mathrm{tr}(RA^2))$. According to (6) we have

$$\bar{x} = \frac{1}{n}\sum_{i=1}^{n} f_i = 0 \qquad \text{and} \qquad \Delta = n\sum_{i=1}^{n} f_i^2 - \left(\sum_{i=1}^{n} f_i\right)^2 = n\mathrm{tr}(RA^2) .$$

From the above identities and (5) we arrive at (4). □

Let us consider some special cases of Theorem 3.1.

- For $F(d_i, d_j) = \sqrt{d_i d_j}$, that is for $TI = RR$, the corresponding adjacency matrix $RA = (r_{ij})$ is defined by

$$r_{ij} = \begin{cases} 1, & \text{if } i \sim j \\ 0, & \text{otherwise} \end{cases} .$$

  Obviously, the matrix RA coincides with ordinary adjacency matrix of G. From (4) we have that for its eigenvalues $\lambda_1 \geq \lambda_2 \geq \cdots \geq \lambda_n$ hold

$$\begin{aligned} \sqrt{\frac{2m}{n(n-1)}} &\leq \lambda_1 \leq \sqrt{\frac{2(n-1)m}{n}} , \\ -\sqrt{\frac{2(i-1)m}{n(n-i+1)}} &\leq \lambda_i \leq \sqrt{\frac{2(n-i)m}{in}}, \quad i = 2, 3, \ldots, n-1 , \\ -\sqrt{\frac{2(n-1)m}{n}} &\leq \lambda_n \leq -\sqrt{\frac{2m}{n(n-1)}} . \end{aligned}$$

  The above inequalities were proven in [15] (see also [6, 8]).

- For $F(d_i,d_j) = d_i d_j$, that is $TI = M_2$, the matrix $RA = (r_{ij})$ is defined as

$$r_{ij} = \begin{cases} \sqrt{d_i d_j}, & \text{if } i \sim j, \\ 0, & \text{otherwise.} \end{cases}$$

For its eigenvalues, $f_1 \geq f_2 \geq \cdots \geq f_n$, the following inequalities are valid

$$\begin{aligned} \sqrt{\frac{2M_2}{n(n-1)}} &\leq f_1 \leq \sqrt{\frac{2(n-1)M_2}{n}}, \\ -\sqrt{\frac{2(i-1)M_2}{n(n-i+1)}} &\leq f_i \leq \sqrt{\frac{2(n-i)M_2}{in}}, \quad i = 2,3,\ldots,n-1, \\ -\sqrt{\frac{2(n-1)M_2}{n}} &\leq f_n \leq -\sqrt{\frac{2M_2}{n(n-1)}}. \end{aligned}$$

- For $F(d_i,d_j) = 1$, the matrix $RA = (r_{ij})$ becomes the Randić matrix [5] (see also [8, 16]). For its eigenvalues, $r_1 \geq r_2 \geq \cdots \geq r_n$, hold

$$\begin{aligned} \sqrt{\frac{2R_{-1}}{n(n-1)}} &\leq r_1 \leq \sqrt{\frac{2(n-1)R_{-1}}{n}}, \\ -\sqrt{\frac{2(i-1)R_{-1}}{n(n-i+1)}} &\leq r_i \leq \sqrt{\frac{2(n-i)R_{-1}}{in}}, \quad i = 2,3,\ldots,n-1, \\ -\sqrt{\frac{2(n-1)R_{-1}}{n}} &\leq r_n \leq -\sqrt{\frac{2R_{-1}}{n(n-1)}}. \end{aligned}$$

- For $F(d_i,d_j) = d_i + d_j$, that is for $TI = M_1$, the matrix $RA = (r_{ij})$ is defined as

$$r_{ij} = \begin{cases} \sqrt{\frac{d_i}{d_j}} + \sqrt{\frac{d_j}{d_i}}, & \text{if } i \sim j, \\ 0, & \text{otherwise.} \end{cases}$$

For its eigenvalues, $f_1 \geq f_2 \geq \cdots \geq f_n$, the following is valid

$$\begin{aligned} \sqrt{\frac{2(SDD+2m)}{n(n-1)}} &\leq f_i \leq \sqrt{\frac{2(n-1)(SDD+2m)}{n}}, \\ -\sqrt{\frac{2(i-1)(SDD+2m)}{n(n-i+1)}} &\leq f_i \leq \sqrt{\frac{2(n-i)(SDD+2m)}{in}}, \quad i = 2,3,\ldots,n-1, \\ -\sqrt{\frac{2(n-1)(SDD+2m)}{n}} &\leq f_n \leq -\sqrt{\frac{2(SDD+2m)}{n(n-1)}}. \end{aligned}$$

- For $F(d_i,d_j) = |d_i - d_j|$, that is $TI = Alb$, matrix $RA = (r_{ij})$ is given by

$$r_{ij} = \begin{cases} \frac{|d_i-d_j|}{\sqrt{d_id_j}}, & \text{if } i \sim j\,, \\ 0, & \text{otherwise}\,. \end{cases}$$

  For its eigenvalues, $f_1 \geq f_2 \geq \cdots \geq f_n$, the following is valid

$$\begin{aligned} \sqrt{\frac{2(SDD-2m)}{n(n-1)}} &\leq f_i \leq \sqrt{\frac{2(n-1)(SDD-2m)}{n}}\,, \\ -\sqrt{\frac{2(i-1)(SDD-2m)}{n(n-i+1)}} &\leq f_i \leq \sqrt{\frac{2(n-i)(SDD-2m)}{in}}\,, \quad i = 2,3,\ldots,n-1\,, \\ -\sqrt{\frac{2(n-1)(SDD-2m)}{n}} &\leq f_n \leq -\sqrt{\frac{2(SDD-2m)}{n(n-1)}}\,. \end{aligned}$$

Theorem 3.2. *For the eigenvalues $f_2 \geq f_2 \geq \cdots \geq f_n$, of matrix RA the following is valid:*

$$\begin{aligned} f_1 &\geq \sqrt{\frac{2}{n(n-1)}}\frac{TI}{\sqrt{M_2}} \\ f_i &\geq -\sqrt{\frac{2(i-1)}{n(n-i+1)}}\frac{TI}{\sqrt{M_2}}, \quad i = 2,3,\ldots,n-1\,, \\ f_n &\geq -\sqrt{\frac{2(n-1)}{n}}\frac{TI}{\sqrt{M_2}}\,. \end{aligned} \tag{8}$$

Proof. Let $a = (a_i)$ and $x = (x_i)$, $i = 1,2,\ldots,n$, be two positive real number sequences. For any real r, $r \geq 0$, holds (see [18])

$$\sum_{i=1}^{n} \frac{x_i^{r+1}}{a_i^r} \geq \frac{(\sum_{i=1}^{n} x_i)^{r+1}}{(\sum_{i=1}^{n} a_i)^r}\,.$$

For $r = 1$, $x_i := F(d_i,d_j)$, $a_i := d_id_j$, where summation is performed over all edges of G, the above inequality transforms into

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

that is

$$\sum_{i\sim j} \frac{F(d_i,d_j)^2}{d_id_j} \geq \frac{TI^2}{M_2}\,. \tag{9}$$

From the above and (2) we have that

$$\operatorname{tr}(RA^2) = 2\sum_{i\sim j} \frac{F(d_i, dj)^2}{d_i d_j} \geq \frac{2TI^2}{M_2}.$$

From the above and (4) we arrive at (8). □

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