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On the Estrada index of signed graphs

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Abstract. Let $\Gamma = (G, \sigma)$ be a signed graph on n vertices with eigenvalues $\mu_1, \mu_2, \ldots, \mu_n$. Then, the Estrada index of Γ is defined as $EE(\Gamma) = \sum_{i=1}^{n} e^{\mu_i}$. In this paper, we characterize unicyclic signed graphs with the maximum Estrada index. Let C_{n+} and C_{n-} be the balanced and unbalanced cycles on n vertices, respectively. We show that the Estrada index of the balanced cycle C_{n+} is almost equal to the Estrada index of the unbalanced cycle C_{n-}. A signed graph Γ is said to have the pairing property if μ is an eigenvalue whenever $-\mu$ is an eigenvalue of Γ and both μ and $-\mu$ have the same multiplicities. If $\Gamma_p^-(n,m)$ denotes the set of all unbalanced connected signed graphs on n vertices and m edges with the pairing property, then we determine the signed graphs having the maximum Estrada index in $\Gamma_p^-(n,m)$, when $m = n$ and $m = n + 1$. Finally, we find signed graphs among all unbalanced complete bipartite signed graphs having the maximum Estrada index.

1. Introduction

A signed graph Γ is an ordered pair (G, σ) in which G is an underlying graph and σ is a function from the edge set $E(G)$ to $\{-1, 1\}$, which is called a signature or a sign function. For a signed graph $\Gamma = (G, \sigma)$ and its subgraph $H \subset G$, we use the notation (H, σ) for writing the signed subgraph of $\Gamma = (G, \sigma)$, where σ is the restriction of the mapping $\sigma : E(G) \to \{-1, 1\}$ to the edge set $E(H)$. The adjacency matrix $A_\Gamma = \left(a_{ij}\right)$ of a signed graph $\Gamma = (G, \sigma)$ naturally arose from the unsigned graph by putting -1 or 1, whenever the corresponding edge is either negative or positive, respectively. The characteristic polynomial, denoted by $\varphi(\Gamma, x) = \det(xI - A_\Gamma)$, is called the characteristic polynomial of the signed graph $\Gamma = (G, \sigma)$. For brevity, the spectrum of the adjacency matrix A_Γ is called the spectrum of the signed graph (G, σ). Let the signed graph Γ on n vertices has distinct eigenvalues $\mu_1(\Gamma), \mu_2(\Gamma), \ldots, \mu_k(\Gamma)$ (we drop Γ where the signed graph is understood) and let their respective multiplicities be $m_1, m_2, \ldots, m_k$. The adjacency spectrum of Γ is written as $Spec(\Gamma) = \{\mu_1^{(m_1)}(\Gamma), \mu_2^{(m_2)}(\Gamma), \ldots, \mu_k^{(m_k)}(\Gamma)\}$. From the definition, it follows that the matrix A_Γ is a real

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symmetric and hence the eigenvalues $\mu_1(\Gamma) \geq \mu_2(\Gamma) \geq \cdots \geq \mu_n(\Gamma)$ of the signed graph Γ are all real numbers. The largest eigenvalue $\mu_1(\Gamma)$ is also known as the index of the signed graph Γ.

The concept of signature switching is necessary when dealing with signed graphs. Let Z be a subset of the vertex set $V(\Gamma)$. The switched signed graph Γ^Z is obtained from Γ by reversing the signs of the edges in the cut $[Z, V(\Gamma)\backslash Z]$. Clearly, we see that the signed graphs Γ and Γ^Z are switching equivalent. The switching equivalence is an equivalence relation that preserves the eigenvalues. The switching class of Γ is denoted by $[\Gamma]$. The sign of a cycle is the product of the signs of its edges. A signed cycle $C_{n\sigma}$ on n vertices is positive (or negative) if it contains an even (or odd) number of negative edges, respectively. A signed graph is said to be balanced if all of its signed cycles are positive, otherwise, it is unbalanced. That is, a signed graph is said to be balanced if it switches to the signed graph with all positive signature. Otherwise, it is said to be unbalanced. By $\sigma \sim +$, we say that the signature σ is equivalent to the all-positive signature, and the corresponding signed graph is equivalent to its underlying graph. In general, the signature is determined by the set of positive cycles. Hence, all trees are switching equivalent to the all-positive signature. Moreover, we can say that the edge signs of bridges are irrelevant. In our drawings of signed graphs, we represent the negative edges with dashed lines and the positive edges with solid lines. A connected signed graph is said to be unicyclic if it has the same number of vertices and edges. If the number of edges is one more than the number of vertices, then it is said to be bicyclic. The girth of a signed graph is the length of the shortest cycle of its underlying graph. For more definitions and notations of graphs, we refer to [18, 21].

A signed graph Γ is said to have the pairing property if μ is an eigenvalue whenever $-\mu$ is an eigenvalue of Γ and both μ and $-\mu$ have the same multiplicities. The signed graph $\Gamma = (G, +)$ with all positive signature has the pairing property if and only if its underlying graph G is bipartite. For any signature σ it is not true. It is essential to note that the pairing property, often referred to as a symmetric spectrum with respect to the origin in the literature.

This paper primarily focuses on comparing the Estrada index within signed graphs that possess the pairing property. The comparison specifically revolves around their largest eigenvalues. If Γ_1 and Γ_2 are two signed graphs with the pairing property, both having the same number of vertices and edges, then Γ_1 has exactly four non-zero eigenvalues while Γ_2 has at least four non-zero eigenvalues. We aim to demonstrate that the Estrada index of Γ_1 is greater than that of Γ_2, given that the largest eigenvalue of Γ_1 surpasses the largest eigenvalue of Γ_2.

The rest of the paper is organized as follows. In Section 2, we characterize the unicyclic signed graphs with the maximum Estrada index. In Section 3, we find the signed graphs in the set of all unbalanced unicyclic and bicyclic signed graphs with the pairing property having the maximal Estrada index.

2. Estrada index in signed graphs

The Estrada index, a graph-spectrum-based structural descriptor, of a graph is defined as the trace of the adjacency matrix exponential and was first proposed by Estrada in 2000. Pena et al. [19] recommended calling it the Estrada index, which has since become widely adopted. This index can be used to measure a range of things, including the degree of protein folding [6–8], the subgraph centrality and bipartivity of complex networks [9, 10]. Because of the graph Estrada index's exceptional use, various Estrada indices based on the eigenvalues of other graph matrices have been investigated. Estrada index-based invariant concerning the Laplacian matrix, signless Laplacian matrix, distance matrix, distance Laplacian matrix and distance signless Laplacian matrix have been studied, see [11]. In social networks, the balance (stability) [12, 13] of a signed network can be quantified by

$$k = \frac{tr(e^{A_{(G,\sigma)}})}{tr(e^{A_{(G,+)}})}, \tag{1}$$

where $tr(X)$ denotes the trace of the matrix X. Motivated by Eq. (1), in [11], the Estrada index for a signed graph is defined in full analogy with the Estrada index for a graph, as

$$EE(\Gamma) = EE((G, \sigma)) = \sum_{i=1}^{n} e^{\mu_i}, \tag{2}$$

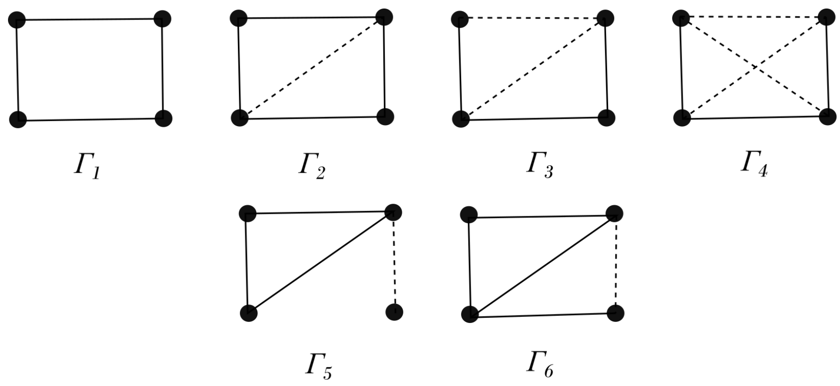

Figure 1: Signed graph $\Gamma_i \quad i = 1, 2, \ldots, 6$.

where $\mu_1, \mu_2, \ldots, \mu_n$ are the eigenvalues of the signed graph Γ. The Seidel matrix S_G of a simple graph G with n vertices and having the adjacency matrix A_G is defined as $S_G = J - I - 2A_G$. Obviously, the Seidel matrix is the adjacency matrix of some signed graph $\Gamma = (K_n, \sigma)$, where K_n is the complete graph on n vertices. Therefore, Eq. (2) is the extension of the Siedel Estrada index [1].

For a non-negative integer k, let $M_k(\Gamma) = \sum_{i=1}^{n} \mu_i^k$ denote the k-th spectral moment of Γ. From the Taylor expansion of e^{μ_i}, $EE(\Gamma)$ in (2) can be rewritten as

$$EE(\Gamma) = \sum_{k=0}^{\infty} \frac{M_k(\Gamma)}{k!}. \tag{3}$$

It is well-known that $M_k(\Gamma)$ is equal to the difference of the number of positive and negative closed walks of length k in Γ. We have

$$M_k(\Gamma) = w^+(k) - w^-(k), \tag{4}$$

where $w^+(k)$ and $w^-(k)$ are, respectively, the number of positive and negative closed walks of length k in Γ. In particular, we have

$$M_0(\Gamma) = n, \ M_1(\Gamma) = 0, \ M_2(\Gamma) = 2m \text{ and } M_3(\Gamma) = 6(t^+ - t^-),$$

where n is the number of vertices, m is the number of edges, t^+ is the number of positive triangles and t^- is the number of negative triangles in the signed graph Γ.

Let Γ_1 and Γ_2 be two signed graphs. If $M_k(\Gamma_1) \geq M_k(\Gamma_2)$ holds for any positive integer k, then by Eq. (3), we get $EE(\Gamma_1) \geq EE(\Gamma_2)$. Further, if the strict inequality $M_k(\Gamma_1) > M_k(\Gamma_2)$ holds for at least one integer k, then $EE(\Gamma_1) > EE(\Gamma_2)$. It is easy to see that if Γ has q connected components $\Gamma_1, \Gamma_2, \ldots, \Gamma_q$, then $EE(\Gamma) = \sum_{i=1}^{q} EE(\Gamma_i)$. So, now onwards, we shall investigate the Estrada index of connected signed graphs. One classical problem of graph spectra is to identify the extremal graphs with respect to the Estrada index in some given class of graphs, for example, see [4, 5, 25]. For a signed tree, all signatures are equivalent. The following result shows that among all signed trees on n vertices, the signed path P_n has the minimum and the signed star S_n has the maximum Estrada index.

Theorem 2.1. [4] *If T_n is an n-vertex tree different from S_n and P_n, then*

$$EE((P_n, \sigma)) < EE((T_n, \sigma)) < EE((S_n, \sigma)).$$

Remark 1.1 Let $\Gamma = (G, +)$ be a connected signed graph on n vertices with all positive signature and e be a positive edge. The signed graph $\Gamma' = \Gamma + e$ is obtained from Γ by adding the edge e. It is easy to see that any self-returning walk of length k of Γ is also a self-returning walk of length k of Γ'. Thus, $M_k(\Gamma') \geq M_k(\Gamma)$ and $EE(\Gamma') \geq EE(\Gamma)$. But in general adding any signed edge between two non-adjacent vertices of a signed graph $\Gamma = (G, \sigma)$ may not increase the Estrada index. Consider the signed graphs Γ_i, $i = 1, 2, \ldots, 6$, as shown in Figure 1. Their spectrum is given by $Spec(\Gamma_1) = \{2, -2, 0^2\}$, $Spec(\Gamma_2) = \{\frac{-1+\sqrt{17}}{2}, 1, 0, \frac{-1-\sqrt{17}}{2}\}$, $Spec(\Gamma_3) = \{2, 1, -1, -2\}$, $Spec(\Gamma_4) = \{\sqrt{5}, 1, -1, -\sqrt{5}\}$, $Spec(\Gamma_5) = \{2.17, 0.31, -1, -1.48\}$ and $Spec(\Gamma_6) = \{2, 1, -1, -2\}$, respectively. The signed graph Γ_2 is obtained from Γ_1 by adding a negative edge between two non-adjacent vertices and clearly $EE(\Gamma_2) = 8.55 < 9.52 = EE(\Gamma_1)$. The signed graph Γ_4 is obtained from Γ_3 by adding a negative edge between two non-adjacent vertices and $EE(\Gamma_4) = 12.54 > 10.61 = EE(\Gamma_3)$. Furthermore, The signed graph Γ_6 is obtained from Γ_5 by adding a positive edge and $EE(\Gamma_5) = 10.71 > 10.61 = EE(\Gamma_6)$. Therefore, the edge addition (deletion) technique cannot be used to compare the Estrada index in signed graphs.

The following result shows that the Estrada index of a signed graph with all positive signature can not be less than the Estrada index of a signed graph with all negative signature.

Theorem 2.2. *Let G be a graph on n vertices. Then $EE((G,+)) \geq EE((G,-))$, with strict inequality if and only if G contains at least one odd cycle.*

Proof. Let G be a graph on n vertices. Put $\Gamma_1 = (G,+)$ and $\Gamma_2 = (G,-)$. Then, by Eq. (2), we have

$$\begin{aligned} EE(\Gamma_1) - EE(\Gamma_2) &= \sum_{i=1}^{n} e^{\mu_i(\Gamma_1)} - \sum_{i=1}^{n} e^{\mu_i(\Gamma_2)} \\ &= \sum_{i=1}^{n} (e^{\mu_i(\Gamma_1)} - e^{\mu_i(\Gamma_2)}). \end{aligned} \tag{5}$$

The signed graph Γ_2 can be obtained from the signed graph Γ_1 by negating each edge. Therefore $Spec(\Gamma_1) = -Spec(\Gamma_2)$. Thus, by rearrangement of Eq. (5) and using Taylor's expansion, we have

$$\begin{aligned} EE(\Gamma_1) - EE(\Gamma_2) &= \sum_{i=1}^{n} (e^{\mu_i(\Gamma_1)} - e^{-\mu_i(\Gamma_1)}) \\ &= 2\sum_{k=0}^{\infty} \frac{M_{2k+1}(\Gamma_1)}{(2k+1)!}. \end{aligned} \tag{6}$$

The signed graph Γ_1 has all positive signature and therefore by Eq. (4), $M_{2k+1}(\Gamma_1) \geq 0$. If Γ_1 has an odd cycle of size l, then $M_l(\Gamma_1) > 0$. Hence the result follows. □

There exist exactly two switching classes on the signings of an odd unicyclic graph (whose unique cycle has odd girth). The cycle with all positive signature and the cycle with all negative signature. The following result is an immediate consequence of Theorem 2.2.

Corollary 2.3. *Let G be an odd unicyclic graph on n vertices and let Γ_1 be any balanced signed graph on G and Γ_2 be any unbalanced one. Then $EE(\Gamma_1) > EE(\Gamma_2)$.*

Let G be a bipartite unicyclic graph on n vertices with girth l and let Γ_1 be any balanced signed graph on G and Γ_2 be any unbalanced one. It is easy to see that $M_{2k+1}(\Gamma_1) = 0 = M_{2k+1}(\Gamma_2)$ for each $k \geq 0$, $M_{2k}(\Gamma_1) = M_{2k}(\Gamma_2)$ for $2k \leq l-2$ and $M_{2k}(\Gamma_1) > M_{2k}(\Gamma_2)$ for $2k \geq l$. In particular, $M_l(\Gamma_1) = M_l(\Gamma_2) + 4l$. Thus, by Eqs. (3) and (4), we have the following lemma.

Lemma 2.4. *Let G be a bipartite unicyclic graph on n vertices and let Γ_1 be any balanced signed graph on G and Γ_2 be any unbalanced one. Then $EE(\Gamma_1) > EE(\Gamma_2)$.*

Let $\Gamma^+(n,l)$ and $\Gamma^-(n,l)$ denote, respectively, the set of balanced and unbalanced unicyclic graphs with n vertices and containing a cycle of length $l \leq n$. Also, we denote by Γ_n^{l+} (respt. Γ_n^{l-}), the signed graph obtained by identifying the center of the signed star S_{n-l+1} with a vertex of positive cycle C_{l+} (respt. negative cycle C_{l-}). Du et al. [5] characterized the unique unicyclic signed graph having all positive signature with the maximum Estrada index and showed the following.

Lemma 2.5. *Let* $\Gamma = (G, +)$ *be a unicyclic graph on* $n \geq 4$ *vertices. Then* $EE(\Gamma) \leq EE(\Gamma_n^{3+})$ *with equality if and only if* Γ *is isomorphic to* Γ_n^{3+}.

The following result is directly obtained from Corollary 2.3 and Lemmas 2.4 and 2.5.

Theorem 2.6. *Let* $\Gamma = (G, \sigma)$ *be a unicyclic signed graph on* $n \geq 4$ *vertices. Then* $EE(\Gamma) \leq EE(\Gamma_n^{3+})$ *with equality if and only if* Γ *is switching equivalent to* Γ_n^{3+}.

Next, we show that the Estrada index of the balanced cycle C_{n+} is almost equal to the Estrada index of the unbalanced cycle C_{n-}.

Theorem 2.7. *Let* C_{n+} *and* C_{n-} *be the balanced and unbalanced cycles on n vertices, respectively. Then* $EE\left(C_{n-}\right) \approx nJ_0 \approx EE\left(C_{n+}\right)$, *where* $J_0 = \sum_{r\geqslant 0} \frac{1}{(r!)^2} = 2.27958530\ldots$. *Also,* $EE\left(C_{n+}\right) = EE\left(C_{n-}\right) + \epsilon_n$, *where* $\epsilon_n \to 0$ *as* $n \to \infty$.

Proof. The Estrada index of the n-vertex signed cycle C_{n+} can be approximated [15] as

$$EE\left(C_{n+}\right) \approx nJ_0, \tag{7}$$

where $J_0 = \sum_{r\geqslant 0} \frac{1}{(r!)^2} = 2.27958530\ldots$.
The eigenvalues of the unbalanced cycle C_{n-} are given by $2\cos\frac{(2r+1)\pi}{n}, \quad r = 0, 1, 2, \ldots, n-1$. Therefore,

$$EE\left(C_{n-}\right) = \sum_{r=0}^{n-1} \mathrm{e}^{2\cos((2r+1)\pi/n)}.$$

The angles $(2r+1)\pi/n$, for $r = 0, 1, 2, \ldots, n-1$, uniformly cover the semi-closed interval $[0, 2\pi)$. Now, using the property of definite integrals as a sum, we have

$$EE\left(C_{n-}\right) = n\left(\frac{1}{n}\sum_{r=0}^{n-1} \mathrm{e}^{2\cos((2r+1)\pi/n)}\right) \approx n\left(\frac{1}{2\pi}\int_0^{2\pi} \mathrm{e}^{2\cos x}\,\mathrm{d}x\right).$$

As $\mathrm{e}^{2\cos x}$ is an even function, therefore

$$\int_0^{2\pi} \mathrm{e}^{2\cos x}\,\mathrm{d}x = 2\int_0^{\pi} \mathrm{e}^{2\cos x}\,\mathrm{d}x = \pi J_0,$$

where J_0 is a special value of the function encountered in the theory of Bessel function and can be seen in [14] as

$$J_0 = \sum_{r=0}^{\infty} \frac{1}{(r!)^2} = 2.27958530\ldots.$$

In view of this,

$$EE\left(C_{n-}\right) \approx nJ_0 = 2.27958530n. \tag{8}$$

Eqs. (7) and (8) give

$$EE\left(C_{n-}\right) \approx nJ_0 \approx EE\left(C_{n+}\right). \tag{9}$$

Note that $M_k(C_{n+}) = M_k(C_{n-})$ for $k \leq n-1$ and $M_k(C_{n+}) \geq M_k(C_{n-})$ for $k \geq n$. In particular, $M_n(C_{n+}) = M_n(C_{n-}) + 4n$. Thus, by Eqs. (3) and (4), we get

$$EE(C_{n+}) - EE(C_{n-}) = \frac{4n}{n!} + \sum_{k=n+1}^{\infty} \frac{M_k(C_{n+}) - M_k(C_{n-})}{k!}. \tag{10}$$

The eigenvalues of C_{n+} and C_{n-} are, respectively, given by $2\cos\frac{2(r-1)\pi}{n}$ and $2\cos\frac{(2r+1)\pi}{n}$, $\quad r = 0, 1, 2, \ldots, n-1$. Therefore,

$$\sum_{k=n+1}^{\infty} \frac{M_k(C_{n+}) - M_k(C_{n-})}{k!} = \sum_{k=n+1}^{\infty} \frac{\sum_{r=0}^{n-1} 2^k(\cos^k \frac{2(r-1)\pi}{n} - \cos^k \frac{(2r+1)\pi}{n})}{k!}. \tag{11}$$

The maximum value of the function $\cos^k \frac{2(r-1)\pi}{n} - \cos^k \frac{(2r+1)\pi}{n}$ is 2. Thus, by Eq. (11), we have

$$\begin{aligned} \sum_{k=n+1}^{\infty} \frac{M_k(C_{n+}) - M_k(C_{n-})}{k!} &\le \sum_{k=n+1}^{\infty} \frac{\sum_{r=0}^{n-1} 2^{k+1}}{k!} \\ &= \sum_{k=n+1}^{\infty} \frac{2^{k+1} n}{k!} \\ &= \frac{2^{n+2} n}{(n+1)!} + \frac{2^{n+3} n}{(n+2)!} + \frac{2^{n+4} n}{(n+3)!} + \cdots \\ &\le \frac{2^{n+2} n}{n!} \left(\frac{1}{(n+1)} + \frac{2}{(n+1)^2} + \frac{2^2}{(n+1)^3} + \cdots \right). \end{aligned} \tag{12}$$

The series $\frac{1}{(n+1)} + \frac{2}{(n+1)^2} + \frac{2^2}{(n+1)^3} + \ldots$ is an infinite geometric progression with common ratio $\frac{2}{(n+1)}$. By inequality (12), we obtain

$$\sum_{k=n+1}^{\infty} \frac{M_k(C_{n+}) - M_k(C_{n-})}{k!} \le \frac{2^{n+2} n}{n!(n-1)}. \tag{13}$$

Eqs. (10) and (13) imply that

$$EE(C_{n+}) - EE(C_{n-}) \le \frac{2^{n+2} n + 4n(n-1)}{n!(n-1)}, \tag{14}$$

where the term $\frac{2^{n+2} n + 4n(n-1)}{n!(n-1)} \sim \frac{2^{n+2}}{n!}$ tends to zero as the girth n becomes large enough. Moreover, the accuracy of the Eq. (9) can be seen from the data given in Table 1. As seen from this data, except for the first few values of n ($n \le 9$), the accuracy is more than sufficient.

Table 1. Approximate and the exact values of the Estrada index of the n-vertex signed cycles (C_{n+}) and (C_{n-}) .

n	$EE\,(C_{n+})$	nJ_0	$EE\,(C_{n-})$
3	8.1248150	6.8387561	5.571899
4	9.5243914	9.1183414	8.7127342
5	11.4961863	11.3979268	11.2993665
6	13.6967139	13.6775122	13.658309
7	15.9602421	15.9570975	15.9533523
8	18.2371256	18.2366829	18.2368574
9	20.5163225	20.5162683	20.5163962
10	22.7958591	22.7958536	22.7958491
11	25.0754389	25.0754390	25.0754200
12	27.3550237	27.3550243	27.3550195
13	29.6346089	29.6346097	29.6345864
14	31.9141942	31.9141951	31.9141892
15	34.1937795	34.1937804	34.1937780

Hence the result follows. □

The main tool used to prove Lemma 2.5 is the construction of mappings which increases the k-th spectral moment for each k and using Eq.(3). For example consider the following result.

Theorem 2.8. [5] *For the all positive signature σ and $4 \leq l \leq n$, we have $EE(\Gamma_n^{(l+1)+}) < EE(\Gamma_n^{l+})$.*

But in unicyclic signed graphs, in general, we cannot construct the mapping which increases the k-th spectral moment for each k. To defend this statement, consider the unicyclic signed graphs Γ_5^{4-} and Γ_5^{5-}. Their spectra is given by $Spec(\Gamma_5^{5-}) = \{\frac{1+\sqrt{5}}{2}^2, \frac{1-\sqrt{5}}{2}^2, -2\}$ and $Spec(\Gamma_5^{4-}) = \{\sqrt{3}, \sqrt{2}, 0, -\sqrt{2}, -\sqrt{3}\}$, respectively. It is easy to see that not only $EE(\Gamma_5^{5-}) = 11.30 > 11.18 = EE(\Gamma_5^{4-})$ but also $M_4(\Gamma_5^{5-}) = 30 > 26 = M_4(\Gamma_5^{4-})$ and $M_5(\Gamma_5^{5-}) = -10 < 0 = M_5(\Gamma_5^{4-})$. Thus the problem of finding the unbalanced unicyclic graphs with extremal Estrada index is interesting.

3. Unbalanced unicyclic and bicyclic signed graphs with the pairing property and with maximal Estrada index

In this section, we first characterize the unbalanced bipartite unicyclic signed graphs with the maximal Estrada index. Given two non-increasing real number sequences $\alpha = \{\alpha_1, \alpha_2, \alpha_3, \ldots, \alpha_n\}$ and $\beta = \{\beta_1, \beta_2, \beta_3, \ldots, \beta_n\}$, we say that α majorizes β, denoted by $\alpha \geq \beta$, if $\sum_{j=1}^{t} \alpha_j \geq \sum_{j=1}^{t} \beta_j$ for each $t = 1, \ldots, n$, with equality for $t = n$. Also, if $\alpha \neq \beta$ then $\alpha > \beta$.

Lemma 3.1. [16] *Let $f : \mathbb{R} \to \mathbb{R}$ be a strictly convex function. If $\alpha \geq \beta$, then $\sum_{i=1}^{n} f(\alpha_i) \geq \sum_{i=1}^{n} f(\beta_i)$. Also, if $\alpha \neq \beta$, then $\sum_{i=1}^{n} f(\alpha_i) > \sum_{i=1}^{n} f(\beta_i)$.*

Let $\Gamma_p(n, m)$ denote the set of all signed graphs on n vertices and m edges with the pairing property. The following results will be useful in the sequel.

Theorem 3.2. *Let Γ_1, $\Gamma_2 \in \Gamma_p(n, m)$ be two signed graphs on n vertices and m edges with the pairing property. If Γ_1 has exactly four non-zero eigenvalues and Γ_2 has at least four non-zero eigenvalues with $\mu_1(\Gamma_1) > \mu_1(\Gamma_2)$, then $EE(\Gamma_1) > EE(\Gamma_2)$.*

Proof. Let $\Gamma_1, \Gamma_2 \in \Gamma_p(n, m)$. Therefore, we have $\sum_{i=1}^{n} \mu_i^2(\Gamma_1) = \sum_{i=1}^{n} \mu_i^2(\Gamma_2) = 2m$. The signed graphs Γ_1 and Γ_2 have the pairing property, so we get $M_{2k+1}(\Gamma_1) = 0 = M_{2k+1}(\Gamma_2)$ for each $k \geq 0$. Let $\mu_1(\Gamma_2) \geq \mu_2(\Gamma_2) \geq \mu_3(\Gamma_2) \geq \cdots \geq \mu_{2r}(\Gamma_2)$, $r \geq 2$, be the non-zero eigenvalues of Γ_2. Thus, by Eq. (3) and the pairing property, we obtain

$$EE(\Gamma_1) = n - 2r + 2\sum_{k=0}^{\infty} \frac{g_k\left(\mu_1^2(\Gamma_1), \mu_2^2(\Gamma_1), 0, \ldots, 0\right)}{(2k)!} \tag{15}$$

and

$$EE(\Gamma_2) = n - 2r + 2\sum_{k=0}^{\infty} \frac{g_k\left(\mu_1^2(\Gamma_2), \mu_2^2(\Gamma_2), \ldots, \mu_r^2(\Gamma_2)\right)}{(2k)!}, \tag{16}$$

where $g_k(x_1, x_2, x_3, \ldots, x_r) = x_1^k + x_2^k + x_3^k + \cdots + x_r^k$, k is a positive integer and $\mu_1^2(\Gamma_1) + \mu_2^2(\Gamma_1) = m = \mu_1^2(\Gamma_2) + \mu_2^2(\Gamma_2) + \cdots + \mu_r^2(\Gamma_2)$. Now, Eqs. (15) and (16) imply that

$$EE(\Gamma_1) - EE(\Gamma_2) = 2\sum_{k=2}^{\infty} \frac{[g_k\left(\mu_1^2(\Gamma_1), \mu_2^2(\Gamma_1), 0, \ldots, 0\right) - g_k\left(\mu_1^2(\Gamma_2), \mu_2^2(\Gamma_2), \ldots, \mu_r^2(\Gamma_2)\right)]}{(2k)!}. \tag{17}$$

We know that the function $f(x) = x^{2k}$ is strictly convex for every positive integer k.
As $\mu_1(\Gamma_1) > \mu_1(\Gamma_2)$ and $\sum_{i=1}^{n} \mu_i^2(\Gamma_1) = \sum_{i=1}^{n} \mu_i^2(\Gamma_2) = 2m$, we conclude that the vector $\alpha = (\mu_1^2(\Gamma_1), \mu_2^2(\Gamma_1), 0, \ldots, 0)$ majorizes $\beta = (\mu_1^2(\Gamma_2), \mu_2^2(\Gamma_2), \cdots, \mu_r^2(\Gamma_2))$, that is $\alpha > \beta$. Thus, by Lemma 3.1, we have

$$g_k\left(\mu_1^2(\Gamma_1), \mu_2^2(\Gamma_1), 0, \ldots, 0\right) > g_k\left(\mu_1^2(\Gamma_2), \mu_2^2(\Gamma_2), \ldots, \mu_r^2(\Gamma_2)\right),$$

for $k \geq 2$. Hence, by Eq. (17), we get $EE(\Gamma_1) > EE(\Gamma_2)$ and the result follows. □

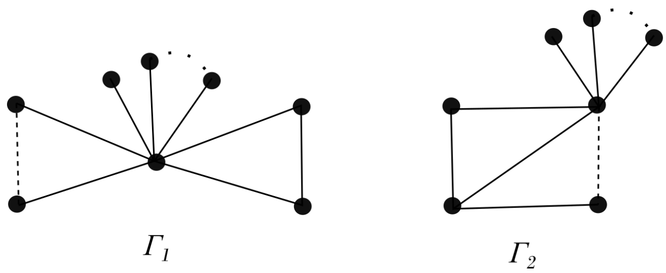

Figure 2: Signed graphs Γ_1 and Γ_2, which are in the statement of Theorem 3.5.

Lemma 3.3. [22] *Let $\Gamma^-(n,l)$ be the set of unbalanced unicyclic signed graphs with n vertices and containing a cycle of length $l \le n$. Then*
(i) for any $\Gamma \in \Gamma^-(n,l)$, we have $\mu_1(\Gamma_n^{l-}) \ge \mu_1(\Gamma)$ with equality if and only if Γ is switching equivalent to Γ_n^{l-};
(ii) $\mu_1(\Gamma_n^{l-}) > \mu_1(\Gamma_n^{(l+1)-})$.

We now recall Schwenk's formula for signed graphs which can be seen in [2]. Let u be any fixed vertex of a signed graph Γ. Then

$$\varphi(\Gamma,x) = x\varphi(\Gamma-u,x) - \sum_{vu\in E(\Gamma)} \varphi(\Gamma-v-u,x) - 2\sum_{Y\in\mathcal{Y}_u} \sigma(Y)\varphi(\Gamma-Y,x),$$

where $\mathcal{Y}_u$ is the set of all signed cycles passing through u, and $\Gamma - Y$ is the graph obtained from Γ by deleting Y.

A unicyclic signed graph has the pairing property if and only if its underlying graph is bipartite because it has a unique cycle. Next, we characterize the unique unbalanced bipartite unicyclic signed graphs with the maximum Estrada index among all unbalanced bipartite unicyclic signed graphs.

Theorem 3.4. *Let $\Gamma_p^-(n,n)$ be the set of all unbalanced bipartite unicyclic signed graphs on n vertices. If $\Gamma \in \Gamma_p^-(n,n)$, then $EE(\Gamma) \le EE(\Gamma_n^{4-})$ with equality if and only if Γ is switching equivalent to Γ_n^{4-}.*

Proof. Let $\Gamma \in \Gamma_p^-(n,n)$ be an unbalanced bipartite unicyclic signed graph on n vertices. By applying Lemma 3.3, we get $\mu_1(\Gamma) \le \mu_1(\Gamma_n^{4-})$ with equality if and only if Γ is switching equivalent to Γ_n^{4-}. Now, by Schwenk's formula, the characteristic polynomial of Γ_n^{4-} is given by

$$\varphi(\Gamma_n^{4-},x) = x^{n-4}\{x^4 - nx^2 + 2(n-2)\}.$$

Clearly, the signed graph Γ_n^{4-} has four non-zero eigenvalues. Let the signed graph Γ, where $\Gamma \in \Gamma_p^-(n,n)$, contains a cycle of length $l \ge 4$. Therefore, the unbalanced cycle C_{l^-} is an induced signed subgraph of Γ. The eigenvalues of C_{l^-} are given by $2\cos\frac{(2r+1)\pi}{l}$, $r = 0,1,2,\ldots,l-1$. Since l is a positive even integer and thus all the eigenvalues of C_{l^-} are non-zero. Hence the result follows by Theorem 3.2 and interlacing theorem for eigenvalues. □

Theorem 3.5. *Let $\Gamma_p^-(n,n+1)$ be the set of all unbalanced bicyclic signed graphs on n ($n \ge 6$) vertices with the pairing property. If $\Gamma \in \Gamma_p^-(n,n+1)\backslash\{\Gamma_1,\Gamma_2\}$, Γ is not switching equivalent to Γ_1 or Γ_2, then $EE(\Gamma_1) > EE(\Gamma_2) > EE(\Gamma)$, where Γ_1 and Γ_2 are the signed graphs on n vertices as shown in Fig.2.*

Proof. By Schwenk's formula, the characteristic polynomials of Γ_1 and Γ_2 are, respectively, given by

$$\varphi(\Gamma_1,x) = x^{n-6}(x^2-1)\{x^4 - nx^2 + n - 5\}$$

and

$$\varphi(\Gamma_2,x) = x^{n-4}\{x^4 - (n+1)x^2 + 2(n-2)\}.$$

It is easy to see that

$$Spec(\Gamma_1) = \{\pm\sqrt{\frac{n \pm \sqrt{n^2-4n+20}}{2}}, 1, 0^{n-6}, -1\}$$

$$\text{and } Spec(\Gamma_2) = \{\pm\sqrt{\frac{n+1 \pm \sqrt{(n+1)^2-8(n-2)}}{2}}, 0^{n-4}\}.$$

Therefore,

$$EE(\Gamma_1) = n-6+e^{\sqrt{\frac{n+\sqrt{n^2-4n+20}}{2}}}+e^{\sqrt{\frac{n-\sqrt{n^2-4n+20}}{2}}}+e^{-\sqrt{\frac{n+\sqrt{n^2-4n+20}}{2}}}+e^{-\sqrt{\frac{n-\sqrt{n^2-4n+20}}{2}}}+e+e^{-1}.$$

Also,

$$EE(\Gamma_2) = n-4+e^{\sqrt{\frac{n+1+\sqrt{(n+1)^2-8(n-2)}}{2}}}+e^{\sqrt{\frac{n+1-\sqrt{(n+1)^2-8(n-2)}}{2}}}+e^{-\sqrt{\frac{n+1+\sqrt{(n+1)^2-8(n-2)}}{2}}}+e^{-\sqrt{\frac{n+1-\sqrt{(n+1)^2-8(n-2)}}{2}}}.$$

For $6 \leq n \leq 35$, we checked with the aid of MATLAB software that $EE(\Gamma_1) > EE(\Gamma_2)$. For $n \geq 36$, we have, $\sqrt{2}-1 < \sqrt{\frac{n-\sqrt{n^2-4n+20}}{2}} < 1$ and $1 < \sqrt{\frac{n+1-\sqrt{(n+1)^2-8(n-2)}}{2}} < \sqrt{2}$. Also, $\sqrt{\frac{n+\sqrt{n^2-4n+20}}{2}} > \sqrt{\frac{n+1+\sqrt{(n+1)^2-8(n-2)}}{2}}$ for $n \geq 36$ ([[17], Lemma 4.5]). Therefore,

$$\begin{aligned}EE(\Gamma_1)-EE(\Gamma_2) &> 2\cosh\left(\sqrt{\frac{n+\sqrt{n^2-4n+20}}{2}}\right)-2\cosh\left(\sqrt{\frac{n+1+\sqrt{(n+1)^2-8(n-2)}}{2}}\right)\\ &+2\cosh\left(\sqrt{2}-1\right)+2\cosh(1)-2\cosh\left(\sqrt{2}\right)-2\\ &> 2\cosh\left(\sqrt{\frac{n+\sqrt{n^2-4n+20}}{2}}\right)-2\cosh\left(\sqrt{\frac{n+1+\sqrt{(n+1)^2-8(n-2)}}{2}}\right)\\ &-1.096>0.\end{aligned}$$

Clearly, $\cosh(x) = \frac{e^x+e^{-x}}{2}$ is an increasing function of $x > 0$ and also it is easy to see that

$$2\cosh\left(\sqrt{\frac{n+\sqrt{n^2-4n+20}}{2}}\right)-2\cosh\left(\sqrt{\frac{n+1+\sqrt{(n+1)^2-8(n-2)}}{2}}\right) > 2$$

for $n \geq 36$. This proves that $EE(\Gamma_1) > EE(\Gamma_2)$ for $n \geq 36$.

Let $\Gamma \in \Gamma_p^-(n, n+1)\backslash\{\Gamma_1, \Gamma_2\}$ be an unbalanced bicyclic signed graph with the pairing property. To prove the result it is enough to show that $EE(\Gamma_2) > EE(\Gamma)$. Since $\mu_1(\Gamma_1) > \mu_1(\Gamma_2)$, for $n \geq 5$, therefore, by [[17], Theorem 3.1], we get $\mu_1(\Gamma_1) > \mu_1(\Gamma_2) > \mu_1(\Gamma)$. The signed graph Γ_2 has four non-zero eigenvalues. Clearly, the signed graph Γ contains a 4-vertex signed path P_4 as an induced subgraph for $n \geq 6$. The characteristic polynomial of P_4 is given by

$$\varphi(P_4, x) = x^4 - 3x^2 + 1.$$

Thus the signed path P_4 has four non-zero eigenvalues. By interlacing theorem for eigenvalues, the signed graph Γ has at least four non-zero eigenvalues. Hence the result follows by Theorem 3.2. □

The following two results will be used in the sequel.

Lemma 3.6. [24] *Let (G, σ) be a connected signed graph. Then, we have $\mu_1((G, \sigma)) \leq \mu_1((G, +))$ with equality if and only if (G, σ) switches to $(G, +)$.*

Lemma 3.7. [23] *For an eigenvalue μ of a connected signed graph Γ, there exists a switching equivalent signed graph Γ', for which the μ-eigenspace contains an eigenvector whose non-zero coordinates are of the same sign.*

Let $\Gamma = (K_{m,n}, \sigma)$ be a complete bipartite signed graph, where $K_{m,n}$ is the complete bipartite graph on $m + n$ vertices. Let $S(K_{m,n}, -)$ be the set of all unbalanced complete bipartite signed graphs on $n+m$ vertices. Also, let Γ^* be an unbalanced complete bipartite signed graph that contains exactly one negative edge. Finally, we characterize the unbalanced complete bipartite signed graphs with the maximum Estrada index.

Theorem 3.8. *Let $S(K_{m,n}, -)$ be the set of all unbalanced complete bipartite signed graphs on $n + m$ vertices. If $\Gamma \in S(K_{m,n}, -)$, then $EE(\Gamma^*) \geq EE(\Gamma)$ with equality if and only if Γ is switching equivalent to Γ^*, where Γ^* is an unbalanced complete bipartite signed graph that contains exactly one negative edge.*

Proof. Let $(\Gamma_1, \Gamma_2, \ldots, \Gamma_k)$ be a sequence consisting of the representatives of all switching equivalence classes of unbalanced complete bipartite signed graphs with $m + n$ vertices such that the representatives are ordered non-increasingly by the largest eigenvalue (index) and chosen in such a way that, for $1 \leq j \leq k$, the $\mu_1(\Gamma_j)$-eigenspace contains an eigenvector whose non-zero coordinates are positive (This existence of Γ_j is provided by Lemma 3.7). By Lemma 3.6, the complete bipartite signed graph with all positive signature has the maximum index. Therefore, by [[3],Theorem 3.2], the signed graph with maximum index among all unbalanced complete bipartite signed graphs on $n + m$ vertices is Γ^* (up to switching), where Γ^* is an unbalanced complete bipartite signed graph that contains exactly one negative edge. That is, for each $\Gamma \in S(K_{m,n}, -)$, we have $\mu_1(\Gamma) \leq \mu_1(\Gamma^*)$ with equality if and only if Γ is switching equivalent to Γ^*. Now, by [[20], Theorem 4.1], the spectrum of the signed graph Γ^* is given by

$$Spec(\Gamma^*) = \{\pm \sqrt{\frac{mn \pm \sqrt{m^2n^2 - 16(m-1)(n-1)}}{2}}, 0^{n-4}\}.$$

Clearly, the signed graph Γ^* has four non-zero eigenvalues. Also, with a suitable labelling of the vertices of $\Gamma \in S(K_{m,n}, -)$, its adjacency matrix is given by

$$A_\Gamma = \begin{pmatrix} O_{m\times m} & B_{m\times n} \\ B^\top_{n\times m} & O_{n\times n} \end{pmatrix},$$

where $B_{m\times n}$ is a matrix whose entries are either 1 or -1. We know that $rank(A_\Gamma) = rank(B_{m\times n}) + rank(B^\top_{m\times n}) = 2rank(B_{m\times n})$. It is easy to see that $rank(A_\Gamma) \geq 4$ because if $rank(B_{m\times n}) = 1$, then Γ is a switching equivalent to a complete bipartite signed graph with all positive signature, which is a contradiction. Thus, the signed graph $\Gamma \in S(K_{m,n}, -)$ has at least four non-zero eigenvalues. Hence the result follows by Theorem 3.2. □

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Data availibility Data sharing is not applicable to this article as no datasets were generated or analyzed during the current study.

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