

UPPER BOUND FOR THE ENERGY OF STRONGLY CONNECTED DIGRAPHS

Singaraj K. Ayyaswamy, Selvaraj Balachandran, Ivan Gutman

The energy of a digraph D is defined as $E(D) = \sum_{i=1}^n |\operatorname{Re}(z_i)|$, where z_1, z_2, \dots, z_n are the (possibly complex) eigenvalues of D . We show that if D is a strongly connected digraph on n vertices, a arcs, and c_2 closed walks of length two, such that $\operatorname{Re}(z_1) \geq (a + c_2)/(2n) \geq 1$, then $E(D) \leq n(1 + \sqrt{n})/2$. Equality holds if and only if D is a directed strongly regular graph with parameters $\left(n, \frac{n + \sqrt{n}}{2}, \frac{3n + 2\sqrt{n}}{8}, \frac{n + 2\sqrt{n}}{8}, \frac{n + 2\sqrt{n}}{8}\right)$. This bound extends to digraphs an earlier result [J. H. KOOLEN, V. MOULTON: *Maximal energy graphs*. Adv. Appl. Math., **26** (2001), 47–52], obtained for simple graphs.

1. INTRODUCTION

The energy $E(G)$ of a graph G is defined to be the sum of absolute values of its eigenvalues [5]. For surveys of the mathematical properties of graph energy see [6, 7]. In the seminal work [8], KOOLEN and MOULTON proved that for all graphs with n vertices and m edges,

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

and

$$(b) \quad E(G) \leq \frac{n}{2}(\sqrt{n} + 1)$$

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and that equality in (b) is attained if and only if G is a strongly regular graph with parameters

$$\left(n, \frac{n + \sqrt{n}}{2}, \frac{n + 2\sqrt{n}}{4}, \frac{n + 2\sqrt{n}}{4} \right).$$

In this work we show how these results can be extended to digraphs.

A digraph (or directed graph) D consists of a nonempty finite set V of elements called vertices and a finite set A of ordered pairs of distinct vertices called arcs. Two vertices are said to be 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 . The in-degree (resp. out-degree) of a vertex v , denoted by $d^-(v)$ (resp $d^+(v)$) is the number of arcs of the form uv (resp. vu), where $u \in V$.

A digraph D is symmetric if for any $uv \in A$ also $vu \in A$, where $u, v \in V$. A one-to-one correspondence between simple 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 $\{v_1, v_2, \dots, v_n\}$ is the $n \times n$ matrix whose (i, j) -entry is defined as

$$a_{ij} = \begin{cases} 1 & \text{if } v_i v_j \in A, \\ 0 & \text{otherwise.} \end{cases}$$

The characteristic polynomial $|zI - A|$ of the adjacency matrix A of D is said to be the characteristic polynomial of D , and it is denoted by $\phi_D = \phi_D(z)$. The eigenvalues z_1, z_2, \dots, z_n of A are the eigenvalues of D and form its spectrum [1, 2]. In the general case, these eigenvalues are complex. They will be labeled so that $\text{Re}(z_1) \geq \text{Re}(z_2) \geq \dots \geq \text{Re}(z_n)$. According to RADA [9], the energy of a digraph D is defined as $E(D) = \sum_{i=1}^n |\text{Re}(z_i)|$.

In this paper we first show that if D is a strongly connected digraph on n vertices, with a arcs and c_2 closed walks of length 2, such that

$$(c) \quad \text{Re}(z_1) \geq \frac{a + c_2}{2n} \geq 1$$

then the inequality

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

holds. Moreover, equality holds if and only if D is either a direct sum of $n/2$ copies of $\overleftrightarrow{K_2}$, $\overleftrightarrow{K_n}$ (or) a non-complete directed strongly regular graph with two non-trivial eigenvalues both with absolute value $\sqrt{\frac{a + c_2}{2} - \left(\frac{a + c_2}{2n} \right)^2} / (n-1)$. Evidently, (d)

is just the digraph-version of inequality (a). Then in a manner analogous to obtaining (b) from (a) (see [8]), we obtain from (d) a sharp upper bound for the energy of strongly connected digraphs in terms of the number of vertices.

2. DEFINITIONS AND KNOWN RESULTS

Let D be a digraph with eigenvalues z_1, z_2, \dots, z_n . It is well known that the number c_s of closed walks in D of length s is equal to $\sum_{i=1}^n (z_i)^s$. Let thus c_2 be the number of closed walks in D of length 2, and let \overleftrightarrow{K}_n be the symmetric digraph on n vertices. With this notation we have:

Lemma 2.1. [9] *Let D be a digraph with n vertices and a arcs. If z_1, z_2, \dots, z_n are the eigenvalues of D , then*

1. $\sum_{i=1}^n (\operatorname{Re}(z_i))^2 - \sum_{i=1}^n (\operatorname{Im}(z_i))^2 = c_2$.
2. $\sum_{i=1}^n (\operatorname{Re}(z_i))^2 + \sum_{i=1}^n (\operatorname{Im}(z_i))^2 \leq a$.

Theorem 2.2. [9] *Let D be a digraph with n vertices and a arcs. Then $E(D) \leq \sqrt{n(a + c_2)/2}$. Equality holds if and only if D is the direct sum of $n/2$ copies of \overleftrightarrow{K}_2 , the directed cycle of length 2.*

Suppose that D is a directed graph on n vertices with adjacency matrix A . We say that D is a directed strongly regular graph with parameters n, k, t, λ, μ if $0 < t < k$, and A satisfies the following matrix equations:

$$(2) \quad JA = AJ = kJ,$$

$$(3) \quad A^2 = tI + \lambda A + \mu(J - I - A),$$

where J is the matrix whose all elements are equal to unity.

Lemma 2.3. [3] *For a directed strongly regular graph with parameters (n, k, t, λ, μ) ,*

$$(4) \quad 0 \leq \lambda < t < k,$$

$$(5) \quad 0 < \mu \leq t < k.$$

Theorem 2.4. [3] *Let A be the adjacency matrix of a directed strongly regular graph with parameters (n, k, t, λ, μ) . Then A has integer eigenvalues $\theta_0 = k$, $\theta_1 = \frac{\lambda - \mu + \delta}{2}$, $\theta_2 = \frac{\lambda - \mu - \delta}{2}$ with multiplicities $m_0 = 1$, $m_1 = -\frac{k + \theta_2(n-1)}{\theta_1 - \theta_2}$ and $m_2 = \frac{k + \theta_1(n-1)}{\theta_1 - \theta_2}$ respectively, provided $\delta = \sqrt{(\mu - \lambda)^2 + 4(t - \mu)}$ is a positive integer.*

Theorem 2.5. [11] *A symmetric regular connected digraph D without loops and multiple arcs of out-degree (or) in-degree k is strongly regular and not a union of complete digraphs if and only if it has exactly three distinct eigenvalues $\lambda^{(1)} = k, \lambda^{(2)}, \lambda^{(3)}$.*

Theorem 2.6. [4] *Let D be a digraph with n vertices and c_2 closed walks of length 2. Then $\operatorname{Re}(z_1) \geq c_2/n$. Equality holds if and only if $D \cong \overleftrightarrow{G} + \{\text{possibly some arcs that do not belong to cycles}\}$, where G is a (c_2/n) -regular graph.*

Theorem 2.7. [4] *Let D be a digraph with n vertices, a arcs and c_2 closed walks of length 2. Then*

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

Equality holds if and only if D is the empty digraph (i.e., the graph consisting of n isolated vertices) or $D \cong \overleftrightarrow{G}$, where

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

Theorem 2.8. [4] *Let D be a digraph with n vertices and symmetry index s (where $s = a - c_2$). Then*

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

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

3. ESTIMATING THE ENERGY OF STRONGLY CONNECTED DIGRAPHS

Theorem 3.1. *If D is a strongly connected digraph on n vertices and a arcs, such that $\operatorname{Re}(z_1) \geq (a + c_2)/(2n) \geq 1$, then the inequality*

$$(6) \quad E(D) \leq \frac{a + c_2}{2n} + \sqrt{(n-1) \left[\frac{a + c_2}{2} - \left(\frac{a + c_2}{2n} \right)^2 \right]}$$

holds. Moreover, equality holds in (6) if and only if D is either a direct sum of $n/2$ copies of $\overleftrightarrow{K_2}$ or $\overleftrightarrow{K_n}$ or is a non-complete directed symmetric strongly regular graph

with two non-trivial eigenvalues both with absolute value $\sqrt{\frac{a+c_2}{2} - \frac{\left(\frac{a+c_2}{2n}\right)^2}{n-1}}$.

Proof. Let z_1, z_2, \dots, z_n be the eigenvalues of D such that $\operatorname{Re}(z_1) \geq \operatorname{Re}(z_2) \geq \dots \geq \operatorname{Re}(z_n)$. By Lemma 2.1,

$$\begin{aligned} \sum_{i=1}^n (\operatorname{Re} z_i)^2 &= c_2 + \sum_{i=1}^n (\operatorname{Im} z_i)^2, \\ \sum_{i=2}^n (\operatorname{Re} z_i)^2 &= c_2 + \sum_{i=1}^n (\operatorname{Im} z_i)^2 - (\operatorname{Re} z_1)^2. \end{aligned}$$

Using this together with the Cauchy–Schwarz inequality, applied to the $(n-1)$ -dimensional vectors $(|\operatorname{Re}(z_2)|, |\operatorname{Re}(z_3)|, \dots, |\operatorname{Re}(z_n)|)$ and $(1, 1, \dots, 1)$, and bearing in mind Lemma 2.1, we obtain the inequality,

$$\begin{aligned} \sum_{i=2}^n |\operatorname{Re}(z_i)| &\leq \sqrt{(n-1) \sum_{i=2}^n |\operatorname{Re}(z_i)|^2} \leq \sqrt{(n-1) \left[c_2 + \sum_{i=1}^n \operatorname{Im}(z_i)^2 - \operatorname{Re}(z_1)^2 \right]} \\ &\leq \sqrt{(n-1) \left[c_2 + \frac{a-c_2}{2} - \operatorname{Re}(z_1)^2 \right]} = \sqrt{(n-1) \left[\frac{a+c_2}{2} - \operatorname{Re}(z_1)^2 \right]}. \end{aligned}$$

Hence,

$$(7) \quad E(D) \leq \operatorname{Re}(z_1) + \sqrt{(n-1) \left[\frac{a+c_2}{2} - \operatorname{Re}(z_1)^2 \right]}.$$

Now, the function $F(x) := x + \sqrt{(n-1) \left(\frac{a+c_2}{2} - x^2 \right)}$ decreases on the interval $\sqrt{\frac{a+c_2}{2n}} < x \leq \sqrt{\frac{a+c_2}{2}}$. From $\frac{a+c_2}{2n} \geq 1$ follows that $\sqrt{\frac{a+c_2}{2n}} \leq \frac{a+c_2}{2n} \leq \operatorname{Re}(z_1)$ must hold. Therefore $F(\operatorname{Re} z_1) \leq F\left(\frac{a+c_2}{2n}\right)$ must hold as well. Hence,

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

For the second part, clearly $D = \bigoplus_{i=1}^{n/2} K_2$ has n vertices and n arcs and n

closed walks of length 2. Consequently,

$$\begin{aligned} E\left(\bigoplus_{i=1}^{n/2} \overleftrightarrow{K}_2\right) &= n = 1 + \sqrt{(n-1)^2} = \frac{n+n}{2n} + \sqrt{(n-1) \left[\frac{n+n}{2} - \left(\frac{n+n}{2n}\right)^2 \right]} \\ &= \frac{a+c_2}{2n} + \sqrt{(n-1) \left[\frac{a+c_2}{2} - \left(\frac{a+c_2}{2n}\right)^2 \right]}. \end{aligned}$$

Since, $D \cong \overleftrightarrow{K}_n$ has n vertices and $n(n-1)$ arcs and $n(n-1)$ closed walks of length 2, we have,

$$\begin{aligned} E\left(\overleftrightarrow{K}_n\right) &= 2(n-1) = (n-1) + \sqrt{(n-1)^2} = \frac{n(n-1) + n(n-1)}{2n} \\ &\quad + \sqrt{(n-1) \left[\frac{n(n-1) + n(n-1)}{2} - \left(\frac{n(n-1) + n(n-1)}{2n}\right)^2 \right]} \\ &= \frac{a+c_2}{2n} + \sqrt{(n-1) \left[\frac{a+c_2}{2} - \left(\frac{a+c_2}{2n}\right)^2 \right]}. \end{aligned}$$

If D is a non-complete directed symmetric strongly regular graph with two non-trivial eigenvalues both with absolute value $\sqrt{\frac{a+c_2}{2} - \left(\frac{a+c_2}{2n}\right)^2} / (n-1)$, then from Theorem 2.4, we get,

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

Since $a = c_2$ for any directed symmetric strongly regular graph, this implies,

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

Conversely, if the equality holds in (6), then $a = c_2$ and by the previous discussion on the function $F(x)$, we see that $\text{Re}(z_1) = a/n$. Hence D is a regular graph with out-degree (or) in-degree a/n . Now, since equality must also hold in the Cauchy-Schwarz inequality given above, we have, $|\text{Re}(z_i)| = \sqrt{a - \left(\frac{a}{n}\right)^2} / (n-1)$, for $2 \leq i \leq n$. Hence the considerations are reduced to three possibilities: either D has two eigenvalues with equal absolute values, in which case D must be $\bigoplus_{i=1}^{n/2} \overleftrightarrow{K}_2$ or D has two eigenvalues with distinct absolute values, in which case D must equal \overleftrightarrow{K}_n , or D has

three eigenvalues with distinct absolute values equal to a/n or $\sqrt{a - \left(\frac{a}{n}\right)^2 / (n-1)}$, in which case, by Theorem 2.5, D must be a non-complete connected symmetric directed strongly regular graph. \square

In [9], RADA proved that if D is a digraph with n vertices and a arcs, then $E(D) \leq \sqrt{\frac{n(a+c_2)}{2}}$. Equality holds if and only if D is either the direct sum of $n/2$ copies of \overleftrightarrow{K}_2 . Since $F\left(\sqrt{\frac{a+c_2}{2n}}\right) = \sqrt{\left(\frac{a+c_2}{2}\right)n}$ holds for the function F defined in the proof of Theorem 3.1, and since F decreases on the interval $\sqrt{\frac{a+c_2}{2n}} < x \leq \sqrt{\frac{a+c_2}{2}}$, from the inequality $\sqrt{\frac{a+c_2}{2n}} \leq \frac{a+c_2}{2n} \leq \operatorname{Re}(z_1)$ we get

$$F\left(\frac{a+c_2}{2n}\right) \leq F\left(\sqrt{\left(\frac{a+c_2}{2n}\right)}\right) = \sqrt{\left(\frac{a+c_2}{2}\right)n}.$$

i.e.,

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

We thus see that (6) is an improvement on the McClelland inequality for the energy of strongly connected digraphs.

Theorem 3.2. *Let D be a strongly connected digraph on n vertices and a arcs, such that $\operatorname{Re}(z_1) \geq (a+c_2)/(2n) \geq 1$. Then*

$$(8) \quad E(D) \leq \frac{n(1+\sqrt{n})}{2}$$

with equality holding if and only if D is a directed strongly regular graph with parameters

$$(9) \quad \left(n, \frac{n+\sqrt{n}}{2}, \frac{3n+2\sqrt{n}}{8}, \frac{n+2\sqrt{n}}{8}, \frac{n+2\sqrt{n}}{8}\right).$$

Proof. Let D be a strongly connected digraph with n vertices and a arcs. Considering the left hand side of (6) as a function of a , we easily calculate that it attains its maximum value for $a = n^2 + n\sqrt{n} - c_2$. Inequality (8) now follows by substituting this value of a into (6).

For the second part, let D be a directed strongly regular graph with parameters $\left(n, \frac{n+\sqrt{n}}{2}, \frac{3n+2\sqrt{n}}{8}, \frac{n+2\sqrt{n}}{8}, \frac{n+2\sqrt{n}}{8}\right)$. The adjacency matrix A of D

satisfies the relation $A^2 = tI + \lambda A + \mu(J - I - A)$, where $0 < t < k$. The eigenvalues of A are $k = \frac{n + \sqrt{n}}{2}$, θ_1, θ_2 where θ_1 and θ_2 are the roots of the quadratic equation

$$(10) \quad x^2 + (\mu - \lambda)x + (\mu - t) = 0.$$

From (9) and (10), we conclude that $\theta_1 = \sqrt{n}/2$ and $\theta_2 = -\sqrt{n}/2$. Using Theorem 2.5, we then get

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

Conversely, if D is a strongly connected digraph with $E(D) = n(1 + \sqrt{n})/2$, then since $a = n^2 + n\sqrt{n} - c_2$, we have, $E(D) = \frac{a + c_2}{2n} + \sqrt{(n - 1) \left[\frac{a + c_2}{2} - \left(\frac{a + c_2}{2n} \right)^2 \right]}$. By Theorem 3.1, D is a non-complete directed symmetric strongly regular graph

with two non-trivial eigenvalues both with absolute value $\sqrt{\frac{a + c_2}{2} - \frac{\left(\frac{a + c_2}{2n} \right)^2}{n - 1}}$.

Since $a = c_2$, the eigenvalues of D are $k = \frac{a}{n} = \frac{n + \sqrt{n}}{2}$, $\theta_1 = \sqrt{\frac{a - \left(\frac{a}{n} \right)^2}{n - 1}}$, and

$\theta_2 = -\sqrt{\left(a - \left(\frac{a}{n} \right)^2 \right) / (n - 1)}$ where θ_1 and θ_2 are the roots of $x^2 + (\mu - \lambda)x + (\mu - t) = 0$. This implies $\mu - t = \theta_1 \theta_2 = -n/4$ and $\mu = \lambda$. Using Lemma 2.3 we get $\mu = \lambda = \frac{n + 2\sqrt{n}}{8}$ and $t = \frac{3n + 2\sqrt{n}}{8}$. Hence D is a directed strongly regular graph with parameters $\left(n, \frac{n + \sqrt{n}}{2}, \frac{3n + 2\sqrt{n}}{8}, \frac{n + 2\sqrt{n}}{8}, \frac{n + 2\sqrt{n}}{8} \right)$. \square

4. CONCLUDING REMARKS AND AN OPEN PROBLEM

The importance of the main result of the present paper, namely of inequality (d), depends on which digraphs satisfy the condition (c). Of course, connected graphs satisfy it, but in that case inequality (d) reduces to the previously known Koolen–Moulton bound (a).

Some less trivial examples in which the condition (c) holds are the following:

- the n -vertex digraph containing $2n - 1$ arcs, obtained by removing one arc from the n -vertex cycle C_n ;
- any strongly connected n -vertex digraph in which at least $\lfloor n/2 \rfloor$ pairs of vertices have arcs in both directions;
- a strongly connected digraph on 14 vertices and five closed walks of length two, designed by RADA [10] (see Fig. 2 in Ref. [10]), for which $\text{Re}(z_1) = \sqrt{5}$ and $(a + c_2)/(2n) = 17/14$.

Characterizing all those strongly connected digraphs with n vertices, a arcs, and c_2 closed walks of length two, for which condition (c) holds remains an open problem.

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Department of Mathematics,
Sastra University of Education,
Thanjavur 613402
India
E-mails: sjcayya@yahoo.co.in,
bala_maths@rediffmail.com

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Faculty of Science,
University of Kragujevac,
P. O. Box 60, 34000 Kragujevac
Serbia
E-mail: gutman@kg.ac.rs