MATCH Communications in Mathematical and in Computer Chemistry

ISSN 0340 - 6253

A Lower Bound for Laplacian Estrada Index of a Graph

Amir Khosravanirad

Department of Mathematics, Saveh Branch, Islamic Azad University, Saveh, Iran

(Received December 10, 2012)

Abstract

Let G be a graph with n vertices and $\mu_1, \mu_2, \ldots, \mu_n$ denote the Laplacian eigenvalues of G. The Laplacian Estrada index of G is defined as $\text{LEE}(G) = e^{\mu_1} + \cdots + e^{\mu_n}$. We show that if G has c connected components and maximum degree Δ , then $\text{LEE}(G) \ge c + e^{\Delta + 1} + (n - c - 1)e^{(2m - \Delta - 1)/(n - c - 1)}$ with equality if and only if G is either a star or the union of c copies of a complete graph on $\Delta + 1$ vertices. This improves a known lower bound.

1 Introduction

Throughout this paper we consider simple graphs, that is finite and undirected graphs without loops and multiple edges. If G is a graph with vertex set $\{1, \ldots, n\}$, the *adjacency matrix* of G is an $n \times n$ matrix $A = [a_{ij}]$, where $a_{ij} = 1$ if there is an edge between the vertices i and j, and 0 otherwise. The *Laplacian matrix* of G is the matrix L = D - Awhere D is a diagonal matrix with (d_1, \ldots, d_n) on the main diagonal in which d_i is the degree of the vertex i. Since L is a real symmetric matrix, its eigenvalues $\mu_1, \mu_2, \ldots, \mu_n$ are real numbers. These are referred to as the Laplacian eigenvalues of G. In what follows we assume that $\mu_1 \ge \mu_2 \ge \cdots \ge \mu_n$. The Laplacian matrix is positive semi-definite matrix, so $\mu_i \ge 0$ and the multiplicity of 0 as an eigenvalue of L is equal to the number of connected components of G. For details on Laplacian eigenvalues of graphs we refer the reader to [3, 15, 16].

e-mail: akh12358@gmail.com

The Estrada index of G defined by E. Estrada [7, 8, 9] as

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

where $\lambda_1, \ldots, \lambda_n$ are the eigenvalues of the adjacency matrix of G. The Estrada index has already found a remarkable variety of applications. Initially it was used to quantify the degree of folding of long-chain molecules, especially proteins [7, 8, 9]; for this purpose the EE-values of pertinently constructed weighted graphs were employed. Another, fully unrelated, application of EE (of simple graphs) was proposed by Estrada and Rodríguez– Velázquez [11, 12]. They showed that EE provides a measure of the centrality of complex (communication, social, metabolic, etc.) networks. In addition to this, in [13] a connection between EE and the concept of extended atomic branching was considered. An application of the Estrada index in statistical thermodynamic has also been reported [10].

Mathematical properties of the Estrada index were studied in a number of recent works [5, 17, 22]; for review see [6].

Quite recently, in analogy to Estrada index, the Laplacian Estrada index of a graph G was introduced in [14] as

$$LEE(G) = \sum_{i=1}^{n} e^{\mu_i}.$$
(1)

Independently the authors [20] defined the Laplacian Estrada index as

$$LEE_{LSC} = LEE_{LSC}(G) = \sum_{i=1}^{n} e^{\mu_i - 2m/n}$$

where the graph G has n vertices and m edges. Since

$$LEE = e^{2m/n} \cdot LEE_{LSC}$$

the two "Laplacian Estrada indices" are essentially equivalent. In what follows we use the definition (1) which looks simpler than LEE_{LSC} .

Various properties of LEE were established in [14, 24] and, of course, in [20]. See also [1, 19, 21, 23, 25] for more recent results.

In this paper we find a lower bound for the Laplacian Estrada index of a graph in terms of its number of vertices, the number of edges and maximum degree. Our bound improves a bound presented in [2].

2 Lower bound for Laplacian Estrada index

In this section we find a lower bound for Laplacian Estrada index of a graph in terms of its number of vertices, number of edges and maximum degree. We denote the complete graph on n vertices by K_n , and the star graph on n vertices by S_n . The nonzero Laplacian eigenvalues of K_n are n with multiplicity n - 1; and those of the star S_n is n with multiplicity 1 and 1 with multiplicity n - 2 (see [15, 16]).

In [2] the following was proved.

Theorem 1. ([2]) Let G be a graph with n vertices, m edges, and c connected components. Then

$$\text{LEE}(G) \ge c + (n-c)e^{2m/(n-c)}$$
 (2)

Equality holds if and only if G is a union of copies of K_s , for some fixed integers s, with (possibly) some isolated vertices.

In Theorem 2, we improve this lower bound. Proposition 1 shows that our bound (3) is always better than (2).

Lemma 1. ([15]) If G is a connected graph with $n \ge 2$ vertices, then $\mu_1 \ge \Delta + 1$; equality holds if and only if $\Delta = n - 1$.

Lemma 2. ([4]) Let G be a connected graph on n vertices with two distinct Laplacian eigenvalues. Then G is a complete graph.

Lemma 3. ([4]) Let G be graph on n vertices with three distinct Laplacian eigenvalues $\theta_1 > \theta_2 > 0$ and let θ_1, θ_2 have multiplicities m_1, m_2 , respectively. Then only two vertex degrees k_1 and k_2 can occur in G. Suppose there are n_1 vertices of degree k_1 and n_2 vertices of degree k_2 . Then

- (i) $\theta_1 + \theta_2 = k_1 + k_2 + 1$
- (*ii*) $m_1\theta_1 + m_2\theta_2 = n_1k_1 + n_2k_2$.

Lemma 4. Let G a graph on n vertices with three distinct Laplacian eigenvalues $\mu_1 > \mu_2 > 0$. If $\mu_1 = n = \Delta + 1$ and μ_1 has multiplicity 1, then G is the star $K_{1,n-1}$.

-178-

Proof. We know $\mu_1 = n$ and G has a vertex of degree n - 1. By Lemma 3, G has only two vertex degrees $k_1 = n - 1$ and k_2 . From Lemma 2(i), we have $\mu_2 = k_2$. Since the multiplicity of μ_2 is n - 2, by Lemma 2(ii), we see $k_2 = 1$. This completes the proof. \Box

Theorem 2. Let G be a graph with n vertices, m edges, c connected components and maximum degree Δ . Then

$$\text{LEE}(G) \ge c + e^{\Delta + 1} + (n - c - 1)e^{\frac{2m - \Delta - 1}{n - c - 1}}.$$
(3)

Equality holds if and only if G is either a star or the union of c copies of a complete graph on $\Delta + 1$ vertices.

Proof. Since G has c connected components, $\mu_n = \cdots = \mu_{n-c+1} = 0$. Therefore,

$$LEE(G) = c + \sum_{i=1}^{n-c} e^{\mu_i}$$

$$\geq c + e^{\mu_1} + (n - c - 1)e^{\frac{\mu_2 + \dots + \mu_{n-c}}{n-c-1}}$$

$$= c + e^{\mu_1} + (n - c - 1)e^{\frac{2m - \mu_1}{n-c-1}}$$
(4)

where (4) is obtained by applying the arithmetic–geometric mean inequality and the last inequality by the fact that $\mu_1 + \mu_2 + \cdots + \mu_{n-c} = 2m$. Now let

$$f(x) := e^x + (n - c - 1)e^{\frac{2m - x}{n - c - 1}}$$

Then $f'(x) = e^x - e^{\frac{2m-x}{n-c-1}}$. So f is increasing for $x \ge \frac{2m}{n-c}$. We claim that $\Delta + 1 \ge \frac{2m}{n-c}$. To prove this, assume that the connected components of G have n_1, \ldots, n_c vertices with maximum degrees $\Delta_1, \ldots, \Delta_c$, respectively. Then

$$2m \le n_1 \Delta_1 + \dots + n_c \Delta_c$$
$$\le (n_1 - 1)\Delta_1 + (n_1 - 1) + \dots + (n_c - 1)\Delta_c + (n_c - 1)\Delta_c$$
$$\le (n - c)\Delta + (n - c)$$

proving the claim. Since $\mu_1 \ge \Delta + 1$ by Lemma 1, we conclude that

$$f(\mu_1) \ge f(\Delta + 1) \tag{5}$$

from which (3) follows.

Now we consider the case of equality. If the equality occurs in (3), then the equalities should occur in both (4) and (5). We may assume that $\Delta = \Delta_1$. Equality in (4) implies $\mu_2 = \cdots = \mu_{n-c}$ and equality in (5) implies $\mu_1 = \Delta_1 + 1 = n_1$ by Lemma 1. First suppose that $\mu_2 = \mu_1$, then each component of G has only two distinct Laplacian eigenvalues, and so by Lemma 2 it must be a complete graph. It turns out that G is a union of some copies of K_{n_1} . Now suppose that $\mu_2 < \mu_1$. From Lemma 4, it follows that one of the components of G is a S_n and also $\mu_2 = 1$. So G cannot have more than one components, and so $G \cong S_n$.

Now we show that the bound (3) is better than (2).

Proposition 1. With the notations of Theorem 2, we have

$$(n-c)e^{\frac{2m}{n-c}} \le e^{\Delta+1} + (n-c-1)e^{\frac{2m-\Delta-1}{n-c-1}}$$

Proof. We have

$$e^{\Delta+1} + (n-c-1)e^{\frac{2m-\Delta-1}{n-c-1}} = e^{\Delta+1} + \sum_{i=1}^{n-c-1} e^{\frac{2m-\Delta-1}{n-c-1}}$$
$$\geq (n-c)e^{\frac{\Delta+1+(n-c-1)\frac{2m-\Delta-1}{n-c}}{n-c}}$$
$$= (n-c)e^{\frac{2m}{n-c}}.$$

Note that second line is obtained by the arithmetic–geometric mean inequality. \Box

References

- S. K. Ayyaswamy, S. Balachandran, Y. B. Venkatakrishnan, I. Gutman, Signless Laplacian Estrada index, MATCH Commun. Math. Comput. Chem. 66 (2011) 785– 794.
- [2] H. Bamdad, F. Ashraf, I. Gutman, Lower bounds for Estrada index and Laplacian Estrada index, Appl. Math. Lett. 23 (2010) 739–742.
- [3] D. Cvetković, P. Rowlinson, S. K. Simić, An Introduction to the Theory of Graph Spectra, Cambridge Univ. Press, Cambridge, 2009.
- [4] E. R. van Dam, Willem H. Haemers, Graphs with constant μ and μ, Discr. Math. 182 (1998) 293–307.
- [5] J. A. de la Peña, I. Gutman, J. Rada, Estimating the Estrada index, *Lin. Algebra Appl.* 427 (2007) 70–76.
- [6] H. Deng, S. Radenković, I. Gutman, The Estrada index, in: D. Cvetković, I. Gutman (Eds.), Applications of Graph Spectra Math. Inst., Belgrade, 2009, pp. 123–140.
- [7] E. Estrada, Characterization of 3D molecular structure, Chem. Phys. Lett. 319 (2000) 713-718.

- [8] E. Estrada, Characterization of the folding degree of proteins, *Bioinformatics* 18 (2002) 697–704.
- [9] E. Estrada, Characterization of the amino acid contribution to the folding degree of proteins, *Proteins* 54 (2004) 727–737.
- [10] E. Estrada, N. Hatano, Statistical-mechanical approach to subgraph centrality in complex networks, *Chem. Phys. Lett.* **439** (2007) 247–251.
- [11] E. Estrada, J. A. Rodríguez–Velázquez, Subgraph centrality in complex networks, *Phys. Rev. E* 71 (2005) 056103.
- [12] E. Estrada, J. A. Rodríguez–Velázquez, Spectral measures of bipartivity in complex networks, *Phys. Rev. E* 72 (2005) 046105.
- [13] E. Estrada, J. A. Rodríguez–Velázquez, M. Randić, Atomic branching in molecules, Int. J. Quantum Chem. 106 (2006) 823–832.
- [14] G. H. Fath-Tabar, A. R. Ashrafi, I. Gutman, Note on Estrada and L-Estrada indices of graphs, Bull. Acad. Serbe Sci. Arts (Cl. Sci. Math.) 139 (2009) 1–16.
- [15] R. Grone, R. Merris, The Laplacian spectrum of a graph II, SIAM J. Discr. Math. 7 (1994) 221–229.
- [16] R. Grone, R. Merris, V. S. Sunder, The Laplacian spectrum of a graph, SIAM J. Matrix Anal. Appl. 11 (1990) 218–238.
- [17] I. Gutman, Lower bounds for Estrada index, Publ. Inst. Math. (Beograd) 83 (2008) 1–7.
- [18] I. Gutman, B. Zhou, Laplacian energy of a graph, Lin. Algebra Appl. 414 (2006) 29–37.
- [19] J. Li, W. C. Shiu, W. H. Chan, Note on the Laplacian Estrada index of a graph, MATCH Commun. Math. Comput. Chem. 66 (2011) 777-784.
- [20] J. Li, W. C. Shiu, A. Chang, On the Laplacian Estrada index of a graph, Appl. Anal. Discr. Math. 3 (2009) 147–156.
- [21] J. Li, J. Zhang, On the Laplacian Estrada index of unicyclic graphs, MATCH Commun. Math. Comput. Chem. 68 (2012) 835–842.
- [22] B. Zhou, On Estrada index, MATCH Commun. Math. Comput. Chem. 60 (2008) 485–492.
- [23] B. Zhou, On sum of powers of Laplacian eigenvalues and Laplacian Estrada index of graphs, MATCH Commun. Math. Comput. Chem. 62 (2009) 611–619.
- [24] B. Zhou, I. Gutman, More on the Laplacian Estrada index, Appl. Anal. Discr. Math. 3 (2009) 371–378.
- [25] B. X. Zhu, On the Laplacian Estrada index of graphs, MATCH Commun. Math. Comput. Chem. 66 (2011) 769–776.