Applied Mathematics and
Computer Science
1 (1) (2016), 9–13

Published by Faculty of Sciences and Mathematics,
University of Niš, Serbia
Available at: http://www.pmf.ni.ac.rs/amcs

Remarks on lower bounds of the general Randić index R_{-1} of graph

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Abstract. Let $G = (V, E)$, $V = \{1, 2, \dots, n\}$ be a simple graph with $n \geq 2$ vertices and m edges with vertex degree sequence $d_1 \geq d_2 \geq \cdots \geq d_n$. Topological degree–based index of graph $R_\alpha = \sum_{i\sim j}(d_i d_j)^\alpha$, where $i \sim j$ denotes that vertices i and j are adjacent, is referred to as general Randić index. We consider the case when $\alpha = -1$ and obtain lower bound for R_{-1} and lower and upper bounds of normalized Laplacian eigenvalues.

1. Introduction

Let $G = (V, E)$ be an undirected simple, connected graph with $n \geq 2$ vertices and m edges, with vertex degree sequence $d_1 \geq d_2 \geq \cdots \geq d_n$, $d_i = d(i)$, $i = 1, 2, \dots, n$. If two vertices are adjacent we denote it as $i \sim j$.

The general Randic index R_α defined by Bollobas and Erdös [1]

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

where α is a given parameter, is generalization of the classic index, where $\alpha = -\frac{1}{2}$, introduced by Randic in 1975 [13]. The Randić index is an important molecular descriptor and has been closely related with many physico-chemical properties of alkanes, such as boiling points, surface areas, energy levels, etc. For details of chemical applications of the general Randić index see for example [7–9, 13, 14]. On other topological degree–based indices of graphs and their applications one can refer to [5, 6, 15].

If $\mathbf{A}$ is the adjacency matrix of graph G and $\mathbf{D} = \mathrm{diag}(d_1, d_2, \dots, d_n)$ the diagonal matrix of order $n \times n$, then $\mathbf{L} = \mathbf{D} - \mathbf{A}$ is the Laplacian matrix od G. Since G is connected, the matrix $\mathbf{D}$ is nonsingular, so $\mathbf{D}^{-1}$ is well defined. Matrix $\mathbf{L}^* = \mathbf{D}^{-1/2}\mathbf{L}\mathbf{D}^{-1/2} = \mathbf{I} - \mathbf{D}^{-1/2}\mathbf{A}\mathbf{D}^{-1/2}$ is called the normalized Laplacian matrix of graph G. Eigenvalues of $\mathbf{L}^*$, $\rho_1 \geq \rho_2 \geq \cdots \geq \rho_{n-1} > \rho_n = 0$, are normalized Laplacian eigenvalues of graph G. Some of their well known properties are [17]

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

2010 *Mathematics Subject Classification*. 05C50.
Keywords. Normalized Laplacian eigenvalues; general Randić index.
Received: 8 May 2016; Accepted: 6 June 2016
Communicated by Dragan S. Djordjevic
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where $R_{-1} = \sum_{i\sim j} \frac{1}{d_i d_j}$ is general Randić index obtained for $\alpha = -1$.

The general Randić index can be exactly determined only for some particular classes of graphs. Therefore, it is important to derive inequalities that set up lower and upper bounds for this invariant, in terms of other graph parameters (see for example [2, 3, 7, 8, 11, 12, 16]). In the present article we establish lower bound for R_{-1}. In addition, we determine lower and upper bounds for the normalized Laplacian eigenvalues of graph, ρ_i, $i = 1, 2, \ldots, n-1$. The obtained results improve the one published in [16].

2. Preliminaries

In the sequel we recall the results from [16] that are of interest for our work.

Lemma 2.1. [16]. *Let G be a simple connected graph on n vertices. If*

$$\rho_1 \leq \frac{2}{\sum_{i=1}^{n} d_i^{-2}}, \tag{2.1}$$

then

$$R_{-1} \geq \frac{n-1}{2(n-2)} \left(\rho_1 - \frac{n}{n-1}\right)^2 + \frac{n}{2(n-1)}. \tag{2.2}$$

Lemma 2.2. [16] *Let G be a simple connected graph. If*

$$R_{-1} \leq 1, \tag{2.3}$$

then

$$\rho_1 \leq \frac{n}{n-1} + \sqrt{\frac{n-2}{n-1}\left(2R_{-1} - \frac{n}{n-1}\right)}. \tag{2.4}$$

In the text that follows we prove the inequality that is more general than (2.2). Then, we prove the inequality that establishes lower and upper bounds for all normalized Laplacian eigenvalues ρ_i, $i = 1, 2, \ldots, n-1$, in terms of n and R_{-1}, and n, d_1 and d_n. The inequality (2.4) will be obtained as a particular case of our results. Also, we prove that conditions (2.1) and (2.3) are needless.

3. Main result

Theorem 3.1. *Let $G = (V, E)$ be a simple connected graph with $n \geq 3$ vertices and m edges. Then, for any real k with the property $\rho_1 \geq k \geq \rho_{n-1}$.*

$$R_{-1} \geq \frac{n-1}{2(n-2)} \left(k - \frac{n}{n-1}\right)^2 + \frac{n}{2(n-1)}. \tag{3.1}$$

equality holds if and only if $k = \frac{n}{n-1}$ and $G \cong K_n$.

Proof In [10], a class $\mathcal{P}_n(a_1, a_2)$ of polynomials, with real roots, of the form

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

was considered, where a_1 and a_2 are fixed real numbers. It was proved that for the roots $x_1 \geq x_2 \geq \cdots \geq x_n$, of that class of polynomials, the following inequalities are valid

$$\bar{x} + \frac{1}{n}\sqrt{\frac{\Delta}{n-1}} \leq x_1 \leq \bar{x} + \frac{1}{n}\sqrt{(n-1)\Delta} \tag{3.2}$$

$$\bar{x} - \frac{1}{n}\sqrt{\frac{i-1}{n-i+1}\Delta} \leq x_i \leq \bar{x} + \frac{1}{n}\sqrt{\frac{n-i}{i}\Delta}, \qquad 2 \leq i \leq n-1 \tag{3.3}$$

$$\bar{x} - \frac{1}{n}\sqrt{(n-1)\Delta} \leq x_n \leq \bar{x} - \frac{1}{n}\sqrt{\frac{\Delta}{n-1}} \tag{3.4}$$

where

$$\bar{x} = \frac{1}{n}\sum_{i=1}^{n} x_i \quad \text{and} \quad \Delta = n\sum_{i=1}^{n} x_i^2 - \left(\sum_{i=1}^{n} x_i\right)^2 . \tag{3.5}$$

Consider now the polynomial

$$\begin{aligned} \varphi(x) &= xP_{n-1}(x) = x\prod_{i=1}^{n-1}(x-\rho_i) = \\ &= x\left(x^{n-1} + a_1x^{n-2} + a_2x^{n-3} + b_3x^{n-4} + \cdots + b_{n-1}\right). \end{aligned}$$

Since

$$\begin{aligned} a_1 &= -\sum_{i=1}^{n-1}\rho_i = -n \quad \text{and} \\ a_2 &= \frac{1}{2}\left(\left(\sum_{i=1}^{n-1}\rho_i\right)^2 - \sum_{i=1}^{n-1}\rho_i^2\right) = \frac{1}{2}(n^2 - n - 2R_{-1}), \end{aligned}$$

the polynomial $P_{n-1}(x)$ belongs to a class $\mathcal{P}_{n-1}\left(-n, \frac{1}{2}(n^2-n-2R_{-1})\right)$. According to (3.5) for $n := n-1$, $x_i = \rho_i$, $i = 1, 2, \ldots, n-1$, we have

$$\bar{x} = \frac{1}{n-1}\sum_{i=1}^{n-1}\rho_i = \frac{n}{n-1}$$

and

$$\Delta = (n-1)\sum_{i=1}^{n-1}\rho_i^2 - \left(\sum_{i=1}^{n-1}\rho_i\right)^2 = 2(n-1)R_{-1} - n.$$

Now, for any k with the property $\rho_1 \geq k \geq \rho_{n-1}$, according to (3.2) we have

$$k \leq \rho_1 \leq \frac{n}{n-1} + \frac{1}{n-1}\sqrt{(n-2)(2(n-1)R_{-1} - n)},$$

i.e.

$$(n-1)k - n \leq \sqrt{(n-2)(2(n-1)R_{-1} - n)}. \tag{3.6}$$

On the other hand, based on (3.4) we have that

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

i.e.

$$n - (n-1)k \leq \sqrt{(n-2)(2(n-1)R_{-1} - n)}. \tag{3.7}$$

According to (3.6) and (3.7) we have that

$$|n - (n-1)k| \leq \sqrt{(n-2)(2(n-1)R_{-1} - n)}$$

wherefrom we obtain the required result.

□

Remark 3.2. *For $k = \rho_1$ from (3.1) the inequality (2.2) follows. Also, for any $k = \rho_i$, $1 \le i \le n-1$,*

$$R_{-1} \ge \frac{n-1}{2(n-2)}\left(\rho_i - \frac{n}{n-1}\right)^2 + \frac{n}{2(n-1)}.$$

Equality holds if and only if $G \cong K_n$. It is easy to conclude that the condition (2.1) in Lemma 2.1 is needless.

For $n := n-1$, $x_i = \rho_i$, $i = 1, 2, \dots, n$, from (3.2), (3.3) (3.4) and (3.5), we obtain the following result:

Theorem 3.3. *Let $G = (V, E)$ be a simple connected graph with $n \ge 3$ vertices and m edges. Then*

$$\begin{aligned} &\frac{n}{n-1} + \frac{1}{n-1}\sqrt{\frac{2(n-1)R_{-1} - n}{n-2}} \le \\ &\le \rho_1 \le \frac{n}{n-1} + \frac{1}{n-1}\sqrt{(n-2)(2(n-1)R_{-1} - n)}, \end{aligned} \tag{3.8}$$

$$\begin{aligned} &\frac{n}{n-1} - \frac{1}{n-1}\sqrt{\frac{i-1}{n-i}(2(n-1)R_{-1} - n)} \le \\ \le\ &\rho_i \le \frac{n}{n-1} + \frac{1}{n-1}\sqrt{\frac{n-i-1}{i}(2(n-1)R_{-1} - n)},\ 2 \le i \le n-2, \end{aligned}$$

$$\begin{aligned} &\frac{n}{n-1} - \frac{1}{n-1}\sqrt{(n-2)(2(n-1)R_{-1} - n)} \le \rho_{n-1} \le \\ &\le \frac{n}{n-1} - \frac{1}{n-1}\sqrt{\frac{2(n-1)R_{-1} - n}{n-2}}. \end{aligned} \tag{3.9}$$

Equalities hold if and only if $G \cong K_n$.

Remark 3.4. *Right-hand side of the inequality (3.8) coincides with (2.4). It is obvious that the condition (2.3), from Lemma 2.2, is needless. Let us note that left-hand side of (3.8) as well as right-hand part of (3.9) were proved in [16].*

The following inequality was proved in [2]:

$$\frac{n}{2d_1} \le R_{-1} \le \frac{n}{2d_n}.$$

Having that in mind, the following corollary of the Theorem 3.3 is obtained.

Corollary 3.5. *Let $G = (V, E)$ be a simple graph with $n \ge 2$ vertices and m edges. Then*

$$\begin{aligned} &\frac{n}{n-1} + \frac{1}{n-1}\sqrt{\frac{n(n-1-d_1)}{(n-2)d_1}} \le \rho_1 \le \\ &\le \frac{n}{n-1} + \frac{1}{n-1}\sqrt{\frac{n(n-2)(n-1-d_n)}{d_n}}, \\ &\frac{n}{n-1} - \frac{1}{n-1}\sqrt{\frac{n(i-1)(n-1-d_n)}{(n-i)d_n}} \le \rho_i \le \\ &\le \frac{n}{n-1} + \frac{1}{n-1}\sqrt{\frac{n(n-i-1)(n-1-d_n)}{id_n}}, \quad 2 \le i \le n-2 \\ &\frac{n}{n-1} - \frac{1}{n-1}\sqrt{\frac{n(n-2)(n-1-d_n)}{d_n}} \le \rho_1 \le \\ &\le \frac{n}{n-1} - \frac{1}{n-1}\sqrt{\frac{n(n-1-d_1)}{(n-2)d_1}}, \end{aligned}$$

equalities hold if and only if $G \cong K_n$.

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