Estrada Index of Graphs

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Abstract

Suppose G is a simple graph. The eigenvalues $\delta_1, \delta_2, \ldots, \delta_n$ of G are the eigenvalues of its adjacency matrix A. The Estrada index of the graph G is defined as $EE = EE(G) = \Sigma_{i=1}^{n} e^{\delta_i}$. In this paper the basic properties of EE are investigated. Moreover, some lower and upper bounds for the Estrada index in terms of the number of vertices, edges and the Randic index are obtained. In addition, some relations between EE and graph energy $E(G)$ are presented.

Keywords: Estrada index, eigenvalue.

1 Introduction

Let $G = (V, E)$ be a simple graph with n vertices and m edges. The eigenvalues of the adjacency matrix $A(G)$ are called the eigenvalues of G and form the spectrum of G. Suppose $\lambda_1, \cdots, \lambda_n$ is the spectrum of G such that $\lambda_1 \lambda_2 \leq \cdots \lambda_n$. The Estrada

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index of the graph G is defined as

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

This spectral quantity is put forward by Estrada [2] in the year 2000. There have been found a lot of chemical and physical applications, including quantifying the degree of folding of long-chain proteins, [2, 3, 4, 8, 9, 10] and complex networks [5, 6, 14, 15, 16, 17]. Mathematical properties of this invariant can be found in e.g. [7, 11, 12, 13, 19, 20, 21].

We now introduce some notation that will be used throughout this paper. The complete graph on n vertices is denoted by K_n. Suppose $\bar{G}$ denotes the complement of G.

Lemma 1.[1] *Let G be a graph of order $n \leq 2$ that contains no isolated vertices. We have*

1. *If G is connected with m edges and diameter D, then $\lambda_2(G) \geq \frac{1}{2mD} > 0$.*
2. *$\lambda_n(G) \geq \frac{n}{n-1}$ with equality if and only if G is the complete graph on n vertices.*

2 Main results

The energy of the graph G is defined as $E(G) = \sum_{i=1}^{n} |\lambda_i|$.

Theorem 1. *If G is connected, then $EE(G) < e(n - 1 + e^{E(G)})$.*

Proof. By definition, we have

$$\begin{aligned} e^{-1}EE(G) &= \sum_{i=1}^{n} e^{\lambda_i - 1} \\ &= \sum_{i=1}^{n}\sum_{k=0}^{\infty} \frac{1}{k!}(\lambda_i - 1)^k \\ &= n + \sum_{i=1}^{n}\sum_{n\geq 2} \frac{1}{k!}(\delta_i - 1)^k \\ &\leq n + \sum_{k\geq 2} \frac{1}{k!}(\sum_{i=1}^{n} |\lambda_i - 1|)^k \\ &= n - 1 + e^{E(G)} \qquad (1) \end{aligned}$$

with equality if and only if $\sum_{i=1}^{n}(\lambda_i - 1)^k = (\sum_{i=1}^{n} |\lambda_i - 1|)^k$ if and only if $\lambda_i = 0$, $1 \leq i \leq n$, if and only if G is an empty graph with n vertices, which is impossible. $\square$

Corollary 1. *If G is connected graph with n vertices, then $EE(G) < e(n - 1 + e^{ER(G)})$, where $ER(G) = \sum_{i=1}^{n} |\delta_i|$, δ_i are the eigenvalues of Randić matrix.*

Theorem 2. *If G is a connected graph with n vertices, then*

$$e^{-1}EE(G) - E(G) < n - 1 - \sqrt{\frac{n}{d_{\min}}} + e^{\sqrt{\frac{n}{d_{\min}}}}. \qquad (2)$$

Proof. In the proof of Theorem 1, the following inequality if proved:

$$e^{-1}EE(G) \leq n + \sum_{i=1}^{n}\sum_{k\geq 1} \frac{\lambda_i^k}{k!}.$$

On the other hand, by definition of the energy,

$$e^{-1}EE(G) \leq n + E(G) + \sum_{i=1}^{n}\sum_{k\geq 2} \frac{\lambda_i^k}{k!}.$$

Thus,

$$\begin{aligned} e^{-1}EE(G)-E(G) &\leq n+\sum_{i=1}^{n}\sum_{k\geq 2}\frac{\lambda_i^k}{k!} \\ &\leq n-1-\sqrt{2R(G)}=e^{\sqrt{2R(G)}}. \end{aligned} \tag{3}$$

The equality holds if and only if $G_n = K_n$, which is impossible. □

Corollary 2. *If G is an r-regular n-vertex graph, then*

$$e^{-1}EE(G)-E(G) < n-1-\sqrt{\frac{n}{r}}+e^{\sqrt{\frac{n}{r}}}, \tag{4}$$

and

$$e^{-1}EE(G)-ER(G) < n-1-\sqrt{\frac{n}{r}}+e^{\sqrt{\frac{n}{r}}}. \tag{5}$$

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