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LOWER BOUNDS FOR THE ESTRADA INDEX USING MIXING TIME AND LAPLACIAN SPECTRUM

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ABSTRACT. The logarithm of the Estrada index has been recently proposed as a spectral measure to characterize the robustness of complex networks. We derive novel analytic lower bounds for the logarithm of the Estrada index based on the Laplacian spectrum and the mixing times of random walks on the network. The main techniques employed are some inequalities, such as the thermodynamic inequality in statistical mechanics, a trace inequality of von Neumann, and a refined harmonic-arithmetic mean inequality.

1. Introduction. Complex networks have recently attracted much interest due to their prevalence in nature and our daily lives. A complex network represents a system whose evolving structure and dynamic behavior contribute to its robustness [**23**]. The classical approaches for determining robustness of networks entail the use of basic concepts from graph theory. For example, the connectivity of a graph is a fundamental measure of robustness of a network. However, the node/edge connectivity only partly reflects the ability of graphs to retain connectedness after deletion. Other improved measures include conditional connectivity [**11**], fault diameter [**16**], toughness [**5**], scattering number [**14**], expansion parameter [**22**], etc. In contrast to node/edge connectivity, these measures treat both the cost to damage a network and how badly the network is damaged. Unfortunately, calculation for these parameters in general graphs is NP-complete. From the perspective of spectral analysis, the second smallest Laplacian eigenvalue (also known as the algebraic connectivity) is treated as a measure of how difficult it is to break a network into independent components [**10**]. However, for all disconnected networks the algebraic connectivity is reduced to zero. Therefore, it is coarse to some extent.

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Recently, the concept of the logarithm of the Estrada index is utilized in [**25, 26, 28**] as a spectral measure of robustness in networks. The Estrada index is expressed in mathematical form as a special case of average eigenvalue, and it characterizes the redundancy of alternative paths by quantifying the weighted number of closed walks of all lengths. It is shown [**26, 28**] that the Estrada index has acute discrimination in measuring the robustness of complex networks and can exhibit the variation of robustness sensitively even for disconnected networks. We mention that the recent work [**27**] has addressed the perturbation of the Estrada index in weighted networks based on some spectral techniques, which are different from those used in the current paper.

In this paper, we further study the logarithm of the Estrada index and provide novel lower bounds based on Laplacian eigenvalues of the network and the mixing times of random walks running on it. The key techniques employed in this paper involve several inequalities: a thermodynamic inequality [**1**], a trace inequality of von Neumann [**20**] and a refined harmonic-arithmetic mean inequality [**19**]. Our result sets up a bridge between the network robustness measure (the Estrada index) and several parameters in dynamical processes on networks (such as Laplacian spectrum, mixing time, Kemeny constant [**17**], etc.)

The rest of the paper is organized as follows. We present some preliminaries for the Estrada index, Laplacian spectrum and mixing times in Section 2. Lower bounds for the logarithm of the Estrada index are given in Section 3.

2. Preliminaries. In this section, we provide some necessary preliminaries leading to the concept of the Estrada index, Laplacian spectrum and mixing times of random walks on graphs.

Let $G = (V, E)$ be an undirected connected graph with $|V| = n$ vertices. Suppose G is a weighted graph with a weight function that assigns a non-negative weight a_{ij} to each pair (i, j) of vertices. The weights satisfy the following properties: $a_{ij} > 0$ if $(i, j) \in E$, $a_{ij} = 0$ if $(i, j) \notin E$, and $a_{ij} = a_{ji}$ for all $i, j \in V$. The degree d_i of vertex $i \in V$ is defined by $d_i = \sum_{j=1}^{n} a_{ij}$. The (weighted) adjacency matrix $A(G) = (a_{ij})$ is the $n \times n$ matrix, with rows and columns indexed by V, whose entries are the edge weights. The degree matrix $D(G) = \mathrm{diag}\,(d_1, \ldots, d_n)$ is the diagonal matrix indexed by V with the vertex degrees on the diagonal. The difference $L(G) = D - A$ is the (combinatorial) Laplacian matrix of G, which is a major tool for enumerating spanning trees and has numerous applications [**2, 21**]. Since L is a positive semi-definite matrix with zero minimum eigenvalue [**21**], we denote the eigenvalues of L by $\mu_1 \geq \mu_2 \geq \cdots \geq \mu_n = 0$. The set $\{\mu_1, \mu_2, \ldots, \mu_n\}$ is called the Laplacian spectrum of the graph G.

Let $\lambda_1 \geq \lambda_2 \geq \cdots \geq \lambda_n$ be the eigenvalues of the adjacency matrix A as it is a real symmetric matrix. A weighted sum of numbers of closed walks is defined in [**28**] by $S = \sum_{k=0}^{\infty} n_k/k!$, where n_k is the number of closed walks of length k in G. Since $n_k = \sum_{i=1}^{n} \lambda_i^k$ [**2**], we have

$$S = \sum_{k=0}^{\infty} \sum_{i=1}^{n} \frac{\lambda_i^k}{k!} = \sum_{i=1}^{n} \sum_{k=0}^{\infty} \frac{\lambda_i^k}{k!} = \sum_{i=1}^{n} e^{\lambda_i}. \tag{1}$$

Note that (1) corresponds to the Estrada index of the graph [**6**], which has been used for the study of bipartivity [**8**] and subgraph centrality [**7, 9**]. The logarithm of the Estrada index of G is then defined as [**7**]

$$\overline{\lambda} = \ln\left(\frac{S}{n}\right) = \ln\left(\frac{1}{n}\sum_{i=1}^{n} e^{\lambda_i}\right), \tag{2}$$

which is dubbed as "natural connectivity" in [**26, 28**] since it corresponds to an average eigenvalue of A recalling that $\lambda_n \leq \overline{\lambda} \leq \lambda_1$.

Let I be the $n \times n$ identity matrix. A simple random walk on G is a finite irreducible Markov chain [**18**] with state space V and with transition probability matrix $T(G) = D^{-1}A$. It follows from the Perron-Frobenius theorem [**24**] that the eigenvalues of T satisfy $1 = \delta_1 > \delta_2 \geq \cdots \geq \delta_n \geq -1$; see also [**18**]. The mixing time, τ, means the expected number of steps for the distribution of the random walk to reach the stationary distribution π with $\pi T = \pi$. Another matrix closely associated with the transition probability matrix T is the normalized Laplacian matrix $\mathcal{L}(G) = I - D^{-1/2}AD^{-1/2} = D^{1/2}(I - T)D^{-1/2}$ which controls the expansion/isoperimetric properties and essentially determines the mixing time of a random walk on the graph G [**4**]. Indeed, the eigenvalues of $\mathcal{L}$ being $0 = 1 - \delta_1 < 1 - \delta_2 \leq \cdots \leq 1 - \delta_n \leq 2$, we have (see, e.g., [**4, 13, 18, 24**])

$$\tau = 1 + \sum_{i=2}^{n} \frac{1}{1 - \delta_i}. \tag{3}$$

3. Main results. The following lemma is a useful result for traces of matrices, which is equivalent to the important Thermodynamic Inequality in statistical mechanics [**12**].

Lemma 1 [**11**]. *Let M and N be two Hermitian matrices. Then*

$$\mathrm{tr}\,(e^{M+N}) \geq \mathrm{tr}\,(e^{M}) e^{\mathrm{tr}\,(Ne^{M})/\mathrm{tr}\,(e^{M})},$$

where $\mathrm{tr}\,(M)$ *is the trace of matrix M.*

Let $d_{\max}$ denote the maximum degree of the graph G. We begin with a lower bound of the natural connectivity $\overline{\lambda}$ based on the Laplacian spectrum of G.

Proposition 1. *Suppose G is a connected weighted graph defined as above. We have*

$$\overline{\lambda} \geq \ln\left(\frac{\sum_{i=1}^{n} e^{d_i}}{n}\right) - \frac{e^{d_{\max}}}{\sum_{i=1}^{n} e^{d_i}} \sum_{i=1}^{n-1} \mu_i,$$

where $\mu_1 \geq \mu_2 \geq \cdots \geq \mu_n = 0$ are the Laplacian eigenvalues of G.

Proof. First, the definition of natural connectivity (2) implies

$$\overline{\lambda} = \ln\left(\frac{1}{n}\mathrm{tr}\,(e^{A})\right) = \ln\left(\frac{1}{n}\mathrm{tr}\,(e^{D-L})\right) \tag{4}$$

by the standard arguments in matrix exponential.

Since both D and L are symmetric matrices, by Lemma 1 we have

$$\begin{aligned}
\mathrm{tr}\,(e^{D-L}) &\geq \mathrm{tr}\,(e^{D}) e^{\mathrm{tr}\,(-Le^{D})/\mathrm{tr}\,(e^{D})} \\
&\geq \left(\sum_{i=1}^{n} e^{d_i}\right) e^{-e^{d_{\max}}\mathrm{tr}\,(L)/\sum_{i=1}^{n} e^{d_i}} \\
&= \left(\sum_{i=1}^{n} e^{d_i}\right) e^{-e^{d_{\max}}\sum_{i=1}^{n-1}\mu_i/\sum_{i=1}^{n} e^{d_i}},
\end{aligned}$$

where the second inequality above holds due to an inequality of von Neumann, cf., [**20**]; the equality holds if and only if e^D is a scalar matrix, in other words, $d_1 = \cdots = d_n$.

Consequently, from (4), we obtain

$$\overline{\lambda} \geq \ln\left(\frac{\sum_{i=1}^n e^{d_i}}{n} \cdot e^{-e^{d_{\max}} \sum_{i=1}^{n-1} \mu_i / \sum_{i=1}^n e^{d_i}}\right),$$

which completes the proof. $\square$

Remark 1. It is easy to see $\lambda_1 \leq d_{\max}$ by the Courant-Fischer theorem [**2**]. Hence, we have an upper bound for the natural connectivity

$$\overline{\lambda} \leq \lambda_1 \leq d_{\max} = \ln\left(\frac{\sum_{i=1}^n e^{d_{\max}}}{n}\right),$$

which is in a comparable form of the lower bound obtained in Proposition 1.

Next, we present the main result of this paper. For a weighted regular graph G, we lower the natural connectivity bound by the mixing time τ of the random walk on G and the second smallest eigenvalue $1 - \delta_2$ of the normalized Laplacian, $\mathcal{L}$.

Theorem 1. *Suppose G is a weighted r-regular graph, that is, $d_1 = \cdots = d_n = r$. Then we have*

(5)

$$\overline{\lambda} \geq r\left(1 - \frac{n-1}{n}\left(\frac{n-1}{\tau-1} + \frac{(\tau-1)(2\tau+3n-5)}{(n-1)^2} \bigvee \frac{4(n-1)}{(\tau-1)(1-\delta_2)^2}\right)\right),$$

where $a \vee b$ represents the maximum of a and b.

Proof. Since we now have the degree matrix $D = rI$ and $I - T = (1/r)L$, the eigenvalues of the Laplacian matrix L are

$$0 = r - r\delta_1 < r - r\delta_2 \leq \cdots \leq r - r\delta_n \leq 2r.$$

From the proof of Proposition 1, we have

$$\begin{aligned} \operatorname{tr}(e^{rI-L}) &\geq \operatorname{tr}(e^{rI}) e^{\operatorname{tr}(-Le^{rI})/\operatorname{tr}(e^{rI})} \\ &= ne^r e^{-e^r \sum_{i=1}^n (r - r\delta_i)/ne^r} \\ &= ne^{r - r\sum_{i=2}^n (1-\delta_i)/n}. \end{aligned}$$

Therefore, by (4) we get

$$\overline{\lambda} \geq \ln\left(e^{r-r\sum_{i=2}^{n}(1-\delta_i)/n}\right) = r\left(1 - \frac{n-1}{n} \cdot \frac{\sum_{i=2}^{n}(1-\delta_i)}{n-1}\right). \tag{6}$$

Now, recall from (3) that $H := (n-1)/(\tau-1)$ is the harmonic mean of a sequence of positive numbers $\{1-\delta_i\}_{i=2}^{n}$, and the expression (6) contains an arithmetic mean of them. Hence, involving a refined inequality of arithmetic-harmonic means (see [**19**, Proposition 4) we derive that

$$\overline{\lambda} \geq r\left(1 - \frac{n-1}{n}\left(H + \frac{\sum_{i=2}^{n} K_i}{n-1}\right)\right), \tag{7}$$

where

$$K_i = \frac{(1-\delta_i-H)^2 \cdot \big(1-\delta_i+2H+(1-\delta_i)\wedge H\big)}{\big(1-\delta_i+(1-\delta_i)\wedge H\big)^2},$$

$a \wedge b$ represents the minimum of a and b, and $H = (n-1)/(\tau-1)$ as mentioned above.

We consider two cases. If $1-\delta_i \geq H$, then

$$K_i \leq \frac{4(1-\delta_i+3H)}{(1-\delta_i+H)^2} \leq \frac{1-\delta_i+3H}{H^2} \leq \frac{2+3H}{H^2}$$

by noting that $0 < 1-\delta_i \leq 2$ for $2 \leq i \leq n$; if $1-\delta_i \leq H$, then

$$K_i = \frac{(1-\delta_i-H)^2 \cdot (1-\delta_i+H)}{2(1-\delta_i)^2} \leq \frac{2(1-\delta_i+H)}{(1-\delta_i)^2} \leq \frac{4H}{(1-\delta_2)^2}.$$

Finally, combining the above discussions with (7), we get

$$\overline{\lambda} \geq r\left(1 - \frac{n-1}{n}\left(H + \frac{2+3H}{H^2} \bigvee \frac{4H}{(1-\delta_2)^2}\right)\right),$$

which readily concludes the proof by some simplifications. $\square$

Remark 2. From Theorem 1, we do not need the complete spectrum to bound the logarithm of the Estrada index $\overline{\lambda}$ as in Proposition 1. Our result sets up a bridge between the Estrada index (network robustness measure) and the mixing time of random walk (dynamical process on networks).

Remark 3. The quantity $\tau - 1$ in (5) is known as the Kemeny constant [**17**], which is used to measure the expected number of links that a surfer on the World Wide Web, located on a random web page, needs to follow before reaching his desired location. For some recent results, we refer the reader to [**3, 15**] and references therein.

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