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On Some new bounds on the spectral radius and the energy of graphs

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ABSTRACT: Let $G = (V, E)$ be a simple connected graph. For any $v \in V$, the maximum neighbourhood degree $m(v)$ is the maximum vertex degree in the neighbourhood $N(v)$. In this paper, we present some new bounds on the spectral radius $\lambda_1(G)$ of G in terms of degrees and maximum neighbourhood degrees of the graph G. Also, we present some new bounds on the energy $E(G)$ of G.

Key Words: Degrees of graphs, maximum neighbourhood degrees, spectral radius, energy of graphs

Contents

1. Introduction

Let $G(V, E)$ be a simple connected graph with the vertex set $V = \{v_1, v_2, ..., v_n\}$. For $v_i \in V$, $(1 \leq i \leq n)$, the neighbourhood $N(v_i)$ is the set of vertices adjacent to v_i and the number of vertices in $N(v_i)$ is the degree of v_i denoted d_i. The maximum vertex degree in $N(v_i)$ is the maximum neighbourhood degree of v_i denoted $m(v_i) = m_i$, $(1 \leq i \leq n)$. Then $MAXNDEG(G) = \{m_1, m_2, ..., m_n\}$ is the maximum neighbourhood degree sequence of the graph G. In network topology, a neighbourhood degree sequence is an important tool for studying the unique characteristics of complex networks. Barrus and Donovan [2] pioneered the study of neighbourhood degree lists (NDL) as a topological invariant of graphs in mathematics. Nishimura and Subramanaya [20] initiated the use of NDL for the combinatorial problem of a graph of changing it into one with given neighbourhood degrees. Amotz Bar-Noy et. al [1] studied neighbourhood degree profiles by dealing with the problem of realizing maximum and minimum neighbourhood degree profiles and gave a complete characterization for $MAXNDEG(G)$ realizable profiles of a graph.

For a graph G with the vertex set $\{v_1, v_2, ..., v_n\}$, the adjacency matrix $A(G) = [a_{ij}]$ of G is a real symmetric matrix of order n such that $a_{ij} = 1$ if v_i and v_j are adjacent and zero otherwise. Let $\lambda_1 \geq \lambda_2 \geq .... \geq \lambda_n$ be the eigenvalues of G. The largest eigenvalue $\lambda_1(G) = \lambda_1$ is the spectral radius of G and the set $\{\lambda_1, \lambda_2, ..., \lambda_n\}$ is referred to as the spectrum of G. Studying the spectral radius of graphs has always been of ample interest in spectral graph theory. For results on the spectral radius, we refer to [4] and [5]. Several bounds on the spectral radius of graphs have been established in [6], [14], [15], [21], etc in terms of various parameters of graphs. The energy $E(G)$ of a graph G is defined as $E(G) = \sum_{i=1}^{n} |\lambda_i|$. This spectrum-based graph parameter is introduced by I. Gutman [10]. It has been studied extensively in mathematics as well as in chemistry. For results on the energy of graphs, we refer to [9], [10], [11], [12], [13], [16] etc.

There are many upper and lower bounds on the spectral radius $\lambda_1(G)$ of a graph G in terms of its degrees. Nevertheless, there are no such bounds in terms of $MAXNDEG(G)$ of G. It is to be noted that $MAXNDEG(G)$ of a graph G is such a tool that reveals many of the structural properties of the graph G. In this paper, we are intending to explore some latent properties of graphs in terms of $MAXNDEG(G)$. Here, we present some new bounds on the spectral radius $\lambda_1(G)$ and the energy $E(G)$ of G in terms of

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its maximum neighbourhood degree profile. In section 2, we present some new bounds on the spectral radius of graphs involving the maximum neighbourhood degree sequence of the graph. In addition, we present some examples of graphs with our bounds on spectral radius $\lambda_1(G)$ in contrast to some other degree-based bounds on spectral radius $\lambda_1(G)$ dealt in [3], [8], [15], [22], etc. In section 3, we investigate some bounds on the energy of graphs in terms of degrees and maximum neighbourhood degrees of G.

2. Bounds on $\lambda_1(G)$ involving degrees and maximum neighbourhood degrees

Let G be a connected graph with n vertices and degree sequence $\{d_1, d_2, ..., d_n\}$. In [3], L. Collatz et. al proved the inequality

$$\lambda_1 \geq \sqrt{\frac{1}{n}\sum_{i=1}^{n} d_i^2} \tag{2.1}$$

with equality in (2.1) if only if G is regular or a semi-regular graph.
In [8], O. Favaron et. al gave the following lower bound on λ_1,

$$\lambda_1 \geq \sqrt{\Delta} \tag{2.2}$$

where Δ is the maximum degree of G. The equality in (2.2) holds if and only if G is $\frac{n}{2}K_2$.
They proved another degree-based lower bound in [8] such as

$$\lambda_1 \geq \frac{1}{e}\sum_{ij\in E}\sqrt{d_i d_j} \tag{2.3}$$

where e is the number of edges in G.
In the year 2004, A. Yu et. al [22] proved the inequality

$$\lambda_1 \geq \sqrt{\frac{\sum_{v_i\in V} d_2^2(v_i)}{\sum_{v_i\in V} d^2(v_i)}} \tag{2.4}$$

where $d_2(v_i) = \sum_{v_j\in N(v_i)} d(v_j), (1 \leq i \leq n)$. The equality in (2.4) holds if and only if G is a pseudo-regular or a strictly pseudo-semi regular graph. Later in the year 2006, Y. Hou et. al [15] generalised the bound (2.4) as follows

$$\lambda_1 \geq \sqrt{\frac{\sum_{v_i\in V} d_{k+1}^2(v_i)}{\sum_{v_i\in V} d_k^2(v_i)}} \tag{2.5}$$

where $d_{k+1}(v_i) = \sum_{v_j\in N(v_i)} d_k(v_j)$, $(1 \leq i, j \leq n)$. The equality in (2.5) holds if and only if $A^{k+2}(G)j = \lambda_1^2(G)A^k(G)j$.
Now, let G be a graph with n vertices and $MAXNDEG(G) = \{m_1, m_2, ..., m_n\}$. Consider the vector $M = (\sqrt{m_1}, \sqrt{m_2}, ..., \sqrt{m_n})^T$ and the diagonal matrix $D = diag(\sqrt{d_1}, \sqrt{d_2}, ..., \sqrt{d_n})$.
Then

$$DM = (\sqrt{d_1 m_1}, \sqrt{d_2 m_2}, ..., \sqrt{d_n m_n})^T$$

If G is a regular graph, $d_i = m_i = \sqrt{d_i m_i}, (1 \leq i \leq n)$. For any vertex $v_i \in V$, $(1 \leq i \leq n)$, by quasi-average d_i' we mean $\frac{\sum_{u_j\in N(u_i)}\sqrt{d_j m_j}}{\sqrt{d_i m_i}}$. If the graph G is such that

$$\frac{\sum_{u_j\in N(u_i)}\sqrt{d_j m_j}}{\sqrt{d_i m_i}} = a(say)$$

for $1 \leq i \leq n$, we call it a quasi-regular graph. A regular graph is quasi-regular. A bipartite graph is $(a-b)$ quasi-regular if each vertex in the same part of the bi-partition has the equal quasi-averages viz: a and b. A graph is called $(a-b)$ semi-regular [15] if $\{d(u_i), d(u_j)\} = \{a, b\}$ holds for any edge $u_i u_j \in E$. A $(a-b)$ semi-regular graph is quasi-regular bipartite.
Now, by Rayleigh's quotient, we have

$$\lambda_1^2 \geq \frac{(D')^T A^2 (D\prime)}{<D',D'>}$$

where $D' = DM$ gives

$$\lambda_1^2 \geq \frac{\sum_{i=1}^{n}\left(\sum_{u_j \in N(u_i)} \sqrt{d_j m_j}\right)^2}{\sum_{i=1}^{n} d_i m_i}$$

Thus we state the following lower bound on the spectral radius λ_1 of G.

Theorem 2.1 *Let G be a graph with n vertices. If $\{d_1, d_2, ..., d_n\}$ and $\{m_1, m_2, ..., m_n\}$ be the degree and the maximum neighbourhood degree sequence of G respectively, then*

$$\lambda_1 \geq \sqrt{\frac{\sum_{i=1}^{n}\left(\sum_{u_j \in N(u_i)} \sqrt{d_j m_j}\right)^2}{\sum_{i=1}^{n} d_i m_i}} \tag{2.6}$$

with the equality if and only if G is a quasi-regular or quasi-regular bipartite graph.

It is to be noted that for a regular graph G, the bound (2.6) gives the bound (2.4).

Corollary 2.1 *Let G be a graph with n vertices and let $\{v_1, v_2, ..., v_r\}$ be the set of all vertices of G such that $d(v_i) = \Delta$, $(1 \leq i \leq r)$. Then*

$$\lambda_1 \geq \sqrt{\frac{\sum_{i=1}^{n}\left(\sum_{u_j \in N(u_i)} d_j m_j\right)^2}{\left(r\Delta^3 + (n - r\Delta)(\Delta')^2\right)}} \tag{2.7}$$

, where Δ' is the second largest of the degrees of G. The equality in (2.7) holds if G is a regular graph.

Proof: Clearly $|\bigcup_{i=1}^{r} N(u_i)| \leq \sum_{i=1}^{r} |N(u_i)| = r\Delta$. Since $m(v) = \Delta$ for any $v \in \bigcup_{i=1}^{r} N(u_i)$ and $m(w) \leq \Delta'$ for any $w \in V \setminus \bigcup_{i=1}^{r} N(u_i)$, therefore $d_1 m_1 + d_2 m_2 + ... + d_n m_n \leq r\Delta\Delta^2 + (n - r\Delta)(\Delta')^2 = r\Delta^3 + (n - r\Delta)(\Delta')^2$ gives the inequality (2.7).
If G is a k-regular graph, $r = n$ and $\Delta = k = \Delta'$ which lead to the equality of the bound (2.7). □

Note that $m_i \leq (n-1)$, $(1 \leq i \leq n)$. Since $\sum_{i=1}^{n} d_i = 2e$, we obtain $d_1 m_1 + d_2 m_2 + ... + d_n m_n \leq 2e(n-1)$. Thus we state the following corollary.

Corollary 2.2 *Let G be a graph with n vertices and e edges. Then*

$$\lambda_1 \geq \sqrt{\frac{\sum_{i=1}^{n}\left(\sum_{u_j \in N(u_i)} \sqrt{d_j m_j}\right)^2}{2e(n-1)}} \tag{2.8}$$

The equality in (2.8) holds if G is a complete graph.

Example 2.1 For the graphs in Figure 1 and Figure 2, in the table 1 we present the following list of values of the spectral radius λ_1 and of the bounds (2.1), (2.2), (2.3), (2.4), (2.6), and (2.8) up to 5 decimal places.

Here we get that our bound (2.6) is better than the bounds (2.1), (2.2), (2.3) and (2.4) for the graphs G_1, G_2, G_3, G_4 and G_5, but it is not always true nevertheless. For example, the bounds (2.3) and (2.4) give stricter value than that of the bound (2.6) in the case of graph G_6. Note that graphs G_1 and G_2 are isomorphic and the values of each of the bounds are equal in the case of graph G_1 and G_2. The values of the bounds (2.6) and (2.8) are equal for each of the graphs G_1, G_2 and G_4.
Now, let G be a graph with n vertices. A k-walks is a sequence of vertices $v_1, v_2, ..., v_k$ such that $v_i v_{i+1} \in E$, $(1 \leq i \leq k-1)$. For any vertex v_i, $W_k(v_i)$ counts the k-walks starting with v_i and $W_k(G) = \sum_{i=1}^{n} W_k(v_i)$ is the count of k-walks of G. In [4], the number of k-walks in terms of the spectrum of the graph is given as follows.

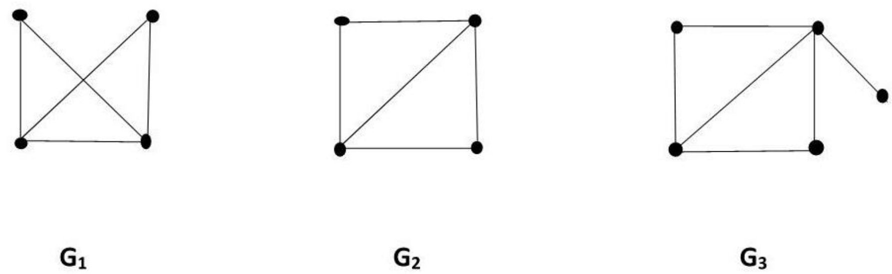

Figure 1:

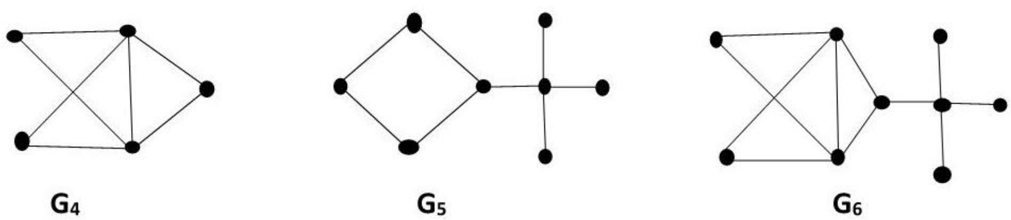

Figure 2:

	λ_1	(2.1)	(2.2)	(2.3)	(2.4)	(2.6)	(2.8)
G_1	2.56155	2.54950	1.73205	2.55959	2.55704	2.56117	2.56117
G_2	2.56155	2.54950	1.73205	2.55959	2.55704	2.56117	2.56117
G_3	2.68554	2.60768	2	2.66998	2.66789	2.67508	2.56119
G_4	3	2.96647	2	2.99579	2.98481	2.99929	2.99929
G_5	2.32684	2.23606	2	2.29538	2.31300	2.31725	1.57894
G_6	3.07247	2.74873	2	2.88236	2.96548	2.88120	1.99047

Table 1:

Theorem 2.2 (4,pp44) *Let G be a graph with n vertices and $v_1, v_2, ..., v_n$ be the orthogonal unit eigen vectors corresponding to the eigen values $\lambda_1, \lambda_2, ..., \lambda_n$, respectively. If $v_i = (v_{i_1}, v_{i_2}, ..., v_{i_n})$, $i \in \{1, 2, ..., n\}$ and $c_i = (\sum_{j=1}^{n} v_{i_j})^2$, then*

$$W_k(G) = c_1\lambda_1^{k-1} + c_2\lambda_2^{k-1} + ... + c_n\lambda_n^{k-1} \tag{2.9}$$

for every $k \geq 1$.

In particular, for $k = 1, 2$ we get $n = c_1 + c_2 + ... + c_n$ and $W_2(G) = c_1\lambda_1 + c_2\lambda_2 + ... + c_n\lambda_n$. Note that if $m(v_i) = d_k$ for some k, $(1 \leq k \leq n)$, then $m(v_i) = w_2(v_i, v_k)$ where $w_2(v_i, v_k)$ is the number of two walks of the type $v_i v_k v_j$ for all $v_j \in N(v_k)$. Thus $d_i m_i \geq W_2(v_i)$. Hence $d_1m_1 + d_2m_2 + ... + d_nm_n \geq W_2(G)$ which gives

$$d_1m_1 + d_2m_2 + ... + d_nm_n \geq c_1\lambda_1 + c_2\lambda_2 + ... + c_n\lambda_n$$

In[19], V. Nikiforov gave the inequality

$$\frac{W_{q+r}(G)}{W_q(G)} \leq \lambda_1^r(G) \tag{2.10}$$

for all $r > 0$ and $q > 0$. Bellow, we state the following arguments borrowed from [19]. If the equality in (2.10) holds,

$$\sum_{i=2}^{n} c_i(\frac{\lambda_i}{\lambda_1})^{q+r-1} = \sum_{i=2}^{n} c_i(\frac{\lambda_i}{\lambda_1})^{q-1} \tag{2.11}$$

Note that if G is a bipartite graph, then the spectrum of G is symmetric to 0. Thus for a bipartite graph G, it follows $M = \phi$ or $M = \{n\}$ where M is the set of all i, $(2 \le i \le n)$ such that $c_i \neq 0$ and $\lambda_i \neq 0$. If $c_n > 0$, (2.11) holds when r is even. Thus from (2.9), we obtain

$$W_3(G) = (c_1 + c_n)\lambda_1^2 \tag{2.12}$$

Now, we state the following estimation on the spectral radius λ_1 for the class of graphs satisfying (2.12).

Theorem 2.3 *Let G be a connected graph with n vertices and e edges. If $W_3(G) = (c_1 + c_n)\lambda_1^2$, then*

$$\lambda_1 \le \sqrt{\frac{n - c_1}{n - c_1 + c_n} 2e} \tag{2.13}$$

Proof: By Cauchy-Schwarz's inequality, $(\sum_{i=2}^{n} c_i^{\frac{1}{2}}|\lambda_i|)^2 \le \sum_{i=2}^{n} c_i \sum_{i=2}^{n} |\lambda_i|^2$. Thus

$$\sum_{i=2}^{n} c_i\lambda_i^2 \le \sum_{i=2}^{n} c_i \sum_{i=2}^{n} \lambda_i^2 \tag{2.14}$$

It is well-known that $\sum_{i=1}^{n} \lambda_i^2 = 2e$. Again $\sum_{i=2}^{n} c_i = n - c_1$ and $\sum_{i=2}^{n} c_i\lambda_i^2 = W_3(G) - c_1\lambda_1^2$. Thus from the equation (2.14), we get $W_3(G) - c_1\lambda_1^2 \le (n - c_1)(2e - \lambda_1^2)$. Substituting $W_3(G) = (c_1 + c_n)\lambda_1^2$, we get the inequality (2.13). □

A clique number in a graph G means a complete subgraph of G. The clique number of G is the number of elements in a maximal clique in G denoted $cl(G)$.

Theorem 2.4 *Let G be a connected graph with n vertices, e edges and $cl(G) \le p$. Then*

$$\lambda_1 \le \sqrt{\frac{p-1}{c_1^2(p+k-1)} \sum_{i=1}^{n} d_i^2 \sum_{i=1}^{n} m_i^2} \tag{2.15}$$

where $k = min\{\frac{c_j^2}{c_1^2} | j = 2, 3, ..., n\}$.

Proof: Since $\sum_{i=1}^{n} d_i m_i \ge c_1\lambda_1 + c_2\lambda_2 + ... + c_n\lambda_n$, therefore by Cauchy-Schwarz's inequality, we obtain

$$\sum_{i=1}^{n} d_i^2 \sum_{i=1}^{n} m_i^2 \ge c_1^2\lambda_1^2 + c_2^2\lambda_2^2 + ... + c_n^2\lambda_n^2$$

which gives

$$\frac{1}{c_1 2} \sum_{i=1}^{n} d_i^2 \sum_{i=1}^{n} m_i^2 \ge \lambda_1^2 + k(\lambda_2^2 + ... + \lambda_n^2) \tag{2.16}$$

Again from V. Nikiforov [19] we have

$$\lambda_1^2 \le (p-1)(\lambda_2^2 + ... + \lambda_n^2) \tag{2.17}$$

Thus from (2.16) and (2.17), we obtain

$$\tfrac{p-1+k}{p-1}\lambda_1^2 \le \tfrac{1}{c_1^2} \sum_{i=1}^{n} m_i^2 \sum_{i=1}^{n} d_i^2$$

which is equivalent to the equation (2.15). □

In particular, for a graph with $c_i = 0$ for some i, $(2 \leq i \leq n)$

$$\lambda_1 \leq \sqrt{\frac{1}{c_1^2}\sum_{i=1}^{n} d_i^2 \sum_{i=1}^{n} m_i^2} \tag{2.18}$$

If G is a regular graph, $d_i = m_i$ for all i, $(1 \leq i \leq n)$ implies that

$$\lambda_1 \leq \frac{1}{c_1}\sum_{i=1}^{n} d_i^2 \tag{2.19}$$

If there exists some c_j, $(2 \leq j \leq n)$ so that $c_1 > c_j$, then we obtain

$$\sum_{i=1}^{n} d_i^2 \sum_{i=1}^{n} m_i^2 \geq c_1^2\lambda_1^2 + c_k^2(2e - \lambda_1^2) \tag{2.20}$$

where $c_k = min\{c_2, c_3, ..., c_n\}$. Note that

$$\sum_{i=1}^{n} d_i^2 \sum_{i=1}^{n} m_i^2 \geq 2ec_k^2 \tag{2.21}$$

Thus we present the following bound on $\lambda_1(G)$.

Theorem 2.5 *Let G be a graph with n vertices and e edges. If there exists some $c_j, (2 \leq j \leq n)$ so that $c_1 > c_j$, then $\lambda_1 \leq \sqrt{\frac{\sum_{i=1}^{n} d_i^2 \sum_{i=1}^{n} m_i^2 - 2ec_k^2}{c_1^2 - c_k^2}}$ where $c_k = min\{c_2, c_3, ..., c_n\}$*

In the year 2003, Vladimir Nikiforov [18] proved the following upper bound of the spectral radius λ_1 in terms of clique number ω which is conjectured by Edward and Elphick [7] in the year 1983.

Theorem 2.6 *Let G be a graph with n vertices and ω be the clique number of G, then*

$$\lambda_1 \leq \sqrt{\frac{\omega - 1}{\omega}2e} \tag{2.22}$$

.

If Δ be the maximal degree of the graph G, by the trivial inequality $\omega \leq \Delta + 1$, we readily obtain $\lambda_1 \leq \sqrt{\frac{\Delta}{\Delta+1}2e}$. Now we deal with the class of graphs with the stricter inequality $\omega \leq \Delta' + 1$ where Δ' is the second-largest degree of G, and present an upper bound on λ_1 involving Δ'.

Theorem 2.7 *Let G be a connected graph with n vertices and e edges. Let C be a maximal clique of G. If there exists a vertex $v \in V \setminus C$ such that $d(v) \geq d(v_k) + 1$, for some $v_k \in C$, then*

$$\lambda_1 \leq \sqrt{2e\frac{\Delta'}{\Delta' + 1}} \tag{2.23}$$

Further

$$\lambda_1^2 \leq \Delta'(\lambda_2^2 + \lambda_3^2 + ... + \lambda_n^2) \tag{2.24}$$

Proof: First we note that $\Delta' + 1 \geq \omega$. If $d(v) = d(v_k) + 1$ for some $v_k \in C$, then $\Delta' \geq d(v_k) \geq \omega - 1$. Assume $d(v) > d(v_k) + 1$ for some $v_k \in C$. If $d(v) = \Delta$, then $d(v) - 1 \geq \Delta' \geq d(v_k) \geq \omega - 1$. If $\Delta > d(v)$, then $\Delta' \geq d(v) > d(v_k + 1) > \omega - 1$. Thus $\Delta' + 1 \geq \omega$. Hence from the inequality (2.22), we get (2.23). Further, putting $2e = \lambda_1^2 + \lambda_2^2 + \lambda_3^2 + ... + \lambda_n^2$ in (2.23), we obtain (2.24).

□

3. Bounds on $E(G)$ involving degrees and maximum neighbourhood degrees

Let G be a connected graph with n vertices and e edges. In [17], McClelland gave the upper bound on $E(G)$ as follows

$$E(G) \leq \sqrt{2ne} \tag{3.1}$$

A. Yu et. al [22] proved a degree-based bound such as

$$E(G) \leq \sqrt{\frac{\sum_{v_i \in V} d_2^2(v_i)}{\sum_{v_i \in V} d^2(v_i)}} + \sqrt{(n-1)\Big(2e - \frac{\sum_{v_i \in V} d_2^2(v_i)}{\sum_{v_i \in V} d^2(v_i)}\Big)} \tag{3.2}$$

where $d_2(v_i) = \sum_{v_j \in N(v_i)} d(v_j), (1 \leq i \leq n)$. The equality in (3.2) holds if and only if $G = \frac{n}{2}k_2$, $G = k_n$ or a non-bipartite connected μ-pseudoregular graph with three distinct eigenvalues μ, $\sqrt{\frac{2e-\mu^2}{n-1}}$, $-\sqrt{\frac{2e-\mu^2}{n-1}}$ where $\mu > \sqrt{\frac{2e}{n}}$. Y. Hou et. al [15] generalised the above inequality as

$$E(G) \leq \sqrt{\frac{\sum_{v_i \in V} d_{k+1}^2(v_i)}{\sum_{v_i \in V} d_k^2(v_i)}} + \sqrt{(n-1)\Big(2e - \frac{\sum_{v_i \in V} d_{k+1}^2(v_i)}{\sum_{v_i \in V} d_k^2(v_i)}\Big)}$$

where $d_2(v_i) = \sum_{v_j \in N(v_i)} d(v_j), (1 \leq i \leq n)$, with the equality if and only if $G = k_n$ or G is a strongly regular graph with two nontrivial eigenvalues with absolute value $\sqrt{\frac{2e-(\frac{2e}{n})^2}{n-1}}$.

Theorem 3.1 *Let G be a graph with n vertices. If $\{d_1, d_2, ..., d_n\}$ and $\{m_1, m_2, ..., m_n\}$ be the degree and the maximum neighbourhood degree sequence of G respectively, then*

$$E(G) \leq \sqrt{\frac{\sum_{i=1}^{n} \big(\sum_{u_j \in N(u_i)} \sqrt{d_j m_j}\big)^2}{\sum_{i=1}^{n} d_i m_i}} + \sqrt{(n-1)\Big(2e - \frac{\sum_{i=1}^{n} \big(\sum_{u_j \in N(u_i)} \sqrt{d_j m_j}\big)^2}{\sum_{i=1}^{n} d_i m_i}\Big)} \tag{3.3}$$

with the equality in (3.3) if and only if G is K_n or quasi-regular with three distinct eigen values λ_1, $\sqrt{\frac{2e-\lambda_1^2}{n-1}}$ and $-\sqrt{\frac{2e-\lambda_1^2}{n-1}}$ where $\lambda_1 > \sqrt{\frac{2e}{n}}$. For regular graph the bound (3.3) gives the bound (3.2).

Example 3.1 The values of $E(G)$ and its bounds (3.2), (3.3) and (3.5) for the graphs in Figure 1 and Figure 2 give Table 2. From the list it is seen that our bound (3.5) is giving stricter upper value than the that of the bounds (3.2) and (3.3) for the graphs G_1, G_2, G_3, G_4 and G_5. However, in the case of the graph G_6, the bound (3.3) gives a stricter value than the value of the bound (3.5).

	$E(G)$	(3.2)	(3.3)	(3.5)
G_1	5.12310	6.32455	6.324 44	6.32439
G_2	5.12310	6.32455	6.324 44	6.32439
G_3	6.04080	7.74596	7.74306	7.74291
G_4	6	8.36660	8.36548	8.36530
G_5	7.86976	11.31370	11.30906	11.30893
G_6	9.90754	14.07124	14.06207	14.06472

Table 2:

Theorem 3.2 *Let G be a connected graph with n vertices and e edges. Let $\lambda_1 \geq \lambda_2 \geq .... \geq \lambda_n$ be the spectrum of G and $v_1, v_2, ..., v_n$ be corresponding orthogonal unit vectors. If $V_i = (v_{i1}, v_{i2}, .., v_{in})$, $1 \leq i \leq n$ and $c_i = (\sum_{i=1}^{n} v_{ij})^2$, then*

$$E(G) \geq \frac{W_2(G)}{n-c_1} + \frac{n-2c_1}{n-c_1}\sqrt{\frac{\sum_{i=1}^{n}\left(\sum_{u_j\in N(u_i)}\sqrt{d_j m_j}\right)^2}{\sum_{i=1}^{n} d_i m_i}} \tag{3.4}$$

Proof: By Cauchy-Schwarz's inequality, $(\sum_{i=2}^{n} c_i \sum_{i=2}^{n} \lambda_i)^{\frac{1}{2}} \geq \sum_{i=2}^{n} c_i^{\frac{1}{2}} |\lambda_i|^{\frac{1}{2}}$. Thus

$$(n-c_1)(E(G) - |\lambda_1|) \geq \textstyle\sum_{i=2}^{n} c_i|\lambda_i| \geq \sum_{i=2}^{n} c_i\lambda_i = W_2(G) - c_1\lambda_1$$

Consider the function $f(x) = \frac{W_2(G)}{n-c_1} + \frac{n-2c_1}{n-c_1}x$. It is to be noted that $f'(x) \geq 0$ for $x \in [0, \infty)$. Thus $f(x)$ is increasing on $x \in [0, \infty)$. Now, from the equation (2.6), we obtain the inequality (3.4). □

Theorem 3.3 *Let G be a graph with $n(\geq 4)$ vertices and e edges. Also, let $\{d_1, d_2, ..., d_n\}$ and $\{m_1, m_2, ..., m_n\}$ be the degrees and maximum neighbourhood degrees of G. Then*

$$\begin{aligned} E(G) \leq \sqrt{\frac{\sum_{i=1}^{n}\left(\sum_{u_j\in N(u_i)}\sqrt{d_j m_j}\right)^2}{\sum_{i=1}^{n} d_i m_i}}\Big\{1 + \frac{1}{4} \\ \left(1 + \sqrt{(n-1)\big(2m\frac{(\sum_{i=1}^{n} d_i m_i)}{\sum_{i=1}^{n}\left(\sum_{u_j\in N(u_i)}\sqrt{d_j m_i}\right)^2} - 1\big)}\right)^2\Big\} \end{aligned} \tag{3.5}$$

The equality in (3.5) holds if G is complete graph K_n.

Proof: It is well-known that for $0 < \alpha < 1$; $a > 0$ and $b > 0$, $a^{\alpha}b^{1-\alpha} \leq \alpha a + (1-\alpha)b$. Setting $a = \sum_{i=2}^{n} |\lambda_i|$, $b = |\lambda_1|$ and $\alpha = \frac{1}{2}$, we get $(\sum_{i=2}^{n} |\lambda_i|)^{\frac{1}{2}}(|\lambda_1|)^{\frac{1}{2}} \leq \frac{1}{2}\sum_{i=2}^{n} |\lambda_i| + \frac{1}{2}|\lambda_1|$. Thus

$$(\textstyle\sum_{i=2}^{n} |\lambda_i|)\lambda_1| \leq \frac{1}{4}\left(|\lambda_1| + \sum_{i=2}^{n} |\lambda_i|\right)^2 \leq \frac{1}{4}\left(|\lambda_1| + \sqrt{(n-1)(2e-\lambda_1^2)}\right)^2$$

gives

$$\sum_{i=2}^{n} |\lambda_i| \leq \frac{1}{4|\lambda_1|}\left(|\lambda_1| + \sqrt{(n-1)(2e-\lambda_1^2)}\right)^2 \tag{3.6}$$

From the equation (3.6), we obtain

$$E(G) \leq |\lambda_1| + \tfrac{1}{4|\lambda_1|}\left(|\lambda_1| + \sqrt{(n-1)(2e-\lambda_1^2)}\right)^2$$

Now, consider the function $f(x) = x + \frac{1}{4x}\left(x + \sqrt{(n-1)(2e-x^2)}\right)^2$. Then

$$f'(x) = 1 + \tfrac{x+\sqrt{(n-1)(2e-x^2)}}{4x^2}\left(\tfrac{x\sqrt{(n-1)(2e-x^2)} - (n-1)(x^2+2e)}{\sqrt{(n-1)(2e-x^2)}}\right)$$

Note that for $n \geq 4$ and $\sqrt{2e} \geq x \geq 0$, $f'(x) \leq 0$. Thus f is decreasing for $n \geq 4$ and $x \geq 0$. Therefore for a graph with $n \geq 4$, from the inequality (2.6) we get the equation (3.5). □

4. Conclusion

In this paper, we obtain some new bounds on spectral radius and energy of graphs involving the maximum neighbourhood degree sequence of the graphs. It seems that the maximum neighbourhood degree sequence of a graph is an important tool for estimation of the spectrum and energy of graphs.

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