

# Lower Bounds for Gaussian Estrada Index of Graphs

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Received: 3 July 2018; Accepted: 6 August 2018; Published: 7 August 2018

**Abstract:** Suppose that  $G$  is a graph over  $n$  vertices.  $G$  has  $n$  eigenvalues (of adjacency matrix) represented by  $\lambda_1, \lambda_2, \dots, \lambda_n$ . The Gaussian Estrada index, denoted by  $H(G)$  (Estrada et al., *Chaos* 27(2017) 023109), can be defined as  $H(G) = \sum_{i=1}^n e^{-\lambda_i^2}$ . Gaussian Estrada index underlines the eigenvalues close to zero, which plays an important role in chemistry reactions, such as molecular stability and molecular magnetic properties. In a network of particles governed by quantum mechanics, this graph-theoretic index is known to account for the information encoded in the eigenvalues of the Hamiltonian near zero by folding the graph spectrum. In this paper, we establish some new lower bounds for  $H(G)$  in terms of the number of vertices, the number of edges, as well as the first Zagreb index.

**Keywords:** Gaussian Estrada index; Zagreb index; lower bound; graph spectrum

## 1. Introduction

Suppose that  $G$  is an undirected, simple graph containing  $n$  vertices and  $m$  edges. Throughout the paper, we will refer to such a graph as an  $(n, m)$ -graph. Denote by  $A = A(G)$  the adjacency matrix of  $G$ . Clearly, it is a real symmetric matrix. The eigenvalues of  $A$ , forming the spectrum of  $G$  [1], can be sorted in a non-increasing order as  $\lambda_1 \geq \lambda_2 \geq \dots \geq \lambda_n$ .

The Estrada index of the graph  $G$  has been defined in [2–7] as

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

As a revealing graph-spectrum-based invariant, it has found numerous applications in chemistry, physics, and complex networks. For example, it has been used to measure the degree of folding of some classes of long-chain molecules, including proteins [2–4]. The folding degree of protein chains can be described by the sum of cosines of dihedral angles of the protein main chain. Remarkably,  $EE$  is shown to distinguish between protein structures where the above sum is identical.  $EE$  also serves as an insightful measure for investigating robustness of complex networks [8–10], for which  $EE$  has an acute discrimination on connectivity and changes monotonically with respect to the removal or addition of edges. There has been a vast literature related to Estrada index and its bounds; see e.g., [11–17]. Other closely related indices include the incidence energy; see e.g., [18].

Please note that  $EE$  is dominated by the largest eigenvalue  $\lambda_1$  if the gap  $\lambda_1 - \lambda_2$  is large. The information of topological properties hidden in the smaller eigenvalues of  $A$  has been overlooked in  $EE$ , and more generally, in matrix functions of the form  $f(A) = \sum_{k=0}^{\infty} c_k A^k$ . Zero eigenvalue and eigenvalues close to zero of  $A$  play a fundamental role in molecular magnetic/stability properties when  $A$  delineates the tight-binding Hamiltonian in the Hückel molecular orbital theory [19,20]. Many chemical reactivities are closely related to the lowest unoccupied molecular orbital (namely, the largest negative eigenvalue of  $A$ ) and the highest occupied molecular orbital (namely, the smallest positive eigenvalue of  $A$ ). For example, electron transfers from the highest occupied molecular orbital of one molecule to the lowest unoccupied molecular orbital of another molecule play a vital part in several

organic chemical reactions; see [20] for a survey. As such, Estrada et al., [21] recently propose to extract key structural information hidden in the eigenvalues in proximity to zero in the spectra of networks by using a Gaussian matrix function. This novel method leads to the Gaussian Estrada index,  $H(G)$ , characterized as follows:

$$H = H(G) = \text{Tr}(e^{-A^2}) = \sum_{i=1}^n e^{-\lambda_i^2}, \quad (2)$$

where  $\text{Tr}(\cdot)$  represents the trace of a square matrix. Since the adjacency matrix  $A$  of a simple graph  $G$  usually contains both positive and negative eigenvalues, the Gaussian Estrada index ideally symbolizes the significance of the eigenvalues in proximity to zero (so called the “middle” part) in the spectrum of graph.

It is worth mentioning that in a network  $G$  of particles governed by the rules of quantum mechanics, the Gaussian Estrada index  $H$  can be viewed as the partition function of the system with Hamiltonian  $A^2$  based on the folded spectrum method [22]. This quantity associated with the time-dependent Schrödinger equation with the squared Hamiltonian reveals information encoded in the eigenvalues near zero. In fact, unlike  $EE$  which gives more weight to the large eigenvalues,  $H$  stresses those close to zero. As shown via numerical simulations in [21],  $H$  is able to distinguish between the dynamics of a particle hopping over a bipartite network from the one hopping over a non-bipartite network. This is impossible for  $EE$  as the large eigenvalues are usually not correlated with the emergence of bipartite structure. Hence, characterization (such as lower and upper bounds) of  $H$  turns out to be highly desirable in quantum information theory.

The Gaussian Estrada index of some simple graphs including complete graphs, paths, cycles, and Erdős-Rényi random graphs as well as BA random networks has been studied in [21]. Signify the star graph on  $n$  vertices by  $K_{1,n-1}$ . Recall that star graphs are the only connected graphs in which at most one vertex has degree greater than one. The following important mathematical property on  $H$  is established.

**Theorem 1** ([21]). *Assume that  $G$  is an  $(n, m)$ -graph. Then*

$$H(G) \leq n - 2 + 2e^{1-n}. \quad (3)$$

*The equality in (3) is attained if and only if  $G = K_{1,n-1}$ .*

To better understand the properties for the Gaussian Estrada index  $H(G)$ , we in this paper aim to establish some new lower bounds for  $H$  in terms of the number of vertices  $n$  and the number of edges  $m$ .

## 2. Results and Discussion

To fix notation, we first introduce some preliminaries. For  $k \geq 0$ , define by  $M_k = M_k(G) = \sum_{i=1}^n \lambda_i^k$  the  $k$ -th spectral moment of the graph  $G$ . It is well-known that  $M_k$  counts the number of self-returning walks of length  $k$  in the graph [1]. A bit of basic algebra leads to the following expression.

$$H = \sum_{k=0}^{\infty} \sum_{i=1}^n \frac{(-\lambda_i^2)^k}{k!} = \sum_{k=0}^{\infty} \frac{(-1)^k}{k!} M_{2k}. \quad (4)$$

By convention,  $K_n$  represents the complete graph over  $n$  vertices and  $\overline{K_n}$  represents its (edgeless) complement.

**Theorem 2.** *Suppose that  $G$  is an  $(n, m)$ -graph. If  $m \leq \frac{n}{2}$ , then we have*

$$H(G) \geq n - 2m. \quad (5)$$

The equality in (5) is attained if and only if  $G = \overline{K_n}$ .

**Proof.** Following (4) and noting that  $M_0 = n$  and  $M_2 = 2m$ , we obtain

$$H(G) = \sum_{i=1}^n \sum_{k=0}^{\infty} \frac{(-\lambda_i^2)^k}{k!} = n - 2m + \sum_{i=1}^n \sum_{k=2}^{\infty} \frac{(-\lambda_i^2)^k}{k!}.$$

Since  $e^{-\lambda_i^2} \geq 1 - \lambda_i^2$  holds for all  $i$ , we observe that  $\sum_{k=2}^{\infty} \frac{(-\lambda_i^2)^k}{k!} \geq 0$ . Hence, for any  $\delta \in [0, 1]$ , we have

$$\begin{aligned} H(G) &\geq n - 2m + \delta \sum_{i=1}^n \sum_{k=2}^{\infty} \frac{(-\lambda_i^2)^k}{k!} \\ &= n - 2m - \delta n + 2m\delta + \delta \sum_{i=1}^n \sum_{k=0}^{\infty} \frac{(-\lambda_i^2)^k}{k!} \\ &= (1 - \delta)n + 2(\delta - 1)m + \delta H(G). \end{aligned}$$

For  $\delta < 1$ , it follows that

$$H(G) \geq \frac{(1 - \delta)n + 2(\delta - 1)m}{1 - \delta} = n - 2m.$$

It is clear that the equality in (5) will be attained if and only if every eigenvalue is equal to zero, namely,  $G = \overline{K_n}$ .  $\square$

Since  $H(G) > 0$  always holds, Theorem 2 is non-trivial when  $m < \frac{n}{2}$ . The next result is also for sparse graphs.

**Theorem 3.** Suppose that  $G$  is an  $(n, m)$ -graph. If  $m \leq \frac{n}{4} + \frac{n(n-1)}{4}e^{-\frac{4m}{n}}$ , then

$$H(G) \geq \sqrt{n - 4m + n(n - 1)e^{-\frac{4m}{n}}}. \tag{6}$$

The equality in (6) is attained if and only if  $G = \overline{K_n}$ .

**Proof.** According to the definition of  $H$ , we obtain

$$H^2 = \sum_{i=1}^n e^{-2\lambda_i^2} + 2 \sum_{1 \leq i < j \leq n} e^{-\lambda_i^2} e^{-\lambda_j^2}. \tag{7}$$

It follows from the Arithmetic-Geometric (A-G) inequality, the symmetry of  $i$  and  $j$ , and  $M_2 = 2m$  that

$$\begin{aligned} 2 \sum_{1 \leq i < j \leq n} e^{-\lambda_i^2} e^{-\lambda_j^2} &\geq n(n - 1) \left( \prod_{1 \leq i < j \leq n} e^{-\lambda_i^2} e^{-\lambda_j^2} \right)^{\frac{2}{n(n-1)}} \\ &= n(n - 1) \left( \prod_{i=1}^n (e^{-\lambda_i^2})^{n-1} \right)^{\frac{2}{n(n-1)}} \\ &= n(n - 1) \left( \prod_{i=1}^n e^{-\lambda_i^2} \right)^{\frac{2}{n}} \\ &= n(n - 1) \left( e^{-\sum_{i=1}^n \lambda_i^2} \right)^{\frac{2}{n}} = n(n - 1)e^{-\frac{4m}{n}}. \end{aligned} \tag{8}$$

Arguing similarly as in Theorem 2, we deduce

$$\sum_{i=1}^n e^{-2\lambda_i^2} = \sum_{i=1}^n \sum_{k=0}^{\infty} \frac{(-2\lambda_i^2)^k}{k!} = n - 4m + \sum_{i=1}^n \sum_{k=2}^{\infty} \frac{(-2\lambda_i^2)^k}{k!} \geq n - 4m. \quad (9)$$

By substituting (8) and (9) into (7), we have

$$H(G) \geq \sqrt{n - 4m + n(n-1)e^{-\frac{4m}{n}}}.$$

The equality in (6) will be attained if and only if every eigenvalue is equal to zero, namely,  $G = \overline{K_n}$ .

□

**Remark 1.** In general, Theorem 2 and Theorem 3 are incomparable in terms of the range of applicability. For example, when  $2m = n$  and  $n \leq 8$ , Theorem 2 is applicable but Theorem 3 is not. On the other hand, when  $m = \frac{n}{4} \ln \ln n$ , Theorem 3 is applicable but Theorem 2 is not. Furthermore, when both theorems can be applied, the results of them are still incomparable generally. For instance, when  $4m = n$ , (5) yields  $H(G) \geq \frac{n}{2}$ . The inequality (6) gives  $H(G) \geq \sqrt{n(n-1)e^{-1}}$ , which is greater than  $\frac{n}{2}$  for  $n \geq 3$ , but smaller than  $\frac{n}{2}$  for  $n \leq 2$ .

Next, we consider the lower bound of  $H$  for denser graphs with  $m \geq \frac{n}{2}$ . The first Zagreb index [23] of the graph  $G$  is defined as  $Zg = Zg(G) = \sum_{i=1}^n d_i^2$ , where  $d_i$  represents the degree of the  $i$ -th vertex in the graph  $G$ . The parameter  $Zg$  has relationship with numerous other graph invariants and has found varied applications in chemical graph theory. It is a useful molecular structure descriptor, characterizing e.g., the degree of branching in the molecular carbon-atom skeleton [24], as well as nanotubes [25].

**Theorem 4.** Suppose that  $G$  is an  $(n, m)$ -graph. If  $m \geq \frac{n}{2}$  and  $n \geq 2$ , then we obtain

$$H(G) \geq e^{-\frac{Zg}{n}} + (n-1)e^{\frac{Zg-2m}{n-1}}. \quad (10)$$

The equality is attained if and only if  $G$  admits  $\lambda_1 = \sqrt{\frac{Zg}{n}}$ ,  $\lambda_2 = \dots = \lambda_k = \frac{1}{n-2k+1} \sqrt{\frac{Zg}{n}}$  and  $\lambda_{k+1} = \dots = \lambda_n = -\frac{1}{n-2k+1} \sqrt{\frac{Zg}{n}}$  for some  $1 \leq k \leq \lfloor \frac{n}{2} \rfloor$ .

**Proof.** In view of the arithmetic-geometric inequality and  $M_2 = 2m$ , we obtain

$$\begin{aligned} H(G) &= e^{-\lambda_1^2} + \sum_{i=2}^n e^{-\lambda_i^2} \\ &\geq e^{-\lambda_1^2} + (n-1) \left( \prod_{i=2}^n e^{-\lambda_i^2} \right)^{\frac{1}{n-1}} \\ &= e^{-\lambda_1^2} + (n-1) e^{\frac{-\sum_{i=2}^n \lambda_i^2}{n-1}} \\ &= e^{-\lambda_1^2} + (n-1) e^{\frac{\lambda_1^2 - 2m}{n-1}}, \end{aligned}$$

with equality if and only if  $\lambda_2^2 = \dots = \lambda_n^2$ .

Since  $\lambda_1 \geq \frac{2m}{n} \geq 1$  [1], we have  $\lambda_1^2 \geq \frac{2m}{n}$ . It is straightforward to see that the mapping  $f(x) := e^{-x} + (n-1)e^{\frac{x-2m}{n-1}}$  is increasing for  $x \geq \frac{2m}{n}$ . Please note that  $\lambda_1 \geq \sqrt{\frac{Zg}{n}}$  with equality attained if and only if every component is either a regular graph of degree  $\lambda_1$  or a bipartite semiregular graph

such that the product of degrees of any two adjacent vertices is equal to  $\lambda_1^2$  based on a symmetry argument [26]. Therefore,  $\lambda_1^2 \geq \frac{Zg}{n} \geq \frac{2m}{n}$  by the definition of  $Zg$  and we have

$$H(G) \geq f\left(\frac{Zg}{n}\right) = e^{-\frac{Zg}{n}} + (n-1)e^{\frac{\frac{Zg}{n}-2m}{n-1}}. \quad (11)$$

If the eigenvalues of  $G$  are  $\lambda_1 = \sqrt{\frac{Zg}{n}}$ ,  $\lambda_2 = \dots = \lambda_k = \frac{1}{n-2k+1}\sqrt{\frac{Zg}{n}}$  and  $\lambda_{k+1} = \dots = \lambda_n = -\frac{1}{n-2k+1}\sqrt{\frac{Zg}{n}}$  for some  $1 \leq k \leq \lfloor \frac{n}{2} \rfloor$ , then the equality holds in (10). Conversely, if the equality is attained in (10), then  $\lambda_1 = \sqrt{\frac{Zg}{n}}$  and  $\lambda_2^2 = \dots = \lambda_n^2$ . We must have  $\lambda_1 > \lambda_2$ . (Otherwise, we have  $G = \overline{K}_n$ , which contradicts the assumptions  $m \geq \frac{n}{2}$  and  $n \geq 2$ .) Since  $\text{Tr}(A) = \sum_{i=1}^n \lambda_i = 0$ ,  $G$  must have the required eigenvalues as above.  $\square$

**Remark 2.** Since  $K_n$  has the eigenvalues  $\lambda_1 = n-1$  and  $\lambda_2 = \dots = \lambda_n = -1$ , it is direct to check that  $G = K_n$  attains the equality in (10). When  $G$  is connected, the equality in (10) implies that  $G$  has diameter less than or equal to two [1]. Also, when  $G$  is regular, the equality in (10) implies that  $G$  is strongly regular [1].

**Remark 3.** If we use  $H(G) \geq f\left(\frac{2m}{n}\right)$  instead in (11), we are led to the following simpler estimation

$$H(G) \geq ne^{-\frac{2m}{n}}, \quad (12)$$

where the equality is attained if and only if  $G = K_2$ .

In fact, to see the equality condition, we have, on one hand,  $H(K_2) = 2e^{-1}$  by direct calculation employing  $\lambda_1 = 1$  and  $\lambda_2 = -1$ . On the other hand, if the equality is attained in (12), then using the same argument as in Theorem 4 we know  $Zg = 2m$  and hence  $d_i = 0$  or  $1$  in  $G$ . Suppose that  $G$  is the union of  $\ell_1$  edges and  $\ell_2$  isolated nodes, namely,  $G = \ell_1 K_2 \cup \ell_2 K_1$  with  $2\ell_1 + \ell_2 = n$ . Please note that  $ne^{-\frac{2m}{n}} \leq ne^{-1} < (n-\ell_2)e^{-1} + \ell_2 = H(\ell_1 K_2 \cup \ell_2 K_1)$ , with both equalities hold if and only if  $\ell_2 = 0$ ,  $n = 2$  and  $m = 1$ . Thus,  $G = K_2$ .

**Remark 4.** It is noteworthy that the gap between upper and lower bounds for the Gaussian Estrada index  $H$  is typically much smaller than that for the Estrada index  $EE$ , especially for sparse graphs when  $m$  scales linearly with  $n$ . For example, when  $m = cn$  for some constant  $c > 1/2$ , it follows from (3) and (12) that  $ne^{-c} \leq H(G) \leq n-2+2e^{1-n}$ . The gap is only represented by a constant multiplier  $e^c$ . Recall that common bounds of  $EE$  (see, e.g., [14], Theorem 1) give  $n \leq EE(G) \leq n + e^{\sqrt{2cn}}$ .

### 3. Conclusions

In this paper, we present some novel  $(n, m)$ -type estimates for the recently introduced Gaussian Estrada index  $H(G)$ . Lower bounds for sparse ( $m \leq \frac{n}{2}$ ) and dense ( $m \geq \frac{n}{2}$ ) graphs are established. The gap between upper and lower bounds of  $H(G)$  is found to be much smaller than that of  $EE(G)$ .

A unique feature of Gaussian Estrada index, as compared to the extensively studied Estrada index, lies in its ability to uncover information encoded in the eigenvalues in proximity to zero.  $H(G)$  can be viewed as the partition function of the system governed by the time-dependent Schrödinger equation based on  $A^2(G)$ . Our results shed light on the understanding of  $H(G)$  and contribute to establishing new inequalities (such as lower and upper bounds) connecting varied interesting network invariants. Notice that the current work only focuses on deterministic graphs without randomness. It would be interesting to derive appropriate estimates for dynamic or random graphs [27,28].

**Funding:** This research was funded by National Natural Science Foundation of China grant number 11505127.

**Acknowledgments:** The author would like to thank the academic editor and the three anonymous referees for their constructive comments that have improved the presentation of this manuscript.

**Conflicts of Interest:** The author declares no conflict of interest.

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