DIMACS Technical Report 99-45
September 1999

The Adjacency Matrix and Spectrum of a Graph with Negative Third Largest Eigenvalue

by

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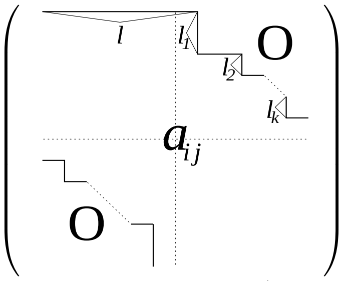
[3]DIMACS Visitor
[4]Research supported in part by XJEC grant of China and RGC CERG grant 652/95E of Hong Kong.

DIMACS is a partnership of Rutgers University, Princeton University, AT&T Labs-Research, Bell Labs, Telcordia Technologies (formerly Bellcore) and NEC Research Institute.

DIMACS is an NSF Science and Technology Center, funded under contract STC–91–19999; and also receives support from the New Jersey Commission on Science and Technology.

ABSTRACT

Let G be a simple connected graph with n vertices, let $\lambda_i(G)$ be the ith largest eigenvalue of G. This paper provides the following results:
1. If $\lambda_3(G) < 0$, then the adjacency matrix of G, $A(G)$ is cogredient to the matrix:



where $a_{ij} = 1$ iff $i \neq j$ and $a_{ij} = 0$ otherwise, and

$$l_1 + l_2 + \ldots + l_k \leq l.$$

Furthermore, if there exists an index i such that $l_i > 1$, then G has the eigenvalue -1 with multiplicity at least $n - 2r - 1$, where $2r$ is the rank of $A(G^c)$.
2. $\lambda_3(G) < 0$ implies that $\lambda_j(G) \geq -1$, $j = 3, 4, \ldots, n - r$, where $2r$ is the rank of the adjacency matrix of the complement of G, $2r \leq n - 1$.

The results presented in [1, 7, 10] are generalized.

1 Introduction and Prelimilaries

All graphs considered here are undirected and simple.

Let G denote a graph with vertex set $\{v_1, v_2, \ldots, v_n\}$. Its *adjacency matrix* $A(G)$ is the $n \times n$ $(0,1)$–matrix (a_{ij}), in which $a_{ij} = 1$ iff v_i is adjacent to v_j, and $a_{ij} = 0$ otherwise. Clearly, $A(G)$ is a symmetric $(0,1)$–matrix with each diagonal entry equal to zero. The *characteristic polynomial* of G, denoted $P(x, G)$, is defined by $\det(xI - A(G))$. Since $A(G)$ is symmetric, its eigenvalues $\lambda_i(A(G))$, $i = 1, 2, \ldots, n$ are real, and may be ordered as $\lambda_1(A(G)) \geq \lambda_2(A(G)) \geq \ldots \geq \lambda_n(A(G))$. For simplicity, we denote the $\lambda_i(A(G))$ by $\lambda_i(G)$ and the complement of the graph G by G^c.

The collection of eigenvalues of G (or $A(G)$) is called the *spectrum* of G. Spectra of graphs appear frequently in the mathematical sciences and chemistry [1]. In quantum chemistry, the skeletons of certain nonsaturated hydrocarbons are represented by graphs. The energy levels of the electrons in such a molecule are the eigenvalues of the corresponding graph. The stability of the molecules as well as other chemically relevant facts are closely related to the graph spectrum. Spectrum techniques are also often used in the proofs of many theorems in matrix theory, graph theory and combinatorics, even though the statements of these theorems do not involve the spectra explicitly [11, 12, 13].

The problem of how to characterize a graph (or a symmetric $(0,1)$–matrix) by its second eigenvalue has been considered by several authors [2, 3, 4, 5]. It is not difficult to show that for a simple connected graph G, $\lambda_2(G) = -1$ or 0 iff G is complete or complete $k-$partite with $2 \leq k \leq n-1$, respectively [1, 6]. For the third largest eigenvalue $\lambda_3(G)$, Dasong Cao and Hong Yuan established in [7] that: (1) $\lambda_3(G) = -1$ iff G^c is isomorphic to the union of a complete biparitite graph and some isolated vertices, (2) there exist no graphs such that $-1 < \lambda_3(G) < -\frac{\sqrt{5}-1}{2}$.

This paper is a continuation of the above work and of [9, 10]. We explore the adjacency matrix $A(G)$ and the eigenvalues of a graph G with $\lambda_3(G) < 0$. In particular, Smith's theorem [1] and Theorem 5, (2) from [7] for the cases of $\lambda_2(G) = -1$ and $\lambda_3(G) = -1$ are also generated.

The techniques and concepts used come from graph theory and the theory of matrices. We recall the following definitions.

Definition 1.1 *Let $A = (a_{ij})$ be an $n \times n$ matrix and $a_{-n+1}, a_{-n+2}, \ldots, a_{n-1}$ be a sequence of numbers. A is a Toeplitz matrix if $a_{ij} = a_{i-j}$, for all $i, j = 1, 2, \ldots, n$.*

Definition 1.2 *Let $A = (a_{ij})$ be a symmetric Toeplitz matrix. If $a_{ij} \neq 0$ iff $0 < |i-j| \leq k$, then A is a symmetric Toeplitz matrix of width k.*

Definition 1.3 *An $n \times n$ $(0,1)$–matrix is a permutation matrix if every row and column contains exactly one non-zero entry.*

Definition 1.4 *An $n \times n$ matrix A is cogredient to a matrix E if for some permutation matrix P, $PAP^T = E$.*

Throughout this paper, the following lemmas are crucial.

Lemma 1.5 *([7]) Let G be a graph with $n \geq 2$ vertices. Then for $k \geq 2$,*

$$\lambda_k(G) + \lambda_{n-k+2}(G^c) \leq -1 \leq \lambda_k(G) + \lambda_{n-k+1}(G^c).$$

Lemma 1.6 *([7]) For every graph G with at least four vertices,*

$$\lambda_3(G) \geq -1.$$

Moreover, if G^c is not bipartite, then $\lambda_3(G) \geq 0$.

Lemma 1.7 *([1]) If G is bipartite, then*

$$\lambda_i(G) = -\lambda_{n-i+1}(G),$$

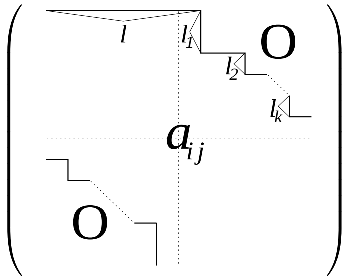
for $1 \leq i \leq n$.

Lemma 1.8 *([1]) Let V be a subgraph of G with k vertices. Then*

$$\lambda_j(G) \geq \lambda_j(V), \quad j = 1, 2, \ldots, k.$$

2 The results

Theorem 2.1 *Let G be a connected graph with n vertices, $n \geq 4$, and $\lambda_3(G) < 0$. Then there exists a permutation matrix P such that*

$PA(G)P^T =$ 

$(\star)$

where $a_{ij} = 1$ iff $i \neq j$, and $a_{ij} = 0$ otherwise, and $l_1 + l_2 + \ldots + l_k \leq l$.

Proof: Taking advantage of Lemma 1.2, $\lambda_3(G) < 0$ implies that G^c is bipartite. So we know that there exists a permutation matrix P_1 such that

$$P_1 A(G) P_1^T = \begin{pmatrix} C_r & B \\ B^T & C_{n-r} \end{pmatrix} \quad (\diamond),$$

where C_i denotes an $i \times i$ matrix with all diagonal entries equal to zero and all off-diagonal entries equal to one. We consider two cases for B:

(i) If B has at most one zero entry, it is easy to see that there exists a permutation matrix P_2 such that $P_2 P_1 A(G) P_1^T P_2^T$ has the form $(\star)$, we then choose $P = P_2 P_1$.

(ii) If B has at least one 2×2 submatrix S_2 such that

$$S_2 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \quad \text{or} \quad S_2 = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}.$$

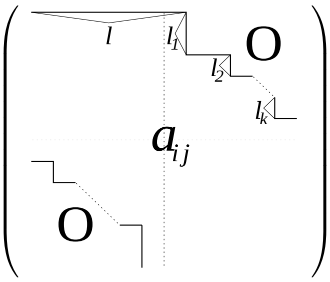
Using $(\diamond)$, we know that $P_1A(G)P_1^T$ has at least one 4×4 principal submatrix S_4 such that

$$S_4 = \begin{pmatrix} 0 & 1 & 1 & 0 \\ 1 & 0 & 0 & 1 \\ 1 & 0 & 0 & 1 \\ 0 & 1 & 1 & 0 \end{pmatrix} \quad \text{or} \quad S_4 = \begin{pmatrix} 0 & 1 & 0 & 1 \\ 1 & 0 & 1 & 0 \\ 0 & 1 & 0 & 1 \\ 1 & 0 & 1 & 0 \end{pmatrix}.$$

Clearly, both cases generate $\lambda_3(S_4) = 0$. By Lemma 1.4, this contradicts our assumption that $\lambda_3(G) < 0$. Therefore, we infer that this case cannot occur.

Consequently, we may conclude that $P_1A(G)P_1^T$ is cogredient to

$$P_2P_1A(G)P_1^TP_2^T =$$



where $a_{ij} = 1$ iff $i \neq j$, and $a_{ij} = 0$ otherwise. Since G^c is bipartite, we have

$$l_1 + l_2 + \ldots + l_k + (n-l) \leq n, \quad \text{or} \quad l_1 + l_2 + \ldots + l_k \leq l.$$

Corollary 2.2 *Let G be a connected graph with n vertices, $n \geq 4$, and $\lambda_3(G) < 0$. Then G has two complete subgraphs, G_1 and G_2 with k_1 and k_2 vertices, respectively, such that $k_1 + k_2 = n$.*

Proof: This is a direct consequence of Theorem 2.1.

Corollary 2.3 *Let G be a connected graph with n vertices, $n \geq 4$. If $\lambda_1(G) \leq \lfloor \frac{n}{2} \rfloor - 1$, then $\lambda_3(G) \geq 0$.*

Proof: If we have $\lambda_3(G) < 0$, then by (2), there exists a permutation matrix P such that

$$PA(G)P^T \geq \begin{pmatrix} C_r & 0 \\ 0 & C_{n-r} \end{pmatrix},$$

where C_i is defined as in Theorem 2.1.

Because G is connected, by the Perron-Frobenius theorem [8],

$$\lambda_1(A(G)) = \lambda_1(G) > \max\{\lambda_1(C_r), \lambda_1(C_{n-r})\} \geq \lfloor \frac{n}{2} \rfloor - 1.$$

Which contradicts our assumption that $\lambda_1(G) \leq \lfloor \frac{n}{2} \rfloor - 1$.

Theorem 2.4 *Let G be a connected graph with n vertices, $n \geq 4$, and $\lambda_3(G) < 0$. Then*
(i) -1 is an eigenvalue of G iff $A(G)$ is not cogredient to the symmetric Toeplitz $(0,1)$–matrix of width $\lfloor \frac{n+1}{2} \rfloor$ (Clearly, there exists only one such matrix for fixed n).
(ii) G has at least $n - 2k - 1$ eigenvalues equal to -1, where $2k$ is the rank of $A(G^c)$.

Proof: *(i)* We consider the matrix $I + PA(G)P^T$, where P is the permutation matrix from Theorem 2.1.

If $\det(I + PA(G)P^T)$ is non-zero, then it is easy to see that

$$l_1 = l_2 = \ldots = l_{\lfloor \frac{n}{2} \rfloor} = 1$$

and $PA(G)P^T$ is the symmetric Toeplitz $(0,1)$–matrix of width $\lfloor \frac{n+1}{2} \rfloor$.

Conversely, if $A(G)$ is cogredient to the symmetric Toeplitz $(0,1)$–matrix of width $\lfloor \frac{n+1}{2} \rfloor$, then

$$\det(I + A(G)) = \det(I + PA(G)P^T) \neq 0,$$

and $P(-1, G) \neq 0$. Thus, -1 is not an eigenvalue of $A(G)$.

(ii) Using $(\star)$ of Theorem 2.1 and by straightforward calculations, we may infer that the rank of the matrix $I + A(G)$ is not greater than $2k + 1$. Thus, -1 is an eigenvalue of G with multiplicity of at least $n - 2k - 1$.

Theorem 2.5 *Let G be a connected graph on n vertices, $n \geq 4$. If $\lambda_3(G) < 0$, then*

$$-1 \leq \lambda_j(G) < 0, \quad j = 3, 4, \ldots, n - r,$$

where $2r$ is the rank of the adjacency matrix $A(G^c)$ of the bipartite graph G^c.

Proof: By Lemma 1.2, $\lambda_3(G) < 0$ implies that G^c is bipartite. So we may assume that $2r$ is the rank of $A(G^c)$.

By Lemma 1.3, $\lambda_{r+1}(G^c) = 0$. Therefore, by Lemma 1.1,

$$\lambda_{n-r}(G) = \lambda_{n-r}(G) + \lambda_{r+1}(G^c) \geq -1.$$

Consequently, we have

$$-1 \leq \lambda_j(G) < 0, \quad j = 3, 4, \ldots, n - r.$$

The following corollary is the main result of [10].

Corollary 2.6 *Let G be a connected graph on n vertices, $n \geq 4$. If $\lambda_3(G) < 0$, and there exists an index k, $2 \leq k \leq \lfloor \frac{n}{2} \rfloor$, such that $\lambda_k(G) = -1$, then*

$$\lambda_j(G) = -1, \quad j = k, k + 1, \ldots, n - r,$$

where $2r$ is the rank of $A(G^c)$ and $r \leq k - 1$.

Proof: If $\lambda_3(G) < 0$, and for an index k, $2 \leq k \leq \lfloor \frac{n}{2} \rfloor$, we have $\lambda_k(G) = -1$. By Theorem 2.5,

$$\lambda_j(G) = -1, \quad j = k, k+1, \ldots, n-r$$

It remains to prove that $r < k$. Since G^c is bipartite, by Lemma 1.3,

$$\begin{aligned} \lambda_j(G^c) &= -\lambda_{n-j+1}(G^c) > 0, \quad j \leq r, \\ \lambda_j(G^c) &= -\lambda_{n-j+1}(G^c) = 0, \quad j > r, \end{aligned}$$

where $2r$ is the rank of matrix $A(G^c)$. Thus the following inequality

$$\lambda_{n-k+1}(G^c) < 0$$

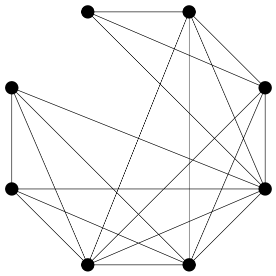
holds for $\lfloor \frac{n}{2} \rfloor \geq r \geq k$. By Lemma 1.1,

$$\begin{aligned} \lambda_k(G) &\geq -1 - \lambda_{n-k+1}(G^c) \\ &> -1, \end{aligned}$$

which contradicts our assertion that $\lambda_k(G) = -1$. Thus, $r \leq k - 1$.

The following example indicates that the equality $r = k - 1$ in Corollary 2.6 does not hold in general.

Example:

$G =$ 

$$A(G) = \begin{pmatrix} 0 & 1 & 1 & 1 & 0 & 0 & 0 & 0 \\ 1 & 0 & 1 & 1 & 1 & 1 & 0 & 0 \\ 1 & 1 & 0 & 1 & 1 & 1 & 0 & 0 \\ 1 & 1 & 1 & 0 & 1 & 1 & 1 & 1 \\ 0 & 1 & 1 & 1 & 0 & 1 & 1 & 1 \\ 0 & 1 & 1 & 1 & 1 & 0 & 1 & 1 \\ 0 & 0 & 0 & 1 & 1 & 1 & 0 & 1 \\ 0 & 0 & 0 & 1 & 1 & 1 & 1 & 0 \end{pmatrix}$$

Using Maple, we obtain that

$$\begin{cases} \lambda_1(G) = 5.24384 \\ \lambda_2(G) = 1.60317 \\ \lambda_3(G) = -0.182062 \\ \lambda_4(G) = -1 \\ \lambda_5(G) = -1 \\ \lambda_6(G) = -1 \\ \lambda_7(G) = -1.53035 \\ \lambda_8(G) = -2.1346. \end{cases}$$

On the other hand, since the rank of the matrix $A(G^c)$ is 4, we infer that

$$\lambda_4(G) = \lambda_5(G) = \lambda_6(G) = -1.$$

Compared with Corollary 2.6, this is the special case that $r = 2, k = 4, n = 8$.

For Corollary 2.6, we consider two special cases:

(*i*) If $\lambda_2(G) = -1$, then $\lambda_j(G) = -1$, $j = 2, 3, \ldots, n-1$. We know $\lambda_1(G) \geq n-1$, as $\lambda_n(G) \leq -1$ and $\sum\limits_{i=1}^{n} \lambda_i(G) = 0$. On the other hand, $\lambda_1(G) \leq n-1$. Hence, $\lambda_1(G) = n-1$. Thus, G is complete. Conversely, if G is complete, then $\lambda_j(G) = -1$, $j = 2, \ldots, n$, and $\lambda_1(G) = n-1$. This is a result presented in [1].

(*ii*) If $\lambda_3(G) = -1$, by Corollary 2.6, we have $r \leq 2$ (since $k = 3$). In the case $r = 2$, by Theorem 2.1, $A(G)$ has a 4×4 principal submatrix S_4, where S_4 is one of these four matrices:

$$\begin{pmatrix} 0 & 1 & 1 & 0 \\ 1 & 0 & 1 & 1 \\ 1 & 1 & 0 & 1 \\ 0 & 1 & 1 & 0 \end{pmatrix}, \begin{pmatrix} 0 & 1 & 1 & 1 \\ 1 & 0 & 1 & 0 \\ 1 & 1 & 0 & 1 \\ 1 & 0 & 1 & 0 \end{pmatrix}, \begin{pmatrix} 0 & 1 & 1 & 0 \\ 1 & 0 & 0 & 1 \\ 1 & 0 & 0 & 1 \\ 0 & 1 & 1 & 0 \end{pmatrix}, \begin{pmatrix} 0 & 1 & 0 & 1 \\ 1 & 0 & 1 & 0 \\ 0 & 1 & 0 & 1 \\ 1 & 0 & 1 & 0 \end{pmatrix}$$

All four matrices have $\lambda_3(S_4) \geq -\frac{\sqrt{5}-1}{2} > -1$, but by Lemma 1.4, we know that $\lambda_3(G) = -1$. Thus, $\lambda_3(G) = -1$ implies that $r \leq 1$.

If $r = 0$, then $A(G^c) = 0$, and therefore G is complete. If $r = 1$, then $A(G^c)$ is cogredient to the following matrix:

$$\widehat{A} = \begin{pmatrix} 0 & J & 0 \\ J^T & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}$$

where J is a matrix whose entries are all equal to one. Consequently, we infer that G^c is the union of a complete bipartite graph and some isolated vertices.

Conversely, if G^c is the union of a complete bipartite graph and some isolated vertices, then, without loss of generality, we may assume that $A(G^c) = \widehat{A}$. Considering the matrix $I + A(G)$, we know that it has rank $t \leq 3$. Therefore, G has at least $n-3$ eigenvalues equal to -1. Since the rank of $A(G^c)$ is 2, $\lambda_3(G) = -1$ by Lemmas 1.1 and 1.3. Noting that G is connected and utilizing Corollary 2.6, this yields

$$\lambda_j(G) = -1, \quad j = 3, 4, \ldots, n-1.$$

Corollary 2.7 *Let G be a connected graph with n vertices, $n \geq 4$, that is not the complete graph. Then*
(*i*) $\lambda_3(G) = -1$ *iff G^c is the union of a complete bipartite graph and some isolated vertices.*
(*ii*) $\lambda_3(G) = -1$ *implies that* $\lambda_j(G) = -1$, $j = 3, 4, \ldots, n-1$.

Corollary 2.7 generalizes Theorem 2.5 in [7] and the corresponding results in [1, 10].

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