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Note on Laplacian Energy of Graphs

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Abstract

Let G be a graph with n vertices and m edges. Denote by $\mu_1, \mu_2, \dots, \mu_n$ the Laplacian eigenvalues of G. Recently, I. Gutman and B. Zhou [17] proposed an energy-like quantity, Laplacian energy, defined to be $LE(G) = \sum_{i=1}^{n} |\mu_i - \frac{2m}{n}|$, and some bounds concerning this quantity have been obtained there. In this note, a few more novel bounds for LE(G) are presented.

INTRODUCTION

The concept of graph energy was introduced by Gutman long time ago. Recently this concept started to attract considerable attention of mathematicians and

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mathematical chemists; for recent mathematical works on the energy of graphs see [11, 12, 13, 14, 15, 16, 19, 20, 21, 22] and the references cited therein.

Let $\mu_1, \mu_2, \dots, \mu_n$ be the Laplacian eigenvalues of G. Recently, Gutman and Zhou [17] proposed an energy-like quantity LE(G), called *Laplacian energy*, which is based on the eigenvalues of the Laplacian matrix of G and defined to be $LE(G) = \sum_{i=1}^{n} |\mu_i - \frac{2m}{n}|$.

In [17], numerous similarities and dissimilarities between the ordinary energy and the Laplacian energy are analyzed. Also, various bounds for LE(G) have been obtained in [17, 18, 23]. In this note, some new bounds for LE(G) have been obtained.

Let G be a simple graph with n vertices and m edges. The ordinary spectrum of G, consisting of the numbers $\lambda_1, \lambda_2, ..., \lambda_n$, is the spectrum of the adjacent matrix A(G) of G. The energy of the graph G is then defined as

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

The Laplacian spectrum of G, consisting of the numbers $\mu_1, \mu_2, \dots, \mu_n$, is the spectrum of the Laplacian matrix L(G) of G. Then

$$LE(G) = \sum_{i=1}^{n} |\gamma_i|, \qquad (2)$$

where

$$\gamma_i = \mu_i - \frac{2m}{n}.\tag{3}$$

The ordinary graph eigenvalues obey the following relations:

$$\sum_{i=1}^{n} \lambda_i = 0 \quad \text{and} \quad \sum_{i=1}^{n} (\lambda_i)^2 = 2m.$$
(4)

Analogous relations hold for the Laplacian energy as given below:

$$\sum_{i=1}^{n} \gamma_{i} = 0 \quad \text{and} \quad \sum_{i=1}^{n} (\gamma_{i})^{2} = 2M.$$
(5)

Here

$$M = m + \frac{1}{2} \sum_{i=1}^{n} (\delta_i - \frac{2m}{n})^2$$
(6)

and δ_i denotes the degree of the i - th vertex of G.

UPPER AND LOWER BOUNDS ON LE(G)

D. de Caen reported the following result in [25].

Lemma 1 Let G be a simple graph with n vertices and m edges. Then

$$\sum_{i=1}^{n} (\delta_i)^2 \le m \left[\frac{2m}{n-1} + n - 2 \right].$$

The following three Lemmas are due to K. C. Das [24].

Lemma 2 Let G be a simple graph with n vertices and m edges. Then

$$\sum_{i=1}^{n} (\delta_i)^2 \le m \left(\frac{2m}{n-1} + n - 2\right) - \delta_1 \left[\frac{4m}{n-1} - 2m_1 - \frac{n+1}{n-1}\delta_1 + (n-1)\right],$$

where δ_1 is the highest degree and m_1 is the average degree of the vertices adjacent to one of the vertices with degree δ_1 .

Lemma 3 Let G be a simple graph with n vertices and m edges. Then

$$\sum_{i=1}^{n} (\delta_i)^2 \le 2mn - n(n-1)\delta_n + 2m(\delta_n - 1),$$

where δ_n is the lowest degree.

Lemma 4 Let G be a simple graph with n vertices and m edges. Then

$$\sum_{i=1}^{n} (\delta_i)^2 \le m(m+1).$$

Now we are ready to give an upper bound on LE(G).

Proposition 5 Let G be a simple graph with n vertices and m edges. Then

$$LE(G) \le \sqrt{mn^2 - \frac{4m^2}{n} + \frac{2nm^2}{n-1}}.$$

Proof. In view of Eq.(6), we obtain

$$M = m + \frac{1}{2} \left(\sum_{i=1}^{n} \delta_i^2 - \frac{4m}{n} \sum_{i=1}^{n} \delta_i + \frac{4m^2}{n^2} \right)$$
$$= \left(m - \frac{2m^2}{n} \right) + \frac{1}{2} \sum_{i=1}^{n} \delta_i^2.$$

Using Cauchy-Schwartz inequality, and bearing in mind Eqs.(2), (3) and (5), we deduce that

$$LE(G) = \sum_{i=1}^{n} |\gamma_i| \leq \sqrt{n \sum_{i=1}^{n} \gamma_i^2} = \sqrt{2nM}.$$

Now applying Lemma 1 gives directly

$$LE(G) \leq \sqrt{2n\left[\left(m-\frac{2m^2}{n^2}\right)+\frac{1}{2}\sum_{i=1}^n \delta_i^2\right]},$$

which implies readily the result of Proposition 5.

Using the same reasoning as employed in Proposition 5, and by Lemmas 2–4, one can obtain the following

Proposition 6 Let G be a simple graph with n vertices and m edges. Then

$$LE(G) \le \sqrt{mn\left(\frac{2m}{n-1} + n\right) - \frac{4m^2}{n} + n\delta_1\left[\frac{4m}{n-1} - 2m_1 - \frac{(n+1)}{n-1}\delta_1 + (n-1)\right]}$$

Proposition 7 Let G be a simple graph with n vertices and m edges. Then

$$LE(G) \le \sqrt{(-n^3 + n^2 + 2mn)\delta_n + 2mn^2 - \frac{4m^2}{n}}.$$

Proposition 8 Let G be a simple graph with n vertices and m edges. Then

$$LE(G) \le \sqrt{3mn + nm^2 - \frac{4m^2}{n}}.$$

In the subsequent part of this section, we introduce some lower bounds for LE(G). As usual, we state some lemmas originated from [24].

Lemma 9 Let G be a simple graph with n vertices and m edges. Then

$$\sum_{i=1}^{n} (\delta_i)^2 \ge (\delta_1)^2 + (\delta_n)^2 + \frac{(2m - \delta_1 - \delta_n)^2}{n - 2},$$

where δ_1 and δ_n denote resp. the maximum and minimum degree of vertices in G.

Lemma 10 Let G be a simple graph with n vertices and m edges. Then

$$\sum_{i=1}^{n} (\delta_i)^2 \ge 2m(2p+1) - pn(1+p),$$

where $p = \left[\frac{2m}{n}\right]$.

Lemma 11 Let G be a simple graph with n vertices and m edges. Then

$$\sum_{i=1}^{n} (\delta_i)^2 \ge (\delta_1 - \delta_n)^2 + \delta_1 + \delta_n (2m - \delta_n).$$

Proposition 12 Let G be a simple graph with n vertices and m edges. Then

$$LE(G) \ge \sqrt{4\left(m - \frac{2m^2}{n^2}\right) + 2\left[\delta_1^2 + \delta_n^2 + \frac{(2m - \delta_1 - \delta_n)^2}{n - 2}\right]}.$$

Proof. Recall that $LE(G) \ge 2\sqrt{M}$ (see [17]). By Eq.(6) and Lemma 9, the result follows immediately.

Similar to Proposition 12, we get

Proposition 13 Let G be a simple graph with n vertices and m edges. Then

$$LE(G) \ge \sqrt{4\left(m - \frac{2m^2}{n^2}\right) + 4m(2p+1) - 2pn(1+p)}$$

where $p = \left[\frac{2m}{n}\right]$.

Proposition 14 Let G be a simple graph with n vertices and m edges. Then

$$LE(G) \ge \sqrt{4\left(m - \frac{2m^2}{n^2}\right) + 2(\delta_1 - \delta_n)^2 + 2\delta_1 + 2\delta_n(2m - \delta_n)}.$$

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References

- I. Gutman, Acyclic systems with extremal Huckel π- electron energy, Theor. Chim. Acta. 45 (1977) 79-87.
- [2] I. Gutman, Total π- electron energy of benzenoid hydrocarbon, Topic. Curr. Chem. 162 (1992) 29-63.
- [3] I. Gutman and O. E. Polansky, Mathematical Concepts in Organic Chemistry (Springer, Berlin, 1986).
- [4] I. Gutman, Acyclic conjugated molecules, trees and their energies, J.Math. Chem. 2 (1987) 123-143.
- [5] I. Gutman, The energy of a graph: old and new results, in: Algebra Combinatorics and Applications eds. A. Betten, A. Kohnert, R. Laue and A. Wassermann (Springer -Verlag, Berlin, 2001), pp. 196-211.
- [6] H. S. Ramane, H. B. Walikar, S. B. Rao, B. D. Acharya, P. R. Hampiholi, S. R. Jog and I. Gutman, Equienergetic graphs, *Kragujevac J. Math.* 26 (2004) 5–13.
- [7] H. S. Ramane, I. Gutman, H. B. Walikar and S. B. Halkarni, Another class of equienergetic graphs, *Kragujevac J. Math.* 26 (2004) 15–18.
- [8] L. Ye and R. Chen, Ordering of trees with a given bipartition by their energies and hosoya indices, MATCH Commun. Math. Comput. Chem. 52 (2004) 193-208.
- [9] H. S. Ramane, H. B. Walikar, S. B. Rao, B. D. Acharya, P. R. Hampiholi, S. R. Jog and I. Gutman, Spectra and energies of iterated line graphs of regular graphs. *Appl. Math. Lett.* 18 (2005) 679–682.

- [10] I. Gutman, Topology and stability of conjugated hydrocarbons. The dependence of total π -electron energy on molecular topology, J. Serb. Chem. Soc. **70** (2005) 441-456.
- [11] B. Zhou and F. Li, On minimal energies of trees of a prescribed diameter, J.Math.Chem. 39 (2006) 465-473.
- [12] A. Yu, M. Lu and F. Tian, New upper bounds for the energy of graphs, MATCH Commun. Math. Comput. Chem. 53 (2005) 441-448.
- [13] W. Yan and L. Ye, On the maximal energy and the Hosoya index of a type of trees with many pendant vertices, MATCH Commun. Math. Comput. Chem. 53 (2005) 449-459.
- [14] W. Lin, X. Guo and H. Li, On the extremal energies of trees with a given maximum degree, MATCH Commun. Math. Comput. Chem. 54 (2005) 363-378.
- [15] F. Li and B. Zhou, Minimal energy of bipartite unicyclic graphs of a given bipartition, MATCH Commun. Math. Comput. Chem. 54 (2005) 379-388.
- [16] G. Indulal and A. Vijayakumar, On a pair of equienergetic graphs, MATCH Commun. Math. Comput. Chem. 55 (2006) 83-90.
- [17] I. Gutman and B. Zhou, Laplacian energy of a graph, *Lin. Algebra Appl.* 414 (2006) 29-37.
- [18] B. Zhou and I. Gutman, On Laplacian energy of graphs, MATCH Commun. Math. Comput. Chem. 57 (2007) 211-220.
- [19] Y. Hou, Z. Teng and C. Woo, On the spectral radius, k-degree and the upper bound of energy in a graph, MATCH Commun. Math. Comput. Chem. 57 (2007) 341-350.
- [20] H. Hua, On minimal energy of unicyclic graphs with prescribed girth and pendent vertices, MATCH Commun. Math. Comput. Chem. 57 (2007) 351-361.
- [21] H. Hua, Bipartite unicyclic graphs with large energy, MATCH Commun. Math. Comput. Chem. 58 (2007) 57-73.
- [22] I. Gutman, B. Furtula and H. Hua, Bipartite unicyclic graphs with maximal, second-maximal and third-maximal energy, MATCH Commun. Math. Comput. Chem. 58 (2007) 75-82.
- [23] B. Zhou and I. Gutman, Nordhaus-Gaddum type relations for the energy and Laplacian energy of graphs, *Bulletin, de l'Acdémie serbe des Sciences et des Arts* (Cl. Math. Natur.), in press.

- [24] Kinkar Ch. Das, Sharp bounds for the sum of the squares of the degrees of a graph, *Kragujevac J. Math.* 25 (2003) 31–49.
- [25] D. de Caen, An upper bound on the sum of squares of degrees in a graph, *Discrete Math.* 185 (1998) 245–248.
- [26] D. Cvetkovic, M. Doob and H. Sachs, Spectra of Graphs, (Academic Press, New York, 1980).