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On Resolvent Estrada Index

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Abstract

Let G be a simple graph with n vertices, and let $\lambda_1(G), \lambda_2(G), \ldots, \lambda_n(G)$ be its eigenvalues. The resolvent Estrada index of G is defined as

$$EE_r(G) = \sum_{i=1}^{n} \left(1 - \frac{\lambda_i(G)}{n-1}\right)^{-1}.$$

In this paper, we show that $EE_r(G)$ can be determined directly by the characteristic polynomial of the graph G. By using this result, we determine the first thirteen trees with the greatest resolvent Estrada index, and characterize the multipartite graphs having the maximal resolvent Estrada index.

1 Introduction

Let $G = (V, E)$ be a simple graph of order n with vertex set $V(G)$ and edge set $E(G)$. A walk W of length k in G is a sequence of vertices $v_0v_1v_2 \cdots v_k$, where v_i is adjacent to v_{i+1} for each $i = 0, 1, \ldots, k-1$. In particular, if $v_0 = v_k$, then W is a closed walk. The adjacency matrix of G, denoted by $A(G)$, is the $n \times n$ matrix (a_{ij}) in which $a_{ij} = 1$ if the vertices v_i and v_j are adjacent, and $a_{ij} = 0$ otherwise. The characteristic polynomial of G, denoted by $\phi(G, \lambda)$, is defined to be the characteristic polynomial of its adjacency matrix, that is, $\phi(G, \lambda) = \det(\lambda I - A(G))$. Observe that $A(G)$ is real and symmetric, so all its eigenvalues $\lambda_1(G), \lambda_2(G), \ldots, \lambda_n(G)$ are real. We assume, without loss of generality, that $\lambda_1(G) \geq \lambda_2(G) \geq \cdots \geq \lambda_n(G)$, and call them the eigenvalues (or spectrum) of G. In particular, $\lambda_1(G)$ is called the largest eigenvalue (or spectral radius) of G. The basic properties of graph eigenvalues can be found in the excellent monograph [4].

For $k \geq 0$, let $M_k(G)$ denote the kth spectral moment of a graph G, namely,

$$M_k(G) = tr(A(G)^k) = \sum_{i=1}^{n} \lambda_i(G)^k,$$

where $tr(\cdot)$ is the trace of a matrix. It is known [4] that $M_k(G)$ is equal to the number of closed walks of length k in G. Thus, the spectral moments become the basis of several structural invariants for graphs, one of which is defined by Estrada [11] as the Taylor expansion of the spectral moments of the form

$$EE(G) = \sum_{k=0}^{\infty} \frac{M_k(G)}{k!}, \tag{1}$$

which has the following closed form in terms of the graph spectrum

$$EE(G) = \sum_{i=1}^{n} e^{\lambda_i(G)}.$$

This exponential-based quantity, later called the Estrada index by de la Peña, Gutman and Rada [6], has found a great deal of applications in various fields. It was initially used to quantify the degree of folding of protein chains [11]. Later, it was exploited to measure the centrality of complex (communication, social, metabolic, *etc.*) networks (in this case it was also called the subgraph centrality) [12]. In addition, a connection between the Estrada index and the concept of extended atomic branching was found in [13]. Due to its extensive applications, the Estrada index has also attracted much attention of mathematicians in the past few years. Various mathematical properties of the Estrada index have been investigated, see [16] for a comprehensive survey.

Recently, Estrada and Higham [14] proposed a general formulation for the invariants of a graph G based on Taylor series expansion of spectral moments

$$EE(G, c) = \sum_{k=0}^{\infty} c_k M_k(G).$$

This general formulation was applied to complex networks by considering the following invariant [14]

$$EE_r(G) = \sum_{k=0}^{\infty} \frac{M_k(G)}{(n-1)^k}, \tag{2}$$

which eventually converges to the trace of the resolvent of the adjacency matrix of a graph G

$$EE_r(G) = tr\left(\mathbf{I} - \frac{1}{n-1}A(G)\right)^{-1} = \sum_{i=1}^{n}\left(1 - \frac{\lambda_i(G)}{n-1}\right)^{-1}, \qquad (3)$$

where $\mathbf{I}$ is the unity matrix of appropriate size. This resolvent-based quantity was later referred to as the resolvent Estrada index by Benzi and Boito [1]. It is worth mentioning that if G is a non-complete graph, then $|\lambda_i(G)| < n-1$ for each $i \in \{1, 2, \ldots, n\}$ (see, *e.g.*, [4]), and hence $EE_r(G)$ is well-defined.

As far as we know, there are few known results for $EE_r(G)$ in the literature, except some upper and lower bounds obtained in [1, 3]. The aim of the present paper is to establish more mathematical properties for $EE_r(G)$. In the next section, we first discuss the similarity between $EE_r(G)$ and $EE(G)$. Then in Section 3, we would focus on the properties of $EE_r(G)$, which are different from those of $EE(G)$. We show that $EE_r(G)$ can be determined directly by the characteristic polynomial of the graph G. This result provides us with a tool to compute $EE_r(G)$ effectively. By utilizing this tool, we determine the first thirteen trees with the greatest resolvent Estrada index among all trees with given number of vertices, and characterize the unique graph having the maximal resolvent Estrada index among all multipartite graphs with given number of vertices.

2 Similarity between EE_r and EE

From (1) and (2), it is evident that both $EE_r(G)$ and $EE(G)$ are "increasing monotonically" with respect to $M_k(G)$. This can be stated formally as follows:

Proposition 1 *For two graphs G_1 and G_2, if $M_k(G_1) \geq M_k(G_2)$ holds for all k, then $EE_r(G_1) \geq EE_r(G_2)$ and $EE(G_1) \geq EE(G_2)$. Moreover, if $M_k(G_1) > M_k(G_2)$ holds for some k, then $EE_r(G_1) > EE_r(G_2)$ and $EE(G_1) > EE(G_2)$.*

For a non-empty graph G, denote by $G - e$ the graph obtained by deleting an edge e from G. Since $M_k(G)$ is equal to the number of closed walks of length k in G, it follows that $M_k(G) \geq M_k(G-e)$ for all $k \geq 0$, and $M_2(G) > M_2(G-e)$. This together with Proposition 1 would yield the following result immediately.

Proposition 2 *Let G be a (non-complete) graph and let e be its arbitrary edge. Then $EE_r(G) > EE_r(G-e)$ and $EE(G) > EE(G-e)$.*

Notice that the result for $EE(G)$ in Proposition 2 was reported by Gutman *et al.* in [15]. In fact, besides this, a great deal of results (mainly the extremal results) for $EE(G)$ were also obtained by means of Proposition 1, see [7, 8, 9, 10, 18, 20] for details. Naturally, all these known results for $EE(G)$, except the case of complete graphs, would be applicable for $EE_r(G)$ as well.

It should be pointed out that although $EE_r(G)$ has many properties analogous to those of $EE(G)$, these two indices are distinct in essence, see [14] for details. We shall add some further evidence to support this point of view in the next section.

3 Main results

In this section we consider the properties of $EE_r(G)$, which are different from those of $EE(G)$. We start with a simple but very useful property of $EE_r(G)$.

Theorem 3 *For any non-complete graph G on n vertices,*

$$EE_r(G) = (n-1)\frac{\mathrm{d}\ln\phi(G,\lambda)}{\mathrm{d}\lambda}\bigg|_{\lambda=n-1} = (n-1)\frac{\phi'(G,n-1)}{\phi(G,n-1)}.$$

Proof. Notice that the characteristic polynomial of G can be written as $\phi(G,\lambda) = \prod_{i=1}^{n}(\lambda - \lambda_i(G))$, where $\lambda_1(G), \lambda_2(G), \ldots, \lambda_n(G)$ are the eigenvalues of G. Then,

$$(n-1)\frac{\mathrm{d}\ln\phi(G,\lambda)}{\mathrm{d}\lambda} = (n-1)\frac{\phi'(G,\lambda)}{\phi(G,\lambda)} = \sum_{i=1}^{n}\frac{n-1}{\lambda-\lambda_i}. \tag{4}$$

By setting $\lambda = n-1$ in (4) and recalling the definition of $EE_r(G)$ (see (3)), we have the desired result, completing the proof. □

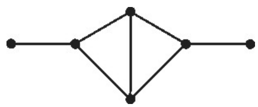

Figure 1. The graph G^*.

Remark. Theorem 3 indicates that $EE_r(G)$ can be determined directly by the characteristic polynomial of the graph G. This result provides us with a tool to compute $EE_r(G)$ effectively. As an instructive example, let G^* be the graph shown in Figure 1. It is easy to check that $\phi(G^*,\lambda) = \lambda^6 - 7\lambda^4 - 4\lambda^3 + 7\lambda^2 + 4\lambda - 1$. Then by Theorem 3, we have

$$EE_r(G^*) = 5 \times \frac{6\lambda^5 - 28\lambda^3 - 12\lambda^2 + 14\lambda + 4}{\lambda^6 - 7\lambda^4 - 4\lambda^3 + 7\lambda^2 + 4\lambda - 1}\bigg|_{\lambda=5} = \frac{1565}{228}.$$

3.1. Trees with maximal EE_r

In this subsection, by means of Theorem 3, we shall determine the first thirteen trees with the greatest resolvent Estrada index among all trees with given number of vertices.

Let T be a tree. Note that $M_{2k+1}(T) = 0$ for all $k \geq 0$, since T is bipartite. Consequently, from (2), we have

$$EE_r(T) = \sum_{k=0}^{\infty} \frac{M_{2k}(T)}{(n-1)^{2k}}. \tag{5}$$

Based on (5), and using the same method as in the proof of Theorem 4 in [21], we obtain the following result.

Lemma 4 *Let T_1 and T_2 be two trees. If T_1 has at most two positive eigenvalues and T_2 has at least two positive eigenvalues with $\lambda_1(T_1) > \lambda_1(T_2)$, then $M_{2k}(T_1) \geq M_{2k}(T_2)$, with the equality if and only if $k = 1$. Consequently, $EE_r(T_1) > EE_r(T_2)$.*

Lemma 5 (see [5]) *Let T be a tree, and let $\theta(T)$ be the maximum number of independent (mutually non-adjacent) edges in T. Then T has exactly $\theta(T)$ positive eigenvalues.*

The next lemma is usually used to calculate the characteristic polynomial of a tree, which can be found in, for instance, [4].

Lemma 6 (see [4]) *Let v be a vertex of degree one in a graph G and u the vertex adjacent to v. Then $\phi(G, \lambda) = \lambda\phi(G\backslash v, \lambda) - \phi(G\backslash\{u, v\}, \lambda)$.*

We are now ready to give the main result of this subsection.

Theorem 7 *Among all n-vertex trees, if $n \geq 12$, then the first thirteen trees with the greatest resolvent Estrada index are, respectively,*

$$S_n^1, S_n^2, S_n^3, S_n^4, S_n^5, S_n^6, S_n^7, S_n^8, S_n^9, S_n^{10}, S_n^{11}, S_n^{12} \text{ and } S_n^{13} \text{ (see Figure 2)}.$$

Proof. It was shown in [17, 2, 19] that among all n-vertex trees, if $n \geq 12$ then the first thirteen trees with the maximal spectral radius are, respectively,

$$S_n^1, S_n^2, S_n^3, S_n^4, S_n^5, S_n^6, S_n^7, S_n^{10}, S_n^8, S_n^{11}, S_n^9, S_n^{12} \text{ and } S_n^{13}.$$

Now, suppose that T is any tree on n vertices different from S_n^i, $i \in \{1, 2, \ldots, 13\}$. Clearly, $\lambda_1(S_n^{13}) > \lambda_1(T)$. Moreover, observing that $\theta(S_n^{13}) = 2$ and $\theta(T) \geq 2$, by Lemma 5, we

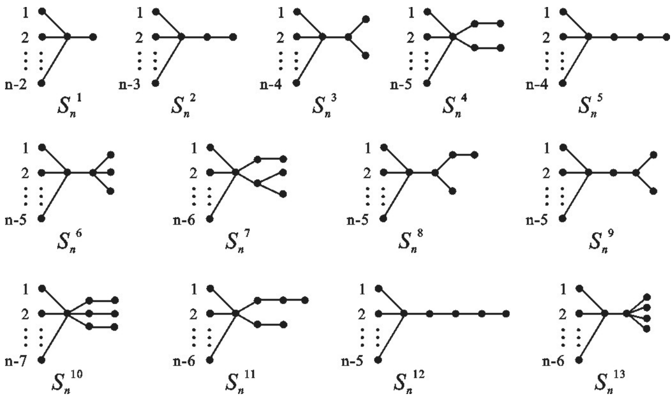

Figure 2. The trees S_n^i, $i \in \{1, 2, \ldots, 13\}$.

know that S_n^{13} has exactly two positive eigenvalues, while T has at least two positive eigenvalues. Consequently, from Lemma 4, we have

$$EE_r(S_n^{13}) > EE_r(T).$$

Next, in order to complete the proof, it suffices to prove that

$$EE_r(S_n^j) > EE_r(S_n^{j+1}) \text{ holds for each } j \in \{1, 2, \ldots, 12\}. \tag{6}$$

For convenience, we partition (6) into the following two claims:

Claim 1. $EE_r(S_n^1) > EE_r(S_n^2) > EE_r(S_n^3) > EE_r(S_n^4)$ and $EE_r(S_n^5) > EE_r(S_n^6) > EE_r(S_n^7)$.

Observe first that $\theta(S_n^1) = 1$, $\theta(S_n^2) = \theta(S_n^3) = \theta(S_n^5) = \theta(S_n^6) = 2$ and $\theta(S_n^4) = \theta(S_n^7) = 3$. On the other hand, we have

$$\lambda_1(S_n^1) > \lambda_1(S_n^2) > \lambda_1(S_n^3) > \lambda_1(S_n^4) > \lambda_1(S_n^5) > \lambda_1(S_n^6) > \lambda_1(S_n^7).$$

Thus, Claim 1 follows directly from Lemmas 4 and 5.

Claim 2. $EE_r(S_n^4) > EE_r(S_n^5)$ and $EE_r(S_n^l) > EE_r(S_n^{l+1})$ for each $l \in \{7, 8, 9, 10, 11, 12\}$.

By Lemma 6 and a direct calculation, we get

$\phi(S_n^4, \lambda) = \lambda^{n-6}[\lambda^6 - (n-1)\lambda^4 + (2n-7)\lambda^2 - (n-5)]$,

$\phi(S_n^5, \lambda) = \lambda^{n-4}[\lambda^4 - (n-1)\lambda^2 + (2n-7)]$,

$\phi(S_n^7, \lambda) = \lambda^{n-6}[\lambda^6 - (n-1)\lambda^4 + (3n-13)\lambda^2 - (2n-12)]$,

$\phi(S_n^8,\lambda) = \lambda^{n-6}[\lambda^6 - (n-1)\lambda^4 + (3n-13)\lambda^2 - (n-5)]$,

$\phi(S_n^9,\lambda) = \lambda^{n-4}[\lambda^4 - (n-1)\lambda^2 + (3n-13)]$,

$\phi(S_n^{10},\lambda) = \lambda^{n-8}[\lambda^8 - (n-1)\lambda^6 + (3n-12)\lambda^4 - (3n-17)\lambda^2 + (n-7)]$,

$\phi(S_n^{11},\lambda) = \lambda^{n-6}[\lambda^6 - (n-1)\lambda^4 + (3n-12)\lambda^2 - (2n-11)]$,

$\phi(S_n^{12},\lambda) = \lambda^{n-6}[\lambda^6 - (n-1)\lambda^4 + (3n-12)\lambda^2 - (n-5)]$,

$\phi(S_n^{13},\lambda) = \lambda^{n-4}[\lambda^4 - (n-1)\lambda^2 + (4n-24)]$.

Since $n \geq 12$, it follows directly from Theorem 3 that $EE_r(S_n^4) > EE_r(S_n^5)$, $EE_r(S_n^7) > EE_r(S_n^8) > EE_r(S_n^9)$ and $EE_r(S_n^{11}) > EE_r(S_n^{12})$.

We finally show that $EE_r(S_n^9) > EE_r(S_n^{10})$, $EE_r(S_n^{10}) > EE_r(S_n^{11})$ and $EE_r(S_n^{12}) > EE_r(S_n^{13})$. Again by Theorem 3, we have,

$$EE_r(S_n^9) - EE_r(S_n^{10}) = \frac{4n(n-2)(n-1)^{2n-12}}{\phi(S_n^9, n-1)\phi(S_n^{10}, n-1)} \times h_1(n)$$

$$EE_r(S_n^{10}) - EE_r(S_n^{11}) = \frac{2n(n-2)(n-1)^{2n-14}}{\phi(S_n^{10}, n-1)\phi(S_n^{11}, n-1)} \times h_2(n)$$

$$EE_r(S_n^{12}) - EE_r(S_n^{13}) = \frac{2(n-1)^{2n-10}}{\phi(S_n^{12}, n-1)\phi(S_n^{13}, n-1)} \times h_3(n)$$

where

$h_1(n) = n^6 - 11n^5 + 65n^4 - 187n^3 + 273n^2 - 168n - 33$,

$h_2(n) = 3n^7 - 38n^6 + 174n^5 - 392n^4 + 450n^3 - 179n^2 - 66n - 6$,

$h_3(n) = 2n^7 - 37n^6 + 194n^5 - 499n^4 + 734n^3 - 631n^2 + 258n + 59$.

For each $i \in \{9, 10, 11, 12, 13\}$, $\phi(S_n^i, n-1) > 0$ always holds since

$$\lambda_1(S_n^i) < \lambda_1(S_n^1) = \sqrt{n-1} < n-1.$$

Moreover, it is easy to verify that,

- if $n \geq 12$, then $h_1(n) = n^5(n-11) + n^3(65n-187) + n(273n - 168 - \frac{33}{n}) > 0$;
- if $n \geq 13$, then $h_2(n) = n^6(3n-38) + n^4(174n-392) + n^2(450n - 179 - \frac{66}{n} - \frac{6}{n^2}) > 0$;
- if $n \geq 18$, then $h_3(n) = n^6(2n-37) + n^4(194n-499) + n^2(734n-631) + 258n + 59 > 0$.

We can further check directly that $h_2(12) > 0$ and $h_3(n) > 0$ for $12 \leq n \leq 18$. Consequently, Claim 2 follows.

This completes the proof. □

Remark. It is worth mentioning that among all n-vertex trees, if $n \geq 12$, then the first six trees with the greatest Estrada index are $S_n^1, S_n^2, S_n^3, S_n^4, S_n^5$ and S_n^6, respectively [8, 21], which coincide the first six trees with the greatest resolvent Estrada index. However, from the numerical results shown in Table 1 (computed by using software Matlab, up to four decimal places), we find that for $23 \leq n \leq 30$ and $n = 40, 50$,

$$EE(S_n^7) > EE(S_n^{10}) > EE(S_n^8) > EE(S_n^{11}) > EE(S_n^9) > EE(S_n^{12}) > EE(S_n^{13}),$$

which provides an example to reveal the difference between these two indices.

On the other hand, as mentioned in [21], it would be of interest to determine the first thirteen trees with the greatest Estrada index.

Table 1. The values of $EE(S_n^l)$, $l \in \{7, 8, 9, 10, 11, 12, 13\}$.

n	$EE(S_n^7)$	$EE(S_n^8)$	$EE(S_n^9)$	$EE(S_n^{10})$	$EE(S_n^{11})$	$EE(S_n^{12})$	$EE(S_n^{13})$
12	31.2169	31.1628	31.0872	31.0112	30.9475	30.8827	30.8071
13	35.4127	35.3463	35.2577	35.2065	35.1305	35.0530	34.6715
14	39.9842	39.9049	39.8028	39.7775	39.6885	39.5978	38.8827
15	44.9630	44.8701	44.7540	44.7557	44.6532	44.5487	43.4702
16	50.3825	50.2755	50.1446	50.1747	50.0580	49.9390	48.4656
17	56.2785	56.1566	56.0104	56.0701	55.9385	55.8045	53.9025
18	62.6888	62.5525	62.3891	62.4798	62.3328	62.1830	59.8166
19	69.6538	69.5002	69.3211	69.4441	69.2809	69.1146	66.2458
20	77.2161	77.0457	76.8490	77.0058	76.8257	76.6422	73.2305
21	85.4211	85.2330	85.0181	85.2102	85.0124	84.8110	80.8133
22	94.3169	94.1104	93.8764	94.1054	93.8891	93.6689	89.0396
23	103.9545	103.7287	103.4747	103.7422	103.5067	103.2669	97.9577
24	114.3876	114.1418	113.8670	114.1747	113.9191	113.6588	107.6182
25	125.6735	125.4067	125.1102	125.4599	125.1833	124.9013	118.0756
26	137.8726	137.5838	137.2647	137.6581	137.3597	137.0558	129.3866
27	151.0486	150.7370	150.3943	150.8334	150.5121	150.1850	141.6117
28	165.2690	164.9336	164.5663	165.0530	164.7079	164.3566	154.8149
29	180.6052	180.2449	179.8520	180.3884	180.0184	179.6419	169.0636
30	197.1323	196.7462	196.3265	196.9147	196.5188	196.1160	184.4291
40	447.7003	446.9875	446.2316	447.4731	446.7504	446.0162	418.2975
50	937.8813	936.6824	935.4279	937.6415	936.4326	935.2062	878.4090

3.2. Multipartite graphs with maximal EE_r

In this subsection we characterize the unique graph having the maximal resolvent Estrada index among all multipartite graphs with given number of vertices.

Denote by $K_{n_1,n_2,\ldots,n_r}$ the complete r-partite graph of order n whose vertex set consists of r parts $V_1, V_2, \ldots, V_r$ with $|V_i| = n_i$, $i \in \{1, 2, \ldots, r\}$, where $2 \le r < n$ and $n_1 + n_2 + \cdots + n_r = n$. We assume, without loss of generality, that $1 \le n_1 \le n_2 \le \cdots \le n_r$. In particular, if $n_i - n_j \le 1$ for $1 \le j < i \le r$, then it is known as the Turán graph $T_r(n)$.

Theorem 8 *For any complete r-partite graph $K_{n_1,n_2,\ldots,n_r}$ of order n,*

$$EE_r(K_{n_1,n_2,\ldots,n_r}) = n - r + \frac{\sum_{k=1}^{r} \frac{(n-1)n_k}{(n-1+n_k)^2}}{1 - \sum_{k=1}^{r} \frac{n_k}{n-1+n_k}} + \sum_{k=1}^{r} \frac{n-1}{n-1+n_k}, \tag{7}$$

and

$$EE_r(K_{1,\ldots,1,n-r+1}) \le EE_r(K_{n_1,n_2,\ldots,n_r}) \le EE_r(T_r(n)),$$

with the left equality if and only if $K_{n_1,n_2,\ldots,n_r} \cong K_{1,\ldots,1,n-r+1}$ and the right if and only if $K_{n_1,n_2,\ldots,n_r} \cong T_r(n)$.

Proof. It is known [4] that

$$\phi(K_{n_1,n_2,\ldots,n_r}, \lambda) = \lambda^{n-r} \left(1 - \sum_{k=1}^{r} \frac{n_k}{\lambda + n_k}\right) \prod_{k=1}^{r} (\lambda + n_k).$$

By Theorem 3 and a direct calculation, (7) follows immediately.

For the second part, we claim that if $n_i - n_j \ge 2$ for $1 \le j < i \le r$, then

$$EE_r(K_{n_1,\ldots,n_j,\ldots,n_i,\ldots,n_r}) < EE_r(K_{n_1,\ldots,n_j+1,\ldots,n_i-1,\ldots,n_r}). \tag{8}$$

Set $f_1(n_i, n_j) = \frac{n_i}{(n-1+n_i)^2} + \frac{n_j}{(n-1+n_j)^2}$, $\overline{f}_1(n_i, n_j) = \sum_{k \ne i,j} \frac{n_k}{(n-1+n_k)^2}$,

$f_2(n_i, n_j) = \frac{n_i}{n-1+n_i} + \frac{n_j}{n-1+n_j}$, $\overline{f}_2(n_i, n_j) = \sum_{k \ne i,j} \frac{n_k}{n-1+n_k}$, and

$f_3(n_i, n_j) = \frac{1}{n-1+n_i} + \frac{1}{n-1+n_j}$.

Noting that $n_i - n_j \ge 2$, we have

$$f_2(n_i - 1, n_j + 1) > f_2(n_i, n_j).$$

Moreover, since $\lambda_1(K_{n_1,n_2,\ldots,n_r}) < \lambda_1(K_n) = n-1$, then $\phi(K_{n_1,n_2,\ldots,n_r}, n-1) > 0$, and hence,

$$0 < 1 - f_2(n_i,n_j) - \overline{f}_2(n_i,n_j) = 1 - \sum_{k=1}^{r} \frac{n_k}{n-1+n_k} < 1.$$

Thus, it follows from (7) that

$$\left(EE_r(K_{n_1,\ldots,n_j+1,\ldots,n_i-1,\ldots,n_r}) - EE_r(K_{n_1,\ldots,n_j,\ldots,n_i,\ldots,n_r})\right)/(n-1)$$

$$= \tfrac{f_1(n_i-1,n_j+1)+\overline{f}_1(n_i,n_j)}{1-f_2(n_i-1,n_j+1)-\overline{f}_2(n_i,n_j)} - \tfrac{f_1(n_i,n_j)+\overline{f}_1(n_i,n_j)}{1-f_2(n_i,n_j)-\overline{f}_2(n_i,n_j)} + f_3(n_i-1,n_j+1) - f_3(n_i,n_j)$$

$$> \tfrac{f_1(n_i-1,n_j+1)+\overline{f}_1(n_i,n_j)}{1-f_2(n_i,n_j)-\overline{f}_2(n_i,n_j)} - \tfrac{f_1(n_i,n_j)+\overline{f}_1(n_i,n_j)}{1-f_2(n_i,n_j)-\overline{f}_2(n_i,n_j)} + f_3(n_i-1,n_j+1) - f_3(n_i,n_j)$$

$$> f_1(n_i-1,n_j+1) - f_1(n_i,n_j) + f_3(n_i-1,n_j+1) - f_3(n_i,n_j)$$

$$= \tfrac{(n_i-n_j-1)g(n-1)}{(n-2+n_i)^2(n+n_j)^2(n-1+n_i)^2(n-1+n_j)^2},$$

where $g(x) = 2x^5 + 2(n_i+n_j)x^4 - 2(2n_in_j + n_i - n_j - 1)x^3$

$$-4(n_i+n_j)(2n_in_j + n_i - n_j - 1)x^2$$

$$-[(n_i-n_j)^3 + 2n_in_j(5n_in_j + 5n_i - 5n_j - 4) + (2n_in_j - 1)(n_i^2 + n_j^2)]x$$

$$-2n_in_j(n_i+n_j)(n_i-1)(n_j+1).$$

In order to prove Inequality (8), it suffices to prove $g(n-1) > 0$. We first show that $g(x)$ is strictly increasing when $x \geq n_i + n_j$. To this end, we consider the fourth derivative of $g(x)$:

$$g^{(4)}(x) = 240x + 48(n_i+n_j) > 0, \quad x \geq n_i + n_j,$$

which implies that $g^{(3)}(x)$ is strictly increasing when $x \geq n_i + n_j$. Therefore,

$$g^{(3)}(x) \geq g^{(3)}(n_i+n_j) = 12(14n_i^2 + 14n_j^2 + 26n_in_j - n_i + n_j + 1) > 0, \quad x \geq n_i + n_j,$$

again implying $g''(x)$ is strictly increasing when $x \geq n_i + n_j$. Repeating this procedure one can finally get that $g(x)$ is strictly increasing when $x \geq n_i + n_j$. As a result, noting that $n-1 \geq n_i + n_j$ and $n_i - n_j \geq 2$, we have

$$g(n-1) \geq g(n_i+n_j) = (n_i+n_j)\big[(n_i-n_j)^3(4(n_i-n_j)-7)$$
$$+18n_in_j(n_i-n_j)(n_i-n_j-2) + 7n_i^2 + 7n_j^2 + 22n_in_j\big] > 0.$$

Thus, our claim follows and from which, Theorem 8 follows immediately. □

By Proposition 2, we know that if a multipartite graph G has the maximal resolvent Estrada index, then G must be a complete multipartite graph. This together with

Theorem 8 yields the following result directly.

Theorem 9 *Among all r-partite graphs with n vertices $(2 \leq r < n)$, the Turán graph $T_r(n)$ is the unique graph having the maximal resolvent Estrada index.*

The chromatic number $\chi(G)$ of a graph G is the minimum number of colors used to assign a color to each of its vertices such that any two adjacent vertices have different colors. This implies that the vertex set $V(G)$ of G can be partitioned into $\chi(G)$ vertex subsets each of which has the same color and therefore, is an independent set, that is, G is a $\chi(G)$-partite graph. Thus, by Theorem 9, we have the following immediate corollary.

Corollary 10 *Among all n-vertex graphs with chromatic number χ $(2 \leq \chi < n)$, the Turán graph $T_\chi(n)$ is the unique graph possessing the maximal resolvent Estrada index.*

Remark. We would like to point out that among all n-vertex graphs with chromatic number χ $(2 \leq \chi < n)$, the extremal graphs possessing the maximal Estrada index have not been determined yet.

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