Proyecciones Journal of Mathematics
Vol. 35, N^o 4, pp. 395-404, December 2016.
Universidad Católica del Norte
Antofagasta - Chile
DOI: 10.4067/S0716-09172016000400003

Energy of strongly connected digraphs whose underlying graph is a cycle

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Received : June 2015. Accepted : July 2016

Abstract

The energy of a digraph is defined as $\mathcal{E}(D) = \sum_{k=1}^{n} |Re(z_k)|$, *where* $z_1, \ldots, z_n$ *are the eigenvalues of the adjacency matrix of* D. *This is a generalization of the concept of energy introduced by I. Gutman in 1978 [3]. When the characteristic polynomial of a digraph* D *is of the form*

$$\phi_D(z) = \sum_{k=0}^{\lfloor \frac{n}{2} \rfloor} (-1)^k b_k(D) z^{n-2k} \tag{0.1}$$

where $b_0(D) = 1$ *and* $b_k(D) \geq 0$ *for all* k, *we show that*

$$\mathcal{E}(D) = \frac{2}{\pi} \int_0^\infty \frac{1}{t^2} ln \left[\sum_{k=0}^{\lfloor \frac{n}{2} \rfloor} b_k(D) t^{2k} \right] dt \tag{0.2}$$

This expression for the energy has many applications in the study of extremal values of the energy in special classes of digraphs. In this paper we consider the set $\mathcal{D}^*(C_n)$ *of all strongly connected digraphs whose underlying graph is the cycle* C_n, *and characterize those whose characteristic polynomial is of the form (0.1). As a consequence, we find the extremal values of the energy based on (0.2).*

Keywords : *digraphs; energy; characteristic polynomial; strongly connected; directed cycles.*

AMS Subject Classification: 05C35; 05C50; 05C90.

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. 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 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 $G \overleftrightarrow{G}$, 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. On the other hand, given a digraph D we denote by $\mathcal{U}(D)$ the underlying graph of D defined as the graph with the same set of vertices as D, and there is an edge between two vertices u and v of $\mathcal{U}(D)$ if and only if uv or vu is an arc of D.

The adjacency matrix of a digraph D with n vertices $\{v_{1,} \ldots, v_n\}$ is defined as the $n \times n$ matrix $A = (a_{ij})$ where

$$\mathrm{a}_{ij} = \begin{cases} 1 & \text{if } v_i v_j \text{ is an arc of } D \\ 0 & \text{if not} \end{cases}$$

The characteristic polynomial of D is the characteristic polynomial of A and we denoted by $\phi_D(z)$. The eigenvalues $z_1, \ldots z_n$ of A are called the eigenvalues of the digraph D. Since A is not necessarily a symmetric matrix, the eigenvalues of D can be complex numbers. The energy of a digraph D is defined as $\mathcal{E}(D) = \sum_{k=1}^{n} |\mathrm{Re}(z_k)|$ [6], a generalization of the energy of a graph introduced by Gutman in 1978 [3] (see also [4] for more details on this concept and its applications to chemistry). Since Coulson's integral formula holds for the energy of a digraph then

$$\mathcal{E}(D) = \frac{2}{\pi} \int_0^{\infty} \frac{1}{t^2} ln \left|\gamma(t)\right| dt \tag{1.1}$$

where $\gamma(t) = t^n \phi_D\left(\frac{i}{t}\right)$ (see ([5] and [6]). When the characteristic polynomial of a digraph D can be expressed as

$$\phi_D(z) = \sum_{k=0}^{\left\lfloor \frac{n}{2} \right\rfloor} (-1)^k b_k(D) z^{n-2k} \tag{1.2}$$

where $b_0(D) = 1$ and $b_k(D) \geq 0$ for all k, we show in Theorem 2.1 that

$$\mathrm{E}(D) = \frac{2}{\pi} \int_0^{\infty} \frac{1}{t^2} \ln \left[\sum_{k=0}^{\lfloor \frac{n}{2} \rfloor} b_k(D)\, t^{2k} \right] dt$$

Consequently, if D_1 and D_2 are digraphs with characteristic polynomials expressed as (1.2), then the energy is increasing with respect to the quasi-order relation $D_1 \preceq D_2$ defined as $b_k(D_1) \le b_k(D_2)$ for all k. This property is essential in order to find extemal values of the energy in special classes of digraphs. So the natural question is: which digraphs satisfy (1.2)?

Let us call Ω_n the set of digraphs with n vertices such that the characteristic polynomial is of the form (1.2). It is well known that the set of bipartite graphs (i.e. bipartite symmetric digraphs) with n vertices is contained in Ω_n. This is not true for general bipartite digraphs. For example, if $\overrightarrow{C_4}$ is the directed cycle of 4 vertices then $\phi_{\overrightarrow{C_4}}(z) = z^4 - 1$ does not alternate signs of the coefficients as in (1.2). It was shown in [7] that the set Δ_n consisting of digraphs with n vertices and such that every cycle has length $\equiv 2(mod4)$ is contained in Ω_n. However it is still an open problem to determine exactly which digraphs belong to Ω_n.

Our interest in this work is to give some insight in this problem. Specifically, we consider the set $\mathcal{D}^*(C_n)$ of strongly connected digraphs whose underlying graph is the cycle C_n. We first characterize such digraphs and then compute its characteristic polynomial (Lemma 2.2 and Theorem 2.3). From this expression of the characteristic polynomial we characterize the digraphs of $\mathcal{D}^*(C_n)$ which belong to Ω_n and then we find the extremal values of the energy (Theorems 2.4 and 2.6).

2. Energy of strongly connected digraphs whose underlying graph is a cycle

Let us define a quasi-order relation over Ω_n as follows: if D_1 and D_2 have characteristic polynomials

$$\phi_{D_i}(z) = \sum_{k=0}^{\lfloor \frac{n}{2} \rfloor} (-1)^k b_k(D_i)\, z^{n-2k}$$

where $b_0(D_i) = 1$ and $b_k(D_i) \ge 0$ for all k $(i = 1, 2)$, then $D_1 \preceq D_2$ if and only if $b_k(D_1) \le b_k(D_2)$ for all k. If further $b_k(D_1) < b_k(D_2)$ for some k then $D_1 \prec D_2$. We first show that the energy is increasing with respect to this quasi-order relation.

Theorem 2.1. *If $D \in \Omega_n$ then* $E(D) = \frac{2}{\pi}\int\limits_0^\infty \frac{1}{t^2} ln \left[\sum\limits_{k=0}^{\lfloor \frac{n}{2} \rfloor} b_k(D)\, t^{2k}\right] dt$

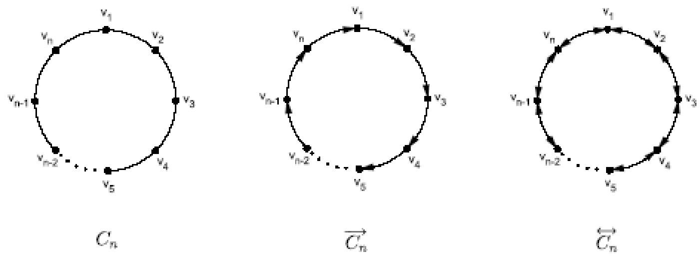

Figure 1: Cycles and directed cycles

In particular, the energy is increasing over Ω_n with respect to the quasi-order relation $\preceq$.

Proof. From (1.1) $\mathrm{E}(D) = \frac{2}{\pi}\int\limits_0^\infty \frac{1}{t^2} ln\left|\gamma(t)\right| dt$
where $\gamma(t) = t^n \phi_D\left(\frac{i}{t}\right)$.

Since $D \in \Omega_n$ we deduce that

$$\begin{aligned} \left|\gamma(t)\right| &= \left|t^n \phi_D\left(\frac{i}{t}\right)\right| = \left|t^n \sum_{k=0}^{\lfloor \frac{n}{2} \rfloor} (-1)^k b_k(D) \left(\frac{i}{t}\right)^{n-2k}\right| \\ &= \sum_{k=0}^{\lfloor \frac{n}{2} \rfloor} b_k(D)\, t^{2k} \end{aligned}$$

and so

$$\mathrm{E}(D) = \frac{2}{\pi}\int\limits_0^\infty \frac{1}{t^2} ln\left|\gamma(t)\right| dt = \frac{2}{\pi}\int\limits_0^\infty \frac{1}{t^2} ln\left[\sum_{k=0}^{\lfloor \frac{n}{2} \rfloor} b_k(D)\, t^{2k}\right] dt$$

It follows easily from this expression that the energy is increasing over Ω_n with respect to the quasi-order relation $\preceq$. $\square$

As we mentioned in the introduction, the set of symmetric bipartite digraphs with n vertices is contained in Ω_n, but for bipartite digraphs in general this is not true. For instance, consider the cycle C_n on n vertices, i.e. the vertex of C_n is $V(C_n) = \{v_1, \ldots, v_n\}$ and the edge set of C_n is

$E(C_n) = \{v_1v_2, v_2v_3, \ldots, v_{n-1}v_n, v_nv_1\}$. Denote by $\overrightarrow{C_n}$ the directed cycle and $\overleftrightarrow{C_n}$ the symmetric digraph of C_n (see Fig. 1). Clearly $\overrightarrow{C_n}$ is a strongly connected bipartite digraph when n is even, and its characteristic polynomial is $\phi_{\overrightarrow{C_n}}(z) = z^n - 1$. Then for every n which is a multiple of 4, $\overrightarrow{C_n} \notin \Omega_n$.

We will investigate which strongly connected digraphs whose underlying graph is C_n belong to Ω_n. Let us denote by $\mathcal{D}(C_n)$ the set consisting of all digraphs D such that $\mathcal{U}(D) = C_n$. Moreover, we define

$\mathrm{D}^*(C_n) = \{U \in \mathcal{D}(C_n) : U \text{ is strongly connected}\}$

Lemma 2.2. *A digraph U belongs to $\mathcal{D}^*(C_n)$ if and only if $U = \overleftrightarrow{C_n}$ or U is obtained from $\overleftrightarrow{C_n}$ by deleting some arcs of the form v_jv_{j-1}, where $j = 1, \ldots, n$ $(v_0 = v_n)$.*

Proof. Assume that $U \in \mathcal{D}^*(C_n)$. Since $\mathcal{U}(D) = C_n$, the only possible directed cycles in U are 2-cycles or $\overrightarrow{C_n}$. If $U \neq \overleftrightarrow{C_n}$ then there exists an arc uv of U such that vu is not an arc of U, in other words, uv does not belong to a 2-cycle. Since U is strongly connected then $\overrightarrow{C_n}$ must be a cycle of U (which contains uv) and so U is obtained from $\overleftrightarrow{C_n}$ by deleting some arcs of the form v_jv_{j-1}, where $j = 1, \ldots, n$ $(v_0 = v_n)$. Conversely, if Y is obtained from $\overleftrightarrow{C_n}$ by deleting some arcs of the form v_jv_{j-1}, then clearly $\mathcal{U}(Y) = C_n$ and every arc of Y is contained in the cycle $\overrightarrow{C_n}$, so Y is strongly connected. □

We next compute the characteristic polynomial of digraphs in $\mathcal{D}^*(C_n)$. Given $U \in \mathcal{D}^*(C_n)$ and p a positive integer, we will denote by $S_p(U)$ the set of p independent 2-cycles of U and $|S_p(U)|$ the number of elements $S_p(U)$ has. For instance, for the digraph Q_8 in Figure 2, $|S_1(Q_8)| = 4$, $|S_2(Q_8)| = 6$, $|S_3(Q_8)| = 4$ and $|S_4(Q_8)| = 1$.

Theorem 2.3. *Let $U \in \mathcal{D}^*(C_n)$.*

1. *If n is odd then*

$$\phi_U(z) = z^n + \sum_{k=1}^{\frac{n-1}{2}} (-1)^k |S_k(U)| z^{n-2k} - 1;$$

2. *If n is even then*

$$\phi_U(z) = \begin{cases} z^n + \sum\limits_{k=1}^{\frac{n}{2}-1} (-1)^k |S_k(U)| z^{n-2k} - \left(1 - \left|S_{\frac{n}{2}}(U)\right|\right) & if \quad n \equiv 0(mod4); \\ z^n + \sum\limits_{k=1}^{\frac{n}{2}-1} (-1)^k |S_k(U)| z^{n-2k} - \left(1 + \left|S_{\frac{n}{2}}(U)\right|\right) & if \quad n \equiv 2(mod4). \end{cases}$$

Proof. Assume that the characteristic polynomial of U is $\phi_U(z) = \sum\limits_{k=0}^{n} a_k z^{n-k}$, where $a_0 = 1$. Then by Sachs Theorem [2], $a_j = \sum\limits_{L \in \mathcal{L}_j} (-1)^{p(L)}$ for every $1 \leq j \leq n$, where $\mathcal{L}_j$ is the set of linear subdigraphs with j vertices and $p(L)$ is the number of components L has. Since $U \in \mathcal{D}^*(C_n)$ has only cycles of length 2 and $\overrightarrow{C_n}$, we can compute the linear subdigraphs of U as follows:

1. If n is odd then

$$\mathcal{L}_k(U) = \begin{cases} \emptyset & if \quad k \text{ is odd, } 1 \leq k \leq n-2 \\ S_{\frac{k}{2}}(U) & if \quad k \text{ is even, } 2 \leq k \leq n-1 \\ \left\{\overrightarrow{C_n}\right\} & if \quad k = n. \end{cases} \tag{2.1}$$

Clearly $a_j = 0$ for all j odd, $1 \leq j \leq n-2$ and $a_n = (-1)^{p\left(\overrightarrow{C_n}\right)} = -1$. When $j \equiv 2(mod4)$ then $\frac{j}{2}$ is odd while $j \equiv 0(mod4)$ implies $\frac{j}{2}$ is even. Hence

$$a_j = \sum_{L \in \mathcal{L}_j} (-1)^{c(L)} = \begin{cases} -\left|S_{\frac{j}{2}}(U)\right| & if \quad j \equiv 2(mod4) \\ \left|S_{\frac{j}{2}}(U)\right| & if \quad j \equiv 0(mod4) \end{cases} \tag{2.2}$$

and consequently

$$\phi_U(z) = \sum_{k=0}^{\frac{n-1}{2}} (-1)^k |S_k(U)| z^{n-2k} - 1.$$

2. If n is even then

$$\mathcal{L}_k(U) = \begin{cases} \emptyset & if \quad k = 1, 3, 5, \ldots, n-1 \\ S_{\frac{k}{2}}(U) & if \quad k = 2, 4, 6, \ldots, n-2 \\ S_{\frac{n}{2}}(U) \cup \left\{\overrightarrow{C_n}\right\} & if \quad k = n. \end{cases} \tag{2.3}$$

Again $a_j = 0$ for all j odd, $1 \leq j \leq n-1$. Similarly, when j is even and $2 \leq j \leq n-2$ then a_j is given by (2.2). Finally,

$$\mathrm{a}_n = \begin{cases} -1 - \left|S_{\frac{n}{2}}(U)\right| & if \quad n \equiv 2(mod4) \\ -1 + \left|S_{\frac{n}{2}}(U)\right| & if \quad n \equiv 0(mod4) \end{cases}$$ and the result follows. □

Now we can determine the digraphs in $\mathcal{D}^*(C_n)$ which belong to Ω_n. For n even, let Q_n be the digraph obtained from $\overrightarrow{C_n}$ by adding the arcs $v_i v_{i-1}$ for all i even $(2 \leq i \leq n-2)$ (see Fig. 2). Clearly by Lemma 2.2, $Q_n \in \mathcal{D}^*(C_n)$ for all positive even integer n.

Theorem 2.4. *Let n be a positive integer.*

1. *If n is odd then no digraph in $\mathcal{D}^*(C_n)$ belongs to Ω_n;*
2. *If $n \equiv 2(mod 4)$ then all digraphs in $\mathcal{D}^*(C_n)$ belong to Ω_n. Moreover, the cycle $\overrightarrow{C_n}$ has the minimal energy and $\overleftrightarrow{C_n}$ has the maximal energy over the set $\mathcal{D}^*(C_n)$;*
3. *If $n \equiv 0(mod 4)$ then a digraph $U \in \mathcal{D}^*(C_n)$ belongs to Ω_n if and only if $U = Q_n$ or U is obtained from Q_n by adding some arcs of the form $v_j v_{j-1}$, where $j = 1, \ldots, n$ $(v_0 = v_n)$. For these digraphs, the minimal energy is attained in Q_n and the maximal energy is attained in $\overleftrightarrow{C_n}$.*

Proof. 1. Note that if n is odd and $U \in \mathcal{D}^*(C_n) \cap \Omega_n$ then $\phi_U(0) = 0$ and by part 1 of Theorem 2.3, $\phi_U(0) = -1$, a contradiction. Hence no digraph in $\mathcal{D}^*(C_n)$ belongs to Ω_n.

2. If $n \equiv 2(mod 4)$ and $U \in \mathcal{D}^*(C_n)$ then by part 2 of Theorem 2.3

$$\phi_U(z) = z^n + \sum_{k=1}^{\frac{n}{2}-1} (-1)^k |S_k(U)| z^{n-2k} - \left(1 + \left|S_{\frac{n}{2}}(U)\right|\right)$$

which clearly satisfies (1.2). Assume that $U \neq \overrightarrow{C_n}$. Then by Lemma 2.2, there exists an arc of the form $v_j v_{j-1}$ in U, for some $j = 1, \ldots, n$ $(v_0 = v_n)$. Let U' be the digraph obtained from U by deleting the arc $v_j v_{j-1}$. Then clearly $U' \in \mathcal{D}^*(C_n)$ and $\mathcal{L}_k(U') \subseteq \mathcal{L}_k(U)$ for all $k \geq 0$. Hence $|S_k(U')| \leq |S_k(U)|$ for all $k = 1, \ldots, \frac{n}{2}$. In other words, $U' \leq U$. Consequently, starting from any digraph $V \in \mathcal{D}^*(C_n)$, we can step by step delete an arc of the form $v_j v_{j-1}$ to obtain a decreasing sequence of digraphs in $\mathcal{D}^*(C_n)$ that ends in $\overrightarrow{C_n}$. Similarly, we construct an increasing sequence of digraphs in $\mathcal{D}^*(C_n)$ by adding arcs that ends in $\overleftrightarrow{C_n}$. Since the energy is increasing with respect to this quasi-order relation by Theorem 2.1, the result follows.

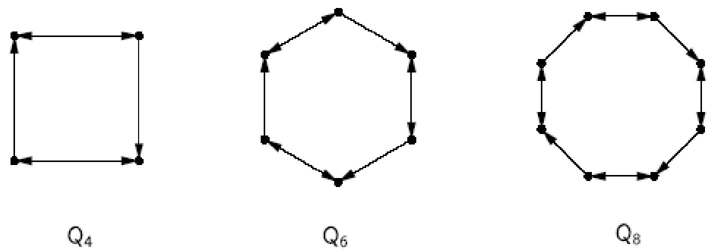

Figure 2: Digraphs in $\mathcal{D}^*(C_n) \cap \Omega_n$ when n is even

3. If $n \equiv 0(mod4)$ and $W \in \mathcal{D}^*(C_n)$ then the characteristic polynomial of W is given by

$$\phi_W(z) = z^n + \sum_{k=1}^{\frac{n}{2}-1} (-1)^k |S_k(W)| z^{n-2k} - \left(1 - \left|S_{\frac{n}{2}}(W)\right|\right)$$

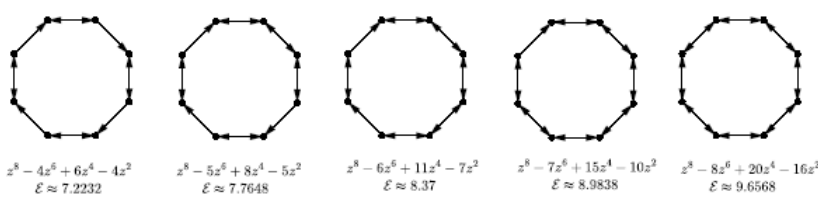

Figure 3: Digraphs in $\Omega_8 \backslash \Delta_8$

Note that when $n \equiv 0(mod4)$ then $\frac{n}{2} - 1$ is odd and so W satisfies (1.2) if and only if $-\left(1 - \left|S_{\frac{n}{2}}(W)\right|\right) \geq 0$, which is equivalent to $S_{\frac{n}{2}}(W) \neq \emptyset$. But clearly $S_{\frac{n}{2}}(W) \neq \emptyset$ if and only if $W = Q_n$ or W is obtained from Q_n by adding some arcs of the form $v_j v_{j-1}$, where $j = 1, \ldots, n$ $(v_0 = v_n)$. Finally if Z is obtained from Q_n by adding some arcs of the form $v_j v_{j-1}$, we proceed as in part 2 to delete arcs of the form $v_j v_{j-1}$ until reaching Q_n. Similarly, adding arcs of this form to Z will end in $\overleftrightarrow{C_n}$. The result follows again by the increasing property of the energy given in Theorem 2.1. $\square$

As we mentioned in the introduction, $\Delta_n \subset \Omega_n$, where Δ_n is the set of digraphs with n vertices and every cycle has length $\equiv 2(\text{mod}4)$ [7]. Note that Theorem 2.4 gives plenty of examples of digraphs in Ω_n which are not in Δ_n.

Example 2.5. *$Q_{4k} \in \Omega_{4k} \backslash \Delta_{4k}$ for every $k \geq 1$ and so does every digraph obtained from Q_{4k} by adding arcs of the form $v_j v_{j-1}$, where $j = 1, \ldots, 4k$ $(v_0 = v_{4k})$. For instance, Q_8 and the derived digraphs shown in Figure 3.*

As we can see in Theorem 2.4, when n is odd no digraph in $\mathcal{D}^*(C_n)$ belongs to Ω_n. However, in this case we still can find the extremal values of the energy over $\mathcal{D}^*(C_n)$.

Theorem 2.6. *If n is odd then $\overrightarrow{C_n}$ has the minimal energy and $\overleftrightarrow{C_n}$ has the maximal energy over the set $\mathcal{D}^*(C_n)$.*

Proof. Let $U \in \mathcal{D}^*(C_n)$. Then by Theorem 2.3

$$\phi_U(z) = z^n + \sum_{k=1}^{\frac{n-1}{2}} (-1)^k |S_k(U)| z^{n-2k} - 1;$$

and so using directly formula (1.1) we deduce that

$$\mathcal{E}(U) = \frac{2}{\pi} \int_0^\infty \frac{1}{t^2} ln |\gamma(t)| \, dt \tag{2.4}$$

where

$$|\gamma(t)| = \left| t^n \phi_U\left(\frac{i}{t}\right) \right| = \left| t^n \left(\left(\frac{i}{t}\right)^n + \sum_{k=1}^{\frac{n-1}{2}} (-1)^k |S_k(U)| \left(\frac{i}{t}\right)^{n-2k} - 1 \right) \right|$$

$$= \left| t^n - i^n \left(1 + \sum_{k=1}^{\frac{n-1}{2}} |S_k(U)| t^{2k} \right) \right|$$

$$= \sqrt{t^{2n} + \left(1 + \sum_{k=1}^{\frac{n-1}{2}} |S_k(U)| t^{2k} \right)^2} \tag{2.5}$$

Hence substituting (2.5) in (2.4) we easily deduce that if $U, U' \in \mathcal{D}^*(C_n)$ are such that $|S_k(U)| \leq |S_k(U')|$ for all $k = 1, \ldots, \frac{n-1}{2}$ then $\mathcal{E}(U) \leq \mathcal{E}(U')$. In particular, $\overrightarrow{C_n}$ has the minimal energy and $\overleftrightarrow{C_n}$ has the maximal energy over the set $\mathcal{D}^*(C_n)$. $\square$

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