On the eigenvalue and energy of extended adjacency matrix

Modjtaba Ghorbani [a,*], Xueliang Li [b], Samaneh Zangi [a], Najaf Amraei [a]

[a] *Department of Mathematics, Faculty of Science, Shahid Rajaee Teacher Training University, Tehran 16785 - 136, Iran*
[b] *Center for Combinatorics, Nankai University, Tianjin 300071, China*

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A B S T R A C T

The extended adjacency matrix of graph G, $\mathcal{A}_{ex}$ is a symmetric real matrix that if $i \neq j$ and $u_i u_j \in E(G)$, then the ijth entry is $d_{u_i}^2 + d_{u_j}^2 / 2d_{u_i} d_{u_j}$, and zero otherwise, where d_u indicates the degree of vertex u. In the present paper, several investigations of the extended adjacency matrix are undertaken and then some spectral properties of $\mathcal{A}_{ex}$ are given. Moreover, we present some lower and upper bounds on extended adjacency spectral radii of graphs. Besides, we also study the behavior of the extended adjacency energy of a graph G.

1. Introduction

In this work, by a graph, we mean a simple, finite and connected one. The symmetric division deg index a graph invariant based on degree of vertices and it is defined as follows:

$$\mathcal{SDD}(G) = \sum_{uv \in E(G)} \frac{d_u^2 + d_v^2}{d_u d_v}, \tag{1}$$

where d_u and d_v denotes the degrees of vertices u and v. Several properties of *sdd*-index are given in [8,11,21–24] as well as [1,9,17].

The inverse symmetric division deg index is defined by Ghorbani et al. in [7] as follows:

$$\mathcal{ISDD}(G) = \sum_{uv \in E(G)} \frac{d_u d_v}{d_u^2 + d_v^2}. \tag{2}$$

The adjacency matrix $A(G)$ of graph G is a matrix that $a_{ij} = 1$ if $v_i v_j \in E(G)$ and zero otherwise. With respect to the symmetric division deg index, the extended adjacency matrix ($\mathcal{A} = \mathcal{A}_{ex}$) is defined as a symmetric real matrix in which the ijth entry is $d_{u_i}^2 + d_{u_j}^2 / 2d_{u_i} d_{u_j}$, when $i \neq j$ and $u_i u_j \in E(G)$, and zero otherwise. It is clear that for a regular graph G, the extended adjacency and the adjacency matrices are the same. For recent research along these lines, see [3,13,25]. Recall that the extended adjacency matrix is just one among a large number of degree-based graph matrices; for details see [4].

* Corresponding author.
E-mail address: mghorbani@sru.ac.ir (M. Ghorbani).

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The structure of this paper is as follows. In continuing this section, we introduce definitions and concepts that we need in this paper. In Section 2, we compute the extended adjacency matrix or $\mathcal{A}$-matrix of well-known graphs together with their characteristic polynomials. In continuing, we will argue about the spectra of certain classes of graphs. In Section 3, we apply algebraic graph theory techniques to explore the $\mathcal{A}$-spectral radii of graphs in general. Finally, in Section 4, the extended adjacency energy of a graph is defined and some bounds are given.

Two graph invariants $M_1(G) = \sum_{uv\in E} d_u + d_v$ and $M_2(G) = \sum_{uv\in E} d_u d_v$ are calles as Zagreb indices and they have been defined in the 1970s, see [16,17]. Also, the forgotten index is defined as [5,6]

$$F(G) = \sum_{uv\in E} d_u^2 + d_v^2.$$

A permutation π on the vertices of a graph G is called an homomorphism, if for an edge $e = xy$ of G, then $\pi(e) = \pi(x)\pi(y)$ is again an edge of G, where the image of edge $e = xy$ is denoted by $\pi(e)$. We say π is an automorphism, if both π and π^{-1} are homomorphism of G. The automorphism group of a graph G is the set $Aut(G) = \{\pi : V(G) \to V(G)$, where π is an automorphism$\}$.

For a given edge $e \in E(G)$, the collection $E_e = \{\ \pi(e)\ ,\ \pi\ \in Aut(G)\ \}$ is an orbit including e. A vertex(edge)-transitive graph is a graph with only one vertex(edge) orbit.

Throughout this paper, for the graph G, the symbol $G \setminus e$ means removing the edge e.

2. Preliminary results

For a graph G of order n and with adjacency matrix $A = A(G)$, the polynomial $\chi_\lambda(G) = \det(\lambda I_n - A)$, where I_n is the identity matrix of order n, is called the characteristic polynomial of G and each root of $\chi_\lambda(G)$ is called an eigenvalue of G. If $\lambda_1, \lambda_2, \ldots, \lambda_s$ are all distinct eigenvalues of G, then the spectrum of G is the multiset $spec(G) = \{[\lambda_1]^{m_1}, \ldots, [\lambda_s]^{m_s}\}$, where m_i $(1 \le i \le s)$ indicates the multiplicity of λ_i. Also, the spectral radius of a graph is the largest absolute value of its eigenvalues.

The eigenvalues of matrix $\mathcal{A} = \mathcal{A}_{ex}$ are shown by $\eta_1, \eta_2, \ldots, \eta_n$ and its spectrum by $spec_{ex}(G)$. It is not difficult to realize that in either a regular graph or a complete bipartite graph, the $\mathcal{A}$-matrix is a multiple of the adjacency matrix. Hence, by having the eigenvalues of the adjacency matrix, we can find the $\mathcal{A}$-eigenvalues, but in general, this problem is more difficult.

Theorem 2.1. *Let G be a graph extended adjacency eigenvalues $\eta_1, \ldots, \eta_n$. Then*

(i) $\sum_{i=1}^{n} \eta_i = tr(\mathcal{A}_{ex}) = 0.$

(ii) $\sum_{i=1}^{n} \eta_i^2 = tr(\mathcal{A}_{ex}^2) = 2\sum_{i,j}((\mathcal{A}_{ex})_{ij})^2 = \frac{1}{2}\sum_{i\sim j}(\frac{d_{u_i}}{d_{u_j}} + \frac{d_{u_j}}{d_{u_i}})^2.$

(iii) $\sum_{i=1}^{n} \eta_i^3 = tr(\mathcal{A}_{ex}^3) = \frac{1}{4}\sum_{i\sim j}\frac{d_{u_i}^2 + d_{u_j}^2}{(d_{u_i}d_{u_j})^2}(\sum_{k\sim i,k\sim j}\frac{(d_{u_i}^2 + d_{u_k}^2)(d_{u_j}^2 + d_{u_k}^2)}{d_{u_k}^2}).$

(iv) $\sum_{i=1}^{n} \eta_i^4 = tr(\mathcal{A}_{ex}^4) = \frac{1}{16}(\sum_{i=1}^{n}(\sum_{i\sim l}(\frac{d_{u_i}}{d_{u_l}} + \frac{d_{u_j}}{d_{u_i}})^2)^2 + \sum_{i\neq j}(\frac{1}{d_{u_i}d_{u_j}}\sum_{l\sim i,l\sim j}\frac{(d_{u_i}^2 + d_{u_l}^2)(d_{u_j}^2 + d_{u_l}^2)}{d_{u_l}^2})^2).$

Proof.

(i) It follows from definition.

(ii) $(\mathcal{A}_{ex}^2)_{ii} = \sum_{j=1}^{n}(\mathcal{A}_{ex})_{ij}(\mathcal{A}_{ex})_{ji} = \sum_{j=1}^{n}((\mathcal{A}_{ex})_{ij})^2 = \sum_{i\sim j}(\mathcal{A}_{ex})_{ij}^2 = \frac{1}{4}\sum_{i\sim j}(\frac{d_{u_i}}{d_{u_j}} + \frac{d_{u_j}}{d_{u_i}})^2$. Therefore,

$$tr(\mathcal{A}_{ex}^2) = \sum_{i=1}^{n}\sum_{i\sim j}(\frac{1}{2}(\frac{d_{u_i}}{d_{u_j}} + \frac{d_{u_j}}{d_{u_i}}))^2 = \frac{1}{2}\sum_{i\sim j}(\frac{d_{u_i}}{d_{u_j}} + \frac{d_{u_j}}{d_{u_i}})^2.$$

(iii) Suppose $i \neq j$. Then

$$\begin{aligned}(\mathcal{A}_{ex}^2)_{ij} &= \sum_{k=1}^{n}(\mathcal{A}_{ex})_{ik}(\mathcal{A}_{ex})_{kj} = \sum_{k\sim i,k\sim j}(\mathcal{A}_{ex})_{ik}(\mathcal{A}_{ex})_{kj} \\ &= \sum_{k\sim i,k\sim j}(\frac{1}{2}(\frac{d_{u_i}}{d_{u_k}} + \frac{d_{u_k}}{d_{u_i}}))(\frac{1}{2}(\frac{d_{u_j}}{d_{u_k}} + \frac{d_{u_k}}{d_{u_j}})) \\ &= \frac{1}{4d_{u_i}d_{u_j}}\sum_{k\sim i,k\sim j}(\frac{(d_{u_i}^2 + d_{u_k}^2)(d_{u_j}^2 + d_{u_k}^2)}{d_{u_k}^2}).\end{aligned}$$

For the matrix $\mathcal{A}_{ex}^3$, we have

$$(\mathcal{A}_{ex}^3)_{ii} = \sum_{j=1}^{n}(\mathcal{A}_{ex})_{ij}(\mathcal{A}_{ex}^2)_{jk} = \sum_{i\sim j}(\frac{1}{2}(\frac{d_{u_i}}{d_{u_j}} + \frac{d_{u_j}}{d_{u_i}}))((\mathcal{A}_{ex})^2)_{jk}$$
$$= \sum_{i\sim j}\frac{d_{u_i}^2 + d_{u_j}^2}{8(d_{u_i}d_{u_j})^2}(\sum_{k\sim i,k\sim j}\frac{(d_{u_i}^2 + d_{u_k}^2)(d_{u_j}^2 + d_{u_k}^2)}{d_{u_k}^2}).$$

Hence

$$tr(\mathcal{A}_{ex}^3) = \sum_{i=1}^{n}\sum_{i\sim j}\frac{d_{u_i}^2 + d_{u_j}^2}{8(d_{u_i}d_{u_j})^2}(\sum_{k\sim i,k\sim j}\frac{(d_{u_i}^2 + d_{u_k}^2)(d_{u_j}^2 + d_{u_k}^2)}{d_{u_k}^2})$$
$$= \frac{1}{4}\sum_{i\sim j}\frac{d_{u_i}^2 + d_{u_j}^2}{(d_{u_i}d_{u_j})^2}(\sum_{k\sim i,k\sim j}\frac{(d_{u_i}^2 + d_{u_k}^2)(d_{u_j}^2 + d_{u_k}^2)}{d_{u_k}^2}).$$

(iv) The trace of $\mathcal{A}_{ex}^4$ is

$$tr(\mathcal{A}_{ex}^4) = \sum_{i,j=1}^{n}(\mathcal{A}_{ex}^2)_{ij}^2 = \sum_{i=j}(\mathcal{A}_{ex}^2)_{ij}^2 + \sum_{i\neq j}(\mathcal{A}_{ex}^2)_{ij}^2$$
$$= \frac{1}{16}(\sum_{i=1}^{n}(\sum_{i\sim l}(\frac{d_{u_i}}{d_{u_l}} + \frac{d_{u_j}}{d_{u_i}})^2)^2$$
$$+ \sum_{i\neq j}(\frac{1}{d_{u_i}d_{u_j}}\sum_{l\sim i,l\sim j}\frac{(d_{u_i}^2 + d_{u_l}^2)(d_{u_j}^2 + d_{u_l}^2)}{d_{u_l}^2})^2).$$

This completes our argument. □

Example 2.1. Theorem 2.1 imlies that if G is r-regular, then clearly $\mathcal{A}_{ex} = A$ and $\mathcal{A}_{ex}^2 = A^2$. On the other hand, $tr(A^2) = nr$ which yields that $tr(\mathcal{A}_{ex}^2) = nr$.

Example 2.2. For the path graph P_n, we obtain

$$\mathcal{A}_{ex}(P_n) = \begin{bmatrix} 0 & \frac{5}{4} & 0 & 0 & \cdots & 0 & 0 \\ \frac{5}{4} & 0 & 1 & 0 & \cdots & 0 & 0 \\ 0 & 1 & 0 & 1 & \ddots & \vdots & \vdots \\ 0 & 0 & 1 & \ddots & \ddots & 0 & 0 \\ \vdots & \vdots & \ddots & \ddots & 0 & 1 & 0 \\ 0 & 0 & \cdots & 0 & 1 & 0 & \frac{5}{4} \\ 0 & 0 & \cdots & 0 & 0 & \frac{5}{4} & 0 \end{bmatrix}$$

The diagonal elements of $\mathcal{A}_{ex}^2(P_n)$ are $\frac{25}{16}, \frac{41}{16}, 2, 2, \cdots, 2, \frac{41}{16}, \frac{25}{16}$. Therefore

$$tr(\mathcal{A}_{ex}^2(P_n)) = \frac{33}{4} + 2(n-4).$$

Theorem 2.2. *Let G be an edge-transitive graph on n vertices. Then*

$$\chi_\eta(\mathcal{A}_{ex}) = \alpha^n\chi_{(\alpha\lambda)}(A),$$

where $\alpha = \frac{a^2+b^2}{2ab}$.

Proof. Since G is edge-transitive, and for each edge $e = uv$, there are two integers a and b such that $a = d_u$ and $b = d_v$. Then

$$\mathcal{A}_{ex}(G) = \frac{a^2+b^2}{2ab}A(G)$$

and we are done. □

Example 2.3. According to Theorem 2.2, for the complete bipartite graph $K_{m,n}$, we obtain

$$\mathcal{A}_{ex}(K_{m,n}) = (\frac{m^2+n^2}{2mn})A(K_{m,n}).$$

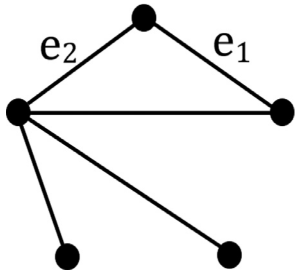

Fig. 1. The graph G.

Hence

$$spec_{ex}(K_{m,n})=\left\{[-\frac{m^2+n^2}{2\sqrt{mn}}]^1,[0]^{m+n-2},[\frac{m^2+n^2}{2\sqrt{mn}}]^1\right\}.$$

Theorem 2.3. *For a regular graph G, we yield that*

$$\chi_\eta(\mathcal{A}_{ex})=\chi_\lambda(A).$$

Proof. It is clear that all non-zero entries of $\mathcal{A}_{ex}$ are 1. This fact and using the definition, would yield the required result. □

3. The spectral radii of extended adjacency matrix of graphs

In this section, we obtain some lower and upper bounds for the spectral radii of extended adjacency matrix of graphs. Here, we show the largest eigenvalue of the adjacency matrix of graph G by $\lambda_1(G)$ (or for simply by λ_1). Also, we denote the largest eigenvalue of extended adjacency matrix of a graph by $\eta_1(G)$ (or for simply by η_1). It is a well-known fact that for the largest ordinary eigenvalue of a graph G, we have $\lambda_1(G)>\lambda_1(G\backslash e)$ [2] but this fact is not true for the largest extended adjacency eigenvalue. For example, consider the graph G as depicted in Fig. 1. It is not difficult to see that $\eta_1(G)=3.65$, $\eta_1(G\backslash e_1)=4.25$ and $\eta_1(G\backslash e_2)=2.65$.

Based on the above facts, we investigate the spectral properties of the largest eigenvalue of extended adjacency matrix of a graph.

Theorem 3.1. *For any graph G, we have $\lambda_1\le\eta_1\le\frac{1}{2}(\frac{\Delta}{\delta}+\frac{\delta}{\Delta})\lambda_1$. The left equality holds if and only if G is a regular graph and the right equality holds if and only if G is a complete bipartite graph.*

Proof. For two arbitrary vertices v_i and v_j $(1\le i,j\le n)$, we have $1\le\frac{1}{2}(\frac{d_{v_i}}{d_{v_j}}+\frac{d_{v_j}}{d_{v_i}})\le\frac{1}{2}(\frac{\Delta}{\delta}+\frac{\delta}{\Delta})$. Consequently, $A(G)\le\mathcal{A}_{ex}(G)\le\frac{1}{2}(\frac{\Delta}{\delta}+\frac{\delta}{\Delta})A(G)$ and thus $\lambda_1\le\eta_1\le\frac{1}{2}(\frac{\Delta}{\delta}+\frac{\delta}{\Delta})\lambda_1$. □

It is well-known that [2,18]

$$\max\{\sqrt{\Delta},\sqrt{\frac{M_1(G)}{n}},\frac{2m}{n},2cos(\frac{\pi}{n+1})\}\le\lambda_1\le\min\{\Delta,n-1\}.$$

This together with the fact that for a tree T, $\lambda_1\le\min\{2\sqrt{\Delta-1},\sqrt{n-1}\}$, we may conclude the following result.

Corollary 3.2.

(i) *For graph G with maximum degree Δ and minimum degree δ*
$\max\{\sqrt{\Delta},\sqrt{\frac{M_1(G)}{n}},\frac{2m}{n},2cos(\frac{\pi}{n+1})\}\le\eta_1\le\frac{1}{2}(\frac{\Delta}{\delta}+\frac{\delta}{\Delta})\min\{\Delta,n-1\}$.

(ii) *For tree T with maximum degree Δ and minimum degree δ*

$$\eta_1\le\frac{1}{2}(\frac{\Delta}{\delta}+\frac{\delta}{\Delta})\min\{2\sqrt{\Delta-1},\sqrt{n-1}\}.$$

It is a well-known fact that among all bipartite graphs of order n, the star graph S_n has the minimum ordinary spectral radius which is $\lambda_1=\sqrt{n-1}$ and the complete bipartite graph $K_{\frac{n}{2},\frac{n}{2}}$ (if n is odd $k_{[\frac{n}{2}],[\frac{n}{2}]+1}$) has the maximum ordinary spectral radius equal to $\lambda_1=\frac{n}{2}$. Thus the next result follows directly.

Corollary 3.3. *Among all bipartite graphs of order n, the star graph S_n has the maximum $\mathcal{A}$-spectral radius $\eta_1=\frac{n^2-2n+2}{2\sqrt{n-1}}$ and the complete bipartite graph $K_{\frac{n}{2},\frac{n}{2}}$ has the minimum $\mathcal{A}$-spectral radius $\eta_1=\frac{n}{2}$.*

For a real vector $x \in \mathbb{R}^n$, the Rayleigh quotient theorem [2] yields that

$$\eta_1 = \sup_{x\neq 0} \frac{x^t \mathcal{A}_{ex} x}{x^t x} = \sup_{x\neq 0} \frac{\sum\limits_{uv\in E(G)} x_u x_v \frac{d_u^2 + d_v^2}{2d_u d_v}}{\sum\limits_{u\in V(G)} x_u^2}.$$

Hence, for $x = \mathbf{j}$, we have

$$\eta_1 \geq \frac{\mathbf{j}^t(\mathcal{A}_{ex}(G))\mathbf{j}}{\mathbf{j}^t\mathbf{j}} = \frac{\mathcal{SDD}(G)}{n}. \tag{3}$$

Consider three following well-known topological indices:

$$R_\alpha(G) = \sum_{uv\in E} (d_u d_v)^\alpha,$$

$$GA(G) = \sum_{uv\in E} \frac{2\sqrt{d_u d_v}}{d_u + d_v},$$

$$ABC(G) = \sum_{uv\in E} \sqrt{\frac{d_u + d_v - 2}{d_u d_v}}.$$

Suppose G has n vertices, m edges and k pendant edges. By [7], the following lower bounds for the spectral radius of $\mathcal{A}_{ex}$ can be explored:

$$\eta_1 \geq \frac{(2m + \frac{2k}{3})}{n}, \tag{4}$$

$$\eta_1 \geq \frac{(m+n)}{n}, \tag{5}$$

$$\eta_1 \geq \frac{\frac{M_1^2(G)}{M_2(G)} - 2m}{n}, \tag{6}$$

$$\eta_1 \geq \frac{\frac{n^2}{R_{-1}(G)} - 2m}{n}, \tag{7}$$

$$\eta_1 \geq \frac{2m^2}{nGA(G)}, \tag{8}$$

$$\eta_1 \geq \frac{3ABC(G)}{2n}, \tag{9}$$

$$\eta_1 \geq \frac{2GA(G)}{n}, \tag{10}$$

$$\eta_1 \geq \frac{4\frac{m^3}{(GA(G))^2} - 2m}{n}, \tag{11}$$

$$\eta_1 \geq \frac{m[(\frac{M_1(G)}{m\Delta})^2 - 2]}{n}. \tag{12}$$

Consider now the real vector $x = (d_{v_i})_i$. Again Rayleigh quotient theorem yields that

$$\frac{x^t(\mathcal{A}_{ex})x}{x^t x} = \frac{\sum\limits_{(v_i,v_j)\in E(G)} ({d_{v_i}}^2 + {d_{v_j}}^2)}{\sum\limits_{k=1}^{n} d_{v_k}^2} = \frac{F(G)}{M_1(G)} \leq \eta_1. \tag{13}$$

Since, $\mathcal{SDD}(G) \geq 2m$, by Eq. (3), we conclude that $\eta_1 \geq \frac{2m}{n}$.

Suppose now $v_k v_s \in E(G)$, is an arbitrary edge. For the non-zero real vector $x = (x)_i$, where

$$x_i = \begin{cases} 1 & i = k, s \\ 0 & otherwise \end{cases},$$

we obtain

$$\frac{x^t(\mathcal{A}_{ex})x}{x^t x} = \frac{1}{2}(\frac{d_k}{d_s} + \frac{d_s}{d_k}) \leq \eta_1 \tag{14}$$

or equivalently $\mathcal{SDD}(G) \leq 2m\eta_1$. Finally, for each vertex $u \in V(G)$, clearly $\delta \leq \deg(u) \leq \Delta$ and thus $\frac{\mathcal{SDD}(G)}{2m} \leq \eta_1$. Hence, we proved the following theorem.

Theorem 3.4. *Let G be a graph on n vertices and m edges. Then*

$$\eta_1 \geq \max\left\{\frac{2m}{n}, \frac{2m + \frac{2k}{3}}{n}, \frac{(m+n)}{n}\right\}.$$

In addition, $\eta_1 = \frac{2m}{n}$ *if and only if G is a regular graph. Applying well-known degree-based topological indices given in Equations* $(4) - (13)$, *we have*

$$\eta_1 \geq \max\left\{\frac{F(G)}{M_1(G)}, \frac{\mathcal{SDD}(G)}{2m}, \frac{\frac{M_1^2(G)}{M_2(G)} - 2m}{n}, \frac{\frac{n^2}{R_{-1}(G)} - 2m}{n}, \frac{2m^2}{nGA(G)}, \frac{3ABC(G)}{2n},\right.$$
$$\left.\frac{2GA(G)}{n}, \frac{\mathcal{SDD}(G)}{n}, \frac{4\frac{m^3}{(GA(G))^2} - 2m}{n}, \frac{m[(\frac{M_1}{m\Delta})^2 - 2]}{n}\right\}.$$

Corollary 3.5. *Suppose G is a graph in which two vertices with degrees* Δ *and* δ *are adjacent. Then*

$$\eta_1 \geq \frac{1}{2}(\frac{\Delta}{\delta} + \frac{\delta}{\Delta}).$$

By using inequality given in Theorem 3.4, one can deduce that for the smallest eigenvalue of $\mathcal{A}_{ex}$, we obtain $\eta_n \leq \frac{\mathcal{SDD}(G)}{n}$. Since

$$\mathcal{SDD}(G) \leq \min\{n\Delta, 2m(1 + I(G)) - n^2, 2m(\frac{kf(G) + n}{n-1}) - n^2\},$$

where $I(G) = \sum_{i=1}^{n} \frac{1}{d_{u_i}}$ and $kf(G) = \sum_{i<j} r_{ij}$, where r_{ij} denotes the resistance-distance between v_i and v_j. We conclude that $\eta_n \leq \frac{1}{n} \times \alpha(G)$, where

$$\alpha(G) = \min\{n\Delta, 2m(1 + I(G)) - n^2, 2m(\frac{kf(G) + n}{n-1}) - n^2\}.$$

Lemma 3.6. *([27]) If* $A_{n\times n}$ *is a Hermitian matrix of order* $n \geq 2$ *with eigenvalues* $\theta_1 \geq \ldots \geq \theta_n$, *then*

$$\theta_1 - \theta_n \geq \frac{|\sum_{i\neq j} a_{ij}|}{n-1}.$$

Theorem 3.7. *If G is r-regular, then* $\lambda_n = \eta_n \leq \frac{r}{1-n}$.

Proof. Since G is r-regular, we conclude that $\mathcal{A}_{ex}(G) = A(G)$, which yield that $\eta_i = \lambda_i$ $(1 \leq i \leq n)$. Specially $\eta_1 = r$. On the other hand, $\sum_{i\neq j}(\mathcal{A}_{ex})_{ij} = nr$ and Lemma 3.6 yields that

$$\eta_1 - \eta_n \geq \frac{nr}{n-1}$$

or equivalently

$$\eta_n \leq \frac{r}{1-n}.$$

□

4. On extended energy of graphs

Let G be a graph with adjacency eigenvalues $\lambda_1, \lambda_2, \cdots, \lambda_n$. The graph energy of G is

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

see [10,12,14,15].

Here, we define the extended energy as the sum of absolute values of the eigenvalues of extended adjacency matrix. More formally, suppose $\eta_1, \eta_2, \cdots, \eta_n$ are the eigenvalues of $\mathcal{A}_{ex}$. It is not difficult to see that these eigenvalues are real numbers and their sum is zero. Hence, the Extended Energy can be defined as $\mathcal{E}_{ex}(G) = \sum_{i=1}^{n} |\eta_i|$, see [4,20].

Theorem 4.1. *Let G be a graph with n vertices. Then*

$$\sqrt{tr(\mathcal{A}_{ex}^2)} \leq \mathcal{E}_{ex}(G) \leq \sqrt{ntr(\mathcal{A}_{ex}^2)}.$$

Proof. The variance of the numbers $|\eta_i|$, $i = 1, 2, \cdots, n$ is equal to

$$\frac{1}{n}\sum_{i=1}^{n} |\eta_i|^2 - \left(\frac{1}{n}\sum_{i=1}^{n} |\eta_i|\right)^2$$

which is greater than or equal to zero. Now, $\sum_{i=1}^{n} |\eta_i|^2 = \sum_{i=1}^{n} \eta_i^2 = tr(\mathcal{A}_{ex}^2)$ and therefore

$$\mathcal{E}_{ex}(G) \leq \sqrt{ntr(\mathcal{A}_{ex}^2)}$$

as we desired. Now by Radon inequality we investigate that

$$\sum_{i=1}^{n} |\eta_i| = \sum_{i=1}^{n} \frac{|\eta_i|^2}{|\eta_i|} \geq \frac{\sum_{i=1}^{n} |\eta_i|^2}{\sum_{i=1}^{n} |\eta_i|}.$$

Hence,

$$\mathcal{E}_{ex}(G) \geq \sqrt{\sum_{i=1}^{n} |\eta_i|^2} = \sqrt{tr(\mathcal{A}_{ex}^2)}$$

□

Theorem 4.2. *Let G be a non-trivial graph. Then*

$$\mathcal{E}_{ex}(G) \geq \sqrt{\frac{tr(\mathcal{A}_{ex}^2)^3}{tr(\mathcal{A}_{ex}^4)}}.$$

Proof. Suppose G has n vertices. The Hölder inequality implies that

$$\sum_{i=1}^{n} a_i b_i \leq \left(\sum_{i=1}^{n} a_i^p\right)^{1/p} \left(\sum_{i=1}^{n} b_i^q\right)^{1/q}$$

where $a_i, b_i \in \mathbb{R}^+ (i = 1, 2, \cdots, n)$. Put $a_i = |\eta_i|^{2/3}, b_i = |\eta_i|^{4/3}$, $p = 3/2$ and $q = 3$, thus we have

$$\sum_{i=1}^{n} |\eta_i|^2 = \sum_{i=1}^{n} |\eta_i|^{2/3}(|\eta_i|^4)^{1/3} \leq (\sum_{i=1}^{n} |\eta_i|)^{2/3}(\sum_{i=1}^{n} |\eta_i|^4)^{1/3}. \tag{15}$$

If Gis not an empty graph, then $\sum_{i=1}^{n} |\eta_i|^4 \neq 0$ and Eq. (15) can be rewritten as

$$\mathcal{E}_{ex}(G) = \sum_{i=1}^{n} |\eta_i| \geq \frac{\sum_{i=1}^{n} (|\eta_i|^2)^{3/2}}{\sum_{i=1}^{n} (|\eta_i|^4)^{1/2}} = \frac{\sum_{i=1}^{n} (\eta_i^2)^{3/2}}{\sum_{i=1}^{n} (\eta_i^4)^{1/2}} = \sqrt{\frac{tr(\mathcal{A}_{ex}^2)^3}{tr(\mathcal{A}_{ex}^4)}}.$$

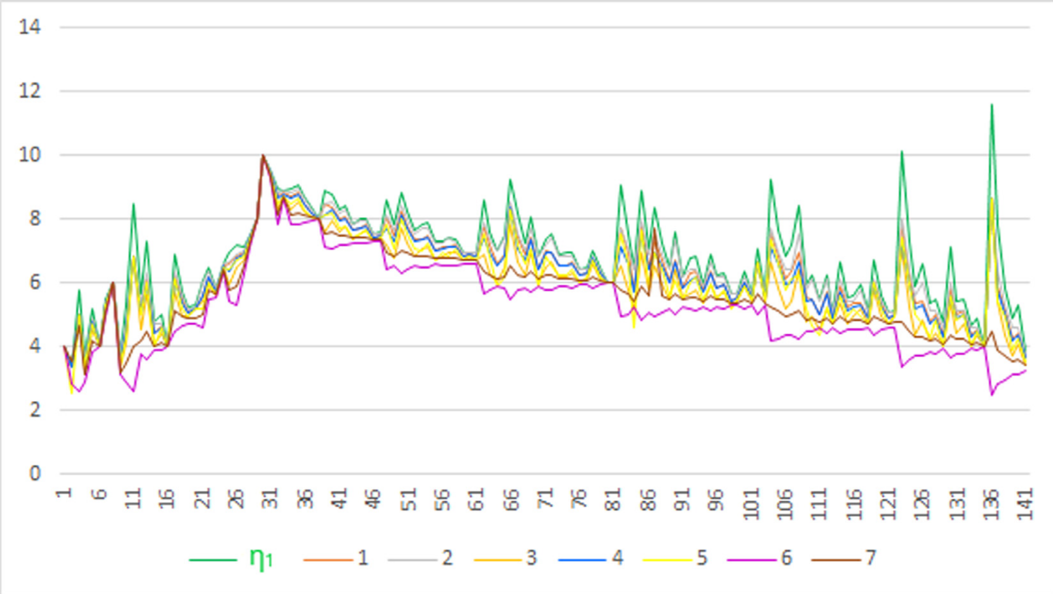

Fig. 2. The correlation between the values of η_1 and other lower bounds.

□

Theorem 4.3. *For the graph G, we have*

$$\mathcal{E}_{ex}(G) \geq 2\eta_1.$$

Proof. It is clear that $\mathcal{E}_{ex}(G) = \sum_{i=1}^{n} |\eta_i|$ and thus

$$\mathcal{E}_{ex}(G) = |\eta_1| + \sum_{i=2}^{n} |\eta_i| \geq |\eta_1| + |\sum_{i=2}^{n} \eta_i|.$$

On the other hand, $\sum_{i=1}^{n} \eta_i = 0$ yields that $\eta_1 = -\sum_{i=2}^{n} \eta_i$, and so $|\eta_1| = |\sum_{i=2}^{n} \eta_i|$. Hence

$$\mathcal{E}_{ex}(G) \geq 2|\eta_1| = 2\eta_1.$$

□

Corollary 4.4. *For the graph G with n vertices, m edges and k pendant edges, we obtain*

$$\mathcal{E}_{ex}(G) \geq 2\max\left\{\frac{2m}{n}, \frac{2m + \frac{2k}{3}}{n}, \frac{(m+n)}{n}\right\}.$$

Moregenerally, comparing with other degree-based topological indices, we have

$$\mathcal{E}_{ex}(G) \geq 2\max\left\{\frac{F(G)}{M_1(G)}, \frac{\mathcal{SDD}(G)}{2m}, \frac{\frac{M_1^2(G)}{M_2(G)} - 2m}{n}, \frac{\frac{n}{R_{-1}(G)} - 2m}{n}, \frac{2m^2 GA(G)}{n}, \frac{3ABC(G)}{2n}\right\}.$$

Proof. Use Theorems 3.4 and 4.3. □

5. Computational experiments

In this section, we present some comparatives examples for different values of n. Considering all graphs of orders 3, 4, 5 and 6, several lower bounds for $\mathcal{A}$-spectral radii in the paper are compared. The analyzing of these graph quantities indicates that the best upper bound for η_1 is as given in Eq. (13). The correlation between the values of η_1 and other lower bounds are given in Fig. 2 and Table 1. By the contents of table, we obtain

$$A_1 = \frac{\mathcal{SDD}(G)}{n}, A_2 = \frac{F(G)}{M_1(G)},$$

Table 1
The correlation between the values of η_1 and other lower bounds.

Corr	A_1	A_2	A_3	A_4	A_5	A_6	A_7
η_1	0.955	0.959	0.906	0.938	0.933	0.558	0.72

$$A_3 = \frac{\frac{M_1^2(G)}{M_2(G)} - 2m}{n}, A_4 = \frac{4\frac{m^3}{(GA(G))^2} - 2m}{n},$$
$$A_5 = \frac{\frac{n^2}{R_{-1}(G)} - 2m}{n}, A_6 = \frac{2GA(G)}{n},$$
$$A_7 = \frac{2m^2}{nGA(G)}.$$

This means that, if n is sufficiently large, then $\eta_1 \approx \frac{F(G)}{M_1(G)}$. The correlations between $\mathcal{A}$-energy and the ordinary and Randic energies of 1000 random graphs of orders 19 and 20 are respectively $corr(\mathcal{E}_{ex}, \mathcal{E}) = -0.41$ and $corr(\mathcal{E}_{ex}, \mathcal{E}_R) = -0.48$. It can be infered that the $\mathcal{A}$-energy has a low correlation with both ordinary and Randic energies.

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