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# *Some Lower Bounds for Estrada Index*

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**ABSTRACT**

For a graph $G$ with $n$ vertices, its Estrada index is defined as $EE(G) = \sum_{i=1}^{n} e^{\lambda_i}$ where $\lambda_1, \lambda_2, \ldots, \lambda_n$ are the eigenvalues of $G$. A lot of properties especially lower and upper bounds for the Estrada index are known. We now establish further lower bounds for the Estrada index.

**Keywords:** Estrada index, eigenvalues (of graph), spectral moments, lower bounds.

## 1 INTRODUCTION

Let $G$ be a simple graph with $n$ vertices. Let $\lambda_1, \lambda_2, \ldots, \lambda_n$ be the eigenvalues of $G$ arranged in a non-increasing order [1]. The Estrada index of the graph $G$ is defined as

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

This graph invariant was proposed as a structure-descriptor, used in the modeling of certain features of the 3D structure of organic molecules [2], in particular of the degree of proteins and other long-chains biopolymers [3,4]. It has also found applications in a large variety of other problems, see, e.g., [5−7]. Lower and upper bounds have been established for the Estrada index, see [8−14]. Some other properties for the Estrada index may be found in [15−19]. Here we present some easily computed lower bounds for the Estrada index.

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## 2 PRELIMINARIES

Let $G$ be a graph with $n$ vertices. For $k = 0,1,2,\ldots,$ denote by $M_k = M_k(G)$ the $k$-th spectral moment of the graph $G$, i.e., $M_k = \sum_{i=1}^{n} \lambda_i^k$. Note that $M_1 = 0$. Then

$$EE(G) = \sum_{i=1}^{n} \sum_{k\geq 0} \frac{\lambda_i^k}{k!} = \sum_{k\geq 0} \frac{M_k}{k!} = n + \sum_{k\geq 2} \frac{M_k}{k!}.$$

The first Zagreb index [20] of the graph $G$ is defined as $Zg(G) = \sum_{u\in V(G)} d_u^2$, where $d_u$ is the degree of vertex $u$ and $V(G)$ is the vertex set of $G$. Let $t(G)$ be the number of triangles in $G$. Recall that $M_k$ is equal to the number of closed walks of length $k$ in the graph [1].

**Lemma 1.** Let $G$ be a graph with $m$ edges. Then for $k \geq 4$, $M_{k+2} \geq M_k$ with equality for all even $k \geq 4$ if and only if $G$ consists of $m$ copies of complete graph on two vertices and possibly isolated vertices, and with equality for all odd $k \geq 5$ if and only if $G$ is a bipartite graph.

**Proof** (i) For even $k \geq 4$, by repeating the first edge twice for a closed walk of length $k$, we get a closed walk of length $k+2$, and then $M_{k+2} \geq M_k$ with equality for all even $k \geq 4$ if and only if $G$ consists of $m$ copies of complete graph on two vertices and possibly isolated vertices.

(ii) For odd $k \geq 5$, by similar considering as above, it is easily seen that $M_{k+2} \geq M_k$ with equality for all odd $k \geq 5$ if and only if $G$ is bipartite. ■

## 3 RESULTS

We now establish several lower bounds for the Estrada index and compare them with the known bounds in the literature.

**Proposition 2.** Let $G$ be a graph with $n$ vertices and $m$ edges. Then

$$EE(G) \geq n + m + t(G) + \frac{1}{2}(e + e^{-1} - 3)M_4 + \frac{1}{2}\left(e - e^{-1} - \frac{7}{3}\right)M_5 \tag{1}$$

$$EE(G) \ge n + m + t(G) + (e + e^{-1} - 3)[Zg(G) - m] + 15\left(e - e^{-1} - \frac{7}{3}\right)t(G) \tag{2}$$

with either equality if and only if $G$ consists of $m$ copies of complete graph on two vertices and possibly isolated vertices.

**Proof.** Note that $M_2 = 2m,\ M_3 = 6t(G).$ By Lemma 1,

$$\begin{aligned} EE(G) &= n + m + t(G) + \sum_{k\ge 2}\frac{M_{2k}}{(2k)!} + \sum_{k\ge 2}\frac{M_{2k+1}}{(2k+1)!} \\ &\ge n + m + t(G) + \sum_{k\ge 2}\frac{M_4}{(2k)!} + \sum_{k\ge 2}\frac{M_5}{(2k+1)!} \\ &= n + m + t(G) + M_4\left(\frac{e+e^{-1}}{2} - 1 - \frac{1}{2!}\right) + M_5\left(\frac{e-e^{-1}}{2} - 1 - \frac{1}{3!}\right) \\ &= n + m + t(G) + \frac{1}{2}(e + e^{-1} - 3)M_4 + \frac{1}{2}\left(e - e^{-1} - \frac{7}{3}\right)M_5 \end{aligned}$$

with equality if and only if $M_k = M_4$ for all even $k \ge 4$ and $M_k = M_5$ for all odd $k \ge 5$, which by Lemma 1, is equivalent to the fact that $G$ consists of $m$ copies of complete graph on two vertices and possibly isolated vertices.

For a fixed vertex $u$, there are at least $d_u^2$ closed walks of length four starting from $u$ and $d_u(d_u - 1)$ closed walks of length four starting from a neighbor of $u$ such that vertices in such walks are only $u$ and its neighbors, and then $M_4 \ge 2Zg(G) - 2m.$ (Actually, $M_4 = 2Zg(G) - 2m + 8q$ where $q$ is the number of quadrangles in $G$, see [21]). Note also that $M_5 \ge 30t(G)$ because there are ten closed walks of length five starting from a fixed vertex on a fixed triangle such that the vertices of the walks are only the vertices of the triangle. (Actually, $M_5 = 30t(G) + 10p + 10r$ where $p$ is the number of pentagons, and $r$ is the number of subgraphs consisting of a triangle with a pendent vertex attached [21]. Now the second inequality follows. ■

**Corollary 3.** Let $G$ be a graph with $n$ vertices and $m$ edges. Then

$$EE(G) \ge n + m + (e + e^{-1} - 3)[Zg(G) - m] \tag{3}$$

with equality if and only if $G$ consists of $m$ copies of complete graphs on two vertices and possibly isolated vertices.

Recently, Das and Lee [14] showed that for a connected graph with $n$ vertices and $m \geq 1.8n+4$ edges, $EE(G) > EE(P_n)$. This may be improved slightly using Corollary 3. Recall that [14] $EE(P_n) < 2.746n+3.569$. If $m \geq 1.4n+2$, then by Corollary 3 and the Cauchy-Schwarz inequality, we have

$$EE(G) \geq n+m+(e+e^{-1}-3)\left(\frac{4m^2}{n}-m\right) > 2.746n+3.569 > EE(P_n).$$

**Remark 4.** For a graph $G$ with $n \geq 2$ vertices, it was shown in [12] that

$$EE(G) \geq e^{\lambda_1}+(n-1)e^{-\frac{\lambda_1}{n-1}} \tag{4}$$

with equality if and only if $G$ is the empty graph or the complete graph. Obviously, (3) and (4) are incomparable.

**Remark 5.** Let $G$ be a graph with $n$ vertices, $m$ edges and nullity (number of zero eigenvalues) $n_0 < n$. Note that $n_0 = n$ if and only if $G$ is an empty graph. Gutman [11] showed that

$$EE(G) \geq n_0 + \frac{n-n_0}{2}(e^a+e^{-a}) \tag{5}$$

with equality if and only if $n-n_0$ is even, $G$ consists of copies of complete bipartite graphs $K_{r_j,t_j}$, $j=1,2,\ldots,(n-n_0)/2$, such that all $r_j t_j$ are equal, and the remaining vertices if exist are isolated vertices, where $a=\sqrt{2m/(n-n_0)}$. A different proof may be found in [12]. For odd cycle $C_n$ with $n \geq 3$, $n_0 = 0$ (see [21]) and $m = n$, we have

$$\begin{aligned} & n+m+(e+e^{-1}-3)[Zg(G)-m]-\left[n_0+\frac{n-n_0}{2}\left(e^a+e^{-a}\right)\right] \\ &= n\left[2+3(e+e^{-1}-3)-\frac{e^{\sqrt{2}}+e^{-\sqrt{2}}}{2}\right] > 0. \end{aligned}$$

Then for odd cycle $C_n$ with $n \geq 3$, the bound in (3) is better than the one in (5), and thus it is easily seen that (3) and (5) are incomparable in general.

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## REFERENCES

1. D. M. Cvetković, M. Doob and H. Sachs, *Spectra of Graphs – Theory and Application*, Johann Ambrosius Barth, Heidelberg, 1995.
2. E. Estrada, Characterization of 3D molecular structure, *Chem. Phys. Lett.* **319** (2000) 713−718.
3. E. Estrada, Characterization of the folding degree of proteins, *Bioinformatics* **18** (2002) 697−704.
4. E. Estrada, Characterization of the amino acid contribution to the folding degree of proteins, *Proteins* **54** (2004) 727−737.
5. E. Estrada and J. A. Rodríguez−Valázquez, Subgraph centrality in complex networks, *Phys. Rev. E* **71** (2005) 056103−1−9.
6. E. Estrada and J. A. Rodríguez-Valázquez, Spectral measures of bipartivity in complex networks, *Phys. Rev. E* **72** (2005) 046105−1−6.
7. E. Estrada, J. A. Rodríguez-Valázquez and M. Randić, Atomic branching in molecules, *Int. J. Quantum Chem.* **106** (2006) 823−832.
8. J. A. de la Peña, I. Gutman and J. Rada, Estimating the Estrada index, *Lin. Algebra Appl.* **427** (2007) 70−76.
9. I. Gutman and S. Radenković, A lower bound for the Estrada index of bipartite molecular graphs, *Kragujevac J. Sci.* **29** (2007) 67−72.
10. I. Gutman, E. Estrada and J. A. Rodríguez−Velázquez, On a graph−spectrum−based structure descriptor, *Croat. Chem. Acta* **80** (2007) 151−154.
11. I. Gutman, Lower bounds for Estrada index, *Publ. Inst. Math. Beograd* (*N.S.*) **83** (2008) 1−7.
12. B. Zhou, On Estrada index, *MATCH Commun. Math. Comput. Chem.* **60** (2008) 485−492.
13. B. Zhou and N. Trinajstić, Estrada index of bipartite graphs, *Int. J. Chem. Model.* **1** (2008) 387−394.

14. K. C. Das and S.–G. Lee, On the Estrada index conjecture, *Lin. Algebra Appl.* **431** (2009) 1351–1359.

15. I. Gutman, S. Radenković, A. Graovac and D. Plavšić, Monte Carlo approach to Estrada index, *Chem. Phys. Lett.* **446** (2007) 233–236.

16. I. Gutman, B. Furtula, V. Marković and B. Glišić, Alkanes with greatest Estrada index, *Z. Naturforsch.* **62a** (2007) 495–498.

17. I. Gutman and A. Graovac, Estrada index of cycles and paths, *Chem. Phys. Lett.* **436** (2007) 294–296.

18. I. Gutman, S. Radenković and B. Furtula, Relating Estrada index with spectral radius, *J. Serb. Chem. Soc.* **72** (2007) 1321–1327.

19. I. Gutman and S. Radenković, Estrada index of benzenoid hydrocarbons, *Z. Naturforsch.* **62a** (2007) 254–258.

20. I. Gutman and K. C. Das, The first Zagreb index 30 years after, *MATCH Commun. Math. Comput. Chem.* **50** (2004) 83–92.

21. D. M. Cvetković, M. Doob, I. Gutman and A. Torgašev, *Recent Results in the Theory of Graph Spectra*, North-Holland, Amsterdam, 1988.