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New Bounds for Estrada Index

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Abstract

An (m, n)-graph G is a simple graph with n vertices and m edges. Let $\lambda_1, \dots, \lambda_n$ be the eigenvalues of its adjacent matrix. The Estrada index of G, denoted by $EE(G)$, is the sum of the terms e^{λ_i}. The first Zagreb index, denoted by $Zg_1(G)$, is the sum of the terms d_i^2, where d_i is the degree of $v_i, i = 1, 2, \dots, n$. In this paper, we prove that $m + n \leq EE(G)$ for every (m, n)-graph, and establish a new upper bound for $EE(G)$ in terms of the first Zagreb index.

1 Introduction

Let G be a graph without loops and multiple edges. Let m and n be, respectively, the number of vertices and edges of G. Such a graph will be referred to as an (m, n)-graph. Let $A(G)$ be the adjacent matrix of G, which is a symmetric $(0; 1)$ matrix. The spectrum of G consists of the eigenvalues of its adjacency matrix, denoted by $\lambda_1, \lambda_2, \dots, \lambda_n$.

A graph–spectrum–based invariant, put forward by Estrada [4], is defined as

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

EE is usually referred as the Estrada index. Although invented in 2000, the Estrada index has found numerous applications. It was used to quantify the degree of folding of long organic molecules, especially proteins [5, 6]. Another, fully unrelated, application of the Estrada index was put forward by Estrada and Rodríguez–Velázquez [7, 8]. They showed that EE provides a measure of the centrality of complex (communication, social, metabolic, etc.) networks. It was also proposed as a measure of molecular branching [9]. Therefore, it is natural to investigate the relations between the Estrada index and the graph–theoretic properties of G.

Some mathematical properties of the Estrada index were established. One of most important properties is the following:

$$EE(G) = \sum_{k \geq 0} \frac{M_k(G)}{k!}$$

where $M_k = M_k(G) = \sum_{i=1}^{n} \lambda_i^k$ is the k-th spectral moment of the graph G. It is well known that $M_k(G)$ is equal to the number of closed walks of length k in G. The question of finding the lower and upper bounds for EE and the corresponding extremal graphs attracted the attention of many researchers.

In [3], the authors established lower and upper bounds for EE in terms of the numbers of vertices and edges, and showed that $\sqrt{m^2+m} \leq EE(G) \leq n-1+e^{\sqrt{2m}}$. The equalities hold if and only if G is an empty graph. In [18], Zhou generalized the above theorem. In [2], the authors showed that $n + (2m/n)^2 + (2m/n)^4/12 \leq EE(G)$. In [1], Bamdad improved the lower bounds, and showed that $\sqrt{m^2+2mn+2nt} \leq EE(G)$, where t is the number of triangles in G.

If graph parameters other than m and n are included into consideration, further bounds for the Estrada index were deduced. In [18], Zhou showed that

$$e^{\sqrt{D/n}} + (n-1)e^{-\frac{1}{n-1}\sqrt{D/n}} \leq EE$$

with equality holds if and only if G is an empty graph or a complete graph, where $D = \sum_{u \in V} d_u^2$. Lower bounds for EE in terms of nullity were also communicated [10, 14].

For a survey on Estrada index see [12].

The first Zagreb index, one of the oldest vertex–degree–based structure descriptors, is defined as $Zg_1 = Zg_1(G) = \sum_{u \in V} d_u^2$.

The first Zagreb index was first considered in [15] and since then studied in numerous paper [11, 13, 16, 17, 19]. It reflects the extent of branching of the molecular carbon–atom skeleton, and can thus be viewed as a molecular structure descriptor. We encourage the readers to consult [11, 13, 15–17, 19] for historical background, computational techniques and mathematical properties of the Zagreb indices.

In this article, we present a new lower bound for EE in terms of the numbers of vertices, edges, triangles, and squares. Also, we obtain a upper bound for EE in terms of $Zg_1(G)$.

2 Main results

First, we list some well known lemmas here, which will be used later.

Lemma 2.1 For any non-negative real x, $e^x \geq 1 + x + \frac{x^2}{2} + \frac{x^3}{3} + \frac{x^4}{4}$. Equality holds if and only if $x = 0$.

Lemma 2.2 Let G be an (m, n)-graph G with eigenvalues $\lambda_1, \ldots, \lambda_n$, with t triangles and h squares. The number of closed walks of length $1, 2, 3, 4$ is

$$M_1 = \sum_{i=1}^{n} \lambda_i = 0, \tag{1}$$

$$M_2 = \sum_{i=1}^{n} \lambda_i^2 = 2m, \tag{2}$$

$$M_3 = \sum_{i=1}^{n} \lambda_i^3 = 6t. \tag{3}$$

$$M_4 = \sum_{i=1}^{n} \lambda_i^4 = 2\sum_{i=1}^{n} d_i^2 - 2m + 8h = 2Zg_1(G) - 2m + 8h = H\,. \tag{4}$$

where d_i is the degree of v_i.

Theorem 2.1 Let G be an (m, n)-graph with t triangles and h squares, then

$$m + n \leq \sqrt{n^2 + 2mn + 2nt + \frac{1}{12}nH + m^2} \leq EE(G) \leq n - 1 + e^{\sqrt[4]{H}}\,.$$

Equalities hold if and only if G is the empty graph $\overline{K_n}$.

Proof. Lower bound:

From Lemma 2.1 and the definition of the Estrada index, we have

$$\begin{aligned}
(EE(G))^2 &= \sum_{i=1}^{n}\sum_{j=1}^{n} e^{\lambda_i + \lambda_j} \\
&\geq \sum_{i=1}^{n}\sum_{j=1}^{n} \left(1 + \lambda_i + \lambda_j + \frac{(\lambda_i + \lambda_j)^2}{2} + \frac{(\lambda_i + \lambda_j)^3}{6} + \frac{(\lambda_i + \lambda_j)^4}{24}\right) \\
&= \sum_{i=1}^{n}\sum_{j=1}^{n} \left(1 + \lambda_i + \lambda_j + \frac{(\lambda_i)^2}{2} + \frac{(\lambda_j)^2}{2} + \lambda_i\lambda_j + \frac{(\lambda_i)^3}{6}\right.
\end{aligned}$$

$$+ \quad \frac{(\lambda_j)^3}{6} + \frac{\lambda_i^2\lambda_j}{2} + \frac{\lambda_i\lambda_j^2}{2} + \frac{\lambda_i^4}{24} + \frac{\lambda_j^4}{24} + \frac{\lambda_i^2\lambda_j^2}{4} + \frac{\lambda_i^3\lambda_j}{6} + \frac{\lambda_i\lambda_j^3}{6}\Bigg).$$

By (1)–(4), we have the following equations:

$$\sum_{i=1}^{n}\sum_{j=1}^{n}(\lambda_i+\lambda_j) = n\sum_{i=1}^{n}\lambda_i + n\sum_{j=1}^{n}\lambda_j = 0$$

$$\sum_{i=1}^{n}\sum_{j=1}^{n}\left(\frac{(\lambda_i)^2}{2}+\frac{(\lambda_j)^2}{2}\right) = 2mn$$

$$\sum_{i=1}^{n}\sum_{j=1}^{n}\lambda_i\lambda_j = \sum_{i=1}^{n}\lambda_i\sum_{j=1}^{n}\lambda_j = 0$$

$$\sum_{i=1}^{n}\sum_{j=1}^{n}\left(\frac{(\lambda_i)^3}{6}+\frac{(\lambda_j)^3}{6}\right) = 2nt$$

$$\sum_{i=1}^{n}\sum_{j=1}^{n}\left(\frac{\lambda_i^4}{24}+\frac{\lambda_j^4}{24}\right) = \frac{1}{12}nH$$

$$\sum_{i=1}^{n}\sum_{j=1}^{n}\frac{\lambda_i^2\lambda_j^2}{4} = m^2$$

$$\sum_{i=1}^{n}\sum_{j=1}^{n}\left(\frac{\lambda_i^3\lambda_j}{6}\right) = \frac{1}{6}\sum_{i=1}^{n}\lambda_i^3\sum_{j=1}^{n}\lambda_j = 0$$

$$\sum_{i=1}^{n}\sum_{j=1}^{n}\left(\frac{\lambda_i\lambda_j^3}{6}\right) = \frac{1}{6}\sum_{i=1}^{n}\lambda_i\sum_{j=1}^{n}\lambda_j^3 = 0\,.$$

From above equations, we get

$$m+n \le \sqrt{n^2+2mn+2nt+\frac{1}{12}nH+m^2} \le EE(G)$$

So the inequalities of left hand hold.

Upper bound:

$$EE(G) = \sum_{i=1}^{n}e^{\lambda_i} = \sum_{i=1}^{n}\sum_{k=0}^{\infty}\frac{\lambda_i^k}{k!} \le n + \sum_{i=1}^{n}\sum_{k=1}^{\infty}\frac{|\lambda_i|^k}{k!} = n + \sum_{k=1}^{\infty}\frac{1}{k!}\sum_{i=1}^{n}(\lambda_i^4)^{\frac{k}{4}}$$

$$\le n + \sum_{k=1}^{\infty}\frac{1}{k!}\Big(\sum_{i=1}^{n}\lambda_i^4\Big)^{\frac{k}{4}} = n + \sum_{k=1}^{\infty}\frac{1}{k!}H^{\frac{k}{4}} = n-1+\sum_{k=0}^{\infty}\frac{\sqrt[4]{H}^k}{k!} = n-1+e^{\sqrt[4]{H}}$$

Equality is attained if and only if $\lambda_i = 0$ for all $i = 1, 2, \ldots, n$, which means that $G \cong \overline{K_n}$. ■

Corollary 2.1 Let G be an (m, n)-graph, and assume that there are no two squares that share one common edge in G, then

$$EE \leq n - 1 + + e^{\sqrt[4]{2Zg_1(G)}}.$$

Proof. Since there are no two squares that share one common edge in G, $m \geq 4h$. Therefore,

$$H = 2Zg_1(G) - 2m + 8h \leq 2Zg_1(G).$$

By Theorem 2.1,

$$EE \leq n - 1 + e^{\sqrt[4]{2Zg_1(G)}}.$$

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