# A unified approach to lower bound on Resolvent Estrada index and Resolvent energy of graphs

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**Abstract.** In this paper, according to symmetric Lanczos algorithm and general Gauss-type quadrature rule, we give some lower bounds on the Resolvent Estrada index $EE_r(G)$ and the Resolvent energy $ER(G)$.
**Keywords**: Resolvent Estrada index; spectral moment; Resolvent energy

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## 1. Introduction

Let $G = (V, E)$ be a simple connected graph with vertex set $V(G) = \{v_1, v_2, \ldots, v_n\}$ and edge set $E(G)$. Graph theoretical terms used but not defined can be found in Bollobás [1]. Let $A(G)$ be the $(0,1)$-adjacency matrix of $G$. The characteristic polynomial $\phi(G; x)$ of $G$ is $|xI - A(G)|$, where $I$ is the unit matrix. We call the eigenvalues $\lambda_1(G) \geq \lambda_2(G) \geq \cdots \geq \lambda_n(G)$ (for short $\lambda_1 \geq \lambda_2 \geq \cdots \geq \lambda_n$) of $A(G)$ the spectrum of $G$. For $k \geq 0$, let $M_k(G)$ denote the $k$-th spectral moment of a graph $G$, namely

$$M_k(G) = tr(A(G)^k) = \sum_{i=1}^{n} \lambda_i^k,$$

where $tr(\cdot)$ is the trace of a matrix.

In [6], Estrada and Higham proposed an invariant of a graph $G$ based on Taylor series expansion of spectral moments

$$EE(G, c) = \sum_{k=0}^{\infty} c_k M_k(G).$$

Obviously, for $c_k = \frac{1}{k!}$, $EE(G, c)$ is the well-known graph invariant, Estrada index, put forward by Estrada [5], which has attracted much attention of mathematicians in the past few years. Various mathematical properties

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of the Estrada index have been investigated, see [7] for a comprehensive survey. For $c_k = \frac{1}{(n-1)^k}$, $EE(G,c)$ is the Resolvent Estrada index, denoted by $EE_r(G)$, defined by Estrada and Higham in [6]. Note that

$$EE_r(G) = EE(G, \frac{1}{(n-1)^k}) = \sum_{k=0}^{\infty} \frac{M_k(G)}{(n-1)^k} = \sum_{i=0}^{n} (1 - \frac{\lambda_i}{n-1})^{-1}.$$

However, the resolvent Estrada index is defined for all graphs but complete graph and this is the main pitfall of this index. In [10], I. Gutman et al gave a novel topological invariant named as the Resolvent energy $ER(G)$ of a graph as following:

$$ER(G) = \frac{1}{n} \sum_{k=0}^{\infty} \frac{M_k(G)}{(n)^k} = \sum_{i=1}^{n} \frac{1}{n - \lambda_i} = \frac{1}{n} \sum_{i=1}^{n} (1 - \frac{\lambda_i}{n})^{-1}.$$

This definition incorporates all graphs.

Recently, some mathematical properties of $EE_r(G)$ and $ER(G)$ have been studied[3, 4, 8, 9, 10]. In this paper, we will give a new lower bound on $EE_r(G)$ and $ER(G)$ by a unified approach.

## 2. Preliminaries

If $A$ is symmetric, then it is possible to find an orthogonal $Q$ such that $A = Q^T \Lambda Q$, where $\Lambda$ is a diagonal matrix consisting of the eigenvalues of $A$ which we order as $\lambda_1 \leq \lambda_2 \leq \ldots \leq \lambda_n$, that is, $\Lambda = diag(\lambda_1, \lambda_2, \ldots, \lambda_n)$. Let $a = \lambda_1, b = \lambda_n$, a real function $f(x)$ is strictly completely monotonic on the interval $[a, b]$ if $f^{(2j)}(x) > 0$ and $f^{(2j+1)}(x) < 0$ for all integers $j \geq 0$, where $f^{(k)}(x)$ denotes the $k$-th derivative of $f(x)$ and $f^{(0)}(x) = f(x)$. For a strictly completely monotonic function $f(x)$ defined on $[a, b]$, define matrix function $f(A) = Q^T f(\Lambda) Q$, where $f(\Lambda) = diag(f(\lambda_1), f(\lambda_2), \ldots, f(\lambda_n))$. For any $u, v \in \mathbb{R}^n$, we have

$$u^T f(A) v = u^T Q^T f(\Lambda) Q v = p^T f(\Lambda) q = \sum_{i=1}^{n} f(\lambda_i) p_i q_i,$$

where $p = Qu, q = Qv$. This sum can be interpreted as a Riemann-Stieltjes integral

$$u^T f(A) v = \int_a^b f(\lambda) d\mu(\lambda), \quad \mu(\lambda) = \begin{cases} 0 & \lambda < a = \lambda_1, \\ \sum_{j=1}^{i} p_j q_j & \lambda_i \leq \lambda < \lambda_{i+1}, \\ \sum_{j=1}^{n} p_j q_j & b = \lambda_n \leq \lambda. \end{cases} \quad (2.1)$$

The general Gauss-type quadrature rule gives in this case:

$$\int_a^b f(\lambda)d\mu(\lambda) = \sum_{j=1}^{k} \omega_j f(t_j) + \sum_{i=1}^{m} v_i f(z_i) + R[f] \tag{2.2}$$

where the nodes $\{t_j\}_{j=1}^k$ and the weights $\{\omega_j\}_{j=1}^k$ are unknown, whereas the nodes $\{z_i\}_{i=1}^m$ are prescribed. We have

(i) $m = 0$ for the Gauss rule;
(ii) $m = 1, z_1 = a$ or $z_1 = b$ for the Gauss-Radau rule;
(iii) $m = 1, z_1 = a$ and $z_2 = b$ for the Gauss-Lobatto rule.

By [2], if $f(x)$ is a strictly completely monotonic on an interval containing the spectrum of $A$, then quadrature rules applied to (2.1) give bounds on $u^T f(A)v$. More precisely, the Gauss rule gives a lower bound, the Gauss-Lobatto rule gives an upper bound, whereas the Gauss-Radau rule can be used to obtain both a lower and an upper bound.

Note that if $u = v$, the remainder in (2.2) can be written as

$$R[f] \quad = \quad \frac{f^{(2n+m)}(\eta)}{(2n+m)!} \int_a^b \prod_{k=1}^{m}(\lambda - z_k)[\prod_{j=1}^{n}(\lambda - s_j)]^2 d\mu(\lambda),$$

for some $\eta \in (a, b)$. For the strictly completely monotonic function $f(x)$ on the interval $[a, b]$, if $m = 0$, then

$$R[f] \quad = \quad \frac{f^{(2n)}(\eta)}{(2n)!} \int_a^b [\prod_{j=1}^{n}(\lambda - s_j)]^2 d\mu(\lambda) \geq 0,$$

further by (2.1) and (2.2), we have

$$u^T f(A)u = \sum_{j=1}^{k} \omega_j f(t_j) + R[f] \geq \sum_{j=1}^{k} \omega_j f(t_j).$$

Especially, we have

$$e_i^T f(A)e_i = (f(A))_{ii} \geq \sum_{j=1}^{k} \omega_j f(t_j). \tag{2.3}$$

Let a tridiagonal matrix

$$J_k = \begin{pmatrix} \omega_1 & \gamma_1 & & & \\ \gamma_1 & \omega_2 & \gamma_2 & & \\ & \ddots & \ddots & \ddots & \\ & & \gamma_{k-2} & \omega_{k-1} & \gamma_{k-1} \\ & & \gamma_{k-1} & \omega_k & \gamma_k \end{pmatrix},$$

where the entries of $J_k$ is obtained by symmetric Lanczos algorithm. The initial vectors are $x_{-1} = 0$ and $x_0 = e_i$, the iteration goes as follows:

$$\begin{aligned} \gamma_j x_j &= r_j = (A - \omega_j I)x_{j-1} - \gamma_{j-1}x_{j-2}, j = 1, 2, \ldots \\ \omega_j &= x_{j-1}^T A x_{j-1} \\ \gamma_j &= \parallel r_j \parallel \end{aligned}$$

From [11], we know that the eigenvalues of $J_k$ are exactly the Gauss nodes $\{t_j\}_{j=1}^k$, whereas the Gauss weights $\{\omega_j\}_{j=1}^k$ are given by the squares of the first entries of the normalized eigenvectors of $J_k$. It follows from (2.1) that the quantity we seek to compute has the form $\sum_{j=1}^k \omega_j f(t_j)$. By [2], we have

$$\sum_{j=1}^{k} \omega_j f(t_j) = e_1^T f(J_k) e_1, \tag{2.4}$$

where $e_1 = (1, \underbrace{0, \ldots, 0}_{k-1})^T$. Therefore, in some cases where $f(J_k)$ is easily computable, we do not need to compute the eigenvalues (that is, Gauss nodes) and eigenvectors (that is, weights) of $J_k$. Then by (2.3) and (2.4), we have

$$(f(A))_{ii} \geq e_1^T f(J_k) e_1. \tag{2.5}$$

# 3. Main results

**Theorem 3.1.** *Let $G = (V, E)$ be a non-complete graph and $d_i$ be the degree of vertex $v_i$ of $G$, then*

$$EE_r(G) \geq \sum_{i=1}^{n} \frac{1 - \frac{2t}{(n-1)d_i}}{1 - \frac{2t}{(n-1)d_i} - \frac{d_i}{(n-1)^2}},$$

*where $t$ is the number of triangles.*

*Proof.* Let $f(x) = x^{-1}$, then $f(x)$ is a strictly completely monotonic function. For the matrix $M = I - \frac{A}{n-1} = (m_{ij})$, then $EE_r(G) = \sum_{i=1}^n f(M)_{ii}$. By symmetric Lanczos algorithm, we have

$$\begin{aligned} \omega_1 &= e_i^T M e_i = 1 - \frac{a_{ii}}{n-1} = 1, \\ r_1 &= (M - \omega_1 I)e_i = (-\frac{A}{n-1})e_i \end{aligned}$$

$$
\begin{aligned}
&= -(\frac{a_{1i}}{n-1},\frac{a_{2i}}{n-1},\ldots,\frac{a_{i-1,i}}{n-1},0,\frac{a_{i+1,i}}{n-1},\ldots,\frac{a_{ni}}{n-1})^T,\\
\gamma_1 &= \sqrt{(\frac{a_{1i}}{n-1})^2+(\frac{a_{2i}}{n-1})^2+\ldots+(\frac{a_{i-1,i}}{n-1})^2+(\frac{a_{i+1,i}}{n-1})^2+\ldots+(\frac{a_{ni}}{n-1})^2}\\
&= \frac{\sqrt{d_i}}{n-1},\\
x_1 &= \frac{-1}{\sqrt{d_i}}(a_{1i},a_{2i},\ldots,a_{i-1,i},0,a_{i+1,i},\ldots,a_{ni})^T,\\
\omega_2 &= x_1^T M x_1 = \frac{1}{d_i}\sum_{k\neq i,l\neq i} m_{kl}a_{ki}a_{li}\\
&= \frac{1}{d_i}[\sum_{k\neq i,l\neq i,k=l} m_{kl}a_{ki}a_{li} + \sum_{k\neq i,l\neq i,k\neq l} m_{kl}a_{ki}a_{li}]\\
&= \frac{1}{d_i}[\sum_{k\neq i} a_{ki}^2 - \frac{1}{(n-1)}\sum_{k\neq i,l\neq i,k\neq l} a_{kl}a_{ki}a_{li}]\\
&= \frac{1}{d_i}[d_i - \frac{2t}{(n-1)}] = 1-\frac{2t}{(n-1)d_i}
\end{aligned}
$$

The tridiagonal matrix is the $2\times 2$ matrix

$$J_2 = \begin{pmatrix} 1 & \frac{\sqrt{d_i}}{n-1} \\ \frac{\sqrt{d_i}}{n-1} & 1-\frac{2t}{(n-1)d_i} \end{pmatrix}$$

$$J_2^{-1} = \frac{1}{1-\frac{2t}{(n-1)d_i}-\frac{d_i}{(n-1)^2}}\begin{pmatrix} 1-\frac{2t}{(n-1)d_i} & -\frac{\sqrt{d_i}}{n-1} \\ -\frac{\sqrt{d_i}}{n-1} & 1 \end{pmatrix}$$

By (2.5), we have

$$f(M)_{ii} = (M^{-1})_{ii} \quad \geq \quad \frac{1-\frac{2t}{(n-1)d_i}}{1-\frac{2t}{(n-1)d_i}-\frac{d_i}{(n-1)^2}}$$

Further,

$$EE_r(G) = \sum_{i=1}^{n} f(M)_{ii} \quad \geq \quad \sum_{i=1}^{n}\frac{1-\frac{2t}{(n-1)d_i}}{1-\frac{2t}{(n-1)d_i}-\frac{d_i}{(n-1)^2}}.$$

□

**Corollary 3.2.** *[3] Let $G=(V,E)$ be a non-complete graph with $n$ vertices and $m$ edges.*

$$EE_r(G) \quad \geq \quad \frac{n^2(n-1)^2}{n(n-1)^2-2m}.$$

*Proof.* Note that

$$\begin{aligned} & \frac{1-\frac{2t}{(n-1)d_i}}{1-\frac{2t}{(n-1)d_i}-\frac{d_i}{(n-1)^2}}-\frac{1}{1-\frac{d_i}{(n-1)^2}} \\ = & \frac{2t}{(1-\frac{2t}{(n-1)d_i}-\frac{d_i}{(n-1)^2})(1-\frac{d_i}{(n-1)^2})(n-1)^3} \geq 0, \end{aligned}$$

then

$$\sum_{i=1}^{n}\frac{1-\frac{2t}{(n-1)d_i}}{1-\frac{2t}{(n-1)d_i}-\frac{d_i}{(n-1)^2}} \geq \sum_{i=1}^{n}\frac{1}{1-\frac{d_i}{(n-1)^2}} = \sum_{i=1}^{n}\frac{(n-1)^2}{(n-1)^2-d_i}. \tag{3.6}$$

Further by Cauchy-Schwarz inequality, we have

$$\sum_{i=1}^{n}(\sqrt{(n-1)^2-d_i})^2\sum_{i=1}^{n}(\frac{1}{\sqrt{(n-1)^2-d_i}})^2 \geq n^2,$$

then

$$\sum_{i=1}^{n}\frac{(n-1)^2}{(n-1)^2-d_i} \geq \frac{n^2(n-1)^2}{\sum_{i=1}^{n}((n-1)^2-d_i)} = \frac{n^2(n-1)^2}{n(n-1)^2-2m}.$$

□

**Corollary 3.3.** *Let $G=(V,E)$ be a bipartite graph, then*

$$EE_r(G) \geq \sum_{i=1}^{n}\frac{(n-1)^2}{(n-1)^2-d_i}.$$

*Proof.* For a bipartite graph, the number of triangles is zero, then by (3.6), we have our desired result. □

**Corollary 3.4.** *Let $G=(V,E)$ be a unicyclic graph, then*

$$EE_r(G) \geq \sum_{i=1}^{n}\frac{(n-1)^2}{(n-1)^2-d_i}.$$

*Proof.* (1) If there is not triangle in $G$, then

$$EE_r(G) \geq \sum_{i=1}^{n}\frac{1}{1-\frac{d_i}{(n-1)^2}} = \sum_{i=1}^{n}\frac{(n-1)^2}{(n-1)^2-d_i}.$$

(2) If there is a triangle $v_l v_j v_k$ in $G$, then $t_l = t_j = t_k = 1$. Note that

$$\frac{1-\frac{2}{(n-1)d_l}}{1-\frac{2}{(n-1)d_l}-\frac{d_l}{(n-1)^2}} > \frac{1}{1-\frac{d_i}{(n-1)^2}}, \frac{1-\frac{2}{(n-1)d_j}}{1-\frac{2}{(n-1)d_j}-\frac{d_j}{(n-1)^2}} > \frac{1}{1-\frac{d_i}{(n-1)^2}},$$
$$\frac{1-\frac{2}{(n-1)d_k}}{1-\frac{2}{(n-1)d_k}-\frac{d_k}{(n-1)^2}} > \frac{1}{1-\frac{d_i}{(n-1)^2}}.$$

Then

$$\begin{aligned}
& EE_r(G) \\
\geq \ & \sum_{i=1, i\neq l,j,k}^{n} \frac{1}{1-\frac{d_i}{(n-1)^2}} + \frac{1-\frac{2}{(n-1)d_l}}{1-\frac{2}{(n-1)d_l}-\frac{d_l}{(n-1)^2}} + \frac{1-\frac{2}{(n-1)d_j}}{1-\frac{2}{(n-1)d_j}-\frac{d_j}{(n-1)^2}} \\
& + \frac{1-\frac{2}{(n-1)d_k}}{1-\frac{2}{(n-1)d_k}-\frac{d_k}{(n-1)^2}} \\
= \ & \sum_{i=1, i\neq l,j,k}^{n} \frac{(n-1)^2}{(n-1)^2-d_i} + \frac{1-\frac{2}{(n-1)d_l}}{1-\frac{2}{(n-1)d_l}-\frac{d_l}{(n-1)^2}} + \frac{1-\frac{2}{(n-1)d_j}}{1-\frac{2}{(n-1)d_j}-\frac{d_j}{(n-1)^2}} \\
& + \frac{1-\frac{2}{(n-1)d_k}}{1-\frac{2}{(n-1)d_k}-\frac{d_k}{(n-1)^2}} > \sum_{i=1}^{n} \frac{(n-1)^2}{(n-1)^2-d_i}.
\end{aligned}$$

Hence we obtain the desirable result. □

Now we consider the lower bound on $ER(G)$. For this topological invariant, we only want to let $M = I - \frac{A}{n}$. Similar to the proof of Theorem 3.1, we have the following results:

**Theorem 3.5.** *Let $G = (V, E)$ be a graph and $d_i$ be the degree of vertex $v_i$ of $G$, then*

$$ER(G) \ \geq \ \frac{1}{n}\sum_{i=1}^{n} \frac{1-\frac{2t}{nd_i}}{1-\frac{2t}{nd_i}-\frac{d_i}{n^2}},$$

*where $t$ is the number of triangles.*

**Corollary 3.6.** *Let $G = (V, E)$ be a non-complete graph with $n$ vertices and $m$ edges.*

$$ER(G) \ \geq \ \frac{n^3}{n^3-2m}.$$

**Corollary 3.7.** *Let $G = (V, E)$ be a bipartite graph, then*

$$ER(G) \geq \sum_{i=1}^{n} \frac{n}{n^2 - d_i}.$$

**Corollary 3.8.** *Let $G = (V, E)$ be a unicyclic graph, then*

$$ER(G) \geq \sum_{i=1}^{n} \frac{n}{n^2 - d_i}.$$

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