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Estimating the Estrada index

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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 graph invariant, defined as $EE = \sum_{i=1}^{n} e^{\lambda_i}$. We establish lower and upper bounds for EE in terms of the number of vertices and number of edges. Also some inequalities between EE and the energy of G are obtained.

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1. Introduction

Let G be a graph without loops and multiple edges. Let n and m be, respectively, the number of vertices and edges of G. Such a graph will be referred to as an (n, m)-graph.

The eigenvalues of the adjacency matrix of G are said to be [1] the eigenvalues of G and to form the spectrum of G. A graph of order n has n (not necessarily distinct, but necessarily real-valued) eigenvalues; we denote these by $\lambda_1, \lambda_2, \ldots, \lambda_n$, and assume to be labelled in a non-increasing manner:

$$\lambda_1 \geqslant \lambda_2 \geqslant \cdots \geqslant \lambda_n.$$

The basic properties of graph eigenvalues can be found in the book [1].

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A graph-spectrum-based invariant, recently put forward by Estrada [2–7], is defined as

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

We propose to call it the *Estrada index*.

Although invented in year 2000 [2], the Estrada index has already found numerous applications. It was used to quantify the degree of folding of long-chain molecules, especially proteins [2–4]; for this purpose the EE-values of pertinently constructed weighted graphs were employed. Another, fully unrelated, application of EE (this time of simple graphs, like those studied in the present paper) was put forward by Estrada and Rodríguez-Velázquez [5,6]. They showed that EE provides a measure of the centrality of complex (communication, social, metabolic, etc.) networks. In addition to this, in a recent work [7] a connection between EE and the concept of extended atomic branching was considered.

Until now only some elementary and easy general mathematical properties of the Estrada index were established. Of these, worth mentioning are only the following three:

1° [5] Denoting by $M_k = M_k(G)$ the kth spectral moment of the graph G,

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

and bearing in mind the power-series expansion of e^x, we have

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

As well known [1], $M_k(G)$ is equal to the number of self-returning walks of length k of the graph G.

2° [8] As a direct consequence of (2), for any graph G of order n, different from the complete graph K_n and from its (edgeless) complement $\overline{K}_n$,

$$EE(\overline{K}_n) < EE(G) < EE(K_n).$$

3° [6] If the graph G is bipartite, and if n_0 is the multiplicity of its eigenvalue zero, then

$$EE(G) = n_0 + 2 \sum_{+} \mathrm{ch}(\lambda_i), \tag{3}$$

where ch stands for the hyperbolic cosine [$\mathrm{ch}(x) = (\mathrm{e}^x + \mathrm{e}^{-x})/2$], whereas $\sum_+$ denotes summation over all positive eigenvalues of the corresponding graph.

In order to contribute towards the better understanding of the properties of the Estrada index $EE(G)$ and, in particular, of its dependence on the structure of the graph G, in this paper we establish lower and upper bounds for EE in terms of n and m. An additional motivation for this was the fact that for an analogous graph-spectrum-based invariant, namely for the graph energy

$$E = E(G) = \sum_{i=1}^{n} |\lambda_i| \tag{4}$$

(n, m)-type estimates have been known for a long time [9]:

$$2\sqrt{m} \leqslant E \leqslant 2m; \quad 2\sqrt{n-1} \leqslant E \leqslant \sqrt{2mn}. \tag{5}$$

2. (n, m)-Type estimates of the Estrada index of general graphs

Theorem 1. *Let G be an (n, m)-graph. Then the Estrada index of G is bounded as*

$$\sqrt{n^2 + 4m} \leqslant EE(G) \leqslant n - 1 + e^{\sqrt{2m}}. \tag{6}$$

Equality on both sides of (6) is attained if and only if $G \cong \overline{K}_n$.

Proof. In the proof of both Theorem 1 and the subsequent estimates we shall frequently use the following well known results for the first few spectral moments of an (n, m)-graph [1]:

$$M_0 = n; \quad M_1 = 0; \quad M_2 = 2m; \quad M_3 = 6t,$$

where t is the number of triangles.

Lower bound. Directly from the definition of the Estrada index, Eq. (1), we get

$$EE^2 = \sum_{i=1}^{n} e^{2\lambda_i} + 2\sum_{i<j} e^{\lambda_i} e^{\lambda_j}. \tag{7}$$

In view of the inequality between the arithmetic and geometric means,

$$\begin{aligned} 2\sum_{i<j} e^{\lambda_i} e^{\lambda_j} &\geqslant n(n-1)\left(\prod_{i<j} e^{\lambda_i} e^{\lambda_j}\right)^{2/[n(n-1)]} \\ &= n(n-1)\left[\left(\prod_{i=1}^{n} e^{\lambda_i}\right)^{n-1}\right]^{2/[n(n-1)]} \\ &= n(n-1)(e^{M_1})^{2/n} = n(n-1). \end{aligned} \tag{8}$$

By means of a power-series expansion, and bearing in mind the properties of M_0, M_1, and M_2, we get

$$\sum_{i=1}^{n} e^{2\lambda_i} = \sum_{i=1}^{n}\sum_{k\geqslant 0} \frac{(2\lambda_i)^k}{k!} = n + 4m + \sum_{i=1}^{n}\sum_{k\geqslant 3} \frac{(2\lambda_i)^k}{k!}. \tag{9}$$

Because we are aiming at a (as good as possible) lower bound, it may look plausible to replace $\sum_{k\geqslant 3} \frac{(2\lambda_i)^k}{k!}$ by $8\sum_{k\geqslant 3} \frac{(\lambda_i)^k}{k!}$. However, instead of $8 = 2^3$ we shall use a multiplier $\gamma \in [0, 8]$, so as to arrive at

$$\begin{aligned} \sum_{i=1}^{n} e^{2\lambda_i} &\geqslant n + 4m + \gamma \sum_{i=1}^{n}\sum_{k\geqslant 3} \frac{(\lambda_i)^k}{k!} \\ &= n + 4m - \gamma n - \gamma m + \gamma \sum_{i=1}^{n}\sum_{k\geqslant 0} \frac{(\lambda_i)^k}{k!}, \end{aligned}$$

i.e.,

$$\sum_{i=1}^{n} e^{2\lambda_i} \geqslant (1-\gamma)n + (4-\gamma)m + \gamma EE. \tag{10}$$

By substituting (8) and (10) back into (7), and solving for EE we obtain

$$EE \geqslant \frac{\gamma}{2} + \sqrt{\left(n - \frac{\gamma}{2}\right)^2 + (4-\gamma)m}. \tag{11}$$

It is elementary to show that for $n \geqslant 2$ and $m \geqslant 1$ the function

$$f(x) := \frac{x}{2} + \sqrt{\left(n - \frac{x}{2}\right)^2 + (4-x)m}$$

monotonically decreases in the interval $[0, 8]$. Consequently, the best lower bound for EE is attained not for $\gamma = 8$, but for $\gamma = 0$.

Setting $\gamma = 0$ into (11) we arrive at the first half of Theorem 1.

Remark. If in Eq. (9) we utilize also the properties of the third spectral moment, we get

$$\sum_{i=1}^{n} \mathrm{e}^{2\lambda_i} = n + 4m + 8t + \sum_{i=1}^{n} \sum_{k\geqslant 4} \frac{(2\lambda_i)^k}{k!}$$

which, in a fully analogous manner, results in

$$EE \geqslant \sqrt{n^2 + 4m + 8t}.$$

Upper bound. Starting with Eq. (2) we get

$$\begin{aligned} EE &= n + \sum_{i=1}^{n} \sum_{k\geqslant 1} \frac{(\lambda_i)^k}{k!} \leqslant n + \sum_{i=1}^{n} \sum_{k\geqslant 1} \frac{|\lambda_i|^k}{k!} \\ &= n + \sum_{k\geqslant 1} \frac{1}{k!} \sum_{i=1}^{n} \left[(\lambda_i)^2\right]^{k/2} \leqslant n + \sum_{k\geqslant 1} \frac{1}{k!} \left[\sum_{i=1}^{n} (\lambda_i)^2\right]^{k/2} \\ &= n + \sum_{k\geqslant 1} \frac{1}{k!} (2m)^{k/2} = n - 1 + \sum_{k\geqslant 0} \frac{(\sqrt{2m})^k}{k!}, \end{aligned}$$

which directly leads to the right-hand side inequality in (6).

From the derivation of (6) it is evident that equality will be attained if and only if the graph G has no non-zero eigenvalues. This, in turn, happens only in the case of the edgeless graph $\overline{K}_n$ [1].

By this the proof of Theorem 1 is completed. □

3. (n, m)-Type estimates of the Estrada index of special types of graphs

Theorem 2. *Let G be a bipartite (n, m)-graph. Then the Estrada index of G is bounded as*

$$\sqrt{n^2 + 4m} \leqslant EE(G) \leqslant n - 2 + 2\,\mathrm{ch}(\sqrt{2m}). \tag{12}$$

Equality on the left-hand side of (12) is attained if and only if $G \cong \overline{K}_n$. Equality on the right-hand side of (12) is attained for graphs possessing no more than one positive eigenvalue, i.e., for the graphs of the form $K_{a,b} \cup \overline{K}_c$, with $a, b, c \geqslant 0$, $a + b + c = n$, $ab = m$.

Proof. In view of Theorem 1 we need to verify only the upper bound. For this we start with Eq. (3) and follow a reasoning fully analogous to that used in the case of the upper bound of

Theorem 1. By n_+ we denote the number of positive eigenvalues of G which is also equal to the number of its negative eigenvalues. Therefore $n_0 + 2n_+ = n$. We thus have

$$EE = n_0 + 2\sum_{+}\sum_{k\geqslant 0}\frac{(\lambda_i)^{2k}}{(2k)!} = n_0 + 2n_+ + 2\sum_{+}\sum_{k\geqslant 1}\frac{(\lambda_i)^{2k}}{(2k)!}$$

$$= n + 2\sum_{k\geqslant 1}\frac{1}{(2k)!}\sum_{+}[(\lambda_i)^2]^k \leqslant n + 2\sum_{k\geqslant 1}\frac{1}{(2k)!}\left[\sum_{+}(\lambda_i)^2\right]^k$$

$$= n + 2\sum_{k\geqslant 1}\frac{m^k}{(2k)!} = n - 2 + 2\sum_{k\geqslant 0}\frac{(\sqrt{m})^{2k}}{(2k)!}$$

i.e.,

$$EE \leqslant n - 2 + 2\,\mathrm{ch}(\sqrt{m}). \qquad \square$$

If the graph G is regular of degree r, then its greatest eigenvalue is equal to r. If, in addition, G is bipartite, then its smallest eigenvalue is equal to $-r$ [1]. Bearing these facts in mind, we can deduce the results stated in the following two theorems. Their proofs are analogous to those of Theorems 1 and 2, and only the crucial details thereof will be indicated.

It should be noted that a regular graph of degree r and order n possesses $m = nr/2$ edges.

Theorem 3. *Let G be a regular graph of degree r and of order n. Then its Estrada index is bounded as*

$$\mathrm{e}^r + \sqrt{n + 2nr - (2r^2 + 2r + 1) + (n-1)(n-2)\mathrm{e}^{-2r/(n-1)}} \leqslant EE(G) \leqslant n - 2 + \mathrm{e}^r + \mathrm{e}^{\sqrt{r(n-r)}}.$$

Proof. In order to obtain the lower bound we consider $(EE - \mathrm{e}^r)^2$ and proceed in the same manner as in Theorem 1. In this case, however, we encounter the term $2\sum_{2\leqslant i<j}\mathrm{e}^{\lambda_i}\mathrm{e}^{\lambda_j}$, whose lower bound (the geometric mean) is

$$(n-1)(n-2)\left(\prod_{i=2}^{n}\mathrm{e}^{\lambda_i}\right)^{2/(n-1)} = (n-1)(n-2)\mathrm{e}^{-2r/(n-1)}$$

because the sum of the eigenvalues λ_i, $i = 2, \ldots, n$ is equal to $-r$.

The upper bound is obtained by estimating $EE - \mathrm{e}^r$ in the same way as in Theorem 1. $\square$

Remark. The lower bound in Theorem 3 can be improved by including into the consideration also the third spectral moment of the graph G:

$$EE(G) \geqslant \mathrm{e}^r + \sqrt{n + 2nr - (2r^2 + 2r + 1) + (n-1)(n-2)\mathrm{e}^{-2r/(n-1)} - \frac{4}{3}(r^3 - 6t)}.$$

In the case of bipartite regular graphs we have to start the considerations with $(EE - \mathrm{e}^r - \mathrm{e}^{-r})^2$ and $EE - \mathrm{e}^r - \mathrm{e}^{-r}$. This time the lower bound is significantly simpler, thanks to the fact that the sum of the eigenvalues λ_i, $i = 2, \ldots, n-1$ is equal to zero.

Theorem 4. *Let G be a bipartite regular graph of degree r and of order n. Then its Estrada index is bounded as*

$$2\,\mathrm{ch}(r)+\sqrt{(n-2)^2+2nr-4r^2}\leqslant EE(G)\leqslant n-4+2\,\mathrm{ch}(r)+2\,\mathrm{ch}\left(\sqrt{nr/2-r^2}\right).$$

4. Bounds for the Estrada index involving graph energy

In the proof of Theorem 1 we arrived at the inequality

$$EE\leqslant n+\sum_{i=1}^{n}\sum_{k\geqslant 1}\frac{|\lambda_i|^k}{k!}. \tag{13}$$

Taking into account the definition of graph energy, Eq. (4), we obtain

$$EE\leqslant n+E+\sum_{i=1}^{n}\sum_{k\geqslant 2}\frac{|\lambda_i|^k}{k!}$$

which, in a way fully analogous to what was used to obtain the upper bound in Theorem 1, leads to

$$EE(G)-E(G)\leqslant n-1-\sqrt{2m}+\mathrm{e}^{\sqrt{2m}}. \tag{14}$$

This inequality holds for all (n, m)-graphs. Equality is attained if and only if $G\cong\overline{K}_n$.

A similar formula is deduced for regular graphs

$$EE(G)-E(G)\leqslant n-2+\mathrm{e}^r-r-\sqrt{r(n-r)}+\mathrm{e}^{\sqrt{r(n-r)}}.$$

Another route to connect EE and E, starting with the inequality (13), is the following:

$$n+\sum_{i=1}^{n}\sum_{k\geqslant 1}\frac{|\lambda_i|^k}{k!}\leqslant n+\sum_{k\geqslant 1}\frac{1}{k!}\left(\sum_{i=1}^{n}|\lambda_i|\right)^k=n+\sum_{k\geqslant 1}\frac{E^k}{k!}=n-1+\sum_{k\geqslant 0}\frac{E^k}{k!}$$

implying

$$EE(G)\leqslant n-1+\mathrm{e}^{E(G)}. \tag{15}$$

Also in this formula equality occurs if and only if $G\cong\overline{K}_n$.

The lower and upper bounds for both the graph energy and the Estrada index of (n, m)-graphs, Eqs. (5) and (6), are increasing functions of the parameters n and m. This fact, together with the inequalities (14) and (15), may give the impression that EE and E depend on the structure of a graph in a similar manner. In particular, one may be tempted to expect that for two graphs G_1 and G_2, the relation $E(G_1) > E(G_2)$ implies $EE(G_1) > EE(G_2)$ and vice versa. This, however, seems to be far from being generally true, as seen from the following two conjectures.

Let S_n and P_n denote, respectively, the n-vertex star and the n-vertex path. Let T_n be any n-vertex tree, different from S_n and P_n. It is known that [9]

$$E(S_n) < E(T_n) < E(P_n).$$

It seems that just the opposite holds for the Estrada index.

Conjecture A. *Among n-vertex trees, the path has minimum and the star maximum Estrada index*:

$$EE(S_n) > EE(T_n) > EE(P_n).$$

Among connected graphs of a given order the star has the minimum energy [9].

Conjecture B. *Among connected graphs of order n, the path has minimum Estrada index.*

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