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Ordering of oriented unicyclic graphs by skew energies

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ABSTRACT

Ordering of the oriented unicyclic graphs with n vertices according to their minimal skew energies is investigated. We derive the first 22 oriented unicyclic graphs for $n \geq 1784$ and a series of oriented unicyclic graphs for $3 \leq n \leq 1783$.

1. Introduction

The energy of a simple undirected graph was introduced by Gutman [1]. The study on the extremal values of energy for graphs is of importance for the chemical graph theory, and a lot of interesting results have been reported [2–7]. For more details on the mathematical concept and properties of the energy of a graph, one can refer to the books [8,9]. For undirected graphs, up to now, there are various generalizations of the graph energy, such as the matching energy [10–12], Laplacian energy [13], incidence energy [14], distance energy [15], and so on. There are some situations when chemists use digraphs rather than graphs. One such situation is, according to Ref. [16], when vertices represent distinct chemical species and arcs represent the direction in which a particular reaction happens between the two corresponding species. So the skew energy was put forward and people hope it will have similar applications as the energy in chemistry.

Let G be a simple undirected graph of order n, and G^σ be an oriented graph obtained from G by assigning an orientation σ to the edge set of G. The skew–adjacency matrix of G^σ is the $n \times n$ matrix $S(G^\sigma) = [s_{pq}]$, where $s_{pq} = 1$ and $s_{qp} = -1$ if the arc $p \to q$ is an arc of G^σ, otherwise $s_{pq} = s_{qp} = 0$. The skew energy of an oriented graph G^σ, denoted by $E_s(G^\sigma)$, is defined as [17]

$$E_s(G^\sigma) = \sum_{i=1}^{n} |\lambda_i|, \tag{1}$$

where $\lambda_1, \ldots, \lambda_n$ are the eigenvalues of $S(G^\sigma)$, namely the n roots of $\phi(G^\sigma, x) = 0$. Here $\phi(G^\sigma, x) = \det[xI - S(G^\sigma)] = \sum_{i=0}^{n} a_i(G^\sigma)x^{n-i}$ is the skew characteristic polynomial of G^σ, where I is the unit matrix of order n, and $a_0, a_1, \ldots, a_n$ are the coefficients of $\phi(G^\sigma, x)$. Since G is a simple graph, G^σ does not have loops and multiple arcs. Hence, $S(G^\sigma)$ is a skewly symmetric real matrix. Therefore λ_i with $1 \leq i \leq n$ are all purely imaginary numbers, and $a_{2i}(G^\sigma) \geq 0$ and $a_{2i+1}(G^\sigma) = 0$ for all $0 \leq i \leq \lfloor n/2 \rfloor$ [17]. Thus we have

$$\phi(G^\sigma, x) = \sum_{i=0}^{\lfloor n/2 \rfloor} a_{2i}(G^\sigma)x^{n-2i}. \tag{2}$$

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By using the coefficients of $\phi(G^\sigma, x)$, Hou et al. [18] expressed the skew energy $E_s(G^\sigma)$ by the following integral formula

$$E_s(G^\sigma) = \frac{2}{\pi}\int_0^{+\infty}\frac{1}{x^2}\log\left[\sum_{i=0}^{\lfloor n/2\rfloor} a_{2i}(G^\sigma)x^{2i}\right]\mathrm{d}x. \tag{3}$$

One can see from (3) that $E_s(G^\sigma)$ is a strictly monotonously increasing function of $a_{2i}(G^\sigma)$ for $0 \le i \le \lfloor n/2\rfloor$. Note that $a_0(G^\sigma) = 1$ and $a_2(G^\sigma)$ equals to the number of the edges in G. Next, we assume $2 \le i \le \lfloor n/2\rfloor$ for $a_{2i}(G^\sigma)$. This provides a useful way for comparing the skew energies of a pair of oriented graphs.

Let $G_1^{\sigma_1}$ and $G_2^{\sigma_2}$ be two oriented graphs of order n. Then

$$a_{2i}(G_1^{\sigma_1}) \le a_{2i}(G_2^{\sigma_2}) \text{ for all } 0 \le i \le \lfloor n/2\rfloor \Rightarrow E_s(G_1^{\sigma_1}) \le E_s(G_2^{\sigma_2}). \tag{4}$$

If $a_{2i}(G_1^{\sigma_1}) = a_{2i}(G_2^{\sigma_2})$ for all $0 \le i \le \lfloor n/2\rfloor$, then we have $E_s(G_1^{\sigma_1}) = E_s(G_2^{\sigma_2})$. For the sake of conciseness, we introduce the symbols "$\rightharpoonup$", "$\rightleftharpoons$" and "$\rightrightarrows$" as follows:

$$\begin{aligned} &E_s(G_1^{\sigma_1}) < E_s(G_2^{\sigma_2}) \iff G_1^{\sigma_1} \rightharpoonup G_2^{\sigma_2}, E_s(G_1^{\sigma_1}) = E_s(G_2^{\sigma_2}) \iff G_1^{\sigma_1} \rightleftharpoons G_2^{\sigma_2},\\ &E_s(G_1^{\sigma_1}) \le E_s(G_2^{\sigma_2}) \iff G_1^{\sigma_1} \rightrightarrows G_2^{\sigma_2}. \end{aligned} \tag{5}$$

The relation (4) will be referred to as the method of coefficient comparison hereinafter, and has successfully been used in the study on the extremal values of skew energy for oriented graphs. For the oriented unicyclic graphs of order n, Hou et al. [18] obtained the oriented graphs with the 1st-minimal, the 2nd-minimal and the maximal skew energies, and Zhu [19] determined the oriented graphs with the first $\lfloor \frac{n-9}{2}\rfloor$ largest skew energies. For the oriented bicyclic graphs, Shen et al. [20] deduced the oriented graphs with the minimal and maximal skew energies, and Wang et al. [21] characterized the oriented graph with the second largest skew energy. For the oriented unicyclic graphs with perfect matchings, Zhu and Yang [22] obtained the oriented graph with the minimal skew energy. For the oriented unicyclic graphs with fixed diameter, Yang et al. [23] determined the oriented graph with the minimal skew energy. Some other results about the extremal skew energies can be found in Refs. [21,24–26]. For a survey on skew energy, one can refer to Ref. [27].

In this paper, we will further study the oriented unicyclic graphs to obtain the increasing order in terms of their minimal skew energies. The set of connected unicyclic graphs on n vertices is denoted by $\mathcal{U}_n$. By various methods, namely the method of coefficient comparison in (4), the integral formula in (10) (in Section 2), and some analytical techniques, we will derive, for $n \ge 1784$, the preceding 22 oriented unicyclic graphs within $\mathcal{U}_n$ in the increasing order according to their minimal skew energies, and obtain, for $3 \le n \le 1783$, a lot of oriented unicyclic graphs within $\mathcal{U}_n$ in the increasing order.

2. Previous results

To deduce the main results of the present paper, some necessary lemmas are simply quoted here and some definitions for certain types of graphs are introduced.

Let $m(G, k)$ be the number of k-matchings in G, where a k-matching is a disjoint union of k edges in G. It is consistent to define $m(G, 0) = 1$ and $m(G, k) = 0$ for $k < 0$.

Lemma 1 [8]. *Let $e = uv$ be an edge of G and k a positive integer. Then we have*

$$m(G, k) = m(G - e, k) + m(G - u - v, k - 1). \tag{6}$$

For two graphs G_1 and G_2, we define a quasi-ordering relation as follows. If $m(G_1, k) \le m(G_2, k)$ holds for all $k \ge 0$, then we write $G_1 \preceq G_2$. If $G_1 \preceq G_2$ and there exists some k_0 such that $m(G_1, k_0) < m(G_2, k_0)$, then we write $G_1 \prec G_2$.

Let P_n be a path with n vertices. The vertices of P_n are labeled consecutively by $v_1, v_2, \ldots, v_n$. Let X_n be the star $K_{1,n-1}$, Y_n the graph obtained from P_4 by attaching $n-4$ pendent edges to v_2, Z_n the graph obtained from P_4 by attaching $n-5$ and one pendent edge to v_2 and v_3, respectively, and W_n the graph obtained from P_5 by attaching $n-5$ pendent edges to v_2.

Lemma 2 [2]. *Let T be a tree with n vertices, where $n \ge 6$. Then $X_n \prec Y_n \prec Z_n \prec W_n \prec T$, where $T \ne X_n, Y_n, Z_n, W_n$.*

Let $B_{n,d}$ be the graph obtained from P_{d+1} by attaching $n-d-1$ pendent edges to v_2 of P_{d+1}, where d is an integer with $n \ge d \ge 1$.

Lemma 3 [3]. *Let d be a positive integer more than one and T a tree with n vertices having diameter at least d. Then $B_{n,d} \preceq T$ with the equality if and only if (iff) $T = B_{n,d}$.*

Let B_n be the graph obtained from P_6 by attaching $n-6$ pendent edges to v_3 of P_6, and D_n the graph obtained from P_6 by attaching $n-7$ and one pendent edge to v_2 and v_5 of P_6, respectively.

Lemma 4 [4]. *Let T be a tree with n vertices having diameter 5, where $n \ge 8$. Then $D_n \prec T$ for $n \ge 8$, where $T \ne B_{n,5}, B_n, D_n$.*

Lemma 5 [5]. *For any real number $x > -1$, we have $\frac{x}{1+x} \le \log(1+x) \le x$.*