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Unicyclic signed graphs with minimal energy☆

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ABSTRACT

A connected signed graph with n vertices is said to be unicyclic if its number of edges is n. The energy of a signed graph S of order n with eigenvalues $x_1, x_2, \ldots, x_n$ is defined as $E(S) = \sum_{j=1}^{n} |x_j|$. We obtain the integral representations for the energy of a signed graph. We show that even and odd coefficients of the characteristic polynomial of a unicyclic signed graph respectively alternate in sign. As an application of integral representation, we compute and compare the energy of unicyclic signed graphs. Finally, we characterize unicyclic signed graphs with minimal energy.

1. Introduction

A signed graph is defined to be a pair $S = (G, \sigma)$, where $G = (V, \mathscr{E})$ is the underlying graph and $\sigma : \mathscr{E} \to \{-1, 1\}$ is the signing function (or signature). The sets of positive and negative edges of S are respectively denoted by $\mathscr{E}^+$ and $\mathscr{E}^-$. Thus $\mathscr{E} = \mathscr{E}^+ \cup \mathscr{E}^-$. Our signed graphs have simple underlying graphs. The dotted edge and the bold edge respectively denote a negative edge and a positive edge. A signed graph is said to be homogeneous if all of its edges have either positive sign or negative sign and heterogeneous, otherwise. A graph can be considered to be a homogeneous signed graph with each edge positive, thus signed graphs become a generalization of graphs. A signed graph is said to be all-positive (respectively, all-negative) if all of its edges are positive (respectively, negative). The sign of a signed cycle is defined as the product of signs of its edges. A signed cycle is said to be positive (respectively, negative) if its sign is positive (respectively, negative) i.e., it contains an even (respectively, odd) number of negative edges. A signed graph is said to be balanced if each of its cycle is positive, and unbalanced otherwise. Throughout this paper, we denote a positive and a negative cycle of length n by C_n and $\mathbf{C}_n$ respectively. A connected signed graph of order n is said to be unicyclic if number of its edges is also n. For other undefined notations and terminology from graph theory, we refer to [20].

The adjacency matrix of a signed graph S whose vertices are $v_1, v_2, \ldots, v_n$ is the $n \times n$ matrix $A(S) = (a_{ij})$, where

$$a_{ij} = \begin{cases} \sigma(v_i, v_j), & \text{if there is an edge from } v_i \text{ to } v_j, \\ 0, & \text{otherwise.} \end{cases}$$

Clearly, $A(S)$ is real symmetric and so all its eigenvalues are real. The characteristic polynomial $|xI - A(S)|$ of the adjacency matrix $A(S)$ of a signed graph S is called the characteristic polynomial of S and is denoted by $\phi_S(x)$. The eigenvalues of $A(S)$ are

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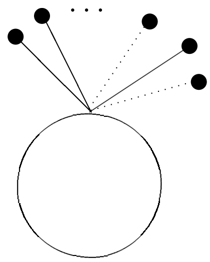

Fig. 1. Signed graph S_n^g (or $\mathbf{S_n^g}$).

called the eigenvalues of S. The set of distinct eigenvalues of S together with their multiplicities is called the spectrum of S. If S is a signed graph of order n having distinct eigenvalues $x_1, x_2, \ldots, x_k$ and their respective multiplicities as $m_1, m_2, \ldots, m_k$, we write the spectrum of S as $spec(S) = \{x_1^{(m_1)}, x_2^{(m_2)}, \ldots, x_k^{(m_k)}\}$.

The following is the coefficient theorem for signed graphs [1].

Theorem 1.1. *If S is a signed graph with characteristic polynomial*

$$\phi_S(x) = x^n + a_1(S)x^{n-1} + \cdots + a_{n-1}(S)x + a_n(S),$$

then

$$a_j(S) = \sum_{L \in \pounds_j} (-1)^{p(L)} 2^{|c(L)|} \prod_{Z \in c(L)} s(Z),$$

for all $j = 1, 2, \ldots, n$, where $\pounds_j$ is the set of all basic figures L of S of order j, $p(L)$ denotes number of components of L, $c(L)$ denotes the set of all cycles of L and $s(Z)$ the sign of cycle Z.

From Theorem 1.1, it is clear that the spectrum of a signed graph remains invariant by changing the signs of non-cyclic edges. The spectral criterion for the balance of signed graphs given by Acharya [1] is as follows.

Theorem 1.2. *A signed graph is balanced if and only if it is co-spectral with the underlying unsigned graph.*

Let S be a signed graph with vertex set V. Switching S by set $X \subset V$ means reversing the signs of all edges between X and its complement. Two signed graphs are said to be switching equivalent if one can be obtained from the other by switching. Switching equivalence is an equivalence relation on the signings of a fixed graph. An equivalence class is called a switching class. A switching class of S is denoted by $[S]$. If S' is isomorphic to a switching of S, we say S and S' are switching isomorphic.

Switching a signed graph does not change the sign of cycles (see [22]), switching equivalent signed graphs have the same set of positive cycles, and they are either both balanced or both unbalanced. By Theorem 1.1, any two switching equivalent signed graphs are co-spectral. The converse of this statement is not true in general, e.g., the signed graphs S_1 and S_2 given in Fig. 2 are co-spectral but not switching equivalent (in fact their underlying graphs are not even isomorphic). We note that there are precisely two switching classes on the signings of a unicyclic graph, the cycle being positive and the cycle being negative and therefore, by Theorem 1.2, two signed graphs on a unicyclic graph are co-spectral if and only if they are switching equivalent. So, as long as spectra is concerned, we often use a single signed graph for a switching class. For a complete bibliography on signed graphs, see [23].

The concept of energy was given by Gutman [8] in 1978. This concept was extended to signed graphs by Germina, Hameed and Zaslavsky [6] and they defined the energy of a signed graph S to be the sum of absolute values of eigenvalues of S. The concept of energy has been extended to digraphs by Pena and Rada [19] and to signed digraphs by the authors [2,21]. For applications of signed graphs in chemistry see [10,11,16].

The girth of a signed graph is the length of its smallest cycle and is denoted by g. Let S_n^g (respectively, $\mathbf{S_n^g}$) denote the balanced (respectively, unbalanced) unicyclic signed graph of order n obtained by identifying the center of the signed star on $n - g + 1$ vertices with a vertex of a positive (respectively, negative) cycle of order g, where $n \geq g \geq 3$ (see Fig. 1) and let $S(n, g)$ denote the set of unicyclic signed graphs of order n and girth g. For unicyclic graphs with minimal energy see [12–15,17,24]. In [4], Caporossi et al. posed the following conjecture based on the results obtained with the computer system AutoGraphix.

Conjecture 1.3. *Among all connected graphs G with $n \geq 6$ vertices and $n-1 \leq m \leq 2(n-2)$ edges, the graphs with minimum energy are stars with $m-n+1$ additional edges all connected to the same vertex for $m \leq n + \lfloor \frac{(n-7)}{2} \rfloor$, and bipartite graphs with two vertices on one side, one of which is connected to all vertices on the other side, otherwise.*

The following result of Hou [12] proves the conjecture for $m = n$.

Theorem 1.4. *Let G be a unicyclic graph with $n \geq 6$ vertices and $G \neq \mathscr{S}_n^3$. Then $E(\mathscr{S}_n^3) < E(G)$, where $\mathscr{S}_n^3$ is the graph obtained from the star graph with n vertices by adding an edge.*

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