ON THE LAPLACIAN SPREAD OF TREES AND UNICYCLIC GRAPHS

MUHUO LIU

ABSTRACT. In this paper, we determine the four trees (resp. the three unicyclic graphs), which share the second to fifth (resp. the second to fourth) largest Laplacian spreads among all the trees (resp. connected unicyclic graphs) on \( n \geq 10 \) (respectively \( n \geq 17 \) vertices).

1. Introduction

Throughout the paper, we only consider the connected undirected simple graphs. Let \( d(u) \) be the degree of vertex \( u \). Especially, \( \Delta(G) \), short for \( \Delta \), indicates the maximum degree of vertices pertaining to \( G \). The notations \( T_n \) and \( U_n \) are used to denote the class of trees and connected unicyclic graphs of order \( n \), respectively. As usual, \( K_{1,n-1} \) denotes the star of order \( n \).

Let \( A(G) \) be the adjacency matrix of \( G \). Since \( A(G) \) is symmetric, the eigenvalues of \( A(G) \) can be arranged as follows:

\[
\lambda_1(G) \geq \lambda_2(G) \geq \ldots \geq \lambda_n(G).
\]

The spread of the graph \( G \) is defined as

\[
S(G) = \lambda_1(G) - \lambda_n(G).
\]

Suppose the degree of vertex \( v_i \) equals \( d(v_i) \) for \( i = 1, 2, \ldots, n \), and let \( D(G) \) be the diagonal matrix whose \((i,i)\)-entry is \( d(v_i) \). The Laplacian matrix of \( G \) is
\[ L(G) = D(G) - A(G), \]
and the Laplacian characteristic polynomial of \( G \) is denoted by \( \Phi(G, x) \), i.e., \( \Phi(G, x) = \det(xI - L(G)) \). It is well known that \( L(G) \) is symmetric and positive semidefinite so that its eigenvalues can be arranged as follows:

\[ 0 = \mu_n(G) \leq \mu_{n-1}(G) \leq \ldots \leq \mu_1(G), \]

where \( \mu_{n-1}(G) > 0 \) if and only if \( G \) is connected and is called the algebraic connectivity of the graph \( G \). The Laplacian spread of the graph \( G \), denoted by \( LS(G) \), is defined to be

\[ LS(G) = \mu_1(G) - \mu_{n-1}(G). \]

Recently, the spread of a graph has received much attention. In [1], Petrović determined all minimal graphs whose spreads do not exceed 4. In [2] and [3], some lower and upper bounds for the spread of a graph were given. After then, the maximal spreads among all unicyclic graphs and all bicyclic graphs were determined in [4] and [5], respectively. For the up to date results on the spread of a graph \( G \), one can refer to [6] and [7]. However, the Laplacian spread seems less well-known because it is conceived somewhat later [6]. Up to now, there are only very limited results on the Laplacian spread. Firstly, the maximal and minimal Laplacian spreads among all trees of given order were identified in [6]. After then, the maximum Laplacian spread among all unicyclic graphs of given order was determined in [7] and [8] by using different methods. Very recently, the minimum Laplacian spread among all unicyclic graphs on \( n \) vertices was determined in [9]. In this paper, by using different methods from [6], [7], [8] and [9], we determine the four trees (resp. the three unicyclic graphs), which share the second to fifth (resp. the second to fourth) largest Laplacian spreads among all the trees (resp. connected unicyclic graphs) of given order.

2. The first to fifth largest Laplacian spreads of trees

Lemma 2.1. [10] Suppose \( G \) is a connected graph, then \( \mu_1(G) \leq \max \{d(v) + m(v) : v \in V\} \), where \( m(v) = \sum_{u \in N(v)} d(u)/d(v) \).

Proposition 2.1. Let \( T \) be a tree on \( n \) vertices with \( \Delta \leq n - 4 \). If \( n \geq 10 \), then \( \mu_1(T) \leq n - 2.5 \).

Proof. By Lemma 2.1, we only need to prove that \( \max \{d(v) + m(v) : v \in V(T)\} \leq n - 2.5 \). Suppose \( \max \{d(v) + m(v) : v \in V(T)\} \) occurs at the vertex \( u \). Three cases arise \( d(u) = 1, d(u) = 2, \) or \( 3 \leq d(u) \leq \Delta \).
Case 1. \( d(u) = 1 \).
Suppose \( v \in N(u) \). Since \( m(u) = d(v) \leq \Delta \leq n - 4 \), thus \( d(u) + m(u) \leq n - 3 < n - 2.5 \).

Case 2. \( d(u) = 2 \).
Suppose that \( v,w \in N(u) \). Note that \( T \) is a tree, then \( |N(v) \cap N(w)| \leq 1 \) and \( |N(v) \cup N(w)| \leq n \). Therefore,

\[
d(u) + m(u) = 2 + \frac{d(v) + d(w)}{2} \leq 2 + \frac{n + 1}{2} \leq n - 2.5.
\]

Case 3. \( 3 \leq d(u) \leq \Delta \).
Note that \( T \) has \( n - 1 \) edges and \( 3 \leq d(u) \leq \Delta \leq n - 4 \), then

\[
d(u) + m(u) \leq d(u) + \frac{2(n - 1) - d(u) - 3}{d(u)} = d(u) - 1 + \frac{2n - 5}{d(u)}.
\]

Next we shall prove that \( d(u) - 1 + \frac{2n - 5}{d(u)} \leq n - 2.5 \), equivalently, \( d(u)(n - 1.5 - d(u)) \geq 2n - 5 \). Once this is proved, we are done. Let \( f(x) = (n - 1.5 - x)x \).

When \( 3 \leq x \leq \frac{n - 1.5}{2} \), since \( f'(x) = n - 1.5 - 2x \geq 0 \), we have \( f(x) \geq f(3) = 3(n - 4.5) > 2n - 5 \).

When \( \frac{n - 1.5}{2} \leq x \leq n - 4 \), since \( f'(x) = n - 1.5 - 2x \leq 0 \), we have \( f(x) \geq f(n - 4) = 2.5(n - 4) \geq 2n - 5 \).

By combining the above arguments, the assertion follows. \( \square \)

\[
\begin{align*}
\begin{array}{c}
\begin{array}{c}
\text{T}_2 \\
\end{array} \quad \begin{array}{c}
\begin{array}{c}
\text{T}_3 \\
\end{array} \quad \begin{array}{c}
\begin{array}{c}
\text{T}_4 \\
\end{array} \quad \begin{array}{c}
\begin{array}{c}
\text{T}_5 \\
\end{array}
\end{array}
\end{array}
\end{array}
\end{align*}
\]

**Figure 1.** The trees \( T_2, T_3, T_4 \) and \( T_5 \)

In the following, let \( T_1 = K_{1,n-1} \) and \( T_2, T_3, \ldots, T_5 \) be the trees of order \( n \geq 10 \) as shown in Figure 1. By an elementary computation, it follows that

(1a) \( \Phi(T_2, x) = x(x - 1)^{n-4}(x^3 - (n + 2)x^2 + (3n - 2)x - n) \).

(2a) \( \Phi(T_3, x) = x(x - 1)^{n-5}(x^4 - (n + 3)x^3 + (5n - 4)x^2 - (6n - 10)x + n) \).

(3a) \( \Phi(T_4, x) = x(x - 1)^{n-4}(x^3 - (n + 2)x^2 + (4n - 7)x - n) \).

(4a) \( \Phi(T_5, x) = x(x - 1)^{n-6}(x^2 - 3x + 1)(x^3 - (n + 1)x^2 + (3n - 5)x - n) \).
Lemma 2.2. If \( n \geq 10 \), then \( LS(T_2) > LS(T_3) > LS(T_4) > LS(T_5) \).

Proof. If \( 10 \leq n \leq 12 \), by equalities (1a)–(4a) we have

<table>
<thead>
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<th>( n )</th>
<th>10</th>
<th>11</th>
<th>12</th>
</tr>
</thead>
<tbody>
<tr>
<td>( LS(T_2) )</td>
<td>8.5826</td>
<td>9.5843</td>
<td>10.5861</td>
</tr>
<tr>
<td>( LS(T_3) )</td>
<td>7.7689</td>
<td>8.7693</td>
<td>9.7705</td>
</tr>
<tr>
<td>( LS(T_4) )</td>
<td>7.7142</td>
<td>8.7070</td>
<td>9.7038</td>
</tr>
<tr>
<td>( LS(T_5) )</td>
<td>7.6660</td>
<td>8.6540</td>
<td>9.6460</td>
</tr>
</tbody>
</table>

It is easily checked that \( LS(T_2) > LS(T_3) > LS(T_4) > LS(T_5) \) holds. Thus, we suppose \( n \geq 13 \) in the following. Let
\[
\varphi_1(x) = x^3 - (n + 2)x^2 + (3n - 2)x - n, \\
\varphi_2(x) = x^4 - (n + 3)x^3 + (5n - 4)x^2 - (6n - 10)x + n, \\
\varphi_3(x) = x^3 - (n + 2)x^2 + (4n - 7)x - n, \\
\varphi_4(x) = x^3 - (n + 1)x^2 + (3n - 5)x - n.
\]
We divide the proof into the next three stages.

(1) \( LS(T_2) > LS(T_3) \).

Since
\[
\varphi_1(0) = -n < 0, \quad \varphi_1(0.5) = 0.25n - 1.375 > 0, \\
\varphi_1(n - 1) = -1 < 0, \quad \varphi_1(n) = n^2 - 3n > 0,
\]
then the three roots of the equation \( \varphi_1(x) = 0 \) lie in \((0, 0.5)\), \((0.5, n - 1)\) and \((n - 1, n)\), respectively. On the other hand, since
\[
\varphi_2(0) = n > 0, \quad \varphi_2(0.24) = 2.13144576 - 0.165824n < 0, \\
\varphi_2(2) = n - 4 > 0, \quad \varphi_2(n - 2) = 4 - n < 0, \\
\varphi_2(n - 1.5) = 0.5n^3 - 4.75n^2 + 12.875n - 8.8125 > 0.5n^3 - 5n^2 > 0,
\]
then the four roots of the equation \( \varphi_2(x) = 0 \) lie in \((0, 0.24), (0.24, 2), (2, n - 2)\) and \((n - 2, n - 1.5)\), respectively.

By equalities (1a) and (2a), we can conclude that
\[
(2.1) \quad 0 < \mu_{n-1}(T_2) < 0.5, \quad n - 1 < \mu_1(T_2) < n. \\
(2.2) \quad 0 < \mu_{n-1}(T_3) < 0.24, \quad n - 2 < \mu_1(T_3) < n - 1.5.
\]

By inequalities (2.1) and (2.2), it follows that
\[
LS(T_2) = \mu_1(T_2) - \mu_{n-1}(T_2) > n - 1 - 0.5 = n - 1.5 - 0 > \mu_1(T_3) - \mu_{n-1}(T_3) = LS(T_3).
\]

(2) \( LS(T_3) > LS(T_4) \).

Recall that \( n \geq 13 \), then
\[
\varphi_3(0.267) = -1.992543837 - 0.003289n < 0,
\]
By Lemmas 2.2 and 2.3, we only need to prove that

\[ \varphi_3(0.34) = 0.2444n - 2.571896 > 0, \quad \varphi_3(n - 2) = -2 < 0, \]
\[ \varphi_3(n - 1.973) = 0.027n^2 - 0.214542n - 1.654812317 > 0.027(n^2 - 8n - 62) > 0. \]

Thus, the three roots of the equation \( \varphi_3(x) = 0 \) lie in \((0.267, 0.34), (0.34, n - 2)\) and \((n - 2, n - 1.973)\), respectively. By equality (3a), it follows that

\[ 0.267 < \mu_{n-1}(T_4) < 0.34, \quad n - 2 < \mu_1(T_4) < n - 1.973. \]

By combining with inequalities (2.2) and (2.3), we can conclude that

\[ \text{LS}(T_4) = \mu_1(T_4) - \mu_{n-1}(T_3) > n - 2 - 0.24 = n - 1.973 - 0.267 > \text{LS}(T_4). \]

(3) \( \text{LS}(T_4) > \text{LS}(T_5) \).

Recall that \( n \geq 13 \), then

\[ \varphi_4(0.38) = -1.989528 - 0.0044n < 0, \]
\[ \varphi_4(0.5) = 0.25n - 2.625 > 0, \quad \varphi_4(n - 2) = -2 < 0, \]
\[ \varphi_4(n - 1.97) = 0.03n^2 - 0.2082n - 1.676273 > 0.03(n^2 - 7n - 56) > 0. \]

Thus, the three roots of the equation \( \varphi_4(x) = 0 \) lie in \((0.38, 0.5), (0.5, n - 2)\) and \((n - 2, n - 1.97)\), respectively. By equality (4a), it follows that

\[ 0.38 < \mu_{n-1}(T_5) < 0.5, \quad n - 2 < \mu_1(T_5) < n - 1.97. \]

By combining with inequalities (2.3) and (2.4), we can conclude that

\[ \text{LS}(T_4) = \mu_1(T_4) - \mu_{n-1}(T_4) > n - 2 - 0.34 > n - 1.97 - 0.38 > \text{LS}(T_5). \]

This completes the proof of this lemma. \( \square \)

The next result determines the largest Laplacian spread in the class of trees on \( n \) vertices

**Lemma 2.3.** [6] If \( n \geq 5 \) and \( T \in T_n \), then \( \text{LS}(T) \leq \text{LS}(T_1) = n - 1 \), where the equality holds if and only if \( T \cong T_1 \).

**Theorem 2.1.** If \( n \geq 10 \) and \( T \in T_n \setminus \{ T_1, T_2, T_3, T_4, T_5 \} \), then

\[ \text{LS}(T_1) > \text{LS}(T_2) > \text{LS}(T_3) > \text{LS}(T_4) > \text{LS}(T_5) > \text{LS}(T). \]

**Proof.** By Lemmas 2.2 and 2.3, we only need to prove that \( \text{LS}(T_5) > \text{LS}(T) \). Since \( T \in T_n \setminus \{ T_1, T_2, T_3, T_4, T_5 \} \), we have \( \Delta(T) \leq n - 4 \). Note that \( \mu_{n-1}(T) > 0 \) because \( T \) is connected, by Proposition 2.1 and inequality (2.4) we have

\[ \text{LS}(T) = \mu_1(T) - \mu_{n-1}(T) < \mu_1(T) \leq n - 2.5 < \mu_1(T_5) - \mu_{n-1}(T_5) = \text{LS}(T_5). \]
This completes the proof of this result.

3. The first to fourth largest Laplacian spreads of unicyclic graphs

Proposition 3.1. Let $G$ be a unicyclic graph with $\Delta \leq n - 3$. If $n \geq 17$, then $\mu_1(G) \leq n - 1.7$.

Proof. By Lemma 2.1, we only need to prove that $\max\{d(v) + m(v) : v \in V\} \leq n - 1.7$. Suppose $\max\{d(v) + m(v) : v \in V\}$ occurs at the vertex $u$. Three cases arise: $d(u) = 1$, $d(u) = 2$, or $3 \leq d(u) \leq \Delta$.

Case 1. $d(u) = 1$.
Suppose $v \in N(u)$. Since $d(v) \leq \Delta \leq n - 3$, thus $d(u) + m(u) = d(u) + d(v) \leq n - 2 < n - 1.7$.

Case 2. $d(u) = 2$.
Suppose $v, w \in N(u)$. Note that $G$ is a unicyclic graph, then $|N(v) \cap N(w)| \leq 2$ and $|N(v) \cup N(w)| \leq n$. Therefore,

$$d(u) + m(u) \leq 2 + \frac{d(v) + d(w)}{2} \leq 2 + \frac{n + 2}{2} < n - 1.7.$$

Case 3. $3 \leq d(u) \leq \Delta$.
Note that $3 \leq d(u) \leq \Delta \leq n - 3$, then

$$d(u) + m(u) \leq d(u) + \frac{2m - d(u) - 2}{d(u)} = d(u) - 1 + \frac{2n - 2}{d(u)}.$$

Let $f(x) = x - 1 + \frac{2n - 2}{x}$, where $3 \leq x \leq n - 3$.
If $3 \leq x \leq \sqrt{2n - 2}$, since $f'(x) \leq 0$, it follows that $f(x) \leq f(3) = 2 + \frac{2n - 2}{3} < n - 1.7$.
If $\sqrt{2n - 2} \leq x \leq n - 3$, since $f'(x) \geq 0$, it follows that $f(x) \leq f(n - 3) = n - 4 + \frac{2n - 2}{n - 3} \leq n - 1.7$.
Recall that $3 \leq d(u) \leq \Delta \leq n - 3$, then $d(u) + m(u) \leq n - 1.7$.
By combining the above discussion, the conclusion follows.

Let $G_1, \ldots, G_4$ be the unicyclic graphs of order $n \geq 17$ as shown in Figure 2.
By an elementary computation, it follows that

(1b) \( \Phi(G_2, x) = x(x - 1)^{n-5}(x - 3)(x^3 - (n + 2)x^2 + (3n - 2)x - n). \)

(2b) \( \Phi(G_3, x) = x(x - 1)^{n-5}(x^4 - (n + 5)x^3 + (6n + 3)x^2 - (9n - 5)x + 3n). \)

(3b) \( \Phi(G_4, x) = x(x - 1)^{n-5}(x - 2)(x^3 - (n + 3)x^2 + (4n - 2)x - 2n). \)

**Lemma 3.1.** If \( n \geq 17 \), then \( LS(G_2) > LS(G_3) > LS(G_4) \).

**Proof.** Let \( f_1(x) = x^3 - (n + 2)x^2 + (3n - 2)x - n, f_2(x) = x^4 - (n + 5)x^3 + (6n + 3)x^2 - (9n - 5)x + 3n, f_3(x) = x^3 - (n + 3)x^2 + (4n - 2)x - 2n \). We divide the proof into the next two stages.

(1) \( LS(G_2) > LS(G_3) \).

Since

\[
 f_1(0) = -n < 0, \quad f_1(0.438) = 0.122156n - 1.175660328 > 0, \\
 f_1(n - 1) = -1 < 0, \quad f_1(n) = n^2 - 3n > 0,
\]

then the three roots of the equation \( f_1(x) = 0 \) lie in \((0, 0.438), (0.438, n - 1)\) and \((n - 1, n)\), respectively. On the other hand, since

\[
 f_2(0.46) = 0.032264n + 2.49289456 > 0, \\
 f_2(0.548) = 2.908261532416 - 0.294742592n < 0, \\
 f_2(2) = n - 2 > 0, \quad f_2(n - 1) = 4 - n < 0,
\]

\[
 f_2(n - 0.98) = 0.02n^3 - 0.1788n^2 - 0.527176n + 3.60952816 \\
 > 0.02(n^3 - 9n^2 - 27n + 180) \\
 > 0,
\]

then the four roots of the equation \( f_2(x) = 0 \) lie in \((0.46, 0.548), (0.548, 2), (2, n - 1)\) and \((n - 1, n - 0.98)\), respectively.
By equalities (1b) and (2b), we can conclude that

\[(3.1) \quad 0 < \mu_{n-1}(G_2) < 0.438, \quad n - 1 < \mu_1(G_2) < n.\]

\[(3.2) \quad 0.46 < \mu_{n-1}(G_3) < 0.548, \quad n - 1 < \mu_1(G_3) < n - 0.98.\]

By inequalities (3.1) and (3.2), it follows that

\[LS(G_2) = \mu_1(G_2) - \mu_{n-1}(G_2) > n - 1 - 0.438 > n - 0.98 - 0.46 > LS(G_3).\]

(2) \(LS(G_3) > LS(G_4).\)

Since

\[f_3(0.585) = -1.996473375 - 0.002225n < 0,\]

\[f_3(0.7) = 0.31n - 2.527 > 0, \quad f_3(n - 1) = -2 < 0,\]

\[f_3(n - 0.965) = 0.035n^2 - 0.20755n - 1.762307125 > 0.035(n^2 - 6n - 51) > 0,\]

then the three roots of the equation \(f_3(x) = 0\) lie in \((0.585, 0.7), (0.7, n - 1)\) and \((n - 1, n - 0.965)\), respectively. By equality (3b), it follows that

\[(3.3) \quad 0.585 < \mu_{n-1}(G_4) < 0.7, \quad n - 1 < \mu_1(G_4) < n - 0.965.\]

By combining with inequalities (3.2) and (3.3), we can conclude that

\[LS(G_3) = \mu_1(G_3) - \mu_{n-1}(G_3) > n - 1 - 0.548 > n - 0.965 - 0.585 > LS(G_4).\]

This completes the proof of this lemma. \(\square\)

In [7] and [8], it has been shown that

\textbf{Lemma 3.2.} [7, 8] If \(n \geq 10\) and \(G \in U_n\), then \(LS(G) \leq LS(G_1) = n - 1\), where the equality holds if and only if \(G \cong G_1\).

\textbf{Theorem 3.1.} If \(n \geq 17\) and \(G \in U_n \setminus \{G_1, G_2, G_3, G_4\}\), then

\[LS(G_1) > LS(G_2) > LS(G_3) > LS(G_4) > LS(G).\]

\textit{Proof.} By Lemmas 3.1 and 3.2, we only need to prove that \(LS(G_4) > LS(G)\). Since \(G \in U_n \setminus \{G_1, G_2, G_3, G_4\}\), then \(\Delta(G) \leq n - 3\). Note that \(\mu_{n-1}(G) > 0\) because \(G\) is connected, by Proposition 3.1 and inequality (3.3) we have

\[LS(G) = \mu_1(G) - \mu_{n-1}(G) < \mu_1(G) \leq n - 1.7 < \mu_1(G_4) - \mu_{n-1}(G_4) = LS(G_4).\]

This completes the proof of this result. \(\square\)
Acknowledgment: The author would like to thank the referee’s many suggestions and comments, which have improved vision of the original manuscript. This work is supported by the fund of South China Agricultural University (No. 4900-k08225).

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DEPARTMENT OF APPLIED MATHEMATICS,
SOUTH CHINA AGRICULTURAL UNIVERSITY,
GUANGZHOU, P. R. CHINA, 510642
E-mail address: liumuhuo@scau.edu.cn