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A lower bound for the spectral radius of a digraph

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Abstract

We show that the spectral radius $\rho(D)$ of a digraph D with n vertices and c_2 closed walks of length 2 satisfies $\rho(D) \geq \frac{c_2}{n}$. Moreover, equality occurs if and only if D is the symmetric digraph associated to a $\frac{c_2}{n}$-regular graph, plus some arcs that do not belong to cycles. As an application of this result, we construct new upper bounds for the low energy of a digraph.

key words. Spectral radius of a digraph. Energy of a digraph. Low energy of a digraph.

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1 Introduction

A directed graph (or just digraph) D consists of a non-empty finite set $\mathcal{V}$ of elements called vertices and a finite set $\mathcal{A}$ of ordered pairs of distinct vertices called arcs. Throughout we assume that D has no loops nor multiple arcs. Two vertices are called adjacent if they are connected by an arc. If there is an arc from vertex u to vertex v we indicate this by writing uv. A walk π of length l from vertex u to vertex v is a sequence of vertices $\pi : u = u_0, u_1, \ldots, u_l = v$, where $u_{t-1}u_t$ is an arc of D for every $1 \leq t \leq l$. If $u = v$ then π is a closed walk. If $u = v$ but $u_i \neq u_j$ for $i \neq j$ $(i, j = 1, \ldots, l)$ then π is a cycle of D.

A digraph D is symmetric if $uv \in \mathcal{A}$ then $vu \in \mathcal{A}$, where $u, v \in \mathcal{V}$. A one to one correspondence between graphs and symmetric digraphs is given by $G \rightsquigarrow \overleftrightarrow{G}$, where $\overleftrightarrow{G}$ has the same vertex set as the graph G, and each edge uv of G is replaced by a pair of symmetric arcs uv and vu. Under this correspondence, a graph can be identified with a symmetric digraph.

The adjacency matrix A of a digraph D whose vertex set is $\{v_1, \ldots, v_n\}$ is the $n \times n$ matrix whose entry a_{ij} is defined as $a_{ij} = 1$ if $v_iv_j \in \mathcal{A}$ and $a_{ij} = 0$ otherwise. The characteristic polynomial $|zI - A|$ of the adjacency matrix A of D is called the characteristic polynomial of D and it is denoted by $\Phi_D = \Phi_D(z)$. The eigenvalues of A are called the eigenvalues of D. Since A

is not necessarily a symmetric matrix, the eigenvalues of A are in general complex numbers. The spectral radius of A (respectively, of D) is denoted by $\rho(A)$ (respectively, $\rho(D)$), and equals to the largest absolute value of an eigenvalue of A. For a recent survey on spectra of digraphs we refer to [1].

The eigenvalues of a graph G with n vertices are real numbers $\lambda_1, \ldots, \lambda_n$. The energy of G, which was introduced by Gutman in [4] and it is extensively studied in chemistry, is defined as $E(G) = \sum_{i=1}^{n} |\lambda_i|$. Recently, Nikiforov ([9],[10]) extended the energy of a graph to general matrices as

$$E(A) = \sum_{i=1}^{n} \sigma_i$$

where $\sigma_1, \ldots, \sigma_n$ are the singluar values of the n by m matrix A. When A is the adjacency matrix of a graph G, then $E(A)$ coincides with $E(G)$.

Another definition for the energy of digraphs was given in [11]. Coulson's integral formula was generalized to digraphs

$$\frac{1}{\pi} \int_{-\infty}^{\infty} \left(n - \frac{ix\Phi_D'(ix)}{\Phi_D(ix)} \right) dx = \sum_{i=1}^{n} |Rez_i|$$

where $z_1, \ldots, z_n$ are the (possibly complex) eigenvalues of the digraph D and Rez_i denotes the real part of z_i. Consequently, the concept of energy was naturally extended to digraphs as

$$e(D) = \sum_{i=1}^{n} |Rez_i|$$

and it is called the low energy of D in [1], to differentiate between the two concepts. For further results in the study of the low energy of digraphs we refer to [8], [11], [12] and [13].

In this paper we use Kolotilina's ideas in the article [6], to find a new lower bound for the spectral radius of a digraph in terms of its number of vertices and number of closed walks of length 2 (see Theorem 2.1). This result generalizes the well known lower bound for the spectral radius of a graph found by L. Collatz and U. Sinogowitz ([2], see also [3, Theorem 3.8]): if G has n vertices and m edges then $\rho(G) \geq \frac{2m}{n}$. Equality holds if and only if G is a $\frac{2m}{n}$-regular graph. As an application of this result, we show in Theorem 3.1 that

$$e(D) \leq \frac{c_2}{n} + \sqrt{(n-1)\left[a - \left(\frac{c_2}{n}\right)^2\right]}$$

where D is a digraph with n vertices, a arcs and c_2 closed walks of length 2. This upper bound for the low energy generalizes the well-known inequality for the energy of a graph given by Koolen and Moulton [7].

Finally, we introduce the symmetry index of a digraph, denoted by s and defined as $s = a - c_2$, which measures how far is a digraph from being symmetric. Then we show in Theorem 3.3 that

$$e(D) \leq \tfrac{n}{2}(1 + \sqrt{n + \tfrac{4s}{n}})$$

generalizing the well known upper bound of the energy of a graph in terms of the number of vertices given in [7, Theorem 3].

2 Lower bound of the spectral radius of a digraph

Recall that the geometric symmetrization of a matrix $A = (a_{ij})$, denoted by $S(A) = (s_{ij})$, is the matrix with entries

$$s_{ij} = \sqrt{a_{ij}a_{ji}}$$

for every $i, j = 1, \ldots, n$. Note that if A is the adjacency matrix of a digraph D with n vertices, then $\sum_{j=1}^{n}\sum_{i=1}^{n} s_{ij} = c_2$, where c_2 denotes the number of walks of length 2 of D. Also, if $\widehat{D}$ is obtained from D by deleting those arcs of D that do not belong to a cycle, then clearly $S(A) = S\left(A\left(\widehat{D}\right)\right)$, where $A\left(\widehat{D}\right)$ is the adjacency matrix of $\widehat{D}$. Moreover, by the coefficient theorem for digraphs [3, Theorem 1.2], D and $\widehat{D}$ have equal characteristic polynomial because they have the same cycle structure.

Theorem 2.1 *Let D be a digraph with n vertices and c_2 closed walks of length 2. Then*

$$\rho(D) \geq \frac{c_2}{n}$$

Equality holds if and only if

$$D = \overleftrightarrow{G} + \{\textit{possibly some arcs that do not belong to cycles}\}$$

where G is a $\frac{c_2}{n}$-regular graph.

Proof. Let A be the adjacency matrix of the digraph D and $S(A) = (s_{ij})$ the geometric symmetrization matrix of A. Clearly $A \geq S(A) \geq 0$ and so by [5, Corollary 8.1.19], $\rho(A) \geq$

$\rho(S(A))$. On the other hand, by Raleigh-Ritz Theorem [5, Theorem 4.2.2],

$$\rho(A) \geq \rho(S(A)) \geq \frac{e^{\top} S(A) e}{n} = \frac{\sum_{i=1}^{n} \sum_{j=1}^{n} s_{ij}}{n} = \frac{c_2}{n} \tag{1}$$

where $e = (1, 1, \dots, 1)^{\top}$.

Now assume that $\rho(A) = \frac{c_2}{n}$. It follows from inequality (1) that

$$\rho(A) = \frac{e^{\top} S(A) e}{n} = \rho(S(A))$$

We consider three cases. (i) D is strongly connected: in this case A is irreducible and so by Perron-Frobenius Theorem, there exists $0 < v = (v_1, \dots, v_n)^{\top} \in \mathbb{R}^n$ such that $Av = \rho(A) v$. Equivalently,

$$\rho(A) = \sum_{j=1}^{n} a_{ij} \frac{v_j}{v_i}$$

for every $i = 1, \dots, n$. Hence by the Geometric-Arithmertic mean inequality,

$$n\rho(A) = \sum_{1 \leq i < j \leq n} \left(a_{ij} \frac{v_j}{v_i} + a_{ji} \frac{v_i}{v_j} \right) \geq 2 \sum_{1 \leq i < j \leq n} \sqrt{a_{ij} a_{ji}} = e^{\top} S(A) e = n\rho(A)$$

which implies

$$a_{ij} \frac{v_j}{v_i} = a_{ji} \frac{v_i}{v_j}$$

for every $i, j = 1, \dots, n$. Since A is a $(0,1)$-matrix and $v > 0$, we deduce that $a_{ij} = 0$ if and only if $a_{ji} = 0$ for every $i, j = 1, \dots, n$. Thus A is a symmetric matrix and so $D = \overleftrightarrow{G}$ for a graph G that has $\frac{c_2}{2}$ edges and n vertices. Since

$$\rho(G) = \rho(A) = \frac{c_2}{n}$$

it follows from [3, Theorem 3.8] that G is a $\frac{c_2}{n}$-regular graph.

(ii) D is the disjoint union of t strongly connected components $D_1, \dots, D_t$: in this case

$$A = \begin{pmatrix} A_1 & 0 & \cdots & 0 \\ 0 & A_2 & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & A_t \end{pmatrix}$$

where each block matrix A_k is the $n_k \times n_k$ adjacency (irreducible) matrix of D_k. Clearly $\sum_{k=1}^{n} n_k = n$. Hence

$$\frac{e^{\top} S(A) e}{n} = \sum_{k=1}^{t} \frac{e_{n_k}^{\top} S(A_k) e_{n_k}}{n_k} \frac{n_k}{n} \leq \sum_{k=1}^{t} \frac{n_k \rho(A_k)}{n} \leq \max_k \rho(A_k) = \rho(A) \tag{2}$$

Since $\rho(A) = \frac{e^{\top} S(A) e}{n}$ we deduce from inequality (2) that $\rho(A) = \rho(A_k) = \frac{e_{n_k}^{\top} S(A_k) e_{n_k}}{n_k}$ for every $k = 1, \ldots, t$, and now applying case (i) it follows that each $D_k = \overleftrightarrow{G_k}$, where G_k is a $\frac{c_2}{n}$-regular graph for every $k = 1, \ldots, t$.

(iii) In the general case, let $\widehat{D}$ be the digraph obtained from D deleting every arc of D which does not belong to a cycle. Then $\widehat{D}$ is the disjoint union of the strongly connected components of D, D and $\widehat{D}$ have equal spectrum and $S(A) = S\left(A\left(\widehat{D}\right)\right)$. Thus

$$\rho\left(\widehat{D}\right) = \rho(D) = \frac{e^{\top} S\left(A\left(\widehat{D}\right)\right) e}{n}$$

Now we apply case (ii) to $\widehat{D}$ to obtain that $\widehat{D} = \overleftrightarrow{G}$ for a $\frac{c_2}{n}$-regular graph G, and consequently

$$D = \overleftrightarrow{G} + \{\text{possibly some arcs that do not belong to cycles}\}$$

■

Note that if G is a graph with m edges and n vertices, then the digraph associated $\overleftrightarrow{G}$ also has n vertices and the number of closed walks of length 2 of $\overleftrightarrow{G}$ is $c_2 = 2m$. Hence

$$\rho(G) = \rho\left(\overleftrightarrow{G}\right) \geq \frac{c_2}{n} = \frac{2m}{n} \tag{3}$$

Moreover, if $\rho(G) = \frac{2m}{n}$ then by inequality (3), $\rho\left(\overleftrightarrow{G}\right) = \frac{c_2}{n}$ and by Theorem 2.1, $\overleftrightarrow{G}$ is a $\frac{c_2}{n}$-regular digraph (every arc of $\overleftrightarrow{G}$ belongs to a cycle) and so G is a $\frac{2m}{n}$-regular graph. Consequently, Theorem 2.1 is a generalization to digraphs of Collatz and Sinogowitz's Theorem.

3 Upper bound for the energy of a digraph

We next apply Theorem 2.1 and the technique used by Koolen and Moulton in [7], to construct new upper bounds for the low energy of a digraph.

Theorem 3.1 *Let D be a digraph with n vertices, a arcs and c_2 closed walks of length 2. Then*

$$e(D) \leq \frac{c_2}{n} + \sqrt{(n-1)\left[a - \left(\frac{c_2}{n}\right)^2\right]} \tag{4}$$

Equality holds if and only if D is the empty digraph (i.e. n isolated vertices) or

$$D = \overleftrightarrow{G} + \{\textit{possibly some arcs that do not belong to cycles}\}$$

where G is one of the following:

1. $G = \frac{n}{2} K_2$;
2. $G = K_n$;
3. *G is a non-complete connected strongly regular graph with two non-trivial eigenvalues both with absolute value* $\sqrt{\frac{a-\left(\frac{c_2}{n}\right)^2}{n-1}}$.

Proof. Let A be the adjacency matrix of D. Since $A \geq 0$ we know that $\rho := \rho(A)$ is an eigenvalue of D. Assume that $\rho = z_1, z_2, \ldots, z_n$ are the eigenvalues of D. By the Cauchy-Schwarz inequality applied to the vectors

$$(|Re(z_2)|, |Re(z_3)|, \ldots, |Re(z_n)|) \text{ and } (1, 1, \ldots, 1)$$

of $\mathbb{R}^{n-1}$ we deduce that

$$\left(\sum_{i=2}^{n} |Re(z_i)|\right)^2 \leq (n-1) \sum_{i=2}^{n} [Re(z_i)]^2$$

From ([12, Lemma 2.2]) we know that

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

Hence

$$e(D) = \rho + \sum_{i=2}^{n} |Re(z_i)| \leq \rho + \sqrt{(n-1)(a-\rho^2)} \tag{6}$$

Consider the function

$$f(x) = x + \sqrt{(n-1)(a-x^2)}$$

defined in the interval $[-\sqrt{a}, \sqrt{a}]$. First we consider the case $c_2 \geq \sqrt{na}$. Then by Theorem 2.1 and inequality (5)

$$\sqrt{\frac{a}{n}} \leq \frac{c_2}{n} \leq \rho \leq \sqrt{a}$$

Since the function f is strictly decreasing in the interval $\left[\sqrt{\frac{a}{n}}, \sqrt{a}\right]$, and bearing in mind inequality (6)

$$e(D) \leq f(\rho) \leq f\left(\frac{c_2}{n}\right) = \frac{c_2}{n} + \sqrt{(n-1)\left[a - \left(\frac{c_2}{n}\right)^2\right]} \tag{7}$$

If $e(D) = \frac{c_2}{n} + \sqrt{(n-1)\left[a - \left(\frac{c_2}{n}\right)^2\right]}$ then by inequality (7), $f(\rho) = f\left(\frac{c_2}{n}\right)$. Since f is strictly decreasing, $\rho = \frac{c_2}{n}$. Again by Theorem 2.1,

$$D = \overleftrightarrow{G} + \{\text{possibly some arcs that do not belong to cycles}\}$$

where G is a $\frac{c_2}{n}$-regular graph with n vertices and $\frac{c_2}{2}$ edges. Further, by [7, Theorem 1] and the fact that $c_2 \leq a$

$$\begin{aligned} e(D) = E(G) &\leq \frac{c_2}{n} + \sqrt{(n-1)\left[c_2 - \left(\frac{c_2}{n}\right)^2\right]} \\ &\leq \frac{c_2}{n} + \sqrt{(n-1)\left[a - \left(\frac{c_2}{n}\right)^2\right]} = e(D) \end{aligned}$$

which implies $c_2 = a$ and

$$E(G) = \tfrac{c_2}{n} + \sqrt{(n-1)\left[c_2 - \left(\tfrac{c_2}{n}\right)^2\right]}$$

Now the result follows from the equality conditions in [7, Theorem 1].

For $c_2 < \sqrt{na}$, we consider two cases:
(a) If $a < n$ then $a \leq \sqrt{(n-1)a}$ and by [12, Theorem 2.5],

$$e(D) \leq a \tag{8}$$

Since f is strictly increasing in $\left[0, \sqrt{\frac{a}{n}}\right]$ and $c_2 < \sqrt{na}$, then $\frac{c_2}{n} \in \left[0, \sqrt{\frac{a}{n}}\right]$ and we have

$$\sqrt{(n-1)a} = f(0) \leq f\left(\frac{c_2}{n}\right) \tag{9}$$

From inequalities (8) and (9) we deduce

$$e(D) \leq \tfrac{c_2}{n} + \sqrt{(n-1)\left[a - \left(\tfrac{c_2}{n}\right)^2\right]}$$

If equality holds, then again from inequalities (8) and (9)

$$e(D) = a = \sqrt{a(n-1)} = f(0) = f\left(\tfrac{c_2}{n}\right)$$

Since f is strictly increasing, $c_2 = 0$. On the other hand by [12, Theorem 2.5], $D = \frac{a}{2} \overleftrightarrow{K}_2$ plus some isolated vertices, which implies that $a = c_2 = 0$. Hence D is the empty digraph.

(b) If $a \geq n$, then it is not difficult to see that

$$\sqrt{\frac{1}{2}n\left(a+c_2\right)} \leq \frac{c_2}{n} + \sqrt{(n-1)\left[a - \left(\frac{c_2}{n}\right)^2\right]}$$

and so by [12, Theorem 2.3]

$$e\left(D\right) \leq \tfrac{c_2}{n} + \sqrt{(n-1)\left[a - \left(\tfrac{c_2}{n}\right)^2\right]}$$

If equality holds, then by [12, Theorem 2.3] $D = \frac{n}{2} \overleftrightarrow{K}_2$.

■

An application of Theorem 3.1 gives an improvement of [7, Theorem 1]. More precisely, if G is a graph with n vertices and m edges, the hypothesis "$2m \geq n$" can be dropped. In fact, consider $\overleftrightarrow{G}$ the digraph associated to G. Then $\overleftrightarrow{G}$ has n vertices and $a = c_2 = 2m$. Now from Theorem 3.1

$$E\left(G\right) = e\left(\overleftrightarrow{G}\right) \leq \frac{2m}{n} + \sqrt{(n-1)\left[2m - \left(\frac{2m}{n}\right)^2\right]} \tag{10}$$

If equality in (10) holds, then again the result follows by the equality conditions in Theorem 3.1.

Koolen and Moulton [7, Theorem 3] also showed that for a graph G with n vertices

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

We next generalize this result for digraphs. Let us first introduce an invariant which measures how far is a digraph from being a symmetric digraph.

Definition 3.2 *Let D be a digraph with a arcs and c_2 closed walks of length 2. The symmetry index of D, denoted by s, is defined as $s = a - c_2$.*

Clearly, $0 \leq s \leq n\left(n-1\right)$ for every digraph D. Also note that a digraph D is symmetric if and only if $s = 0$.

Theorem 3.3 *Let D be a digraph with n vertices and symmetry index s. Then*

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

Proof. Consider the function $g(x) = \frac{x}{n} + \sqrt{(n-1)\left(x + s - \left(\frac{x}{n}\right)^2\right)}$ defined in the interval $I = \left[\frac{n^2}{2} - \frac{n}{2}\sqrt{n^2+4s}, \frac{n^2}{2} + \frac{n}{2}\sqrt{n^2+4s}\right]$. Using routine calculus we can see that g attains its maximum in $x_0 = \frac{n^2}{2} + \frac{n}{2}\sqrt{n + \frac{4s}{n}} \in I$. Then by Theorem 3.1 and the fact that $c_2 \in I$ because

$$c_2 \leq n(n-1) \leq \frac{n^2}{2} + \frac{n}{2}\sqrt{n^2+4s}$$

we deduce

$$e(D) \leq g(c_2) \leq g(x_0) = \frac{n}{2}\left(1 + \sqrt{n + \frac{4s}{n}}\right)$$

■

Note that Theorem 3.3 is a generalization of [7, Theorem 3] since $s = 0$ for symmetric digraphs.

It is reasonable to compare the generalized McClelland bound

$$M = \sqrt{\frac{1}{2}n(a + c_2)}$$

given in [12, Theorem 2.3] with the new bound

$$K = \frac{c_2}{n} + \sqrt{(n-1)\left[a - \left(\frac{c_2}{n}\right)^2\right]}$$

given in Theorem 3.1. It was shown in [7, Inequality (4) and Theorem 2] that if D is a symmetric digraph then $K \leq M$. In the general situation this is not always true, as we can see in the proof of Theorem 3.1 when $a \geq n$ and $c_2 < \sqrt{na}$. However, we show in our next result a large class of non-symmetric digraphs where $K \leq M$.

Proposition 3.4 *Let D be a digraph with $n \geq 6$ vertices, c_2 closed walks of length 2 and symmetry index s. If $c_2 \geq \frac{n^2}{2} + \frac{n}{2}\sqrt{n + \frac{4s}{n}}$ then $K < M$.*

Proof. Consider the functions

$$M(x) = \sqrt{\tfrac{n}{2}(2x + s)} \quad \text{and} \quad K(x) = \tfrac{x}{n} + \sqrt{(n-1)\left(x + s - \left(\tfrac{x}{n}\right)^2\right)}$$

which are well defined in the interval $I = [0, n(n-1)]$. Since $M'(x) > 0$ for every $x \in I$ then M is strictly increasing in I. On the other hand, $K(x)$ attains its maximum in $x_0 = \frac{n^2}{2} + \frac{n}{2}\sqrt{n + \frac{4s}{n}}$ ($x_0 \in I$ when $n \geq 6$), and it is strictly decreasing in the interval $[x_0, n(n-1)]$ (see Figure 1).

It is easy to see that

$$K(x_0) = \frac{n}{2}\left(1 + \sqrt{n + \frac{4s}{n}}\right) < \sqrt{\frac{n}{2}(n^2 + n\sqrt{n + \frac{4s}{n}} + s)} = M(x_0).$$

Hence $K(x) < M(x)$ for every $x \in [x_0, n(n-1)]$. In particular, if $c_2 \geq x_0$ (note that in any digraph $c_2 \leq n(n-1)$) then $K = K(c_2) < M(c_2) = M$. ∎

Example 3.5 *Table 1 shows examples of non-symmetric digraphs with n vertices, symmetry index s and c_2 closed walks of length 2 such that $K \leq M$.*

Table 1:

n	10	20	50	100
c_2	68	252	1436	5520
s	4	32	53	200
K	21,11	61,38	209,11	569,61
M	26,17	73,21	270,41	749,66

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