J Math Chem (2008) 44:373–378
DOI 10.1007/s10910-007-9314-y

ORIGINAL PAPER

Smooth function topological structure descriptors based on graph-spectra

Ramon Carbó-Dorca

Received: 4 July 2007 / Accepted: 15 August 2007 / Published online: 1 November 2007

Abstract The spectral topological indices: energy and Estrada index of a graph are generalized for any smooth function. The smooth function indices are introduced for this purpose as well as, via positive definite square summable functions, the Shannon entropy of a graph. Some comparative values are given between linear chains and cycles.

Keywords Adjacency matrix spectrum · Topological indices · Energy index · Estrada index

1 Introduction

Recently, there have been studied and compared two structural indices related to the spectra of the adjacency matrix of a given graph [1].

Throughout this paper it will be employed the adjacency matrix as the source of the eigenvalues leading to spectral indices, but the extensive definition of derived topologically related matrices [2] precludes that other topologically related matrix forms can be employed for the same purpose.

These structural indices can be easily generalized and extended. Such is the purpose of this paper.

R. Carbó-Dorca (✉)
Department of Inorganic and Physical Chemistry, Ghent University, Krijgslaan 281, Gent 9000, Belgium
e-mail: quantumqsar@hotmail.com

R. Carbó-Dorca
Institut de Química Computacional, Universitat de Girona, Girona, Catalonia 17071, Spain

Suppose that one represents by a diagonal matrix:

$$\Lambda(G) \equiv \Lambda = \mathrm{Diag}\{\lambda_I \,| I = 1, N\}$$

the spectrum of the adjacency matrix $\mathbf{A}(G) \equiv \mathbf{A} = \{a_{\mathrm{IJ}}\}$, of a given graph G, possessing N vertices.

The energy [3] of the graph G is defined by:

$$E(G) \equiv E = \langle \Lambda \rangle = \sum_I |\lambda_I|$$

and the so-called Estrada index [4] has been described as:

$$\mathrm{EE}(G) \equiv \mathrm{EE} = \sum_I \exp(\lambda_I).$$

Both indices are just particular cases of a straightforward general definition, which can be based on the eigensystem of the adjacency matrix of a known graph or to any of the possible transformed matrices. The Estrada index is quite interesting, as has been successfully employed in a large variety of problems [5], among others protein folding and complex networking.

2 Eigensystem of the adjacency matrix: applications

Indeed, as the adjacency matrix of a graph is real and symmetric, there always exists an orthogonal transformation:$\mathbf{U}$, such that:

$$\mathbf{U}\mathbf{U}^T = \mathbf{U}^T\mathbf{U} = \mathbf{I}$$

which transforms the adjacency matrix into a diagonal form containing its eigenvalues as elements:

$$\mathbf{U}^T\mathbf{A}\mathbf{U} = \Lambda.$$

On the other hand, given a continuous smooth real function: $\varphi(x)$, it can be defined the matrix of the same function of the adjacency matrix, $\varphi(\mathbf{A})$ by means of:

$$\varphi(\mathbf{A}) = \mathbf{U}\varphi(\Lambda)\mathbf{U}^T$$

with the diagonal matrix $\varphi(\Lambda)$ easily defined as:

$$\varphi(\Lambda) = \mathrm{Diag}\{\varphi(\lambda_I)\,| I = 1, N\}.$$

Defining now the trace of an adjacency matrix as:

$$\mathrm{Tr}(\mathbf{A}) = \sum_I a_{II}$$

it is trivial to demonstrate the following property:

$$\mathrm{Tr}(\mathbf{A}) = \langle \Lambda \rangle,$$

and in general:

$$\mathrm{Tr}(\varphi(\mathbf{A})) = \langle \varphi\,(\Lambda) \rangle\,.$$

Therefore the graph energy can be rewritten as:

$$E(G) = \langle |\Lambda| \rangle = \mathrm{Tr}\,(|\mathbf{A}|)$$

and the Estrada index by means of:

$$\mathrm{EE}(G) = \left\langle e^{\Lambda} \right\rangle = \mathrm{Tr}\left(e^{\mathbf{A}}\right).$$

3 Smooth function topological indices and weighted spectral moments of a graph

In this manner one can define a large class of topological indices, based on smooth functions of the adjacency matrix:

$$\mathrm{SF}(G) = \langle \varphi\,(\Lambda) \rangle = \mathrm{Tr}\,(\varphi\,(\mathbf{A}))\,.$$

Also, smooth functions can be expressed in terms of the specific corresponding Taylor series:

$$\varphi(x) = \sum_{K=0}^{\infty} \theta_K \frac{x^K}{K!},$$

where it is needed the definition of a set of coefficients: $\left\{\theta_K = \frac{d^{(K)}\varphi(0)}{\mathrm{d}x^K}\right\}$, associated to the K-th derivative of the function $\varphi(x)$ computed at the zero value of the variable, with the convention: $\theta_0 = \varphi(0)$.

Then, one can also use the weighted spectral moments of the graph G, see reference [1] for example, within the definition of the $\mathrm{SF}(G)$ index. This can be easily realized, just writing:

$$\mathrm{SF}(G) = \sum_{K=0}^{\infty} \frac{\theta_K}{K!} \left\langle \Lambda^K \right\rangle$$

due that M_K, the K-th spectral moment of the graph G, can be simply defined as:

$$M_K = \left\langle \Lambda^K \right\rangle.$$

Of course, the values of any SF(G) index for the two extreme graphs: O_N, made by N isolated vertices and K_N, possessing $N(N-1)/2$ edges, can be easily computed as:

$$\mathrm{SF}\left(O_N\right) = N\varphi(0)$$

and

$$\mathrm{SF}\left(K_N\right) = \varphi(N-1) + (N-1)\varphi(-1),$$

respectively.

4 Comparison of two graphs employing their spectral moments up to a fixed order

Spectral moments can be used to compare two diverse graphs, even possessing a different number of vertices. Indeed, using the symbol:

$$\left\langle M^P(G)\right\rangle = \left\{M_K(G)\left|K = 1, P\right.\right\}$$

to denote a P-dimensional column array containing the first P spectral moments of a given graph G, then two graphs can be compared by means of a similarity measure:

$$\begin{aligned} &C\left(G_A, G_B\right) = \\ &\left(\left\langle M^P\left(G_A\right)\middle|M^P\left(G_A\right)\right\rangle\left\langle M^P\left(G_B\right)\middle|M^P\left(G_B\right)\right\rangle\right)^{-\frac{1}{2}}\left\langle M^P\left(G_A\right)\middle|M^P\left(G_B\right)\right\rangle \end{aligned}$$

or a dissimilarity measure like:

$$\begin{aligned} &D\left(G_A, G_B\right) = \\ &\left(\left\langle M^P\left(G_A\right)\middle|M^P\left(G_A\right)\right\rangle + \left\langle M^P\left(G_B\right)\middle|M^P\left(G_B\right)\right\rangle - 2\left\langle M^P\left(G_A\right)\middle|M^P\left(G_B\right)\right\rangle\right)^{\frac{1}{2}} \end{aligned}$$

where by the symbol:$\left\langle M^P\left(G_A\right)\middle|M^P\left(G_B\right)\right\rangle$ is denoted the scalar product of the two vectors of spectral moments:

$$\left\langle M^P\left(G_A\right)\middle|M^P\left(G_B\right)\right\rangle = \sum_{K=1}^{P} M_K\left(G_A\right)M_K\left(G_B\right).$$

5 Probability function topological indices and Shannon entropy of a graph

Moreover, it is interesting to choose as a generating smooth function topological index any probability density function: $\rho(x)$, which can be constructed from any smooth function possessing a summable square module, even if the smooth function is defined in the complex field, as in the usual quantum mechanical lore:

$$\rho(x) = |\varphi(x)|^2$$

with the additional Minkowski normalization condition:

$$\langle\rho\rangle = \int_D \rho(x)\mathrm{d}x = 1.$$

Then, for a given spectrum of the adjacency matrix, the diagonal matrix can be computed:

$$\rho(\Lambda) = \{\rho(\lambda_I)|I = 1, N\}$$

which can be normalized, employing the straightforward procedure:

$$\nu = \langle\rho\,(\Lambda)\rangle = \sum_I \rho\,(\lambda_I) \rightarrow \rho_\nu\,(\Lambda) = \nu^{-1}\rho\,(\Lambda) = \left\{\nu^{-1}\rho\,(\lambda_I)\,|I = 1, N\right\}$$
$$\rightarrow \langle\rho_\nu\,(\Lambda)\rangle = \nu^{-1}\,\langle\rho\,(\Lambda)\rangle = 1$$

The Minkowski norm above being the Estrada index for the probability density function and from there one can easily define a graph (Shannon) entropy topological index as:

$$S(G) = -\,\langle\rho_\nu(\Lambda)\log\left(\rho_\nu(\Lambda)\right)\rangle = -\nu^{-1}\sum_I \rho\,(\lambda_I)\log\left(\nu^{-1}\rho\,(\lambda_I)\right).$$

6 Tests

It is a simple matter to set up straightforward computational tests, in order to evaluate the behavior of some of the proposed indices; for example: comparing graphs of linear and cyclic polyenes.

When the absolute value is employed as smooth function index, the linear chains produce lesser values of the graph energy than cycles and the Shannon entropy follows the same trend.

When the exponential function e^x is employed in the evaluation of the smooth function index, the linear chains possess a lesser Estrada index than cycles although this situation is reversed when computing the Shannon entropy: cycles present slightly lower values than linear chains. However if one uses: x^2e^x, both parameters for cycles are slightly superior than in linear chains. Moreover, when using: $x^{-2}e^{x}$, then the smooth function index is greater for cycles but the Shannon entropy is larger in linear graphs up to eight vertices where its value goes slightly under the corresponding cycle.

For a smooth function like a Gaussian: e^{x^2}, unfolding a cycle produces an decrease of the smooth function topological index, while Shannon entropy computed from renormalization of the same smooth function is greater for linear chains up to 10 vertex graphs; after this vertex number, the cycle's entropy becomes slightly larger.

For the hyperbolic cosine, the smooth function index for cycles is greater than for linear graphs while in the Shannon entropy values this tendency is reversed giving slightly greater values for linear structures than for cycles.

For the hyperbolic secant from five vertex graphs and up, the smooth function index and Shannon entropy are greater for linear structures than for circles.

When increasing the number of vertices, smooth function indices tend to become equal for both structures and entropy also becomes a similar number as well.

7 Conclusions

A general smooth function family of topological indices has been studied. The well known energy and Estrada indices of a graph can be seen as nothing else but particular definitions of the proposed general structure. The described framework permit to extend the smooth function topological indices to probability functions and via a simple renormalization, the Shannon entropy of a graph can be also computed. Spectral moments play a leading role in the developed theoretical definitions and can be employed to set similarity and dissimilarity indices between two different graphs.

Acknowledgements The author wants to acknowledge the Spanish Ministerio de Educación y Ciencia for a grant, ref.: CTQ2006-04410/BQU, which partially sponsored this work and also the Catalan AGAUR for a fellowship, ref: 2006 BE-2, Expedient #10154, which has allowed the author to perform during 2007 a stage at Ghent University.

References

1. I. Gutman, E. Estrada, J.A. Rodríguez-Velázquez, Croat. Chim. Acta **80**, 151 (2007)
2. D. Jacenic, A. Milicevic, S. Nikolic, N. Trinajstic, *Graph Theoretical Matrices in Chemistry*. (Mathematical Chemistry Monographs 3, University of Kragujevac, Faculty of Science, Kragujevac, 2007)
3. I. Gutman, J. Serb. Chem. Soc. **70**, 441 (2005)
4. E. Estrada, Chem. Phys. Lett. **319**, 713 (2000)
5. (a) E. Estrada, Bioinformatics **18**, 697 (2002), (b) E. Estrada, Proteins **54** 727 (2004), c) E. Estrada, J.A. Rodríguez-Velázquez, Phys. Rev. **E71**, 056103 (2005), (d) E. Estrada, J.A. Rodríguez-Velázquez, Phys. Rev. **E72** 046105 (2005), (e) E. Estrada, J.A. Rodríguez-Velázquez, M. Randic, Intl. J. Quantum Chem. **106**, 823 (2006)