Available online at www.sciencedirect.com
ScienceDirect
Chemical Physics Letters 436 (2007) 294–296
CHEMICAL PHYSICS LETTERS
www.elsevier.com/locate/cplett

Estrada index of cycles and paths

Ivan Gutman [a,*], Ante Graovac [b]

[a] Faculty of Science, University of Kragujevac, P.O. Box 60, 34000 Kragujevac, Serbia and Montenegro
[b] The Rugjer Bošković Institute, Bijenička c. 54, 10000 Zagreb, Croatia

Received 26 December 2006; in final form 11 January 2007
Available online 18 January 2007

Abstract

Let G be a graph on n vertices, and let $\lambda_1, \lambda_2, \ldots, \lambda_n$ be its eigenvalues. The Estrada index of G is a recently introduced molecular structure descriptor, defined as $EE(G) = \sum_{i=1}^{n} e^{\lambda_i}$. We show that the Estrada indices of the n-vertex cycle C_n and the n-vertex path P_n can be approximated as $EE(C_n) \approx n\, I_0$ and $EE(P_n) \approx (n+1)I_0 - \cosh(2)$, where $I_0 = \sum_{k \geqslant 0} 1/(k!)^2 = 2.27958530\ldots$. The precision of these approximations is remarkably good.

1. Introduction

Let G be a simple graph, n the number of its vertices, and $\lambda_1, \lambda_2, \ldots, \lambda_n$ its eigenvalues (forming the spectrum of G) [1–3]. A graph-spectrum-based molecular structure descriptor, recently put forward by Estrada [4–9], is defined as

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

Recall that the adjacency matrix $\mathbf{A}(G)$ of the graph G is the square matrix of order n whose (i, j)-entry is 1 if the ith and jth vertices of G are adjacent, and 0 otherwise. The characteristic polynomial $\phi(G, \lambda)$ is the polynomial of degree n, defined as $\det[\lambda \mathbf{I}_n - \mathbf{A}(G)]$, where $\mathbf{I}_n$ is the unit matrix of order n. The spectrum of G is formed by the n solutions of the equation $\phi(G, \lambda) = 0$. All the eigenvalues of a graph are real-valued numbers, and their sum is equal to zero. More data on graph spectra can be found in the standard monograph [1].

Although invented only a few years ago [4], the Estrada index has already found numerous applications. It was used to quantify the degree of folding of long-chain molecules, especially proteins [4–6]; for this purpose the EE-values of pertinently constructed weighted graphs were employed. Another, fully unrelated, application of EE (this time of simple graphs) was put forward by Estrada and Rodríguez-Velázquez [7,8]. They showed that EE provides a measure of the centrality of complex (reaction, metabolic, communication, social, etc.) networks. In addition to this, in a recent work [9] a connection between EE and the concept of extended atomic branching was pointed out.

Until now only some elementary general properties of the Estrada index were established [10,11]. In order to contribute towards its better understanding, in this Letter we examine two simple and frequently encountered (molecular) graphs – the cycle C_n and the path P_n, whose spectra are well known [1–3].

In Fig. 1 are plotted the Estrada indices of C_n and P_n versus n. 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. The two straight lines are apparently parallel.

In what follows we find analytical (yet approximate) expressions for $EE(C_n)$ and $EE(P_n)$, corroborating and quantifying the regularities seen in Fig. 1.

2. Estrada index of the cycle

The spectrum of the cycle C_n consists of the numbers [1–3]:

* Corresponding author. Fax: +381 34 335 040.
E-mail address: gutman@knez.uis.kg.ac.yu (I. Gutman).

0009-2614/$ - see front matter © 2007 Elsevier B.V. All rights reserved.
doi:10.1016/j.cplett.2007.01.044

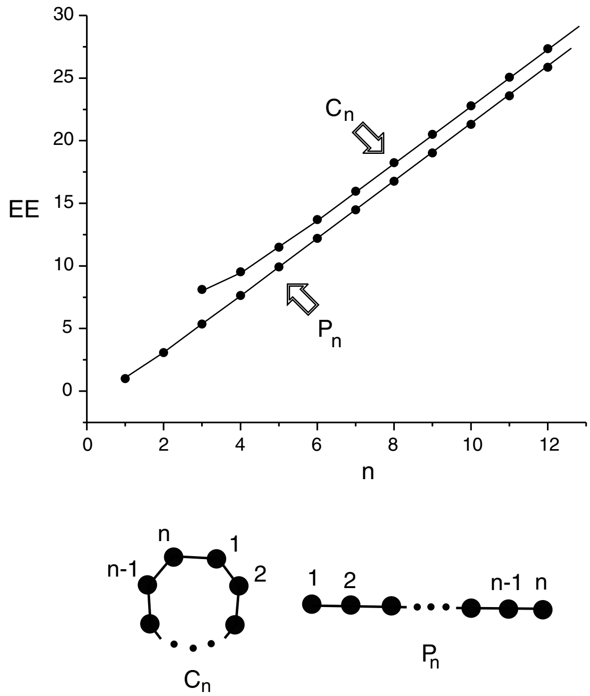

Fig. 1. The Estrada indices of the n-vertex cycle (C_n) and n-vertex path (P_n), plotted versus n. Except for the first few values of n the two lines are straight and mutually parallel.

$$2\cos\frac{2k\pi}{n}, \quad k = 1, 2, \ldots, n$$

implying

$$EE(C_n) = \sum_{k=1}^{n} e^{2\cos(2k\pi/n)}.$$

For $k = 1,2, \ldots ,n$ the angles $2k\pi/n$ uniformly cover the interval [0, 2π], thus enabling the usage of the following integral approximation:

$$EE(C_n) = n\left(\frac{1}{n}\sum_{k=1}^{n} e^{2\cos(2k\pi/n)}\right) \approx n\left(\frac{1}{2\pi}\int_0^{2\pi} e^{2\cos x}\,dx\right).$$

Now,

$$\int_0^{2\pi} e^{2\cos x}\,dx = 2\int_0^{\pi} e^{2\cos x}\,dx = \pi I_0$$

where I_0 (or more precisely: $I_0(z)$ for $z = 2$) is a particular value of a function encountered in the theory of Bessel function. It is known [12,13] that

$$I_0 = \sum_{k=0}^{\infty} \frac{1}{(k!)^2} = 2.27958530\ldots$$

In view of this,

$$EE(C_n) \approx nI_0 = 2.27958530n. \qquad (1)$$

The precision of the approximate expression (1) can be checked from the data given in Table 1. As seen from these

Table 1
Exact and approximate values of the Estrada index of the n-vertex cycle (C_n) and of the n-vertex path (P_n)

n	$EE(C_n)$	$EE(C_n)_{\text{approx}}$	$EE(P_n)$	$EE(P_n)_{\text{approx}}$
1			1.0000000	0.7969750
2			3.0861613	3.0765604
3	8.1248150	6.8387561	5.3563671	5.3561458
4	9.5243914	9.1183414	7.6357338	7.6357311
5	11.4961863	11.3979268	9.9153162	9.9153165
6	13.6967139	13.6775122	12.1949014	12.1949018
7	15.9602421	15.9570975	14.4744867	14.4744872
8	18.2371256	18.2366829	16.7540720	16.7540726
9	20.5163225	20.5162683	19.0336573	19.0336579
10	22.7958591	22.7958536	21.3132426	21.3132433
11	25.0754389	25.0754390	23.5928279	23.5928286
12	27.3550237	27.3550243	25.8724132	25.8724140
13	29.6346089	29.6346097	28.1519985	28.1519994
14	31.9141942	31.9141951	30.4315838	30.4315847
15	34.1937795	34.1937804	32.7111691	32.7111701
16	36.4733648	36.4733658	34.9907544	34.9907555
17	38.7529501	38.7529511	37.2703398	37.2703408
18	41.0325354	41.0325365	39.5499251	39.5499262
19	43.3121207	43.3121219	41.8295104	41.8295115
20	45.5917060	45.5917072	44.1090957	44.1090969
21	47.8712913	47.8712926	46.3886810	46.3886823
22	50.1508767	50.1508780	48.6682663	48.6682676
23	52.4304620	52.4304633	50.9478516	50.9478530
24	54.7100473	54.7100487	53.2274369	53.2274383
25	56.9896326	56.9896340	55.5070222	55.5070237
26	59.2692179	59.2692194	57.7866074	57.7866091
27	61.5488032	61.5488048	60.0661928	60.0661944
28	63.8283885	63.8283901	62.3457781	62.3457798
29	66.1079738	66.1079755	64.6253634	64.6253652
30	68.3875591	68.3875608	66.9049487	66.9049505

$EC(C_n)_{\text{approx}}$ and $EC(P_n)_{\text{approx}}$ pertain to the right-hand sides of Eqs. (1) and (2), respectively.

data, except for the first few values of n, formula (1) reproduces the Estrada index of the cycle with a remarkable accuracy: on two, four, and six decimal places for, respectively, $n \geqslant 6$, $n \geqslant 9$, and $n \geqslant 12$. This accuracy is more than sufficient for any (hitherto reported) application of EE.

3. Estrada index of the path

In the case of the path P_n the considerations are analogous, yet somewhat more complicated. The spectrum of P_n consists of the numbers [1–3]:

$$2\cos\frac{k\pi}{n+1}, \quad k = 1, 2, \ldots, n$$

implying

$$EE(P_n) = \sum_{k=1}^{n} e^{2\cos(kr/(n+1))}.$$

This time, however, the angles $k\pi/(n+1)$ do not cover the entire interval [0, π]. Therefore, when employing an integral approximation one needs to compensate for the missing near-zero and near-π contributions. This is done as follows:

$$
\begin{aligned}
EE(P_n) &= \frac{1}{2}\sum_{k=0}^{n} e^{2\cos(k\pi/(n+1))} + \frac{1}{2}\sum_{k=1}^{n+1} e^{2\cos(k\pi/(n+1))} - \frac{1}{2}(e^2+e^{-2}) \\
&= \frac{n+1}{2}\left(\frac{1}{n+1}\sum_{k=0}^{n} e^{2\cos(k\pi/(n+1))}\right) + \frac{n+1}{2}\left(\frac{1}{n+1}\sum_{k=1}^{n+1} e^{2\cos(k\pi/(n+1))}\right) \\
&\quad - \frac{1}{2}(e^2+e^{-2}) \\
&\approx \frac{n+1}{2}\left(\frac{1}{\pi}\int_0^{\pi} e^{2\cos x}\,dx\right) + \frac{n+1}{2}\left(\frac{1}{\pi}\int_0^{\pi} e^{2\cos x}\,dx\right) - \frac{1}{2}(e^2+e^{-2}) \\
&= \frac{n+1}{\pi}\int_0^{\pi} e^{2\cos x}\,dx - \frac{1}{2}(e^2+e^{-2}) = (n+1)I_0 - \frac{1}{2}(e^2+e^{-2})
\end{aligned}
$$

which finally yields

$$
\begin{aligned}
EE(P_n) &\approx nI_0 - \left(\frac{e^2+e^{-2}}{2} - I_0\right) \\
&= 2.27958530n - 1.48261039
\end{aligned}
$$

or, in a more compact form,

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

The (excellent) precision of the approximation (2) can also be seen from the data given in Table 1. By comparing (1) and (2) it is evident that the lines shown in Fig. 1 are parallel (both slopes being equal to I_0).

The main conclusion of this work is that although in general the Estrada index depends on the structure of a (molecular) graph in an involved way, this index is outstandingly simple to calculate in the case of cycle and path graphs.

References

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

[2] N. Trinajstić, Chemical Graph Theory, CRC Press, Boca Raton, 1983.

[3] I. Gutman, O.E. Polansky, Mathematical Concepts in Organic Chemistry, Springer, Berlin, 1986.

[4] E. Estrada, Chem. Phys. Lett. 319 (2000) 713.

[5] E. Estrada, Bioinformatics 18 (2002) 697.

[6] E. Estrada, Proteins 54 (2004) 727.

[7] E. Estrada, J.A. Rodríguez-Velázquez, Phys. Rev. E 71 (2005) 056103.

[8] E. Estrada, J.A. Rodríguez-Velázquez, Phys. Rev. E 72 (2005) 046105.

[9] E. Estrada, J.A. Rodríguez-Velázquez, M. Randić, Int. J. Quantum. Chem. 106 (2006) 823.

[10] I. Gutman, E. Estrada, J.A. Rodríguez-Velazquez, Croat. Chem. Acta 79 (2006) 000.

[11] J.A. de la Peña, I. Gutman, J. Rada, Lin. Algebra Appl., in press.

[12] I.S. Gradshteyn, I.M. Ryzhik, Tables of Integrals, Series, and Products, Academic Press, New York, 1965.

[13] I.N. Sneddon, Special Functions of Mathematical Physics and Chemistry, Longman Group, London, 1980.