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Bicyclic digraphs with maximal energy

Juan Monsalve, Juan Rada*

Instituto de Matemáticas, Universidad de Antioquia Medellín, Colombia

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ABSTRACT

If D is a digraph with n vertices then the energy of D is defined as $\mathcal{E}(D) = \sum_{k=1}^{n} |\mathrm{Re}(z_k)|$, where Re $(z_1), \ldots,$ Re(z_n) are the real parts of the eigenvalues $z_1, \ldots, z_n$ of D. In this paper we solve a problem proposed in Khan et al. (2015), we find the maximal value of the energy over the set of all bicyclic digraphs $\mathcal{B}_n$ with n vertices.

1. Introduction

A directed graph (or just digraph) D consists of a non-empty finite set $\mathcal{V}_D$ of elements called vertices and a finite set $\mathcal{A}_D$ of ordered pairs of distinct vertices called arcs. If (u, v) is an arc we indicate this by simply writing uv, and we say that u and v are adjacent vertices. A digraph D is symmetric if $uv \in \mathcal{A}_D$ then $vu \in \mathcal{A}_D$. A one to one correspondence between graphs and symmetric digraphs is given by $G \rightsquigarrow \overline{G}$, where $\overline{G}$ 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 of a digraph D with n vertices $\{v_1, \ldots, v_n\}$ is defined as the $n \times n$ matrix $A = (a_{jk})$ where

$$a_{jk} = \begin{cases} 1 & \text{if } v_j v_k \text{ is an arc of } D \\ 0 & \text{otherwise} \end{cases}$$

The characteristic polynomial of D is the characteristic polynomial of A and we denote it by $\phi_D(z)$, i.e., $\phi_D(z) = det(zI - A)$, where I is the $n \times n$ identity. The eigenvalues of D are the eigenvalues of the adjacency matrix of D.

The energy of a simple graph G with n vertices was introduced by Gutman [1] as $\mathcal{E}(G) = \sum_{k=1}^{n} |\lambda_k|$, where $\lambda_1, \ldots, \lambda_n$ are the eigenvalues of G. The motivation comes from theoretical chemistry, within the Hückel molecular orbital (HMO) approximation, the energy levels of the π-electrons in molecules of conjugated hydrocarbons are related to the energy of the molecular graphs. Details on the development of the graph energy concept and its associated chemistry applications can be seen in the recent book [7]. A generalization of the energy to digraphs was proposed in [11]: if D is a digraph with n vertices then $\mathcal{E}(D) = \sum_{k=1}^{n} |\mathrm{Re}(z_k)|$, where Re $(z_1), \ldots,$ Re(z_n) are the real parts of the eigenvalues $z_1, \ldots, z_n$ of D. The energy defined so satisfies Coulson's integral formula [10,11]

$$\mathcal{E}(D) = \frac{2}{\pi} \int_0^{\infty} \frac{1}{x^2} \ln|\gamma_D(x)| dx, \tag{1}$$

where $\gamma_D(x) = x^n \phi_D(\frac{i}{x})$. For further results on the mathematical properties of the energy of digraphs we refer to [2] and the recent survey [13].

* Corresponding author. Tel.: +57 42198648.
E-mail addresses: jdmonsal@gmail.com (J. Monsalve), pablo.rada@udea.edu.co (J. Rada).

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One of the fundamental problems in the theory of digraph energy is to find extremal values of the energy over a significant set of digraphs (see [12]). The extremal values of the energy over the set of all unicyclic digraphs with n vertices was determined in [11], see also [2]:

Theorem 1.1. *[12] Among all unicyclic digraphs with n vertices, the minimal energy is attained in digraphs which contain a cycle of length* 2, 3 *or* 4. *The maximal energy is attained in the directed cycle* $\overrightarrow{C}_n$ *of n vertices.*

A significant set of digraphs are the bicyclic digraphs ([3,8,9,14]. See also [4] and [5] in the case of graphs). Recently, Khan et al. [6] considered the problem of finding the minimal and maximal energy over the set $\mathcal{CC}_n$ of bicyclic digraphs with n vertices such that the directed cycles are vertex-disjoint. We denote by $CC[k, l]$ the disjoint union of cycles of length $2 \leq k, l$. If $D \in \mathcal{CC}_n$ then its strong components are $CC[k, l]$, where $2 \leq k, l \leq n-2$ such that $k+l \leq n$, and $n-(k+l)$ isolated vertices.

Theorem 1.2. *[7]* $\mathcal{E}(D) \leq \mathcal{E}(CC[n-2, 2])$ *for every* $D \in \mathcal{CC}_n$.

In this paper we solve a problem proposed in [6], we find the maximal value of the energy over the set $\mathcal{B}_n$ of all bicyclic digraphs with n vertices.

2. Maximal energy of bicyclic digraphs

In order to compare energies of digraphs we will frequently use the following application of Coulson's integral formula (1).

Lemma 2.1. *Let* D_1, D_2, D_3 *and* D_4 *digraphs. Then*

1. *If* $\left|\gamma_{D_1}(x)\right| \leq \left|\gamma_{D_2}(x)\right|$ *for all* $x \in [0, +\infty)$ *then* $\mathcal{E}(D_1) \leq \mathcal{E}(D_2)$;
2. *If* $\left|\gamma_{D_2}(x)\right| \cdot \left|\gamma_{D_3}(x)\right| \leq \left|\gamma_{D_1}(x)\right| \cdot \left|\gamma_{D_4}(x)\right|$ *for all* $x \in [0, +\infty)$ *then*

$$\mathcal{E}(D_3) - \mathcal{E}(D_4) \leq \mathcal{E}(D_1) - \mathcal{E}(D_2).$$

Proof.

1. Direct consequence of formula (1).
2. It follows from the fact that:

$$\begin{aligned}\mathcal{E}(D_2) + \mathcal{E}(D_3) &= \frac{2}{\pi}\int_0^\infty \frac{1}{x^2}\ln\left(|\gamma_{D_2}(x)| \cdot |\gamma_{D_3}(x)|\right)dx \\ &\leq \frac{2}{\pi}\int_0^\infty \frac{1}{x^2}\ln(|\gamma_{D_1}(x)| \cdot |\gamma_{D_4}(x)|)dx \\ &= \mathcal{E}(D_1) + \mathcal{E}(D_4)\end{aligned}$$

□

Let P_n denote the directed path with n vertices. The θ-digraph with parameters a, b, c where a, b, c are positive integers such that $a \geq b$ and $(a, b) \neq (1, 1)$, denoted by $\theta[a, b, c]$, consists of three directed paths P_a, P_b and P_c such that the initial vertex of P_a and P_b is the terminal vertex of P_c, and the initial vertex of P_c is the terminal vertex of P_a and P_b. A ∞-digraph with parameters k, l, where $k \geq l \geq 2$, denoted by $\infty[k, l]$, consists of two directed cycles of lengths k and l, with exactly one common vertex. Finally we denote by $CC[k, l]$ the digraph with two disjoint directed cycles, one of length k and the other of length l (see Fig. 1). Note that $CC[k, l]$ has $k+l$ vertices, $\infty[k, l]$ has $k+l-1$ vertices and $\theta[a, b, c]$ has $a+b+c-1$ vertices. Their characteristic polynomials are given by

$$\phi(D, z) = \begin{cases} z^{k+l} - z^k - z^l + 1, & D = CC[k, l] \\ z^{k+l-1} - z^{k-1} - z^{l-1}, & D = \infty[k, l] \\ z^{a+b+c-1} - z^{a-1} - z^{b-1}, & D = \theta[a, b, c] \end{cases} \tag{2}$$

We will denote by $\mathcal{B}_n$ the set of bicyclic digraphs with n vertices. Digraphs in $\mathcal{B}_n$ are classified in three categories:

1. Its strong components are $CC[k, l]$ and $n-(k+l)$ vertices;
2. Its strong components are $\infty[k, l]$ and $n-(k+l-1)$ vertices;
3. Its strong components are $\theta[a, b, c]$ and $n-(a+b+c-1)$ vertices.

Since the energy of a digraph is the sum of the energies of its strong components [11], then the problem reduces to computing the energy of $CC[k, l]$ when $k+l \leqslant n$, $\infty[k, l]$ when $k+l-1 \leq n$ and $\theta[a, b, c]$ when $a+b+c-1 \leq n$. Moreover, the energy of a θ-digraph is equal to the energy of a ∞-digraph as we can see in our next result.