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On a Graph-Spectrum-Based Structure Descriptor*

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The structure descriptor *EE*, put forward in 2000 by one of the present authors, is equal to the sum of the terms $\exp(\lambda_i)$ over all eigenvalues λ_i of the underlying (molecular) graph. Some basic properties of the *EE*-index are determined: lower and upper bounds for *EE* are obtained (valid for *n*-vertex graphs and for (*n,m*)-graphs), and the corresponding extremal graphs are characterized. Some relations between *EE* and graph energy are established.

INTRODUCTION

A few years ago, one of the present authors[1] conceived the molecular structure descriptor *EE*, based on the spectrum of the adjacency matrix of a pertinently weighted molecular graph, capable of measuring the 3D folding of long-chain molecules. It proved to be particularly convenient for ranking proteins according to their degree of folding:[1–3] *EE* assumes the maximum value for the most folded protein chain. The same quantity (computed for non-weighted graphs) was eventually shown to provide a measure of centrality of complex networks (such as neural, social, metabolic, or protein-protein interaction networks, as well as the Internet and the World Wide Web).[4,5] Quite recently, *EE* was proposed to be used (also) as a graph-theoretic measure of extended atomic branching, accounting for the effects of all atoms in the molecule, giving higher weight to the nearest neighbors.[6]

The definition of the *EE*-index is simple: Let G be an *n*-vertex (molecular) graph, and let $\lambda_1, \lambda_2, \ldots, \lambda_n$ be its eigenvalues (*i.e.,* eigenvalues of the adjacency matrix of G).[7–10] Then:

$$EE = EE(\mathrm{G}) = \sum_{i=1}^{n} \exp(\lambda_i) \qquad (1)$$

By means of a power-series expansion of the function $\exp(x)$ we immediately have:

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

where M_k is the *k*-th spectral moment[10] of graph G:

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

* Dedicated to Professor Haruo Hosoya in the happy celebration of his 70th birthday.

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In spite of the numerous (and quite different) applications of the *EE*-index, its basic (mathematical) properties have not been investigated so far. The present paper is aimed at partially filling this gap.

In the subsequent section, we provide answers to some simple questions in the theory of the *EE*-index. In particular, we determine the interval (depending on n) to which the *EE*-values of n-vertex graphs belong. In the next section, we establish relations between *EE* and the graph energy *E*.

BOUNDS FOR THE *EE*-INDEX

It is evident from Eq. (2) that if graph G can be transformed into another graph G', such that $M_k(G) \geq M_k(G')$ holds for all values of k, and $M_k(G) > M_k(G')$ holds for at least some values of k, then $EE(G) > EE(G')$. Now, graph transformation G $\rightarrow$ G' of the required type is when G' is obtained by deleting an edge from G. Indeed, as well known,[10,11] M_k is equal to the number of closed walks of length k. Therefore, by deleting an edge from G, the number of closed walks of length k will certainly not increase, and in some cases (*e.g.*, for $k = 2$) will strictly decrease.

Bearing the above in mind, we readily conclude that the n-vertex graph with as few as possible and as many as possible edges has, respectively, the minimum and the maximum *EE*-value. In other words, we have:

Proposition 1. – (a) Among n-vertex graphs, graph O_n consisting of n isolated vertices (and thus possessing no edges) has minimum *EE*. (b) Among n-vertex graphs, the complete graph K_n (possessing $n(n-1)/2$ edges) has maximum *EE*.

The spectra of O_n and K_n are well known.[8,10] From these and Eq. (1), we readily compute that:

$$EE(O_n) = n$$

and

$$EE(K_n) = e^{n-1} + (n-1)\frac{1}{e}.$$

Hence, for any n-vertex graph G, different from O_n and K_n:

$$n < EE(G) < e^{n-1} + (n-1)\frac{1}{e}.$$

Without proof we state another related, result:

Proposition 2. – Among connected n-vertex graphs, the path-graph P_n has minimum *EE*.

Recall that according to Proposition 1, among connected n-vertex graphs, the complete graph K_n has maximum *EE*.

A graph possessing n vertices and m edges will be referred to as an (n,m)-graph.

We now attack a significantly more difficult problem: finding (n,m)-graphs with maximum and minimum *EE*-index.

Let G be an (n,m)-graph. Bearing in mind that:[8,10]

$$\sum_{i=1}^{n} \lambda_i = 0 \quad \text{and} \quad \sum_{i=1}^{n} (\lambda_i)^2 = 2m$$

we may apply the Lagrange-multiplier technique. For this, consider the expression:

$$L = \sum_{i=1}^{n} \exp(\lambda_i) - A\left[\sum_{i=1}^{n} \lambda_i\right] - \frac{B}{2}\left[\sum_{i=1}^{n} (\lambda_i)^2 - 2m\right]$$

whose value, irrespective of the choice of multipliers A and B is equal to *EE*. Imposing the conditions $\partial L / \partial \lambda_i = 0$ for $i = 1,2,...,n$, by direct calculation, we arrive at:

$$\exp(\lambda_i) - A - B\lambda_i = 0.$$

Depending on the actual values of parameters A and B, an equation of the form:

$$\exp(x) = A + Bx \qquad (3)$$

has either no real solution, or a single real solution, or two real solutions.

If Eq. (3) has no real solution, then our Lagrange-multiplier approach does not work, since the graph eigenvalues are necessarily real numbers.[8]

If Eq. (3) has a single solution, then the graph with extremal *EE* must have all eigenvalues mutually equal. This happens only in the case of the edgeless graph[8] O_n, which, according to Proposition 1, is indeed extremal. However, this case does not offer anything new.

The case when Eq. (3) has two different real solutions remains. It corresponds to graphs possessing exactly two distinct eigenvalues. Graphs with this spectral property are those[8] consisting of a number of copies (say p) of mutually isomorphic complete graphs (say K_q). If so, then $n = pq$ and $m = pq(q-1)/2$. This, in turn implies:

Proposition 3. – Let G be an (n,m)-graph. If the quantities p and q:

$$p = \frac{n^2}{2m+1} \text{ and } q = \frac{2m}{n} + 1$$

are integers, and if G $\neq p\ K_q$, then $EE(G) > EE(p\ K_q)$.

Recall that:

$$EE(pK_q) = p\left[e^{q-1} + (q-1)\frac{1}{e}\right].$$

Characterization of (n,m)-graphs in other cases, namely when p and q are not integers, seems to be much more difficult and remains a task for the future.

Let G be an (n,m)-graph. Then one can always find integers h and k, such that:

$$m = \frac{k(k-1)}{2} + h \; ; \quad 0 \le h < k \; .$$

Integers k and h are determined uniquely by these relations.

For given n and m, construct graph $G_{k,h}$ as follows. Start with the complete graph K_k. Attach a new vertex to exactly h vertices of K_k. The graph thus obtained has m edges and $k + 1$ vertices. If $n > k + 1$, then add additional $n - (k + 1)$ isolated vertices and then the construction of the graph $G_{k,h}$ is complete.

By numerical testing we found that the following result holds. Its proof has not been achieved so far.

Proposition 4. – For any n and m, among (n,m)-graphs, graph $G_{k,h}$ has the greatest *EE*-index.

RELATING *EE* WITH GRAPH ENERGY

A much-studied graph-spectrum-based molecular structure descriptor is the graph energy E, defined as:

$$E = E(G) = \sum_{i=1}^{n} |\lambda_i| .$$

For details on graph energy see the reviews,[12,13] recent papers,[14–22] and the references quoted therein. It should be noted that both E and EE are symmetric functions of the graph eigenvalues (thus expressible in terms of spectral moments),[23,24] and therefore both may possess similar properties. On the other hand, whereas $\exp(x)$ is a monotonically increasing function of x, this is not the case with $|x|$, which monotonically increases only for $x > 0$ (and decreases for $x < 0$). For both reasons, it seems interesting to examine the relations between E and EE.

Let G be an n-vertex graph, such that n_+ of its eigenvalues are positive, n_- are negative, and n_0 are equal to zero, $n_+ + n_- + n_+ = n$. Denote by $\sum_+$ and $\sum_-$ the summation over positive and negative eigenvalues, respectively. Then, in view of Eq. (1):

$$EE = n_0 + \sum_{+} \exp(\lambda_i) + \sum_{-} \exp(\lambda_i) .$$

Because of the inequality between the arithmetic and geometric means:

$$\frac{1}{n_+} \sum_{+} \exp(\lambda_i) \ge \left[\prod_{+} \exp(\lambda_i) \right]^{1/n_+} = \left[\exp \sum_{+} \lambda_i \right]^{1/n_+} = \left[\exp\left(\frac{1}{2} E \right) \right]^{1/n_+}$$

and

$$\frac{1}{n_-} \sum_{-} \exp(\lambda_i) \ge \left[\prod_{-} \exp(\lambda_i) \right]^{1/n_-} = \left[\exp \sum_{-} \lambda_i \right]^{1/n_-} = \left[\exp\left(\frac{1}{2} E \right) \right]^{1/n_-}$$

resulting in

$$EE \ge n_0 + n_+ \cdot \exp\left(\frac{E}{2n_+} \right) + n_- \cdot \exp\left(\frac{E}{2n_-} \right). \quad (4)$$

For many (but certainly not all!) molecular graphs, $n_0 = 0$ and $n_+ = n_- = n/2$. If so, then the right-hand side of the above inequality reduces to a remarkably simple expression:

$$EE \ge n \; \mathrm{ch}(E / n) \quad (5)$$

where ch stands for the hyperbolic cosine, $\mathrm{ch}(x) = [\exp(x) + \exp(-x)] / 2$.

Equality in (4) occurs if all positive eigenvalues of G coincide, and if the same is the case also of negative eigenvalues. There are two types of such graphs. The first are of the form $p\ K_q$ (as described above) plus an arbitrary number of isolated vertices. The second consists of copies of complete bipartite graphs $K_{a,b}$, such that product ab is the same for all copies, plus an arbitrary number of isolated vertices. Equality in (5) occurs either for graph O_n without edges, or for the graph whose all components are isomorphic to K_2.

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SAŽETAK

O jednom strukturnom deskriptoru zasnovanom na spektru grafa

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Strukturni deskriptor *EE*, koji je 2000. godine koncipirao jedan od autora, jednak je zbroju izraza $\exp(\lambda_i)$ preko svih vlastitih vrijednosti λ_i odgovarajućeg (molekulskog) grafa. Određena su neka osnovna svojstva indeksa *EE*: nađene su donje i gornje granice za *EE* (koje vrijede za grafove s n vrhova, te za (n,m)-grafove), i okarakterizirani su odgovarajući ekstremalni grafovi. Nađene su i relacije između *EE* i energije grafa.