Some sharp bounds for the spectral radius and energy of digraphs

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Abstract

For a simple digraph D with n vertices, the energy of D is defined as $E(D) = \sum_{i=1}^{n} |\mathrm{Re}(z_i)|$, where $z_1, z_2, ..., z_n$ are the eigenvalues of D. This paper first gives an improved lower bound on the spectral radius of D, which is used to obtain some upper bounds for the energy $E(D)$. These results improve and generalize some known results on upper bounds of the energy of digraphs.

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1. Introduction

Assume that D is a simple digraph with n vertices and Γ is the set of arcs, which consisting of ordered pairs of distinct vertices. Two vertices u and v of D are adjacent if they are connected by an arc. If the arc is from u to v, then we write the arc by (u, v).

A walk of length 2 from vertex u to vertex v is a sequence of vertices $\pi : u, w, v$, where (u, w) and (w, v) are arcs of D. If $u = v$, then π is called a closed walk of length 2. We denote the number of all closed walks of length 2 associated with vertex $v_i \in V$ by $c_2^{(i)}$. The sequence $\left(c_2^{(1)}, c_2^{(2)}, ..., c_2^{(n)}\right)$ is called closed walk sequence of length 2 of D. Thus $c_2 = c_2^{(1)} + c_2^{(2)} + \cdots + c_2^{(n)}$ is the number of all closed walks of length 2 of D [12].

A digraph D is *symmetric* if for any $(u, v) \in \Gamma$ also $(v, u) \in \Gamma$, where $u, v \in V$. A one-to-one correspondence between a graph and a symmetric

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digraph is given by $G \rightsquigarrow \overleftrightarrow{G}$, where $\overleftrightarrow{G}$ and G has the same vertex set, every edge uv of G is replaced by a pair of symmetric arcs (u, v) and (v, u). Hence, a graph can be identified with a symmetric digraph, see [5, 12].

A graph G is called *regular* if every vertex of G has equal degree. A bipartite graph is called *semiregular* if each vertex in the same part of a bipartition has the same degree. A graph G is called *pseudo-regular* if every vertex of G has equal average-degree. A bipartite graph is called *pseudo-semiregular* if each vertex in the same part of a bipartition has the same average-degree, see [10].

The adjacency matrix $A = (a_{ij})$ of D is the $n \times n$ matrix, defined by $a_{ij} = 1$ for $(v_i, v_j) \in \Gamma$; 0 otherwise. The eigenvalues $z_1, z_2, \ldots, z_n$ of A are called the *eigenvalues* of D and form the *spectrum* of D. The eigenvalues of D are in general complex numbers because of the adjacency matrix A of D is not necessarily a symmetric matrix. The *spectral radius* of D, denoted by $\rho(D)$, equals to the largest absolute value of the eigenvalues of D, see [2, 7]. The energy of a digraph (see [7]) is defined by $E(D) = \sum_{i=1}^{n} |\mathrm{Re}(z_i)|$ where z_i is the eigenvalue of the digraph D and $\mathrm{Re}(z_i)$ denotes the real part of z_i, $i = 1, 2, ..., n$. For more details about the spectral radius and the energy of digraphs, see [2, 3, 5, 7, 8, 9, 12] and the references therein.

In this paper, we first give an improved lower bound for the spectral radius of a digraph D. Applying this result, we obtain some sharp upper bounds on the energy of D and characterize some extreme digraphs which attain these upper bounds. We also show that our results improve and generalize some known results in [5, 9, 12]. For the remaining basic terminology and notation used throughout the paper we refer the book [1].

2. A lower bound of the spectral radius of digraphs

Recall that for an $n \times n$ matrix $A = (a_{ij})$, its geometric symmetrization, denoted by $S = (s_{ij})$, is a matrix with entries $s_{ij} = \sqrt{a_{ij}a_{ji}}$ for any $i, j = 1, 2, ..., n$. Obviously, $c_2^{(j)} = \sum_{i=1}^{n} s_{ij}$ for any vertex v_j of V for a digraph D.

Theorem 1. *Let D be a simple digraph with n vertices and at least a closed walk of length 2. Also let $\left(c_2^{(1)}, c_2^{(2)}, ..., c_2^{(n)}\right)$ be the closed walk sequence of length 2 of D. Assume that $t_j = \sum_{i=1}^{n} c_2^{(i)} s_{ij}$ for any $j = 1, 2, ..., n$. Then*

$$\rho(D) \geq \sqrt{\frac{\sum_{i=1}^{n} (t_i)^2}{\sum_{i=1}^{n} \left(c_2^{(i)}\right)^2}} \qquad (1)$$

with equality in (1) if and only if $D = \overleftrightarrow{G}$+{*possibly some arcs that do not belong to cycles*}, *where each connected component of G is either an r-pseudo-regular graph or an* (r_1, r_2)*-pseudo-semiregular bipartite graph, satisfying* $r^2 = r_1 r_2 = \frac{\sum_{i=1}^{n}(t_i)^2}{\sum_{i=1}^{n}\left(c_2^{(i)}\right)^2}$.

Proof. Let A be the adjacency matrix of the digraph D and $S(A) = (s_{ij})$. Observe that $A \geq S(A) \geq 0$. From Corollary 2.15 in [1], $\rho(A) \geq \rho(S(A))$. By the Rayleigh-Ritz Theorem, it must be that

$$\rho(A) \geq \rho(S(A)) = \sqrt{\rho\left(S(A)^2\right)} = \sqrt{\max_{x\neq 0} \frac{x^T S(A)^2 x}{x^T x}} \geq \sqrt{\frac{c^T S(A)^2 c}{c^T c}}, \quad (2)$$

where $c = \left(c_2^{(1)}, c_2^{(2)}, ..., c_2^{(n)}\right)^T$. By a simple calculation,

$$S(A)c = \left(\sum_{i=1}^{n} c_2^{(i)} s_{i1}, \sum_{i=1}^{n} c_2^{(i)} s_{i2}, ..., \sum_{i=1}^{n} c_2^{(i)} s_{in}\right)^T = (t_1, t_2, ..., t_n)^T.$$

Hence,

$$\rho(D) = \rho(A) \geq \rho(S(A)) = \sqrt{\rho\left(S(A)^2\right)} \geq \sqrt{\frac{\sum_{i=1}^{n}(t_i)^2}{\sum_{i=1}^{n}\left(c_2^{(i)}\right)^2}}. \quad (3)$$

If the equality in (1) holds, then the above equalities in both (2) and (3) hold. Thus c is a positive eigenvector of $S(A)^2$ corresponding to $\rho\left(S(A)^2\right)$, which implies that the multiplicity of $\rho\left(S(A)^2\right)$ is either one or two. Note that the following proof is similar to these of Theorem 1 in [12] and Theorem 2.1 in [5]. Next we consider three cases.

Case (i): D is strongly connected, in consequence A is an irreducible matrix. Moreover, if $A > S(A)$, then $\rho(A) > \rho(S(A))$, which is a contradiction with $\rho(A) = \rho(S(A))$. Hence $A = S(A)$, which implies that $D = \overleftrightarrow{G}$ and G is a connected simple graph. From the proof of Theorem 4 in [10], we have G is either an r-pseudo-regular graph or an (r_1, r_2)-pseudo-semiregular bipartite graph, satisfying $r^2 = r_1 r_2 = \frac{\sum_{i=1}^{n}(t_i)^2}{\sum_{i=1}^{n}\left(c_2^{(i)}\right)^2}$.

Case (ii): D is the direct sum of its t disjoint strongly connected components $D_1, D_2, ..., D_t$. Let A_k be the $n_k \times n_k$ adjacency matrix of D_k such that $\sum_{k=1}^{t} n_k = n$. In this case $A = A_1 \oplus A_2 \oplus \cdots \oplus A_t$. Since the equality in (2) holds. Then we have

$$\rho(A) = \rho(S(A)) = \sqrt{\frac{c^T S(A)^2 c}{c^T c}} = \sqrt{\sum_{k=1}^{t} \frac{c_{n_k}^T S(A_k)^2 c_{n_k}}{c_{n_k}^T c_{n_k}} \frac{c_{n_k}^T c_{n_k}}{c^T c}}$$

$$\leq \sqrt{\sum_{k=1}^{t} \frac{\rho(S(A_k)^2)c_{n_k}^T c_{n_k}}{c^T c}} \leq \sqrt{\max_k \rho\left(S(A_k)^2\right)}$$

$$= \max_k \rho\left(S\left(A_k\right)\right) = \rho\left(S\left(A\right)\right) = \rho\left(A\right),$$

which implies that, for every $k = 1, 2, ..., t$,

$$\rho\left(A\right) = \rho\left(A_k\right) = \rho\left(S\left(A_k\right)\right) = \sqrt{\sum_{k=1}^{t} \frac{c_{n_k}^T S(A_k)^2 c_{n_k}}{c_{n_k}^T c_{n_k}}}.$$

It follows, from Case (i), that each $D_k = \overleftrightarrow{G_k}$, where each connected component G_k is either an r-pseudo-regular graph or an (r_1, r_2)-pseudo-semiregular bipartite graph, satisfying $r^2 = r_1 r_2 = \frac{\sum_{i=1}^{n}(t_i)^2}{\sum_{i=1}^{n}\left(c_2^{(i)}\right)^2}$.

Case (iii): In the general case, let $\widetilde{D}$ be the digraph obtained from D by deleting those arcs of D that do not belong to any cycle. Then $S(A) = S(A(\widetilde{D}))$. Noting that $\widetilde{D}$ and D have the same cycle structure. From Theorem 1.2 in [4], $\widetilde{D}$ and D have equal characteristic polynomial and the same eigenvalues. Since $\widetilde{D}$ is direct sum of its some disjoint strongly connected components. Then above Case (ii) implies that $\widetilde{D} = \overleftrightarrow{G}$ and each connected component of G is either an r-pseudo-regular graph or an (r_1, r_2)-pseudo-semiregular bipartite graph, satisfying $r^2 = r_1 r_2 = \frac{\sum_{i=1}^{n}(t_i)^2}{\sum_{i=1}^{n}\left(c_2^{(i)}\right)^2}$. Hence, $D = \overleftrightarrow{G} + \{$possibly some arcs that do not belong to cycles$\}$.

Conversely, suppose that $D = \overleftrightarrow{G} + \{$possibly some arcs that do not belong to cycles$\}$, where each connected component of G is either an r-pseudo-regular graph or an (r_1, r_2)-pseudo-semiregular bipartite graph, satisfying $r^2 = r_1 r_2 = \frac{\sum_{i=1}^{n}(t_i)^2}{\sum_{i=1}^{n}\left(c_2^{(i)}\right)^2}$. From the proof of Theorem 4 in [10], the equality in (1) holds. The proof is completed. □

The following Corollary 1 indicates that Theorem 1 is an improvement on Theorem 2.1 in [12].

Corollary 1[12]. *Let D be a simple digraph with n vertices, at least a closed walk of length 2 and $\left(c_2^{(1)}, c_2^{(2)}, ..., c_2^{(n)}\right)$ the closed walk sequence of length 2 of D. Then*

$$\rho\left(D\right) \geq \sqrt{\frac{\sum_{i=1}^{n}\left(c_2^{(i)}\right)^2}{n}}$$

with equality if and only if $D = \overleftrightarrow{G} + \{$possibly some arcs that do not belong to cycles$\}$, where G is an r-regular graph or an (r_1, r_2)-semiregular bipartite

graph, satisfying $r = \sqrt{r_1 r_2} = \sqrt{\frac{\sum_{i=1}^{n}\left(c_2^{(i)}\right)^2}{n}}$.
Proof. By Theorem 1 and the Cauchy-Schwarz inequality, we obtain

$$\rho(D) \geq \sqrt{\frac{\sum_{i=1}^{n}(t_i)^2}{\sum_{i=1}^{n}\left(c_2^{(i)}\right)^2}} \geq \sqrt{\frac{\left(\sum_{i=1}^{n} t_i\right)^2}{n\sum_{i=1}^{n}\left(c_2^{(i)}\right)^2}} = \sqrt{\frac{\left(\sum_{i=1}^{n}\left(c_2^{(i)}\right)^2\right)^2}{n\sum_{i=1}^{n}\left(c_2^{(i)}\right)^2}}$$
$$= \sqrt{\frac{\sum_{i=1}^{n}\left(c_2^{(i)}\right)^2}{n}},$$

with the equality holds if and only if G is either a pseudo-regular graph or a pseudo-semiregular bipartite graph with $t_1 = t_2 = \cdots = t_n$. From the proof of Corollary 6 in [10], it must be that G is a regular graph or a semiregular bipartite graph, satisfying $r = \sqrt{r_1 r_2} = \sqrt{\frac{\sum_{i=1}^{n}\left(c_2^{(i)}\right)^2}{n}}$. □

3. Some upper bounds of the energy of digraphs

In this section, applying the lower bound (1), we obtain some upper bounds on the energy of a digraph D and characterize some graphs which attain these upper bounds. Now we state the following lemma about the eigenvalues of digraphs.
Lemma 1[9]. *Let D be a simple digraph with n vertices, a arcs, and c_2 closed walks of length 2. If $z_1, z_2, ..., z_n$ are the eigenvalues of D, then*

$$(i)\sum_{i=1}^{n}(\mathrm{Re}\,(z_i))^2-\sum_{i=1}^{n}(\mathrm{Im}\,(z_i))^2 = c_2;\quad (ii)\sum_{i=1}^{n}(\mathrm{Re}\,(z_i))^2+\sum_{i=1}^{n}(\mathrm{Im}\,(z_i))^2 \leq a.$$

Theorem 2. *Let D be a simple digraph with n vertices, a arcs and at least a closed walk of length 2. Also let $\left(c_2^{(1)}, c_2^{(2)}, ..., c_2^{(n)}\right)$ be closed walk sequence of length 2 of D and $t_j = \sum_{i=1}^{n} c_2^{(i)} s_{ij}$ for $j = 1, 2, ..., n$. Then*

$$E(D) \leq \sqrt{\frac{\sum_{i=1}^{n}(t_i)^2}{\sum_{i=1}^{n}\left(c_2^{(i)}\right)^2}} + \sqrt{(n-1)\left(a - \frac{\sum_{i=1}^{n}(t_i)^2}{\sum_{i=1}^{n}\left(c_2^{(i)}\right)^2}\right)}. \qquad (4)$$

The equality holds in (4) if and only if $D = \overleftrightarrow{G}$, where G is either $\frac{n}{2}K_2, K_n$ or a non-bipartite connected ρ-pseudo-regular graph with three distinct eigenvalues $\left(\rho, \sqrt{\frac{a-\rho^2}{n-1}}, -\sqrt{\frac{a-\rho^2}{n-1}}\right)$, where $\rho = \sqrt{\frac{\sum_{i=1}^{n}(t_i)^2}{\sum_{i=1}^{n}\left(c_2^{(i)}\right)^2}}$.

Proof. Let $\rho = z_1, z_2, ..., z_n$ be the eigenvalues of D such that $\mathrm{Re}(z_1) \geq \mathrm{Re}(z_2) \geq ... \geq \mathrm{Re}(z_n)$. From the (ii) of Lemma 1, it must be that

$$\sum_{i=2}^{n} (\mathrm{Re}(z_i))^2 \leq a - \rho^2. \tag{5}$$

Thus, by the Cauchy-Schwarz inequality,

$$\sum_{i=2}^{n} |\mathrm{Re}(z_i)| \leq \sqrt{(n-1)\sum_{i=2}^{n} (\mathrm{Re}(z_i))^2} \leq \sqrt{(n-1)(a-\rho^2)}.$$

Hence, $E(D) \leq \rho + \sqrt{(n-1)(a-\rho^2)}$. Take the function $f(x) = x + \sqrt{(n-1)(a-x^2)}$, for $x \in [0, \sqrt{a}]$. First assume that $\sqrt{\frac{\sum_{i=1}^{n}(t_i)^2}{\sum_{i=1}^{n}\left(c_2^{(i)}\right)^2}} \geq \sqrt{\frac{a}{n}}$. Then by Theorem 1 and (5),

$$\sqrt{\frac{a}{n}} \leq \sqrt{\frac{\sum_{i=1}^{n}(t_i)^2}{\sum_{i=1}^{n}\left(c_2^{(i)}\right)^2}} \leq \rho \leq \sqrt{a}.$$

It is easy to verify that the function $f(x)$ decreases strictly on the interval $\left[\sqrt{\frac{a}{n}}, \sqrt{a}\right]$. Thus $f(\rho) \leq f\left(\sqrt{\frac{\sum_{i=1}^{n}(t_i)^2}{\sum_{i=1}^{n}\left(c_2^{(i)}\right)^2}}\right)$, which implies that the inequality (4) holds.

Now assume that the equality in (4) holds. Then $f(\rho) = f\left(\sqrt{\frac{\sum_{i=1}^{n}(t_i)^2}{\sum_{i=1}^{n}\left(c_2^{(i)}\right)^2}}\right)$, which implies $\rho = \sqrt{\frac{\sum_{i=1}^{n}(t_i)^2}{\sum_{i=1}^{n}\left(c_2^{(i)}\right)^2}}$ because of $f(x)$ decreases strictly in $\left[\sqrt{\frac{a}{n}}, \sqrt{a}\right]$. Again by Theorem 1, $D = \overleftrightarrow{G} + \{$possibly some arcs that do not belong to cycles$\}$, where each connected component of G is either an r-pseudo-regular graph or an (r_1, r_2)-pseudo-semiregular bipartite graph, satisfying $r^2 = r_1 r_2 = \frac{\sum_{i=1}^{n}(t_i)^2}{\sum_{i=1}^{n}\left(c_2^{(i)}\right)^2}$.

Since $c_2 \leq a$, Theorem 2.1 in [11] implies

$$\begin{aligned} E(D) = E(G) &\leq \sqrt{\frac{\sum_{i=1}^{n}(t_i)^2}{\sum_{i=1}^{n}\left(c_2^{(i)}\right)^2}} + \sqrt{(n-1)\left(c_2 - \frac{\sum_{i=1}^{n}(t_i)^2}{\sum_{i=1}^{n}\left(c_2^{(i)}\right)^2}\right)} \\ &\leq \sqrt{\frac{\sum_{i=1}^{n}(t_i)^2}{\sum_{i=1}^{n}\left(c_2^{(i)}\right)^2}} + \sqrt{(n-1)\left(a - \frac{\sum_{i=1}^{n}(t_i)^2}{\sum_{i=1}^{n}\left(c_2^{(i)}\right)^2}\right)} = E(D), \end{aligned}$$

which implies that $a = c_2$ and

$$E(G) = \sqrt{\frac{\sum_{i=1}^{n}(t_i)^2}{\sum_{i=1}^{n}\left(c_2^{(i)}\right)^2}} + \sqrt{(n-1)\left(c_2 - \frac{\sum_{i=1}^{n}(t_i)^2}{\sum_{i=1}^{n}\left(c_2^{(i)}\right)^2}\right)}.$$

Hence, from the equality conditions of Theorem 2.1 in [11], we obtain the required results.

If $\sqrt{\frac{\sum_{i=1}^{n}(t_i)^2}{\sum_{i=1}^{n}\left(c_2^{(i)}\right)^2}} < \sqrt{\frac{a}{n}}$, then by the proof of Corollary 1,

$$0 \le \sqrt{\frac{\sum_{i=1}^{n}\left(c_2^{(i)}\right)^2}{n}} \le \sqrt{\frac{\sum_{i=1}^{n}(t_i)^2}{\sum_{i=1}^{n}\left(c_2^{(i)}\right)^2}} < \sqrt{\frac{a}{n}},$$

which implies that $f\left(\sqrt{\frac{\sum_{i=1}^{n}\left(c_2^{(i)}\right)^2}{n}}\right) \le f\left(\sqrt{\frac{\sum_{i=1}^{n}(t_i)^2}{\sum_{i=1}^{n}\left(c_2^{(i)}\right)^2}}\right)$ because of $f(x)$ increases strictly in the interval $\left[0, \sqrt{\frac{a}{n}}\right]$. Therefore, by Theorem 2 in [12], the inequality (4) holds. If the equality in (4) holds, then $E(D) = f\left(\sqrt{\frac{\sum_{i=1}^{n}\left(c_2^{(i)}\right)^2}{n}}\right) = f\left(\sqrt{\frac{\sum_{i=1}^{n}(t_i)^2}{\sum_{i=1}^{n}\left(c_2^{(i)}\right)^2}}\right)$. Hence, from the equality conditions of Theorem 2 in [12], we obtain the required results. □

Remark 1. If $na \le c_2^2$, then

$$\sqrt{\frac{a}{n}} \le \frac{c_2}{n} \le \sqrt{\frac{\sum_{i=1}^{n}\left(c_2^{(i)}\right)^2}{n}} \le \sqrt{\frac{\sum_{i=1}^{n}(t_i)^2}{\sum_{i=1}^{n}\left(c_2^{(i)}\right)^2}} \le \rho \le \sqrt{a}.$$

Since the function $f(x) = x + \sqrt{(n-1)(a - x^2)}$ decreases strictly in the interval $\left[\sqrt{\frac{a}{n}}, \sqrt{a}\right]$, we get

$$E(D) \le f(\rho) \le f\left(\sqrt{\frac{\sum_{i=1}^{n}(t_i)^2}{\sum_{i=1}^{n}\left(c_2^{(i)}\right)^2}}\right) \le f\left(\sqrt{\frac{\sum_{i=1}^{n}\left(c_2^{(i)}\right)^2}{n}}\right).$$

Hence the bound (4) improves that of Theorem 2 in [12], for some cases.

Theorem 3. *Let D be a simple digraph with n vertices, a arcs and at least a closed walk of length 2. Also let $\left(c_2^{(1)}, c_2^{(2)}, \ldots, c_2^{(n)}\right)$ be closed walk* *sequence of length 2 of* D *and* $t_j = \sum_{i=1}^{n} c_2^{(i)} s_{ij}$ *for each* $j = 1, 2, ..., n$. *If* $\sqrt{\frac{\sum_{i=1}^{n}(t_i)^2}{\sum_{i=1}^{n}\left(c_2^{(i)}\right)^2}} \geq \sqrt{\frac{a+c_2}{2n}}$, *then*

$$E(D) \leq \sqrt{\frac{\sum_{i=1}^{n}(t_i)^2}{\sum_{i=1}^{n}\left(c_2^{(i)}\right)^2}} + \sqrt{(n-1)\left(\frac{a+c_2}{2} - \frac{\sum_{i=1}^{n}(t_i)^2}{\sum_{i=1}^{n}\left(c_2^{(i)}\right)^2}\right)}. \quad (6)$$

The equality holds in (6) if and only if $D = \overleftrightarrow{G}$, *where* G *is either* $\frac{n}{2}K_2, K_n$ *or a non-bipartite connected* ρ*-pseudo-regular graph with three distinct eigenvalues* $\left(\rho, \sqrt{\frac{\frac{a+c_2}{2}-\rho^2}{n-1}}, -\sqrt{\frac{\frac{a+c_2}{2}-\rho^2}{n-1}}\right)$, *where* $\rho = \sqrt{\frac{\sum_{i=1}^{n}(t_i)^2}{\sum_{i=1}^{n}\left(c_2^{(i)}\right)^2}}$.

Proof. Let $\rho = z_1, z_2, ..., z_n$ be the eigenvalues of D such that $\operatorname{Re}(z_1) \geq \operatorname{Re}(z_2) \geq ... \geq \operatorname{Re}(z_n)$. It follows from Lemma 1 that

$$\sum_{i=2}^{n} (\operatorname{Re}(z_i))^2 \leq \frac{a+c_2}{2} - \rho^2. \quad (7)$$

From the inequality (7) and the Cauchy-Schwarz inequality, it must be that

$$\sum_{i=2}^{n} |\operatorname{Re}(z_i)| \leq \sqrt{(n-1)\sum_{i=2}^{n}(\operatorname{Re}(z_i))^2} \leq \sqrt{(n-1)\left(\frac{a+c_2}{2} - \rho^2\right)}.$$

Hence,

$$E(D) \leq \rho + \sqrt{(n-1)\left(\frac{a+c_2}{2} - \rho^2\right)}. \quad (8)$$

Consider the function $g(x) = x + \sqrt{(n-1)\left(\frac{a+c_2}{2} - x^2\right)}, x \in [0, \sqrt{\frac{a+c_2}{2}}]$. Since $\sqrt{\frac{\sum_{i=1}^{n}(t_i)^2}{\sum_{i=1}^{n}\left(c_2^{(i)}\right)^2}} \geq \sqrt{\frac{a+c_2}{2n}}$. Then by Theorem 1,

$$\sqrt{\frac{a+c_2}{2n}} \leq \sqrt{\frac{\sum_{i=1}^{n}(t_i)^2}{\sum_{i=1}^{n}\left(c_2^{(i)}\right)^2}} \leq \rho \leq \sqrt{\frac{a+c_2}{2}}.$$

Since $f(x)$ decreases strictly in the interval $\left[\sqrt{\frac{a+c_2}{2n}}, \sqrt{\frac{a+c_2}{2}}\right]$. Then $g(\rho) \leq g\left(\sqrt{\frac{\sum_{i=1}^{n}(t_i)^2}{\sum_{i=1}^{n}\left(c_2^{(i)}\right)^2}}\right)$, which implies that the inequality (6) holds.

If the equality in (6) holds, then $g(\rho) = g\left(\sqrt{\frac{\sum_{i=1}^{n}(t_i)^2}{\sum_{i=1}^{n}\left(c_2^{(i)}\right)^2}}\right)$. Hence, $\rho = \sqrt{\frac{\sum_{i=1}^{n}(t_i)^2}{\sum_{i=1}^{n}\left(c_2^{(i)}\right)^2}}$ because of the function $g(x)$ decreases strictly. At this point we continue using the same techniques used in the proof of Theorem 2, we obtain the required results. □

Remark 2. Observe that $c_2 \leq a$, the upper bound (6) in Theorem 3 is an improvement on the upper bound (4) in Theorem 2 whenever $\sqrt{\frac{\sum_{i=1}^{n}(t_i)^2}{\sum_{i=1}^{n}\left(c_2^{(i)}\right)^2}} \geq \sqrt{\frac{a+c_2}{2n}}$. On the other hand, from the proof of Theorem 3,

$$E(D) \leq g(\rho) \leq g\left(\sqrt{\frac{\sum_{i=1}^{n}(t_i)^2}{\sum_{i=1}^{n}\left(c_2^{(i)}\right)^2}}\right) \leq g\left(\sqrt{\frac{a+c_2}{2n}}\right) = \sqrt{\frac{1}{2}n(a+c_2)}.$$

Hence, the bound (6) in Theorem 3 is also an improvement on the generalized McClelland bound given in ([9], see Theorem 2.3) for some cases.

Corollary 2. *Let D be a digraph with n vertices, a arcs and c_2 closed walks of length 2. If $\frac{a+c_2}{2} \leq \frac{c_2^2}{n}$, then*

$$E(D) \leq \frac{c_2}{n} + \sqrt{(n-1)\left(\frac{a+c_2}{2} - \left(\frac{c_2}{n}\right)^2\right)}. \qquad (9)$$

Equality in (9) holds if and only if $D = \overleftrightarrow{G}$, where G is either $\frac{n}{2}K_2$, K_n or a non-bipartite connected strongly regular graph with two non-trivial eigenvalues both with absolute value $\sqrt{\left(\frac{a+c_2}{2} - \left(\frac{c_2}{n}\right)^2\right)/(n-1)}$, or nK_1.

Proof. If $\frac{a+c_2}{2} \leq \frac{c_2^2}{n}$. By Corollary 1 and the Cauchy-Schwarz inequality,

$$\sqrt{\frac{a+c_2}{2n}} \leq \frac{c_2}{n} \leq \sqrt{\frac{\sum_{i=1}^{n}\left(c_2^{(i)}\right)^2}{n}} \leq \sqrt{\frac{\sum_{i=1}^{n}(t_i)^2}{\sum_{i=1}^{n}\left(c_2^{(i)}\right)^2}} \leq \rho \leq \sqrt{\frac{a+c_2}{2}}.$$

From the proof of Theorem 3, we obtain

$$E(D) \leq g(\rho) \leq g\left(\sqrt{\frac{\sum_{i=1}^{n}(t_i)^2}{\sum_{i=1}^{n}\left(c_2^{(i)}\right)^2}}\right) \leq g\left(\sqrt{\frac{\sum_{i=1}^{n}\left(c_2^{(i)}\right)^2}{n}}\right) \leq g\left(\frac{c_2}{n}\right),$$

which implies that the inequality (9) holds. The rest of proof is similar to Theorem 2 in [12], omitted. □

Remark that if $c_2 \leq a$, the upper bound (9) of Corollary 2 improves that of Theorem 3.1 in [5] whenever $\frac{a+c_2}{2} \leq \frac{c_2^2}{n}$.

Let D be a digraph with n vertices, a arcs and c_2 closed walks of length 2. The *symmetry index* of D, denoted by s, is defined as $s = a - c_2$. In [5], Gudiño and Rada proved that

$$E(D) \leq \frac{n}{2}\left(1+\sqrt{n+\frac{4s}{n}}\right).$$

The following Theorem 4 is a slight improvement on above result.

Theorem 4. *Let D be a digraph with n vertices, c_2 closed walks of length 2 and symmetry index s. If $s \leq 2\left(\frac{c_2^2}{n} - c_2\right)$, then*

$$E(D) \leq \frac{n}{2}\left(1+\sqrt{n+\frac{2s}{n}}\right). \tag{10}$$

The equality holds in (10) if and only if $D = \overleftrightarrow{G}$ where G is a strongly regular graph with parameters $\left(n, \frac{n+\sqrt{n}}{2}, \frac{n+2\sqrt{n}}{4}, \frac{n+2\sqrt{n}}{4}\right)$.

Proof. The following proof is similar to that of Theorem 3.3 in [5]. Consider the function

$$h(x) = \frac{x}{n} + \sqrt{(n-1)\left(x+\frac{s}{2}-\left(\frac{x}{n}\right)^2\right)}, \quad x \in \left[0, \frac{n^2}{2}+\frac{n}{2}\sqrt{n^2+2s}\right].$$

It is easy to see that $h(x)$ attains its maximum in $x_0 = \frac{n^2}{2} + \frac{n}{2}\sqrt{n^2+2s}$. Observe that $c_2 \leq n(n-1) \leq \frac{n^2}{2} + \frac{n}{2}\sqrt{n^2+2s}$. By Corollary 2, we obtain

$$E(D) \leq h(c_2) \leq h(x_0) = \frac{n}{2}\left(1+\sqrt{n+\frac{2s}{n}}\right), \tag{11}$$

which proves (10).

Now assume that the equality in (10) holds. Then by (11), we have

$$E(D) = h(c_2) = \frac{c_2}{n} + \sqrt{(n-1)\left(\frac{a+c_2}{2}-\left(\frac{c_2}{n}\right)^2\right)}.$$

Corollary 2 implies that $D = \overleftrightarrow{G}$, that is, $s = 0$. Therefore, by (11)

$$E(G) = E(D) = \frac{n}{2}\left(1+\sqrt{n}\right).$$

The result follows from the equality conditions of Theorem 3 in [6]. □

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References

[1] A. Berman, R.J. Plemmons. Nonnegative matrices in the mathematical sciences. Academic, New York, 1979 (SIAM, Philadelphia, PA, 1994).

[2] R. Brualdi. Spectra of digraphs. Linear Algebra Appl. 432 (2010) 2181-2213.

[3] Ş.B. Bozkurt, D. Bozkurt, X.D. Zhang. On the spectral radius and the energy of a digraph. Linear and Multilinear Algebra. 63 (2015) 2009-2016.

[4] D. Cvetković, M. Doob, H. Sachs, Spectra of Graphs: Theory and Application, Academic press, New York, 1980.

[5] E. Gudiño, J. Rada. A lower bound for the spectral radius of a digraph. Linear Algebra Appl. 433 (2010) 233-240.

[6] J.H. Koolen, V. Moulton. Maximal energy graphs. Adv. Appl. Math. 26 (2001) 47-52.

[7] I. Peña, J. Rada. Energy of digraphs. Linear Multilinear Algebra. 56 (2008) 565-579.

[8] J. Rada. Bounds for the energy of normal digraphs. Linear Multilinear Algebra. 60 (2012) 323-332.

[9] J. Rada. The McClelland inequality for the energy of digraphs. Linear Algebra Appl. 430 (2009) 800-804.

[10] A.M. Yu, M. Lu, F. Tian. On the spectral radius of graphs. Linear Algebra Appl. 387 (2004) 41-49.

[11] A.M. Yu, M. Lu, F. Tian. New upper bounds for the energy of graphs. Match Commun. Math. Comput. Chem. 53 (2005) 441-448.

[12] G.X. Tian, S.Y. Cui. On upper bounds for the energy of digraphs. Linear Algebra Appl. 438 (2013) 4742-4749.