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Resolvent Estrada Index – Computational and Mathematical Studies

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Abstract

The resolvent Estrada index of a (non-complete) graph G of order n is defined as $EE_r = \sum_{i=1}^{n} \left(1 - \frac{\lambda_i}{n-1}\right)^{-1}$, where $\lambda_1, \lambda_2, \ldots, \lambda_n$ are the eigenvalues of G. Combining computational and mathematical approaches, we establish a number of properties of EE_r. In particular, any tree has smaller EE_r-value than any unicyclic graph of the same order, and any unicyclic graph has smaller EE_r-value than any tricyclic graph of the same order. The trees, unicyclic, bicyclic, and tricyclic graphs with smallest and greatest EE_r are determined.

1 Introduction

In this paper we are concerned with simple graphs, that is graphs without directed, multiple, or weighted edges, and without self–loops. Let G be such a graph, possessing n vertices and m edges.

Let $\lambda_1, \lambda_2, \ldots, \lambda_n$ be the eigenvalues of G, that is the eigenvalues of the adjacency matrix of G. These eigenvalues form the spectrum of G [4, 5].

The k-th spectral moment of the graph G is defined as

$$M_k = M_k(G) = \sum_{i=1}^{n} (\lambda_i)^k \ . \tag{1}$$

As well known [4,5], $M_0 = n$, $M_1 = 0$, $M_2 = 2m$, and M_k is equal to the number of closed walks in G of length k.

Around year 2000, in order to model certain geometric characteristics of biologically important molecules, Ernesto Estrada [6] introduced the quantity

$$EE = EE(G) = \sum_{k=0}^{\infty} \frac{M_k(G)}{k!} \tag{2}$$

which eventually was named *Estrada index*. This graph–spectrum–based invariant found noteworthy applications, both in biochemistry [6–8] and in the theory of complex networks [9, 10, 12]. Its mathematical properties are nowadays well understood, see [14] and the references cited therein. Here we only mention the formula

$$EE = \sum_{i=1}^{n} e^{\lambda_i} \tag{3}$$

which immediately follows from Eqs. (1) and (2).

Recently, Estrada and Higham [11] considered a new variant of the index EE, defined as

$$EE_r = EE_r(G) = \sum_{k=0}^{\infty} \frac{M_k(G)}{(n-1)^k} \tag{4}$$

which should be compared with Eq. (2). In the few hitherto published papers on EE_r [1–3, 13] it is called *resolvent Estrada index*.

An equivalent way of expressing the resolvent Estrada index is

$$EE_r = \sum_{i=1}^{n} \frac{1}{1 - \frac{\lambda_i}{n-1}} = (n-1) \sum_{i=1}^{n} \frac{1}{n-1-\lambda_i} \tag{5}$$

which should be compared with Eq. (3).

The spectrum of the complete graph K_n consists of the numbers $n-1$ and -1 (with multiplicity $n-1$). All eigenvalues of all other n-vertex graphs are less than $n-1$ [4, 5]. Bearing this in mind, from Eq. (5) is seen that the definition (4) of the resolvent Estrada index can be applied to all simple graphs, except to the complete graphs.

In what follows we state a few previously established results on the resolvent Estrada index, which we will need in the present considerations.

Lemma 1. [3] *Let $G - e$ be the graph obtained by deleting the edge from the graph G. Then*

$$EE_r(G - e) < EE_r(G)\,.$$

From Lemma 1 it immediately follows that among graphs of fixed order n, the edgeless graph $\overline{K}_n$ has minimal, whereas the graph $K_n - e$ has maximal resolvent Estrada index. (Recall that the resolvent Estrada index of the complete graph K_n is not defined.) From Lemma 1 it also follows that among connected graphs of fixed order n, the graph with minimal EE_r-value is a tree.

Let, as usual, P_n and S_n denote the path and star on n vertices. Denote by P_n^* the tree obtained by attaching a pendent vertex to the second vertex of the path P_{n-1}. Denote by S_n^* the tree obtained by attaching a pendent vertex to a pendent vertex of the star S_{n-1}.

Lemma 2. [13] *Among trees of order n, the path P_n has smallest and the tree P_n^* second–smallest resolvent Estrada index. Among trees of order n, the star S_n has greatest and the tree S_n^* second–greatest resolvent Estrada index.*

Lemma 3. [2] *Let G be a graph with n vertices and m edges. Then*

$$EE_r(G) \geq \frac{n^2\,(n-1)^2}{n(n-1)^2 - 2m}\,.$$

Equality is attained if and only if either $G \cong \overline{K}_n$ or (provided n is even) $G \cong \frac{n}{2}\,K_2$.

Lemma 4. [2] *Let G be a bipartite graph with n vertices ($n \geq 3$) and m edges. Then*

$$EE_r(G) \leq n + \frac{2m}{(n-1)^2 - m}\,. \tag{6}$$

Equality is attained if and only if either $G \cong \overline{K}_n$ or $G \cong K_{a,b} \cup \overline{K}_{n-a-b}$, where $K_{a,b}$ is a complete bipartite graph such that $ab = m$.

2 Computational studies

In order to gain a better insight into the properties of the resolvent Estrada index, we have undertaken extensive computer–aided studies. The EE_r-values of all trees and connected unicyclic, bicyclic, and tricyclic graphs up to 15 vertices were computed, and the structure of the extremal members of these classes was established. Thus our examination embraced over ten million graphs. The main conclusions gained within these studies are the following.

First of all, the earlier known results stated as Lemma 2 were confirmed.

Observation 5. We refer to the graphs whose structure is depicted in Fig. 1. Among connected unicyclic graphs of order n, $n \geq 4$, the cycle C_n has smallest and the graph C_n^* second–smallest resolvent Estrada index. Among these graphs of order n, $n \geq 5$, the graphs X_n and X_n^* have, respectively, greatest and second–greatest resolvent Estrada index.

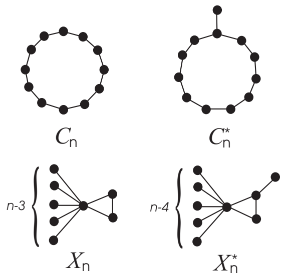

Fig. 1. Unicyclic graphs with extremal resolvent Estrada indices; for details see Observation 5.

Observation 6. We refer to the graphs whose structure is depicted in Fig. 2. Among connected bicyclic graphs of order n, those with the smallest resolvent Estrada indices are:

$$\begin{array}{lll} B_{p-1,p-1,p} & \text{if} & n = 3p\,,\ p \geq 2 \\ B_{p-1,p,p} & \text{if} & n = 3p+1\,,\ p \geq 1 \\ B_{p,p,p} & \text{if} & n = 3p+2\,,\ p \geq 1\,. \end{array} \tag{7}$$

The graphs with second–smallest resolvent Estrada index are

$$\begin{array}{lll} B_{p-2,p,p} & \text{if} & n = 3p\,,\ p \geq 2 \\ B_{p-1,p-1,p+1} & \text{if} & n = 3p+1\,,\ p \geq 2 \\ B_{p-1,p,p+1} & \text{if} & n = 3p+2\,,\ p \geq 1\,. \end{array}$$

Among these graphs of order n, $n \geq 5$, the graph Y_n has greatest resolvent Estrada index. For $n \geq 9$, the graph Y_n^* has second–greatest resolvent Estrada index, whereas Y_5^*, Y_6^*, Y_7^*, and Y_8^* are exceptions.

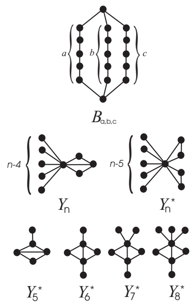

Fig. 2. Bicyclic graphs with extremal resolvent Estrada indices; for details see Observation 6.

Observation 7. We refer to the graphs whose structure is depicted in Fig. 3. Among connected tricyclic graphs of order n , $n \geq 5$, the graph Z_n has greatest resolvent Estrada index. For $n \geq 6$, the graph Z_n^* has second–greatest resolvent Estrada index, whereas Z_5^* is an exception.

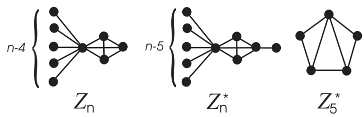

Fig. 3. Tricyclic graphs with greatest resolvent Estrada indices; for details see Observation 7.

Observation 8. The structural regularity obeyed by the connected tricyclic graphs with smallest EE_r is not easy to envisage. These graphs of order n , $5 \leq n \leq 15$, are depicted in Fig. 4.

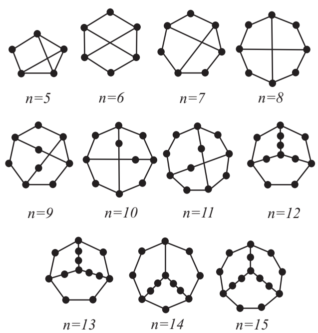

Fig. 4. Tricyclic graphs of order n , $5 \leq n \leq 15$, with smallest resolvent Estrada indices.

Observation 9. The inequality $EE_r(S_n) < EE_r(C_n)$ holds for all $n \geq 4$. Consequently, any tree has smaller EE_r-value than any unicyclic graph of the same order.

For $B_{a,b,c}$ specified by Eq. (7), the inequality $EE_r(X_n) < EE_r(B_{a,b,c})$ holds only until $n = 6$ and is violated for all $n \geq 7$. Consequently, it is not true that any unicyclic graph has smaller EE_r-value than any bicyclic graph of the same order. The same applies also to the relation between EE_r of bicyclic and tricyclic graphs. On the other hand, any unicyclic graph has smaller EE_r-value than any connected tricyclic graph of the same order.

Observation 10. Evidently, cospectral graphs have equal EE_r-values. Until now, we did not detect pairs of (connected) non-cospectral graphs with equal EE_r-values. However, there exist non-cospectral graphs whose EE_r-values are different, but remarkably close. For instance, $EE_r(B_{3,4,4}) = 13.199203763$ whereas $EE_r(B_{3,3,5}) = 13.199203796$, and $EE_r(B_{4,4,5}) = 15.16613306697$ whereas $EE_r(B_{3,5,5}) = 15.16613306703$. These findings resemble the existence of the earlier discovered almost–equienergetic graphs [15–17].

3 Mathematical studies

We first provide a partial proof of Observation 9.

Let G_1 be a bipartite graph with $n \geq 3$ vertices and m edges. Let G_2 be a non-complete graphs with n vertices and $m + k$ edges, $k \geq 1$. Then in view of Lemmas 3 and 4, a sufficient (but not necessary) condition for the inequality $EE_r(G_1) < EE_r(G_2)$ is

$$n + \frac{2m}{(n-1)^2 - m} < \frac{n^2\,(n-1)^2}{n(n-1)^2 - 2(m+k)} \,. \tag{8}$$

Because $(n-1)^2 - m > 0$ holds for all $n \geq 3$, and because for non-complete graphs with n vertices and $m + k$ edges, $n(n-1)^2 - 2(m+k) > 0$, inequality (8) is transformed into

$$(n-2)m^2 < \big[n(n-1)^2 - (n-2)m\big]k \,. \tag{9}$$

Bearing in mind that $m \leq n(n-1)/2$, it is easy to verify that $n(n-1)^2 - (n-2)m > 0$, and thus relation (9) yields

$$k > \frac{(n-2)m^2}{n(n-1)^2 - (n-2)m} \tag{10}$$

which will be the starting point for our analysis.

It is obvious that if some integer $k = k_0$ satisfies the condition (10), then also any integer greater than k_0 satisfies this condition. Therefore, we will be interested in the smallest (integer) value of k, for which inequality (10) holds.

What next should be observed is that for any graph-theoretically meaningful values of the parameter n, the expression

$$\frac{(n-2)m^2}{n(n-1)^2-(n-2)m} \tag{11}$$

is monotonically increasing in the variable m.

Consider now two special cases.

Case 1: $m = n-1$. A connected graph with $n-1$ edges is a tree and is thus necessarily bipartite. Then

$$\frac{(n-2)m^2}{n(n-1)^2-(n-2)m} = \frac{n^2-3n+2}{n^2-2n+2}$$

which evidently is less than 1. Therefore, in this case, $k = 1$ satisfies inequality (10).

As a direct consequence, we obtain:

Theorem 11. *The resolvent Estrada index of any tree is smaller than the resolvent Estrada index of any connected unicyclic graph of the same order.*

Theorem 12. *The resolvent Estrada index of any tree is smaller than the resolvent Estrada index of any connected graph of the same order, with cyclomatic number k , $k > 1$.*

Case 2: $m = n$. Then

$$\frac{(n-2)m^2}{n(n-1)^2-(n-2)m} = \frac{n^2-2n}{n^2-3n+2} \ .$$

It is easy to verify that for $n \geq 3$,

$$1 < \frac{n^2-2n}{n^2-3n+2} < 2 \ .$$

Therefore, in this case, $k = 1$ does not satisfy inequality (10), but $k = 2$ does. From this result we obtain:

Theorem 13. *The resolvent Estrada index of any connected bipartite n-vertex unicyclic graph is smaller than the resolvent Estrada index of any connected tricyclic graph.*

Theorem 14. *The resolvent Estrada index of any connected bipartite n-vertex unicyclic graph is smaller than the resolvent Estrada index of any connected graph of the same order, with cyclomatic number k , $k > 3$.*

Note that Theorems 11–14 fully agree with what above was stated as Observation 9, but are somewhat weaker than what we established in our computational studies.

The upper bound (6), earlier obtained in [2], is restricted to bipartite graphs. We now show how it can be modified so as to hold for all graphs.

Theorem 15. *Let G be a non-complete graph with n vertices ($n > 3$) and m edges. Then*

$$EE_r(G) \leq n + \frac{4m}{(n-1)^2 - 2m} \,. \tag{12}$$

Proof. Start with Eq. (4) which can be rewritten as

$$\begin{aligned} EE_r(G) &= \sum_{k\geq 0} \frac{M_{2k}}{(n-1)^{2k}} + \sum_{k\geq 0} \frac{M_{2k+1}}{(n-1)^{2k+1}} \\ &= n + \sum_{k\geq 1} \frac{M_{2k}}{(n-1)^{2k}} + \sum_{k\geq 1} \frac{M_{2k+1}}{(n-1)^{2k+1}} \end{aligned}$$

in view of $M_0 = n$ and $M_1 = 0$. Taking into account Eq. (1), we arrive at

$$\begin{aligned} EE_r(G) &= n + \sum_{k\geq 1} \frac{\sum_{i=1}^{n} \lambda_i^{2k}}{(n-1)^{2k}} + \sum_{k\geq 1} \frac{\sum_{i=1}^{n} \lambda_i^{2k+1}}{(n-1)^{2k+1}} \\ &\leq n + \sum_{k\geq 1} \frac{\sum_{i=1}^{n} \lambda_i^{2k}}{(n-1)^{2k}} + \sum_{k\geq 1} \frac{\sum_{i=1}^{n} |\lambda_i|^{2k+1}}{(n-1)^{2k+1}} \\ &\leq n + \sum_{k\geq 1} \frac{\sum_{i=1}^{n} \lambda_i^{2k}}{(n-1)^{2k}} + \sum_{k\geq 1} \frac{\sum_{i=1}^{n} |\lambda_i|^{2k}}{(n-1)^{2k}} \end{aligned}$$

where we have used the fact that all eigenvalues of all non-complete graphs are less than $n-1$, and therefore $|\lambda_i|^{2k+1} < (n-1)\,|\lambda_i|^{2k} = (n-1)\,\lambda_i^{2k}$. Thus,

$$EE_r(G) \leq n + 2 \sum_{k\geq 1} \frac{\sum_{i=1}^{n} \lambda_i^{2k}}{(n-1)^{2k}} \,.$$

Using the well known analytical inequality $\sum_i a_i^p \leq \big(\sum_i a_i\big)^p$, we get

$$EE_r(G) \leq n + 2 \sum_{k\geq 1} \left[\frac{\sum_{i=1}^{n} \lambda_i^2}{(n-1)^2} \right]^k = n + 2 \sum_{k\geq 1} \left[\frac{2m}{(n-1)^2} \right]^k$$

which now straightforwardly leads to inequality (12).

It is easy to see that equality in (12) holds if and only if $\lambda_i = 0$ for all $i = 1, 2, \ldots, n$, i.e., if and only if G is the edgeless graph $\overline{K}_n$. ■

4 Summary and Conclusion

In this paper, we established a number of properties of the resolvent Estrada index EE_r . A few of these were proven by mathematical arguments and stated as Theorems 11–15. Most of our results, stated here as Observations 5–10, should be considered as conjectures, awaiting to be verified or (what we deem to be less likely) refuted. We believe that these will invite other colleagues to undertake additional research of this newly conceived graph–spectrum–based structure descriptor.

Another topic that calls for investigation are the relations between the two Estrada indices EE (Eqs. (2), (3)) and EE_R (Eqs. (4), (5)). Such relations certainly exist, and earlier works [3, 11] have revealed a great deal of parallelism between EE and EE_r . In order that EE_r gets applications independent of EE (especially in network science), of paramount importance would be to have cases in which its structure–dependence is significantly different from that of EE. In our future studies, we intend to pay particular attention on discovering and characterizing such properties of the resolvent Estrada index.

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