de Caen’s inequality and bounds on the largest Laplacian eigenvalue of a graph

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Received 1 May 2000; accepted 18 October 2000

Submitted by R.A. Brualdi

Abstract

In this paper we determine the extremal graphs for which equality in de Caen’s inequality holds and then apply the inequality to give an upper bound for the largest Laplacian eigenvalue \( \lambda_1(G) \) of a graph. In addition, we give two other types of upper bound for \( \lambda_1(G) \) and determine the extremal graphs which achieve the bounds. © 2001 Elsevier Science Inc. All rights reserved.

AMS classification: 15A18; 05C50

Keywords: Graph; Laplacian matrix; Largest eigenvalue; Upper bound

1. Introduction

Let \( G = (V(G), E(G)) \) be a connected graph with vertex set \( V(G) = \{v_1, v_2, \ldots, v_n\} \) and edge set \( E(G) = \{e_1, e_2, \ldots, e_m\} \). Assume that the vertices are ordered such that \( d_1 \geq d_2 \geq \cdots \geq d_n \), where \( d_i \) is the degree of \( v_i \) for \( i = 1, 2, \ldots, n \). The Laplacian matrix of \( G \) is \( L(G) = D(G) - A(G) \), where \( D(G) = \text{diag}(d_1, d_2, \ldots, d_n) \), and \( A(G) \) is the adjacency matrix of \( G \). It is known that \( L(G) \) is a positive semidefinite, symmetric and singular. Hence we may assume that \( \lambda_1(G) \geq \lambda_2(G) \geq \cdots \geq \lambda_{n-1}(G) \geq \lambda_n(G) = 0 \) are the eigenvalues of \( L(G) \). Moreover it is known that the
multiplicity of 0 as the eigenvalue of $L(G)$ is equal to the number of connected components of $G$. So a graph $G$ is connected if and only if $\lambda_{n-1}(G) > 0$. The eigenvalues of the Laplacian matrix are important in graph theory, because they have relations to numerous graph invariants including connectivity, expanding property, isoperimetric number, maximum cut, independence number, genus, diameter, mean distance, and bandwidth-type parameters of a graph (see, for example, [2,3,8,10] and the references therein). Especially, the largest and the second smallest eigenvalues of $L(G)$ (for instance [2,3,8,10]) are probably the most important information contained in the spectrum of a graph, they play the central role in our fundamental understanding of graphs. Since $\lambda_{n-1}(G) = n - \lambda_1(\overline{G})$, where $\overline{G}$ is the complement of $G$, it is not surprising at all that the importance of one of these eigenvalues implies the importance of the other.

In many applications one needs good bounds for the largest Laplacian eigenvalue $\lambda_1(G)$ (for instance [2,3,8,10]). Anderson and Morley [1] proved that

$$\lambda_1(G) \leq \max\{d_i + d_j; v_iv_j \in E(G)\}. \quad (1)$$

Li and Zhang [6] improved the upper bound (1) as follows:

$$\lambda_1(G) \leq 2 + \sqrt{(r - 2)(s - 2)}, \quad (2)$$

where $r = \max\{d_i + d_j; v_iv_j \in E(G)\} = d_k + d_l$ for some $v_kv_l \in E(G)$, and $s = \max\{d_i + d_j; v_iv_j \in E(G) - v_kv_l\}$. Merris [9] gave a bound as follows:

$$\lambda_1(G) \leq \max\{d_i + m_i; v_i \in V(G)\}, \quad (3)$$

where $m_i$ is the average of the degrees of the vertices adjacent to $v_i$ ($d_i m_i$ is the “2-degree” of $v_i$). Li and Zhang [7] presented the following result:

$$\lambda_1(G) \leq \max \left\{ \frac{d_i(d_i + m_i) + d_j(d_j + m_j)}{d_i + d_j}; v_iv_j \in E(G) \right\}. \quad (4)$$

It is easy to see that the upper bound (4) is an improvement of (3). Recently, de Caen [4] gave an inequality concerning the sum of squares of degrees in a graph. The inequality is a powerful tool for establishing an upper bound of the largest Laplacian eigenvalue of a graph. In this paper, we determine the extremal graphs for which equality in de Caen’s inequality holds, and give upper bounds for the largest eigenvalue of the Laplacian matrix of a graph.

2. **On de Caen’s inequality**

In this section, we determine the extremal graphs for which equality in de Caen’s inequality holds.

**Theorem 2.1** [4]. *Let $G$ be a simple graph with $n$ vertices and $m$ edges, and let $\pi = (d_1, d_2, \ldots, d_n)$ be the degree sequence of $G$. Then,*
\[ d_1^2 + d_2^2 + \cdots + d_n^2 \leq m \left( \frac{2m}{n-1} + n - 2 \right). \] (5)

Recently, van Dam [5] proved the following.

**Theorem 2.2** [5]. Let \( X = (X_{ij}) \) be an \( m \times n \) real matrix. Then

\[
\left( \sum_{i=1}^{m} \sum_{j=1}^{n} X_{ij} \right)^2 + mn \sum_{i=1}^{m} \sum_{j=1}^{n} X_{ij}^2 \\
\geq m \sum_{i=1}^{m} \left( \sum_{j=1}^{n} x_{ij} \right)^2 + n \sum_{j=1}^{n} \left( \sum_{i=1}^{m} x_{ij} \right)^2,
\] (6)

with equality if and only if \( X_{ij} = y_i + z_j \) for some real vectors \( y \) and \( z \), and all \( i \) and \( j \).

van Dam pointed out that the matrix inequality (6) and de Caen’s inequality are equivalent in the following sense. When Theorem 2.2 is applied to the symmetric \( n \times n \) matrix \( Z \) for which

\[ Z_{ii} = \frac{2}{n-2} \sum_{j \neq i} Z_{ij} - \frac{2}{(n-1)(n-2)} \sum_{j<k} Z_{jk}, \]

then the following is obtained.

**Theorem 2.3** [4]. Let \( Z = (Z_{ij}) \) be an \( n \times n \) real matrix. Then

\[
\left( \sum_{i<j} Z_{ij} \right)^2 + \left( \frac{n-1}{2} \right) \sum_{i<j} Z_{ij}^2 \geq \frac{n-1}{2} \sum_{i} \left( \sum_{j \neq i} Z_{ij} \right)^2.
\] (7)

Using these above results, we can prove the following.

**Theorem 2.4.** Let \( G \) be a connected graph with \( n \) vertices and \( m \) edges. Then equality in (5) holds if and only if \( G \) is a star graph \( K_{1,n-1} \) or a complete graph \( K_n \).

**Proof.** It is easy to verify that equality in (5) is satisfied by the graphs \( K_{1,n-1} \) and \( K_n \).

Now suppose that \( G \) is a connected graph for which equality in (5) holds and \( A = (a_{ij}) \) is the adjacency matrix of \( G \). If \( n = 2 \), it is easy to see that \( G = K_2 \) and (5) becomes equality. Hence we can assume that \( n \geq 3 \). van Dam pointed out that by using Theorem 2.2 to the \( n \times n \) symmetric matrix \( X = (X_{ij}) \) defined by \( X_{ij} = a_{ij} \) if \( i \neq j \) and
we can obtain (7) and (5). Hence, if equality in (5) holds, then \( X_{ij} = y_i + z_j \) for some real vectors \( y \) and \( z \), and all \( i \neq j \). Therefore

\[
A = \begin{pmatrix}
0 & y_1 + z_2 & \cdots & y_1 + z_n \\
y_2 + z_1 & 0 & \cdots & y_2 + z_n \\
\vdots & \vdots & \ddots & \vdots \\
y_n + z_1 & y_n + z_2 & \cdots & 0
\end{pmatrix},
\]

where \( y_i + z_j = 0 \) or 1 \((i, j = 1, 2, \ldots, n)\). Without loss of generality, we can arrange the vertices of \( G \) such that \( d_i \) is the \( i \)th row sum of \( A \), and \( d_1 \geq d_2 \geq \cdots \geq d_n \geq 1 \). Now assume \( d_1 < n - 1 \). Then there is an integer \( 1 < j \leq n \) such that \( a_{1j} = y_1 + z_j = 0 \). Since \( d_j \geq 1 \), there must be an integer \( 1 < k \leq n \) such that \( a_{kj} = y_k + z_j = 1 \). Hence \( y_k = a_{kj} - z_j + a_{1j} = 1 - z_j + y_1 + z_j = y_1 + 1 \). Therefore for any \( s \neq k \), \( a_{ks} = y_k + z_s = y_1 + 1 + z_s = 1 + a_{1s} \). So, \( a_{1s} = 0 \) and \( a_{ks} = 1 \). In other words, \( d_1 = d_2 = \cdots = d_n = 1 \). Hence \( 2m = n \). Since \( G \) is connected, \( m = n/2 \geq n - 1 \). It follows that \( n \leq 2 \), impossible. Hence \( d_1 = n - 1 \). If \( d_2 < n - 1 \), then there must be an integer \( j > 2 \) such that \( a_{2j} = 0 \). Hence \( y_1 + z_j = y_2 + z_j = 1 \), i.e., \( y_2 = y_1 - 1 \). Therefore, \( a_{2j} = y_2 + z_j = y_1 - 1 + z_j = a_{1j} - 1 = 0 \) for \( j \geq 3 \). Hence \( d_2 = 1 \). Thus \( G \) is a star graph. If \( d_2 = n - 1 \), then for \( j \geq 3 \), \( a_{2j} = 1 = a_{21} \), i.e., \( z_j = z_1 \). So, for \( i \geq 3 \) and \( j \neq i \), \( a_{ij} = y_i + z_j = y_i + z_1 = a_{i1} = a_{1i} = 1 \). Hence \( G \) is a complete graph. □

3. Main results

In this section, we will give three upper bounds for the largest Laplacian eigenvalue of a graph. Firstly, we apply de Caen’s inequality to give the upper bound as follows.

**Theorem 3.1.** Let \( G \) be a connected graph with \( n \) vertices and \( m \) edges. Then,

\[
\lambda_1(G) \leq \frac{2m + \sqrt{(n - 2)m(n(n - 1) - 2m)}}{n - 1},
\]

with equality if and only if \( G \) is one of \( K_{1,n-1} \) and \( K_n \).

**Proof.** Clearly,

\[
\lambda_1(G) + \lambda_2(G) + \cdots + \lambda_{n-1}(G) = \text{Tr}(L(G)) = \sum_{v \in V(G)} d_v,
\]

\[
\lambda_1^2(G) + \lambda_2^2(G) + \cdots + \lambda_{n-1}^2(G) = \text{Tr}(L^2(G)) = \sum_{v \in V(G)} (d_v^2 + d_v),
\]
where $\text{Tr}(L(G))$ is the trace of $L(G)$. By the Cauchy–Schwarz inequality, we have

$$(n - 2)(\lambda_2^2(G) + \lambda_3^2(G) + \cdots + \lambda_{n-1}^2(G))$$

$$\geq (\lambda_2(G) + \lambda_3(G) + \cdots + \lambda_{n-1}(G))^2.$$  

Hence,

$$(n - 2) \left( \sum_{v \in V(G)} (d_v^2 + d_v) - \lambda_1^2(G) \right) \geq \left( \sum_{v \in V(G)} d_v - \lambda_1(G) \right)^2.$$  

Therefore,

$$\lambda_1(G) \leq \frac{\sum_{v \in V(G)} d_v + \sqrt{(n - 2)((n - 1) \sum_{v \in V(G)} (d_v^2 + d_v) - (\sum_{v \in V(G)} d_v)^2) / n - 1}}{n - 1}.$$  

Thus (8) comes from (5).

Now suppose equality in (8) holds for the graph $G$. Then de Caen’s inequality must be equality. By Theorem 2.4, $G$ is $K_{1,n-1}$ or $K_n$.

Conversely, it is easy to verify that equality in (8) holds for $K_{1,n-1}$ and $K_n$.  

The following are two other types of upper bounds for $\lambda_1(G)$.

**Theorem 3.2.** Let $G$ be a connected graph with $n$ vertices and $m$ edges. Then

$$\lambda_1(G) \leq \sqrt{2d_1^2 + 4m - 2d_n(n - 1) + 2d_1(d_n - 1)},$$

with equality if and only if $G$ is a bipartite regular graph.

**Proof.** Suppose that $x = (x_1, x_2, \ldots, x_n)^T$ is an eigenvector with unit length corresponding to $\lambda_1(G)$. Then $L(G)x = \lambda_1(G)x$. Hence, for $u \in V(G)$,

$$\lambda_1(G)x_u = d_u x_u - \sum_{v \in V(G)} a_{uv} x_v,$$

where $A = (a_{uv})$ is the adjacency matrix of $G$. Therefore,

$$\lambda_1(G)x_u = \sum_{v \sim u} (x_u - x_v),$$

where $v \sim u$ means that $v$ and $u$ are adjacent. By the Cauchy–Schwarz inequality, we have

$$\lambda_1^2(G)x_u^2 \leq \left( \sum_{v \sim u} 1^2 \right) \sum_{v \sim u} (x_u - x_v)^2.$$
\[ = d_u \left( \sum_{v \sim u} x_u^2 - 2x_u \sum_{v \sim u} x_v + \sum_{v \sim u} x_v^2 \right). \]

Observe that
\[-2x_u \sum_{v \sim u} x_v \leq \sum_{v \sim u} (x_u^2 + x_v^2) = d_u x_u^2 + \sum_{v \sim u} x_v^2. \quad (11)\]

Hence,
\[\lambda_1^2(G) x_u^2 \leq 2d_u^2 x_u^2 + 2d_u \sum_{v \sim u} x_v^2. \quad (12)\]

Consequently,
\[\lambda_1^2(G) = \lambda_1^2(G) \sum_{u \in V(G)} x_u^2 \leq 2d_u^2 x_u^2 + 2 \sum_{u \in V(G)} d_u \sum_{v \sim u} x_v^2 \leq 2d_1^2 + 2 \sum_{u \in V(G)} d_u \sum_{v \sim u} x_v^2.\]

Now let \( v \not\sim u \) mean that \( v \) and \( u \) are not adjacent. Then
\[
\sum_{v \not\sim u} d_u \sum_{v \not\sim u} x_v^2 = \sum_{u \in V(G)} d_u \left( 1 - \sum_{v \not\sim u} x_v^2 \right) = 2m - \sum_{u \in V(G)} d_u \sum_{v \not\sim u} x_v^2
\]
\[= 2m - \left( \sum_{u \in V(G)} d_u x_u^2 + \sum_{u \in V(G)} d_u \sum_{v \not\sim u \sim u} x_v^2 \right) \leq 2m - \left( \sum_{u \in V(G)} d_u x_u^2 + \sum_{u \in V(G)} d_n \sum_{v \not\sim u \not\sim u} x_v^2 \right)
= 2m - \left( \sum_{u \in V(G)} d_u x_u^2 + \sum_{u \in V(G)} d_n (n - d_u - 1)x_u^2 \right)
= 2m - \left( d_n (n - 1) - (d_n - 1) \sum_{u \in V(G)} d_u x_u^2 \right)
= 2m - d_n (n - 1) + (d_n - 1) \sum_{u \in V(G)} d_u x_u^2
\leq 2m - (n - 1)d_n + d_1 (d_n - 1).
\]

Hence
\[\lambda_1^2(G) \leq 2d_1^2 + 4m - 2d_n (n - 1) + 2d_1 (d_n - 1).\]

Thus (9) holds.
Now suppose that equality in (9) holds. Then all inequalities in the above argument must be equalities. In particular, we have from (11) that
\[ -2x_u \sum_{v \sim u} x_v = d_u x_u^2 + \sum_{v \sim u} x_v^2. \]
Hence,
\[ \sum_{v \sim u} (x_u + x_v)^2 = 0. \]
Therefore \(-x_v = x_u\) for each \(v \sim u\). Since \(G\) is connected, every component of \(x\) is non-zero. Denote
\[ V_1 = \{ u \in V(G) \mid x_u > 0 \}, \quad V_2 = \{ u \in V(G) \mid x_u < 0 \}. \]
Then \(V_1, V_2\) is a partition of \(V(G)\). Clearly, there is no pair of two vertices in \(V_1\) or \(V_2\) which is an edge. Thus \(G\) is a bipartite graph. Moreover, for each \(u \in V(G)\), it follows by (10) that
\[ (d_u - \lambda_1(G))x_u = \sum_{v \sim u} x_v = d_u x_v = -d_u x_u. \]
Hence, \(2d_u = \lambda_1(G)\) for \(u \in V(G)\). Thus \(G\) is regular.

Conversely, it is easy to verify that equality in (9) holds for bipartite regular graphs. □

**Theorem 3.3.** Let \(G\) be a connected graph. Then
\[ \lambda_1(G) \leq \max \{ \sqrt{2d_u(d_u + m_u)} : u \in V(G) \}, \]
with equality if and only if \(G\) is a bipartite regular graph.

**Proof.** It follows from (12) that
\[ \lambda_1^2(G) \leq 2 \sum_{u \in V(G)} d_u^2 x_u^2 + 2 \sum_{u \in V(G)} x_u^2 \left( \sum_{v \sim u} d_v \right) \]
\[ = 2 \sum_{u \in V(G)} (d_u^2 + m_u d_u) x_u^2. \]
Thus (13) holds.

If equality in (13) holds, then equality in (11) holds. By the proof of Theorem 3.2, \(G\) is a bipartite regular graph. Conversely, we can easily verify that equality in (13) holds for bipartite regular graphs. □

**Remark.** The three bounds (8), (9), and (13) are incomparable. Moreover, there is no comparability between any one of them and any one of the upper bounds (1), (2), (3) and (4). However, the upper bound (13) is better than the bounds (3) and (4) in some cases. As an illustration, let us consider the graph \(G\) presented in Fig. 1. By an elementary calculation, we have
\begin{align*}
\max\{d_i + d_j : v_i v_j \in E(G)\} &= 2 + \sqrt{(r-2)(s-2)} = 9. \\
\max\{d_u + m_u : u \in V(G)\} &= \max \left\{ \frac{d_i (d_i + m_i) + d_j (d_j + m_j)}{d_i + d_j} : v_i v_j \in E(G) \right\} \\
&= 8.75 > 8.37 = \sqrt{70} \\
&= \max\{\sqrt{2d_u(d_u + m_u)} : u \in V(G)\}.
\end{align*}

Acknowledgment

We would like to thank the referee for valuable comments on our paper.

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