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Resolvent Estrada Index of Cycles and Paths

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Abstract: Let G be a simple graph of order n. The resolvent Estrada index of G 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. Formulas for computing EE_r of the cycle C_n and the path P_n are derived. The precision of these approximations are shown to be excellent. We also examine the difference and relations between the Estrada index and the resolvent Estrada index of C_n and P_n.

Keywords: Resolvent Estrada index, Estrada index, spectrum (of graph), cycle, path.

1 Introduction

Let G be a simple graph of order n with vertex set $\{v_1, v_2, \ldots, v_n\}$. The adjacency matrix of G, is the square matrix $\mathbf{A} = (a_{ij})$ of order n, in which $a_{ij} = 1$ if the vertices v_i and v_j are adjacent, and $a_{ij} = 0$ otherwise. The characteristic polynomial $\phi(G, \lambda)$ of the graph G is the polynomial of degree n, defined as $\det(\lambda\, \mathbf{I}_n - \mathbf{A})$, where $\mathbf{I}_n$ is the unit matrix of order n. Since $\mathbf{A}$ is real and symmetric, all its eigenvalues $\lambda_1, \lambda_2, \ldots, \lambda_n$ are real. These form the spectrum of the graph G.

For an integer $k \geq 0$, the k-th spectral moment of G is defined as

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

In this paper, we are concerned with two simple and frequently encountered graphs – the cycle C_n and the path P_n . Recall that C_n is the connected graph of order n in which all vertices have degree 2. The path P_n is the tree (= connected acyclic graph) of order n in

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which exactly two vertices have degree 1 (whereas all other vertices have degree 2). The spectra of C_n and P_n are well known [4] (see below).

In 2000, Ernesto Estrada introduced a structural invariant based on the spectral moments, defined as [6]

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

which eventually was named "*Estrada index*" [14]. Applications of the Estrada index range from the description of folding of protein molecules [6, 7] to measuring the centrality of complex (communication, social, metabolic, etc.) networks [9, 8]. This graph–spectrum–based invariant was also subject of extensive mathematical studies, for review see [10].

Recently, Estrada and Higham [8] modified the quantity occurring on the right–hand side of Eq. (1), and considered the spectrum–based invariant

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

Bearing in mind that $|\lambda_i| < n-1$ holds for for all eigenvalues of all graphs of order n, except in the case of the n-vertex complete graph [4], the right–hand side summation in Eq. (2) is convergent. Thus, EE_r is well defined for all graphs, except for the complete graphs. It is easy to verify that

$$EE_r = \sum_{i=1}^{n} \frac{n-1}{n-1-\lambda_i} = \sum_{i=1}^{n} \left(1 - \frac{\lambda_i}{n-1}\right)^{-1} . \tag{3}$$

The expression on the right–hand side of Eq. (3) indicates that EE_r is a resolvent–operator–based quantity [1], in view of which EE_r has been named *resolvent Estrada index*.

Although EE_r has many properties analogous to those of EE, the two indices are distinct in essence [8, 3]. In what follows, we will show additional evidence to support this view.

At the present moment, there are only a few mathematical and computational studies of the resolvent Estrada index [3, 2, 11, 12]. Some of the basic properties of EE_r have been established, but numerous open problems (many stated in form of conjectures [12]) await to be solved in the future. The present work is aimed at contributing towards partially filling this gap.

Cycles and paths play an important role in researching the resolvent Estrada index. In particular, we have:

Theorem 1 [11] *Among all connected graphs of order n $(n \geq 1)$, the path P_n has minimal resolvent Estrada index.*

In order to find the graph with second–minimal EE_r-value, the tree $P_{n-1}(j)$ had to be considered [5, 11], where $P_(n-1)(j)$ is obtained by attaching a pendent vertex at position j of the path P_{n-1} . Then it follows:

Theorem 2 [11] *Among all connected graphs of order n* $(n \geq 4)$*, the tree* $P_{n-1}(2)$ *has the second–minimal resolvent Estrada index.*

For a complete proof of Theorem 2, it was necessary to show that [11]

$$EE_r(P_{n-1}(2)) < EE_r(C_n)\,.$$

The latter inequality holds because C_n possesses many more self-returning walks than $P_{n-1}(2)$ and some of the odd spectral moments of C_n are greater than zero if n is odd. Similarly, when $j \geq 3$, the condition $EE_r(P_{n-1}(j)) < EE_r(C_n)$ is necessary for establishing the j-th minimal resolvent Estrada index among all connected graphs of order n [11].

In [12], based on extensive computer work, it has been shown that the cycle C_n has smallest EE_r-value among all connected unicyclic graphs of order n $(n \geq 3)$.

Motivated by the above results, we now offer a simple method for computing the resolvent Estrada indices of P_n and C_n. Before presenting it, we outline the analogous formulas for the ordinary Estrada index.

2 Estrada indices of cycles and paths

Graovac and one of the present authors [13] showed that the Estrada indices of the cycles and paths can be approximated as

$$EE(C_n) \approx n\,I_0 \tag{4}$$

and

$$EE(P_n) \approx (n+1)I_0 - \cosh(2) \tag{5}$$

where $I_0 = \sum\limits_{k \geq 0} 1/(k!)^2 = 2.27958530\ldots$. Hence, in the case of cycles and paths, EE can be calculated easily.

In Fig. 1 are presented the $EE(C_n)$- and $EE(P_n)$-values for $1 \leq n < 16$. As it can be seen, except for the first few values of n, the plots of $EE(C_n)$ and $EE(P_n)$ are practically parallel, and $EE(C_n)$ is always greater than $EE(P_n)$. This is in full agreement with Eqs. (4) and (5).

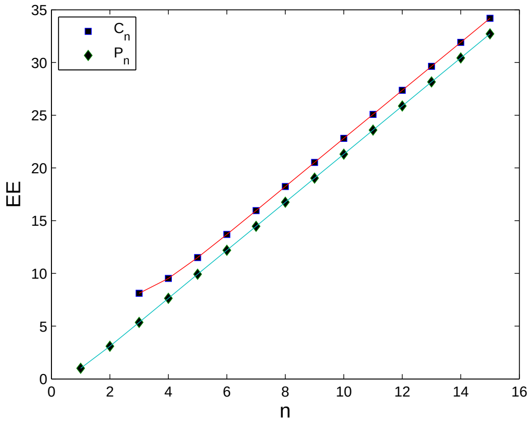

Fig. 1. $EE(C_n)$ (upper) and $EE(P_n)$ (lower), plotted versus n.

3 Resolvent Estrada index of cycles

It is well known [4] that the spectrum of the cycle C_n consists of the numbers $2\cos(2i\pi/n)$, $i = 1,2,\ldots,n$. In view of this,

$$
\begin{aligned}
EE_r(C_n) &= \sum_{i=1}^{n}\left(1-\frac{2\cos\frac{2i\pi}{n}}{n-1}\right)^{-1} \\
&= \sum_{i=1}^{n}\left[1+\frac{2\cos\frac{2i\pi}{n}}{n-1}+\left(\frac{2\cos\frac{2i\pi}{n}}{n-1}\right)^{2}+\left(\frac{2\cos\frac{2i\pi}{n}}{n-1}\right)^{3}\right. \\
&+ \left.\left(\frac{2\cos\frac{2i\pi}{n}}{n-1}\right)^{4}+\left(\frac{2\cos\frac{2i\pi}{n}}{n-1}\right)^{5}+\left(\frac{2\cos\frac{2i\pi}{n}}{n-1}\right)^{6}+\cdots\right]
\end{aligned}
$$

One can see that the angles $2i\pi/n$ uniformly cover the interval $[0,2\pi]$ when $i = 1,2,\ldots,n$.

Thus, the following integral approximation is applicable:

$$\begin{aligned}
EE_r(C_n) &= n + \sum_{i=1}^{n} \frac{2\cos\frac{2i\pi}{n}}{n-1} + \sum_{i=1}^{n}\left(\frac{2\cos\frac{2i\pi}{n}}{n-1}\right)^2 + \sum_{i=1}^{n}\left(\frac{2\cos\frac{2i\pi}{n}}{n-1}\right)^3 \\
&+ \sum_{i=1}^{n}\left(\frac{2\cos\frac{2i\pi}{n}}{n-1}\right)^4 + \sum_{i=1}^{n}\left(\frac{2\cos\frac{2i\pi}{n}}{n-1}\right)^5 + \sum_{i=1}^{n}\left(\frac{2\cos\frac{2i\pi}{n}}{n-1}\right)^6 + \cdots \\
&\approx n + \frac{n}{2\pi(n-1)}\int_0^{2\pi} 2\cos x\, dx + \frac{n}{2\pi(n-1)^2}\int_0^{2\pi}(2\cos x)^2\, dx \\
&+ \frac{n}{2\pi(n-1)^3}\int_0^{2\pi}(2\cos x)^3\, dx + \frac{n}{2\pi(n-1)^4}\int_0^{2\pi}(2\cos x)^4\, dx \\
&+ \frac{n}{2\pi(n-1)^5}\int_0^{2\pi}(2\cos x)^5\, dx + \frac{n}{2\pi(n-1)^6}\int_0^{2\pi}(2\cos x)^6\, dx\,.
\end{aligned}$$

By direct computation, we obtain

$$EE_r(C_n) \approx n + \frac{2n}{(n-1)^2} + \frac{6n}{(n-1)^4} + \frac{20n}{(n-1)^6}\,. \tag{6}$$

The precision of the approximate expression (6) can be seen from the data in Table 1. Except for the first few values of n, the resolvent Estrada indices of cycles are excellently reproduced by Eq. (6). Thus, its accuracy is on two, four, and six decimal places for, respectively, $n \geq 5$, $n \geq 7$, and $n \geq 11$. This is more than sufficient for any standard application of $EE_r(C_n)$.

4 Resolvent Estrada index of paths

In a similar way as in the case of C_n, yet somewhat more complicated, we get an approximate expression for $EE_r(P_n)$. The spectrum of P_n consists of the numbers $2\cos[i\pi/(n+$

n	$EE_r(C_n)$	$EE_r(C_n)_{approx}$	$EE_r(P_n)$	$EE_r(P_n)_{approx}$
3			5.0000025	4.7500000
4	5.6000000	5.2949246	4.9090909	4.8888889
5	5.7894737	5.7666016	5.5948719	5.5917969
6	6.5476190	6.5452800	6.4471502	6.4464640
7	7.4246863	7.4242970	7.3602814	7.3600823
8	8.3479907	8.3478823	8.3025966	8.3025270
9	9.2951602	9.2951202	9.2612890	9.2612610
10	10.2564519	10.2564349	10.2301490	10.2301366
11	11.2268280	11.2268200	11.2057821	11.2057760
12	12.2034043	12.2034003	12.1861666	12.1861635
13	13.1844062	13.1844042	13.1700201	13.1700183
14	14.1686808	14.1686780	14.1564870	14.1564860
15	15.1554446	15.1554438	15.1449742	15.1449736
16	16.1441471	16.1441466	16.1350567	16.1350563
17	17.1343895	17.1343892	17.1264217	17.1264215
18	18.1258756	18.1258755	18.1188337	18.1188335
19	19.1183810	19.1183811	19.1121118	19.1121117
20	20.1117327	20.1117326	20.1061149	20.1061148
21	21.1057942	21.1057941	21.1007309	21.1007309
22	22.1004571	22.1004571	22.0958701	22.0958700
23	23.0956344	23.0956345	23.0914592	23.0914592
24	24.0912551	24.0912551	24.0874383	24.0874383
25	25.0872602	25.0872603	25.0837577	25.0837577
26	26.0836015	26.0836015	26.0803757	26.0803757
27	27.0802379	27.0802379	27.0772573	27.0772573
28	28.0771351	28.0771351	28.0743727	28.0743727
29	29.0742640	29.0742639	29.0716965	29.0716965
30	30.0715991	30.0715991	30.0692068	30.0692068

Table 1. Exact and approximate values of resolvent Estrada indices of C_n and P_n.

$1)]$, $i = 1,2,\ldots,n$ [4]. In view of this,

$$\begin{aligned} EE_r(P_n) &= \sum_{i=1}^{n} \left(1 - \frac{2\cos\frac{i\pi}{n+1}}{n-1}\right)^{-1} \\ &= \sum_{i=1}^{n} \left[1 + \left(\frac{2\cos\frac{i\pi}{n+1}}{n-1}\right) + \left(\frac{2\cos\frac{i\pi}{n+1}}{n-1}\right)^2 + \left(\frac{2\cos\frac{i\pi}{n+1}}{n-1}\right)^3 \right. \\ &+ \left. \left(\frac{2\cos\frac{i\pi}{n+1}}{n-1}\right)^4 + \left(\frac{2\cos\frac{i\pi}{n+1}}{n-1}\right)^5 + \left(\frac{2\cos\frac{i\pi}{n+1}}{n-1}\right)^6 + \cdots \right]. \end{aligned}$$

Since the angles $i\pi/(n+1)$ do not cover the entire interval $[0,\pi]$, the missing near–zero and near-π contributions need to be compensated when applying an integral approximation. Bearing this in mind, we can proceed as follows. Let $m > 0$ be an integer. Then,

$$\begin{aligned}
\sum_{i=1}^{n}\left(\frac{2\cos\frac{i\pi}{n+1}}{n-1}\right)^m &= \frac{1}{2}\sum_{i=0}^{n}\left(\frac{2\cos\frac{i\pi}{n+1}}{n-1}\right)^m + \frac{1}{2}\sum_{i=1}^{n+1}\left(\frac{2\cos\frac{i\pi}{n+1}}{n-1}\right)^m \\
&- \frac{1}{2}\left[\left(\frac{2}{n-1}\right)^m + \left(\frac{-2}{n-1}\right)^m\right] \\
&\approx \frac{n+1}{2\pi(n-1)^m}\int_0^\pi (2\cos x)^m\,dx + \frac{n+1}{2\pi(n-1)^m}\int_0^\pi (2\cos x)^m\,dx \\
&- \frac{1}{2}\left[\left(\frac{2}{n-1}\right)^m + \left(\frac{-2}{n-1}\right)^m\right] \\
&= \frac{n+1}{\pi(n-1)^m}\int_0^\pi (2\cos x)^m\,dx - \frac{1}{2}\left[\left(\frac{2}{n-1}\right)^m + \left(\frac{-2}{n-1}\right)^m\right].
\end{aligned}$$

Note that $\sum_{i=1}^{n}\left(\frac{2\cos\frac{i\pi}{n+1}}{n-1}\right)^m$ is approximately equal to 0 when m is odd. Therefore,

$$\begin{aligned}
EE_r(P_n) &\approx n + \frac{n+1}{\pi(n-1)^2}\int_0^\pi (2\cos x)^2\,dx - \frac{2^2}{(n-1)^2} + \frac{n+1}{\pi(n-1)^4}\int_0^\pi (2\cos x)^4\,dx \\
&- \frac{2^4}{(n-1)^4} + \frac{n+1}{\pi(n-1)^6}\int_0^\pi (2\cos x)^6\,dx - \frac{2^6}{(n-1)^6}.
\end{aligned}$$

This finally yields

$$EE_r(P_n) \approx n + \frac{2n-2}{(n-1)^2} + \frac{6n-10}{(n-1)^4} + \frac{20n-44}{(n-1)^6}. \tag{7}$$

In Table 1 are also given the exact and approximate values of $EE_r(P_n)$. We see that the precision of the approximation (7) is remarkably good. Comparing the values of $EE_r(C_n)$ and $EE_r(P_n)$, it becomes evident that, except for the first few values of n, these two resolvent Estrada indices are almost equal. The very same conclusion is obtained by comparing the expressions (6) and (7).

5 Comparing Estrada and resolvent Estrada indices

In this section, we examine the relations and difference between the Estrada index and the resolvent Estrada index in the case of C_n and P_n .

As seen from Eqs. (1) and (2), the resolvent Estrada index depends on all eigenvalues or all spectral moments of the underlying graph. Yet, as shown by our formulas (6) and (7), in the case of cycles and paths this index can be calculated (approximately, but with very high precision) from just the number of vertices, n.

In Fig. 2 are shown $EE_r(C_n)$ and $EE_r(P_n)$ for $2 < n < 16$. We see that, except for the first few values of n, $EE_r(C_n)$ and $EE_r(P_n)$ are almost equal. This finding is in full agreement with the approximate expressions deduced in Sections 3 and 4.

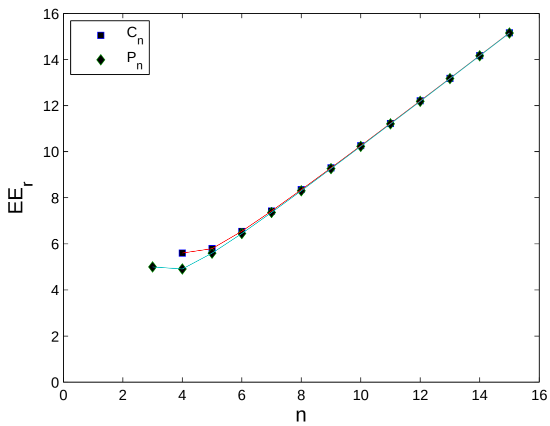

Fig. 2. $EE_r(C_n)$ and $EE_r(P_n)$, plotted versus n.

By comparing Figs. 1 and 2, a remarkable difference is envisaged between the Estrada index and the resolvent Estrada index in the case of cycles and paths. The reason for this difference can be explained as follows.

From the expressions (4) and (5), it is immediately seen that, except for the first few values of n, $EE(C_n)$ and $EE(P_n)$ are linear functions of n. Due to the same slope I_0 of Eqs. (4) and (5), the two lines shown in Fig. 1 are parallel. The difference between the two lines is given by the term $\cosh(2) - I_0$, which is a fixed constant, and is approximately equal to 1.4826.

On the other hand, the expressions (6) and (7) for the resolvent Estrada indices of C_n and P_n are non-linear functions of n, although their deviation from linearity rapidly vanishes with increasing n. The difference between (6) and (7) is

$$\frac{2}{(n-1)^2}+\frac{10}{(n-1)^4}+\frac{44}{(n-1)^6}$$

which rapidly tends to zero for $n\to\infty$. This implies that the two lines presented in Fig. 2 gradually tend to become linear and tend to coincide as n increases. That this happens very fast is seen from Fig. 2 and the data given in Table 1.

By comparing expressions (4) and (6) and bearing in mind that $I_0\approx 2.27958530$, we easily see that

$$EE_r(C_n)<EE(C_n) \tag{8}$$

holds provided $n\geq 4$.

Indeed, if $n\geq 4$, then

$$\frac{2n}{(n-1)^2}+\frac{6n}{(n-1)^4}+\frac{20n}{(n-1)^6}\leq 3\,.$$

and then by (4) and (6),

$$n+\frac{2n}{(n-1)^2}+\frac{6n}{(n-1)^4}+\frac{20n}{(n-1)^6}\leq n+3\leq 2n<n\,I_0$$

implying the inequality (8).

In an analogous manner, for $n\geq 3$, we get

$$EE_r(P_n)<EE(P_n)\,. \tag{9}$$

Inequalities (8) and (9) shed some light on the relations between the Estrada and the resolvent Estrada indices. It remains a challenge for the future to investigate whether the inequality $EE_r(G)<EE(G)$ holds for other graphs G, or – perhaps – for all graphs. If not, then it would be interesting to find graphs for which $EE_r(G)=EE(G)$.

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References

[1] M. Benzi, P. Boito, *Quadrature rule–based bounds for functions of adjacency matrices*, Lin. Algebra Appl., Vol. 433, (2010), 637–652.

[2] X. Chen, J. Qian, *Bounding the resolvent Estrada index of a graph*, J. Math. Study, Vol. 45, 2 (2012), 159–166.

[3] X. Chen, J. Qian, *On resolvent Estrada index*, MATCH Commun. Math. Comput. Chem., Vol. 73, 1 (2015), 163–174.

[4] D. Cvetković, M. Doob, H. Sachs, *Spectra of Graphs – Theory and Application*, Academic Press, New York, 1980.

[5] H. Deng, *A note on the Estrada index of trees*, MATCH Commun. Math. Comput. Chem., Vol. 62, 3 (2009), 607–610.

[6] E. Estrada, *Characterization of 3D molecular structure*, Chem. Phys. Lett., Vol. 319, (2000), 713–718.

[7] E. Estrada, *Characterization of the folding degree of proteins*, Bioinformatics, Vol. 18, (2002), 697–704.

[8] E. Estrada, D. J. Higham, *Network properties revealed through matrix functions*, SIAM Rev., Vol. 52 (2010) 696–714.

[9] E. Estrada, J. A. Rodríguez–Velázquez, *Subgraph centrality in complex networks*, Phys. Rev. E, Vol. 71, (2005), 056103.

[10] I. Gutman, H. Deng, S. Radenković, *The Estrada index: An updated survey*, in: D. Cvetković, I. Gutman (Eds.), *Selected Topics on Applications of Graph Spectra*, Math. Inst., Beograd, 2011, pp. 155–174.

[11] I. Gutman B. Furtula, X. Chen, J. Qian, *Graphs with smallest resolvent Estrada indices*, MATCH Commun. Math. Comput. Chem., Vol. 73, 1 (2015), 267–270.

[12] I. Gutman, B. Furtula, X. Chen, J. Qian, *Resolvent Estrada index – computational and mathematical studies*, MATCH Commun. Math. Comput. Chem., Vol. 74, 3 (2015), 431–440.

[13] I. Gutman, A. Graovac, *Estrada indices of cycles and paths*, Chem. Phys. Lett., Vol. 463, (2007), 294–296.

[14] J. A. de la Peña, I. Gutman, J. Rada, *Estimating the Estrada index*, Lin. Algebra Appl., Vol. 427, (2007), 70–76.