 Bounds On The Second Stage Spectral Radius Of Graphs

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Abstract—Let G be a graph of order n. The second stage adjacency matrix of G is the symmetric $n \times n$ matrix for which the $ij^{th}$ entry is 1 if the vertices $v_i$ and $v_j$ are of distance two; otherwise 0. The sum of the absolute values of this second stage adjacency matrix is called the second stage energy of G. In this paper we investigate a few properties and determine some upper bounds for the largest eigenvalue.

Keywords—Second stage spectral radius; Irreducible matrix; Derived graph.

I. INTRODUCTION

Let G be a connected graph with vertex set $V(G) = \{v_1, v_2, ..., v_n\}$. The second stage adjacency matrix is denoted by $A_2(G)$ and the second stage energy by $E_2(G)$. As it is symmetrical it will be an adjacency matrix for some graph $G'$ which we call the derived graph of G. If $\Delta'$ is the maximum degree of $G'$ then clearly $\Delta' \leq \Delta$. Irreducibility of the adjacency matrix is related to the property of connectedness[2]. Hence $A_2(G)$ is irreducible if and only if the derived graph $G'$ is connected. Proposition 2.1 guarantees plenty of graphs for which their derived graphs are connected, for example, the Peterson graph whose derived graph is a 6-regular graph. In this paper we consider only those graphs for which $A_2(G)$ is irreducible.

II. SOME PROPERTIES

The derived graph of any odd cycle $C_{2m-1} = v_1, v_2, ..., v_{2m-1}$ is the odd cycle $C_{2m-1} = v_1, v_2, ..., v_{2m-1}, v_{2m-2}, ..., v_1$. This motivates to enunciate the following proposition:

Proposition 2.1. Let G be a graph having $C_{2m-1} = v_1, v_2, ..., v_{2m-1}$ as an induced subgraph for some $m \geq 3$. If (i) $\Delta \leq n - 2$ and

(ii) for every $u \in V(G) - V(C_{2m-1})$, there exist at least one $v_j \notin N(u), j \in \{1, 2, ..., 2m - 1\}$, then the derived graph is connected.

Proof: As mentioned above the induced subgraph $v_1, v_2, ..., v_{2m-1}$ is connected in $G'$. Choose any vertex $u \neq v_i$ for all $i = 1, 2, ..., 2m - 1$ and let $v_j$ be a vertex in $C_{2m-1}$ which is not in $N(u)$.

Case 1. $N(u) \cap \{v_1, v_2, ..., v_{2m-1}\} = \phi$. Let $u = u_1u_2...u_r = v_i$ be the shortest path from u to $C_{2m-1}$ of length r.

Case 1.1. r is even, then we have $d(u = u_1, u_3) = d(u_3, u_5) = \ldots = d(u_{r-2}, u_r = v_i) = 2$ and so the derived graph has the path $uu_2uu_3...uu_{r-2}v_i$.

Case 1.2. r is odd, then we have $uu_2uu_3...uu_{r-1}v_i$ is a path in the derived graph.

Case 2. $N(u) \cap \{v_1, v_2, ..., v_{2m-1}\} \neq \phi$. Choose a vertex $v_k \in N(u) \cap \{v_1, v_2, ..., v_{2m-1}\}$ such that $v_k$ is nearest to $v_j$. If $k = j \pm 1$, then $d(u, v_j) = 2$. Otherwise $v_i$ is of distance two from u where $l = k \pm 1$, ie., $d(u, v_l) = 2$.

Proposition 2.2. Let G be a r-regular graph with order n such that $n = 2r + 1$. Then the derived graph $G'$ of G is also r-regular.

Proof: Clearly r is even. Choose any vertex $v_i$. Let $v_k$ be a vertex such that $v_k \in N(v_i)$. Let $v_k \notin N(v_j)$ for all $v_j \in N(v_i)$. This implies $deg(v_k) \leq (2r+1) - (r+2) = r-1$, which is a contradiction since $deg(v_k) = r$.

Remark: Converse of the above proposition is not true. For example, consider any odd cycle other than $C_5$. It is 2-regular and its derived graph being an odd cycle is also 2-regular. But $n \neq 2r + 1$.

Proposition 2.3. The derived graph of circulant graph is a circulant graph.

Proof: Let G be a circulant graph formed by the set $S \subseteq \{1, 2, ..., n\}$. Then $\epsilon \in S$ if and only if $n - \epsilon \in S [1]$. Consider a vertex $v_i$. Let $v_k \in D(v_i)$. Then there exists a vertex $v_j$ such that $v_j$ is adjacent to $v_i$ and $v_k$. Then by the definition of circulant graph, $v_{n-k}$ is also adjacent to $v_j$ and so $v_{n-k} \in D(v_i)$. Thus, $G'$ is formed by a set $S' \subseteq \{1, 2, ..., n\}$ such that $k \in S'$ if and only if $n - k \in S'$ and hence $G'$ is also circulant.

Proposition 2.4. Given any positive integer n of the form $p^r$ where p is a prime number and r is a positive integer, there exists a graph G for which the second stage energy is $2(p - 1)p^{r-1}$.

Proof: Let G be the complement of the circulant graph H formed by the set $S = \{\alpha_1, \alpha_2, ..., \alpha_k\}$ where $\alpha_i$'s are all numbers less than n and prime to n. Then the derived graph of G is the circulant graph H whose energy is $2(p - 1)p^{r-1}$ [1]. Hence $E_2(G) = E(H) = 2(p - 1)p^{r-1}$.

Theorem 2.5. Let $D(v_i) = \{v_j : d(v_i, v_j) = 2\}$. Then for each fixed $i = 1, 2, ..., n$, $|D(v_i)| = S_1 - S_2$, where
$S_1 = \sum_{v_i \text{adj} v_j \text{nonpendent}} |N(v_i)| - |N(v_j)|$ and $S_2 = \sum_{v_i \text{adj} v_j \text{nonpendent}} (l_k - 1)$ where $l_k$ is the number of vertices which are adjacent to both $v_i$ and $v_k$.

Proof: If we take any vertex $v_i$ adjacent to $v_j$, then all members of $N(v_j)$ need not be in $D(v_i)$, because some neighbours of $v_j$ may be neighbours of $v_i$ and so $v_j$ can contribute only $|N(v_j)| - |N(v_i) \cap N(v_j)|$ number of members to $D(v_j)$. Similarly for all other neighbours of $v_j$. Therefore, the total number of members contributed by the neighbours of $v_j$ is

$$\sum_{v_i \text{adj} v_j \text{nonpendent}} (|N(v_j)| - |N(v_i) \cap N(v_j)|),$$

which can be written as

$$S_1 = \sum_{v_i \text{adj} v_j \text{nonpendent}} |N(v_i)| - |N(v_j)|.$$  

Among these $S_1$ members, some may appear more than once. For example, a member $v_k$ of $D(v_i)$ may have neighbours $v_i, v_j, \ldots, v_k$ which all are in turn neighbours of $v_i$ also. Thus, $v_k$ is repeated say $k_i$ times in $S_1$. But it should be taken only once. Thus we get the required result.

Corollary 2.6. If the second stage adjacency matrix is irreducible, then $|D(v_j)| \leq 2m - 2d_i - \delta + \epsilon + \frac{n}{m}$, where $\epsilon$, and $\delta$ is the number of pendant vertices adjacent to $v_i$.

Proof: We observe that $v_i$ is included as many times as $d_i - \epsilon$, in $\sum_{v_i \text{adj} v_j \text{nonpendent}} (|N(v_i)|)$.

Hence

$$|D(v_i)| = \sum_{v_i \text{adj} v_j \text{nonpendent}} |N(v_i)| \geq d_i.$$

Therefore

$$D(v_i) \leq S \leq \sum_{v_i \text{adj} v_j \text{nonpendent}} (|N(v_i)|) - d_i + \epsilon + \delta.$$  

(1)

Since the second stage adjacency matrix is irreducible, for each vertex $v_i$, there is atleast one vertex $v_k$ which is non-adjacent to $v_i$.

Therefore

$$\sum_{v_i \text{adj} v_j \text{nonpendent}} |N(v_i)| \leq 2m - d_i - \delta.$$  

(2)

Combining (1) and (2), we get $D(v_i) \leq 2m - 2d_i - \delta + \epsilon + \delta$.

III. BOUNDS FOR THE LARGEST EIGENVALUE

Theorem 3.1. Let $G$ be a graph with minimum degree $\delta \geq 1$ and maximum degree $\Delta$. Then

$$\rho(G) \leq \sqrt{2\Delta(m + n - \delta - 1)} - 4m + \delta(2 - \delta) + A,$$

where $A = \epsilon + \delta(2 \Delta + \delta + 1)$ and $\epsilon + \delta$ is the number of pendant vertices of $G$.

Proof: Let $D(v_i) = \{v_j : d(v_i, v_j) = 2\}$. Let $D_i(v_i) = \{v_j : d(v_i, v_j) \neq 2\}$ and $D_i(v_i) = D_i(v_i) - \{v_i\}$. Let $x = (x_1, x_2, \ldots, x_n)^T$ be the unit eigenvector corresponding to $\rho(G)$. Then $\rho(G)x_i = \sum_{v_i \text{adj} v_j \text{adj} v_j} \alpha_{ij}x_j$. By Cauchy–Schwarz inequality,

$$\rho^2(A)x_i^2 = \sum_{v_i \text{adj} v_j \text{adj} v_j} \alpha_{ij}x_j$$

$$\leq \sum_{v_i \text{adj} v_j \text{adj} v_j} \sum_{j=1}^n (a_{ij}x_j)^2$$

$$\leq (2m - (2d_i - \delta + \epsilon + \Delta)) \sum_{j=1}^n x_j^2,$$

by using corollary 2.6.

Hence

$$\rho(G)^2 = \sum_{j=1}^n \rho(G)^2x_j^2$$

$$\leq \sum_{j=1}^n (2m - (2d_i - \delta + \epsilon + \Delta)) \sum_{j=1}^n x_j^2$$

$$= \sum_{j=1}^n (2m - (2d_i + \delta - \epsilon - \Delta)) \sum_{j=1}^n x_j^2$$

$$= 2mn - 4m - n\delta + \epsilon + \frac{n}{m} (2m - (2d_i + \delta - \epsilon - \Delta) \sum_{j=1}^n x_j^2$$

In (3), we estimate, $\sum_{j=1}^n (2m - (2d_i + \delta - \epsilon - \Delta)) \sum_{j=1}^n x_j^2$

$$= \sum_{j=1}^n 2m - \sum_{j=1}^n (2d_i - \delta + \epsilon - \Delta) \sum_{j=1}^n x_j^2$$

(4)

Now, consider

$$\sum_{j=1}^n (2d_i + \delta - \epsilon - \Delta) \sum_{j=1}^n x_j^2$$

$$= \sum_{j=1}^n 2d_i + \delta - \epsilon - \Delta \sum_{j=1}^n x_j^2 + \sum_{j=1}^n \delta \sum_{j=1}^n \epsilon \sum_{j=1}^n x_j^2$$

$$- \sum_{j=1}^n \epsilon \sum_{j=1}^n \sum_{j=1}^n \sum_{j=1}^n \delta \sum_{j=1}^n x_j^2$$

$$\leq \sum_{j=1}^n 2d_i + \delta - \epsilon - \Delta \sum_{j=1}^n x_j^2 + \sum_{j=1}^n \delta \sum_{j=1}^n \sum_{j=1}^n \epsilon \sum_{j=1}^n x_j^2$$

$$\leq \sum_{j=1}^n 2d_i + \delta - \epsilon - \Delta \sum_{j=1}^n x_j^2 + \sum_{j=1}^n \delta \sum_{j=1}^n \sum_{j=1}^n \epsilon \sum_{j=1}^n x_j^2$$

(5)

In a similar fashion, we have $-\sum_{j=1}^n 2m \sum_{j=1}^n \sum_{j=1}^n \epsilon \sum_{j=1}^n x_j^2$

$$= -\sum_{j=1}^n 2m \sum_{j=1}^n \sum_{j=1}^n \sum_{j=1}^n \epsilon \sum_{j=1}^n x_j^2$$

$$= -2m - 2m \sum_{j=1}^n \sum_{j=1}^n \sum_{j=1}^n \epsilon \sum_{j=1}^n x_j^2$$

$$= -2m - 2m \sum_{j=1}^n \sum_{j=1}^n \sum_{j=1}^n \epsilon \sum_{j=1}^n x_j^2$$
\[ \begin{align*}
&\leq -2m - 2m \sum_{i=1}^{n} (n - d_i - 1)x_i^2 \\
&= -2m - 2m \sum_{i=1}^{n} m_i x_i^2 + 2m \sum_{i=1}^{n} d_i x_i^2 + 2m \sum_{i=1}^{n} x_i^2 \\
&= -2m - 2m + 2m \sum_{i=1}^{n} d_i x_i^2 + 2m \\
&\leq -2m + 2m \Delta \\
\end{align*} \tag{6} \]

From (3), (4), (5), (6), we get,
\[ \rho(G)^2 \leq (2m - 4m - n - n + \epsilon_F) + (2(\Delta - 1) - \delta(n - 2 - 1) + \delta(n - 2 + 1) + \epsilon_F(2 \Delta + 1) + 2m \Delta \\
= -4m - n + \epsilon_F + 2\Delta(n - 1) + \delta(n - 2(\Delta - 1) - \delta + \epsilon_F(2 \Delta + 1) + 2m \Delta \\
= -4m + 2m \Delta + 2\Delta(n - 1) - \delta(2\Delta - 1) + \delta(2\Delta - 1) + \epsilon_F(2 \Delta + 1) + 2m \Delta \\
= -4m + 2m \Delta + 2\Delta(n - 2 - 2\Delta + 2\Delta - \delta^2 + \epsilon_F(2 \Delta + 1) + 2m \Delta \\
= -4m + 2\Delta(m - n - \delta) + (2\delta - \delta^2) + \epsilon_F(2 \Delta + 1) + 2m \Delta. \\
\]

Hence
\[ \rho(G) \leq \sqrt{2\Delta(m + n - \delta - 4m + \delta(2 - \delta) + A}, \text{ where } A = \epsilon_F(2 \Delta + 1). \]

Let B be an \( n \times n \) matrix and let \( S_i(B) \) denote the \( i^{th} \) row sum of B, i.e., \( S_i(B) = \sum_{j=1}^{n} B_{ij} \), where \( 1 \leq i \leq m \).

Lemma 3.2. Let G be a connected \( n \)-vertex graph and \( A_2 \) its second stage adjacency matrix, with spectral radius \( \rho \).

Let P be any polynomial. If \( A_2 \) is irreducible, then,
\[ \min_{v \in V(G)} S_i(P(A_2)) = \rho(P) \leq \max_{v \in V(G)} S_i(P(A_2)) \]

Moreover, if the row sums of \( P(A_2) \) are not all equal then both inequalities are strict.

Proof: Since \( A_2 \) is irreducible, the proof is just analogous to that of Lemma 2.2 in [4].

Lemma 3.3. For each fixed \( i=1,2, \ldots, n \),
\[ S_i(A_2^2) = |D(v)| + \sum_{i \neq j} |\{v_k : d(v_k, v_i) = 2 \text{ and } d(v, v_j) = 2\}| \]

Proof: \( i^{th} \) entry in \( b_{ij} \) in \( A_2^2 = \sum_{k=1}^{n} a_{ik} a_{kj} \)
\[ \text{Case 1. Let } i = j, \text{ then } b_{ii} = \sum_{k=1}^{n} a_{ik} a_{ki} = \sum_{k=1}^{n} |D(v)| \]
\[(7) \]

\[ \text{Case 2. Let } i \neq j, a_{ik} a_{kj} = 1 \text{ and only if } a_{ik} = 1 \text{ and } a_{kj} = 1 \]
\[ a_{ik} a_{kj} = 1 \text{ and only if } d(v_k, v_i) = 2 \text{ and } d(v, v_j) = 2. \]

Therefore
\[ b_{ij} = \sum_{k} \{v_k : d(v_k, v_i) = 2 \text{ and } d(v, v_j) = 2\} \]
\[ \text{Case 2. Let } i \neq j, a_{ik} a_{kj} = 1 \text{ and only if } a_{ik} = 1 \text{ and } a_{kj} = 1 \]
\[ a_{ik} a_{kj} = 1 \text{ and only if } d(v_k, v_i) = 2 \text{ and } d(v, v_j) = 2. \]
\[ \]

\[ S_i(A_2^2) = b_{ii} + \sum_{i \neq j} b_{ij} = |D(v)| + B \text{ where } B = \sum_{i \neq j} \{v_k : d(v_k, v_i) = 2 \text{ and } d(v, v_j) = 2\}. \]

Using (7) and (8),
\[ \text{Lemma 3.4. Let } G \text{ be a simple graph with } n \text{ vertices and } m \text{ edges. Let } \Delta = \Delta(G) \text{ be the maximum degree of vertices of } G \text{ and } \rho(G) \text{ be the spectral radius of the second stage adjacency matrix } A_2 \text{ of } G. \text{ Then } \rho(G) \leq (1 + \sqrt{4(n - 1)\Delta + 2})/2. \]

Proof: Since \( S_i(A_2^2) = |D(v)| + \sum_{i \neq j} \{v_k : d(v_k, v_i) = 2 \text{ and } d(v, v_j) = 2\} \)
\[ S_i(A_2^2) - S_i(A_2) = \sum_{i \neq j} \{v_k : d(v, v_j) = 2 \text{ and } d(v_k, v_i) = 2\} \]
\[ \leq \rho(n - 1) \Delta. \]

As this holds for every vertex \( v \in V(G) \).

Lemma 3.2 implies that \( \rho(G) = (1 + \Delta(G))^2 \leq (1 + \sqrt{4(n - 1)\Delta + 2})/2. \)

For a non regular graph, many upper bounds for the largest eigenvalue of adjacency matrix are found. One such upper bound is
\[ \lambda_1 \leq \Delta - (1/2\Delta(n - 1)\Delta^2) \]
In the following theorem we find a similar upper bound for our second stage concept.

Theorem 3.5. If G is connected and not regular, then
\[ \lambda_1 \leq \Delta - (1/4\Delta^2(n - 2\Delta - 3\Delta + \epsilon_F)) \]
Proof: Let x be a positive unit eigenvector of \( A_2 \) corresponding to \( \lambda_1 \). We have that \( \lambda_1 = |\lambda_1 ||x|^2 \)
\[ \lambda_1 = \lambda_1 \sum_{v \in V} x_{v}^2 \]
\[ = 2 \sum_{v \in V} x_{v}^2 \]
Since the maximum degree of G is \( \Delta \) and G is not regular, we have
\[ \Delta = |D(v)| \geq 2m - 2d_i - \delta + \epsilon_F \]
and hence \( \sum_{v \in V} x_{v}^2 \geq (1/|D(v)|) \sum_{v \in V} x_{v}^2 \geq (1/2m - 2d_i - \delta + \epsilon_F) \sum_{v \in V} x_{v}^2 \geq (1/2m - 2d_i - \delta + \epsilon_F) \sum_{v \in V} x_{v}^2 \geq (1/2m - 3\Delta + \epsilon_F) \sum_{v \in V} x_{v}^2 \]
Let u and v be the vertices of derived graph G such that \( x_u = \max_{v \in V} x_v \) and \( x_v = \min_{v \in V} x_v \) and let \( u = w_0 w_1 \ldots w_k = v \) be a path between u and v in the derived graph G. Then
\[ \sum_{v \in E} x_{v} \geq x_{u} \geq x_{w_0} \]
We have \( \Delta - \lambda_1 \geq (1/2m - 3\Delta + \epsilon_F)(x_{u} - x_v) \). It remains to estimate \( x_{u} - x_v \). Since \( \sum_{v \in V} x_{v}^2 = 1 \), we have \( x_{u} \geq 1/\sqrt{n} \) and \( x_v \leq 1/\sqrt{n} \).

There are three cases to consider.

Case 1a: \( x_u \geq 1/\sqrt{n} + c \). Then \( x_v = 1/\sqrt{n} \) and again \( \Delta - \lambda_1 \geq (c^2/2m - \delta + \epsilon_F) \). Case 1b: \( x_v \leq 1/\sqrt{n} - c \). Then \( x_u = 1/\sqrt{n} \) and again \( \Delta - \lambda_1 \geq (c^2/2m - \delta + \epsilon_F) \). Case 2: \( 1/\sqrt{n} - c < x_v < x_u < 1/\sqrt{n} + c \). Then \( x_v = 1/\sqrt{n} - c = 1/\sqrt{n} + c \). Then \( x_u \in (1/\sqrt{n} - c, 1/\sqrt{n} + c) \). Then \( x_v \in (1/\sqrt{n} - c, 1/\sqrt{n} + c) \) holds for each \( v_i \in V \), and by choosing \( s \in V' \) with \( d_s < \Delta - 1 \), which is regular, we get
\[ \lambda_1(1/\sqrt{n} - c) < \lambda_1 x_v \]
\[\sum_{(s,t) \in E'} x_t < (\Delta' - 1)(1/\sqrt{n} + c)\]

where \(\Delta' = \max D(v_i), i = 1, 2, ..., n\) and \(E'\) is the edge set of \(G'\) which implies,

\[\lambda_1 < (\Delta' - 1)(1 + c\sqrt{n}/1 - c\sqrt{n}).\]

In order for the expression on the RHS to be useful, it must be less than \(\Delta'\), which is satisfied for \(c < 1/(2\Delta' - 1)\). Put \(c = 1/2\Delta'\sqrt{n}\) in cases Ia and Ib, we get,

\[
\Delta - \lambda_1 > 1/(2m - 3\delta + \epsilon_F)4(\Delta')^2 n
\]

\[\lambda_1 < \Delta - (1/(2m - 3\delta + \epsilon_F)4(\Delta')^2 n)\]

While in \(\lambda_1 < (\Delta' - 1)(1 + \sqrt{n}/2\Delta'\sqrt{n}/1 - \sqrt{n}/2\Delta'\sqrt{n})\)

\[
< (\Delta' - 1)(2\Delta' + 1/2\Delta' - 1)
\]

\[= (2\Delta^2 + \Delta' - 2\Delta' - 1/2\Delta' - 1)\]

\[= \Delta' - (1/2\Delta' - 1)\]

This implies \(\lambda_1 < \Delta' - (1/2\Delta' - 1)\)

\[
< \Delta - (1/4(\Delta')^2(2m - 3\delta + \epsilon_F))
\]

\[< \Delta - (1/4(\Delta)^2 n(2m - 3\delta + \epsilon_F))\]

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