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Some results on the Laplacian eigenvalues of unicyclic graphs ☆

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ABSTRACT

In this paper, we provide the smallest value of the second largest Laplacian eigenvalue for any unicyclic graph, and find the unicyclic graphs attaining that value. And also give an "asymptotically good" upper bounds for the second largest Laplacian eigenvalues of unicyclic graphs. Using this results, we can determine unicyclic graphs with maximum Laplacian separator. And unicyclic graphs with maximum Laplacian spread will also be determined.

1. Introduction

Let $G=(V,E)$ be a connected graph with vertex set $V=\{v_1,v_2,\ldots,v_n\}$ and edge set E. Let $A(G)$ be the adjacency matrix of G. Since $A(G)$ is symmetric, its eigenvalues are real. Without loss of generality, they can be written in descendant order as $\lambda_1(G)\geqslant\lambda_2(G)\geqslant\cdots\geqslant\lambda_n(G)$ and called the *eigenvalues* of G. Denote the degree of vertex v_i by $d(v_i)$. Let $\delta(G)$ and $\Delta(G)$ be the minimum degree and the maximum degree of the vertices of G, respectively. The *Laplacian matrix* $L(G)$ is defined as $D(G)-A(G)$, where $D(G)=\mathrm{diag}(d(v_1),d(v_2),\ldots,d(v_n))$ is the diagonal matrix of the vertex degrees of G. It is obvious that $L(G)$ is positive semidefinite symmetric and singular. Moreover, since G is connected, $L(G)$ is irreducible. We denote its eigenvalues by

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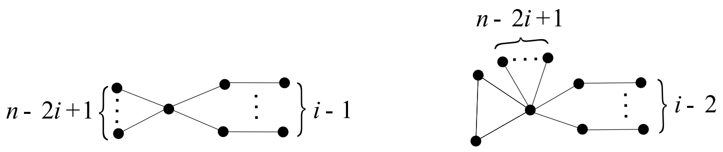

Fig. 1. Tree T_n^i and unicyclic graph U_n^i.

$$\mu_1(G) \geqslant \mu_2(G) \geqslant \cdots \geqslant \mu_n(G) = 0$$

and call $\mu_k(G)$ the *kth largest Laplacian eigenvalue* of G. The eigenvalues $\mu_1(G)$ and $\mu_{n-1}(G)$ are called the *Laplacian spectral radius* and the *algebraic connectivity* of the graph G, respectively.

The study of the eigenvalues of the Laplacian matrix have long been attracting researcher's attention, and there are several monographs and a lot of research papers published continually (see [1,3–5] and their cited references). The eigenvalues of $L(G)$ can be used in various areas of mathematics, mainly discrete mathematics and combinatorial optimization, with interpretation in several physical and chemical problems [12,13,18]. In many applications, good lower bound and upper bound of the kth largest eigenvalue of $L(G)$ are essential.

In [19], Pati explored the relationship between the third smallest Laplacian eigenvalue and the graph structure. Let $\overline{G}$ denote the complement of the graph G. Since $L(G) + L(\overline{G}) = nI - J$, where I and J denote the identity matrix and the matrix with all entries equal to 1, respectively. Clearly, $\mu_2(G) + \mu_{n-2}(\overline{G}) = n$. Thus, while studying the third smallest Laplacian eigenvalue of a graph G, some information about the second largest Laplacian eigenvalue of its complement $\overline{G}$ is useful. There is another motivation for studying the second largest Laplacian eigenvalue of G. Guo [9] investigated the second largest Laplacian eigenvalue of trees, provided the smallest three values of the second largest Laplacian eigenvalue for any tree, and characterize the trees attaining those values. However, there are only very limited results on the unicyclic graphs.

Throughout this paper, we denote the set of trees and unicyclic graphs of order n by $\mathscr{T}_n$ and $\mathcal{U}_n$, respectively. Let T_n^i $(2 \leqslant 2i \leqslant n+1)$ denote the tree obtained from the star $K_{1,n-i}$ by joining $i-1$ pendant vertices of $K_{1,n-i}$ to $i-1$ edges (obvious $K_{1,n-1} = T_n^1$). Let U_n^i $(4 \leqslant 2i \leqslant n+1)$ denote the unicyclic graph of order n obtained from C_3 by attaching $n-2i+1$ pendant edges and $i-2$ paths of length 2 together to one of three vertices of C_3. Both T_n^i and U_n^i are shown in Fig. 1.

We also denote by $\Phi(B) = \Phi(B; x) = \det(xI - B)$ the characteristic polynomial of the matrix B. Other undefined notations are referred to [2].

The rest of this paper is organized as follows. In Section 2, we present some properties of the Laplacian spectral radii of graphs. In Section 3, as motivated by [9], we discuss the second largest Laplacian eigenvalue of unicyclic graphs and show that $\mu_2(U) \geqslant 3$ for all unicyclic graphs U except two graphs, and characterize all unicyclic graphs with $\mu_2(U) = 3$. We also give an "asymptotically good" upper bound for the second largest Laplacian eigenvalue of unicyclic graphs. In Section 4, we use the results obtained in Section 3 to show that U_n^2 is the unique graph with maximum (Laplacian) separator among all graphs in $\mathscr{U}_n$. Moreover, trees with maximum (Laplacian) separator will also be discussed in this section. In Section 5, we determine U_n^2 is the unique graph with maximum Laplacian spread among all graphs in $\mathscr{U}_n$. The definitions of (Laplacian) separator and (Laplacian) spread will be introduced in Sections 4 and 5, respectively.

2. Laplacian spectral radii of graphs

Let G be a graph of order n and let $G' = G + e$ be the graph obtained from G by adding a new edge e to G. Then $L(G') = L(G) + zz^T$, where z is a column n-vector with two non-zero entries 1 and -1 in the corresponding places and z^T is the transpose of z. The next lemma follows the well-known Courant–Weyl inequalities (see [4, p. 51, Theorem 2.1]) and the fact that $\mu_n(zz^T) = 0$.

Lemma 2.1. *For $e \notin E(G)$, the Laplacian eigenvalues of G and $G' = G + e$ interlace, i.e.,*

$$\mu_1(G') \geqslant \mu_1(G) \geqslant \mu_2(G') \geqslant \mu_2(G) \geqslant \cdots \geqslant \mu_n(G') = \mu_n(G) = 0.$$

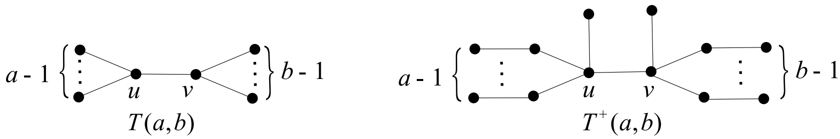

Fig. 2. Trees $T(a,b)$ and $T^+(a,b)$.

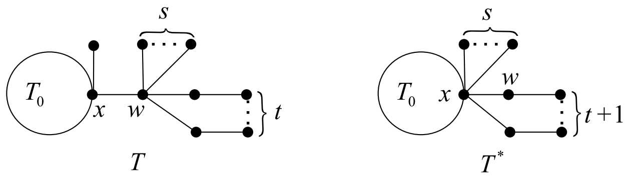

Fig. 3. Trees T and T^*.

Lemma 2.2 [12]. *Let G be a graph containing at least one edge. Then $\mu_1(G) \geqslant \Delta(G)+1$. Moreover, for G connected on $n>1$ vertices, the equality holds if and only if $\Delta(G)=n-1$.*

Lemma 2.3 [1]. *Let G be a graph. Then $\mu_1(G) \leqslant \max\{d(u)+d(v)|uv \in E(G)\}$.*

2.1. Results on trees

Let $T \in \mathscr{T}_n$ $(n \geqslant 4)$, and $e=uv$ be a non-pendant edge of T. Suppose X and Y are the two components of $T-e$ such that $u \in X$ and $v \in Y$. We define T_0 to be the graph obtained from T in the following ways:

Contract the edge e such that u and v are identified to form a new vertex w, and then add a pendant edge to w. This procedure is called the *Edge-Growing Transformation of T* (on the edge e), or *EGT of T* (on the edge e) for short.

Proposition 2.4 [15]. *Let $T \in \mathscr{T}_n(n \geqslant 4)$ be a tree with at least one non-pendant edge $e=uv$. If T_0 is obtained from T by an EGT on e, then $\mu_1(T) < \mu_1(T_0)$.*

The following lemma can be obtained directly from Proposition 2.4.

Lemma 2.5. *Let T be a tree and $uv \in E(T)$. Suppose a and b are orders of the two components of $T-uv$. Then $\mu_1(T) \leqslant \mu_1(T(a,b))$, where $T(a,b)$ is shown in Fig. 2. Moreover, the equality holds if and only if $T \cong T(a,b)$.*

Lemma 2.6 [8]. *Let T and T^* be the trees in Fig. 3, where T_0 is a tree with at least two vertices, $s \geqslant 2, t \geqslant 0$, or $s=1, t \geqslant 1$. Then $\mu_1(T) < \mu_1(T^*)$.*

Making use of Lemmas 2.5 and 2.6, we establish the following proposition for trees with perfect matchings.

Proposition 2.7. *Let T be a tree and $uv \in E(T)$. Suppose T_1 and T_2 are the two components of $T-uv$ such that both of them contain perfect matchings. Suppose T_1 and T_2 are of orders $2a$ and $2b$, respectively. Then $\mu_1(T) \leqslant \mu_1(T^+(a,b))$ ($T^+(a,b)$ is shown in Fig. 2). Moreover, the equality holds if and only if $T \cong T^+(a,b)$.*

Proof. Let M_1 and M_2 be perfect matchings of T_1 and T_2, respectively. Then $|M_1|=a$ and $|M_2|=b$. Let $M=M_1 \cup M_2$. Note that $uv \notin M$. If M contains a non-pendent edge xy of T, then let T_0 be the tree obtained from T by performing EGT on xy. Then T_0 contains a perfect matching $M_0 = M \cup \{e_0\} \setminus \{xy\}$, where e_0 is the new edge added into T after performing EGT. Repeat this procedure until there is no non-pendent edge in the most updated perfect matching. Let T' be the resulting tree and the corresponding perfect matching be M'. By Proposition 2.4 we have $\mu_1(T) \leqslant \mu_1(T')$. Note that the equality does not hold if at least one EGT is preformed. Moreover, each edge in M' is a pendent edge.

Claim 1. $\deg_{T'}(u) = 2$ *(resp.* $\deg_{T'}(v) = 2$*) if and only if* $a = 1$ *(resp.* $b = 1$*).*

Claim 2. *If there are two adjacent vertices of degree 2 in T', then $T' = T \cong T^+(1, 1)$.*

If $a = b = 1$, then by Claims 1 and 2 we have $\mu_1(T) = \mu_1(T^+(1, 1))$. When $a > 1$ ($b > 1$), by Claim 1, we have $\deg_{T'}(u) \geqslant 3$ ($\deg_{T'}(v) \geqslant 3$). Suppose there is a vertex of at least degree 3 in $V(T') \setminus \{u, v\}$. Without loss of generality, we assume that T_1 contains such vertex. Let $w \in V(T_1)$ of degree at least 3 such that the distance between u and w is maximum. Let $u \cdots xw$ be the path between u and w. Note that $\deg_{T'}(x) \geqslant 3$ and x is incident with a pendent edge. By Lemma 2.6, we obtain the tree T^* from T' (in this case, $s = 1$). Then $\mu_1(T^*) < \mu_1(T')$. Note that the number of vertices of degree at least 3 in T^* is one less than that in T' and M' is still a perfect matching of T^*. Applying Lemma 2.6 repeatedly, until there is no vertex of degree at least 3 except u and v. Then the resulting tree is $T^+(a, b)$. Combining the previous results, we have $\mu_1(T) \leqslant \mu_1(T') \leqslant \mu_1(T^+(a, b))$.

Proof of Claim 1. It is because that if an EGT is performed in T_1, then the degree of u will increase by one.

Proof of Claim 2. Suppose there are two vertices of degree 2 in T', say x' and y'. Let $N_{T'}(x') = \{y', w\}$ and $N_{T'}(y') = \{x', z\}$, where x', y', w and z are distinct. Since each edge in M' is a pendent edge, $x'y' \notin M'$. Since M' is perfect, $x'w, y'z \in M'$. Then w and z are pendents. Hence the order of T' is of order 4. Then we have the claim, and the proof is complete. □

With Proposition 2.7, the Corollary 6 in [10] becomes an obvious corollary.

Corollary 2.8 [10]. *Let T be a tree on $n = 2k$ vertices with a perfect matching. Then $\mu_1(T) \leqslant \mu_1(T^k_{2k})$, and the equality holds if and only if $T = T^k_{2k}$.*

2.2. Results on unicyclic graphs

A matching of a graph G with maximum cardinality is called a *maximum matching* in G. The cardinality of a maximum matching of G is called the *matching number* of G and denoted by $\beta(G)$.

Lemma 2.9 [22]. *Let $U \in \mathscr{U}_n$ with matching number $\beta(U) = i$. Then $\mu_1(U) \leqslant r$, where r is the maximum root of the equation*

$$x^3 - (n - i + 5)x^2 + (3n - 3i + 7)x - n = 0,$$

and the equality holds if and only if $U \cong U^i_n$.

Corollary 2.10. *Let U be a unicyclic graph on $n = 2t$ vertices with a perfect matching. Then $\mu_1(U) \leqslant r$, where r is the maximum root of the equation*

$$x^3 - (t + 5)x^2 + (3t + 7)x - 2t = 0,$$

and the equality holds if and only if $U \cong U^t_{2t}$.

Proposition 2.11. *The Laplacian spectral radius of the unicyclic graph U^i_n is a decreasing function on i, i.e.,*

$$n = \mu_1(U^2_n) > \mu_1(U^3_n) > \cdots > \mu_1\left(U_n^{\lfloor \frac{n+1}{2} \rfloor}\right).$$

Proof. Since $\Delta(U^i_n) = n - i + 1$, by Lemmas 2.2 and 2.3, we have $\mu_1(U^i_n) > n - i + 2$ and $\mu_1(U^{i+1}_n) \leqslant n - i + 2$ for $i = 2, 3, \ldots, \lfloor \frac{n-1}{2} \rfloor$. Moreover, when $i = 2$, $\mu_1(U^2_n) = n$. Hence the assertion holds. □

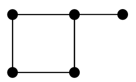

Fig. 4. Unicyclic graph C_4^1.

By using Lemma 2.9 and Proposition 2.11 we have

Corollary 2.12. *Let $U \in \mathscr{U}_n$, then $\mu_1(U) \leqslant n$, with the equality holds if and only if $U \cong U_n^2$.*

3. The second largest Laplacian eigenvalues of unicyclic graphs

It is easy to see that $\delta(U) \leqslant 2$ for all $U \in \mathscr{U}_n$ with $n \geqslant 3$. Moreover, $\delta(U) = 2$ if and only if $U = C_n$.

Lemma 3.1 [4]. *For $n \geqslant 3$,*

$$\mu_2(C_n) = \begin{cases} 2\left(1+\cos\frac{\pi}{n}\right) & \text{if } n \text{ is odd,} \\ 2\left(1+\cos\frac{2\pi}{n}\right) & \text{if } n \text{ is even.} \end{cases}$$

By Lemma 3.1, we have $\mu_2(C_n) \geqslant 3$ $(n \neq 4)$ and $\mu_2(C_n) = 3$ if and only if $n = 3, 6$.

So, the second largest Laplacian eigenvalue of unicyclic graph with minimum degree 2 is totally determined. In the following, for considering the lower bound of the second largest Laplacian eigenvalue of unicyclic graph $U \in \mathscr{U}_n$ with $n \geqslant 4$, we assume $\delta(U) = 1$. For convenience, we let $\mathcal{U}_n^+$ be the set of unicyclic graphs of order n with minimum degree 1.

Lemma 3.2. *For $i \geqslant 2$, $\mu_2(U_n^i) = 3$.*

Proof. For $i = 2$, the characteristic polynomial of $L(U_n^2)$ is

$$\Phi(L(U_n^2), x) = x(x-3)(x-n)(x-1)^{n-3}.$$

Hence $\mu_2(U_n^2) = 3$.

For $i \geqslant 3$, by some computations, the characteristic polynomial of $L(U_n^i)$ is equal to

$$\Phi(L(U_n^i), x) = x(x-3)(x-1)^{n-2i+1}(x^2-3x+1)^{i-3} \times [x^3-(n-i+5)x^2+(3n-3i+7)x-n].$$

Let $f(x) = x^3-(n-i+5)x^2+(3n-3i+7)x-n$. We have

$$f(n) = (i-2)(n^2-3n) > 0 \quad (\text{since} \quad i \geqslant 3, n \geqslant 2i-1 \geqslant 5),$$
$$f(3) = 3-n < 0,$$
$$f(2) = n-2i+2 > 0 \quad (n \geqslant 2i-1),$$
$$f\left(\frac{1}{3}\right) = -\frac{1}{9}n - \frac{8}{9}i + \frac{1}{27} - \frac{5}{9} + \frac{7}{3} \leqslant -\frac{2}{9}i + \frac{1}{9} - \frac{8}{9}i + \frac{1}{27} - \frac{5}{9} + \frac{7}{3} \leqslant -\frac{8}{27} < 0.$$

So, the three roots of equation $f(x) = 0$ lie in $(3, n)$, $(2, 3)$ and $\left(\frac{1}{3}, 2\right)$, respectively.

And the equation $x^2-3x+1 = 0$ has two roots $\frac{3+\sqrt{5}}{2}$ and $\frac{3-\sqrt{5}}{2}$ which are less than 3.

Hence $\mu_2(U_n^i) = 3$. $\square$

From the tables of the Laplacian spectra of all unicyclic graphs of order n $(3 \leqslant n \leqslant 6)$ in [4], we know that $\mu_2(U) \geqslant 3$ for $U \in \mathscr{U}_n^+$ except $U \cong C_4^1$ (see Fig. 4) and the equality holds if and only if U is isomorphic to one of graphs, H_i $(1 \leqslant i \leqslant 5)$ (see Fig. 5), and U_n^i $(i \geqslant 2)$.

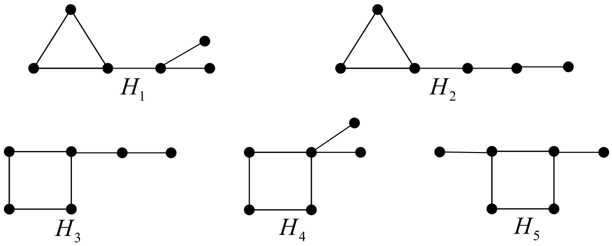

Fig. 5. Unicyclic graphs H_i $(1 \leqslant i \leqslant 5)$.

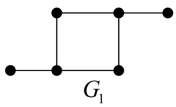

Fig. 6. Unicyclic graph G_1.

Thus, from now on, we only consider the cases of $n \geqslant 7$.

Theorem 3.3. *For $n \geqslant 7, \mu_2(U) \geqslant 3$ for $U \in \mathscr{U}_n^+$; and the equality holds if and only if $U \cong U_n^i (2 \leqslant i \leqslant \lfloor \frac{n+1}{2} \rfloor)$.*

Proof. Let C_l be the unique cycle in $U, l \geqslant 3$.

If $l \neq 4$, then U contains $C_l + N_{n-l}$ as a spanning subgraph, where N_m is the null graph of order m. By Lemmas 2.1 and 3.1, we have $\mu_2(U) \geqslant \mu_2(C_l + N_{n-l}) \geqslant 3$.

If $l = 4$, then U contains one of the graphs $H_i + N_{n-6}$ $(i = 3, 4, 5)$ or $G_1 + N_{n-6}$ as a spanning subgraph, where H_i $(i = 3, 4, 5)$ are shown in Fig. 5 and G_1 is shown in Fig. 6. Since $\mu_2(H_3 + N_{n-6}) = \mu_2(H_4 + N_{n-6}) = \mu_2(H_5 + N_{n-6}) = 3$ and $\mu_2(G_1 + N_{n-6}) \doteq 3.414$. By Lemma 2.1, we have $\mu_2(U) \geqslant \min_{3 \leqslant i \leqslant 5}\{\mu_2(H_i + N_{n-6}), \mu_2(G_1 + N_{n-6})\} = 3$.

Hence we have $\mu_2(U) \geqslant 3$.

In the following, we shall show that for each $U \in \mathscr{U}_n^+$, $\mu_2(U) = 3$ if and only if $U \cong U_n^i$ for some i.

From Lemma 3.2, we know that $\mu_2(U_n^i) = 3$ for $n \geqslant 7$.

Let C_l be the unique cycle in U. Then $C_l + N_{n-l}$ is a spanning subgraph of U, $n \geqslant 7$ and $n > l \geqslant 3$. By Lemma 2.1, $\mu_2(U) \geqslant \mu_2(C_l + N_{n-l}) = \mu_2(C_l)$. Since $\mu_2(U) = 3$, by Lemma 3.1 we have $l = 3, 4$ or 6.

Suppose $l = 6$. Since $n \geqslant 7$, $C_6^1 + N_{n-7}$ is a spanning subgraph of U. By Lemma 2.1 again, $3 = \mu_2(U) \geq \mu_2(C_6^1 + N_{n-7}) = \mu_2(C_6^1) \doteq 3.414 > 3$. It is impossible.

If $l = 4$, then U contains one of the graphs $G_1 + (n-6)K_1$ or $G_i + (n-7)K_1$ $(i = 2, 3, 4, 5, 6)$ as a spanning subgraph, where G_1 is shown in Fig. 6 and G_i $(i = 2, 3, 4, 5, 6)$ are shown in Fig. 7. By Lemma 2.1, we have $\mu_2(U) \geqslant \min_{2 \leqslant i \leqslant 6}\{\mu_2(G_1 + (n-6)K_1), \mu_2(G_i + (n-7)K_1)\} = \mu_2(G_4 + (n-7)K_1) \doteq 3.058$. It is impossible too.

Suppose $l = 3$. If $U \ncong U_n^i$, then U contains one of the graphs $G_7 + (n-5)K_1$ or $G_i + (n-7)K_1$ $(i = 8, 9, 10, 11)$ as a spanning subgraph $(n \geqslant 7)$, where G_i $(i = 7, 8, 9, 10, 11)$ are shown in Fig. 8. By Lemma 2.1, we have $\mu_2(U) \geqslant \min_{8 \leqslant i \leqslant 11}\{\mu_2(G_7 + N_{n-5}), \mu_2(G_i + N_{n-7})\} = \mu_2(G_9 + N_{n-7}) \doteq 3.117$. It is impossible. So by Lemma 3.2, for any $U \in \mathscr{U}_n^+$, if $\mu_2(U) = 3$, then $U \cong U_n^i$.

From the above discussions, the proof is completed. □

Consequently, the second largest Laplacian eigenvalues of all unicyclic graphs of order $n \geqslant 3$ except C_4 and C_4^1 are at least 3. Furthermore, the second largest Laplacian eigenvalue equal to 3 if and only if the unicyclic graph is isomorphic to one of graphs, H_i $(1 \leqslant i \leqslant 5)$, U_n^i $(i \geqslant 2)$, C_3 and C_6.

In the following, we will give an "asymptotically good" upper bound for the second largest Laplacian eigenvalue of unicyclic graph in $\mathscr{U}_n$. We then begin with introducing some useful results as follows.

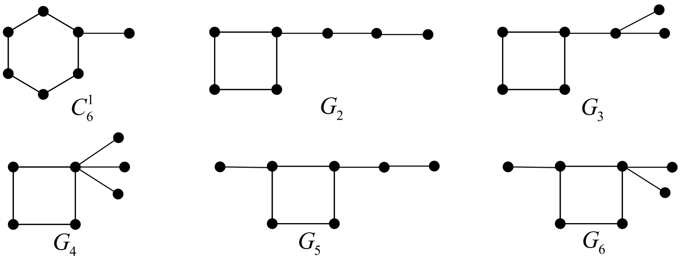

Fig. 7. Unicyclic graphs, C_6^1 and G_i $(2 \leqslant i \leqslant 6)$.

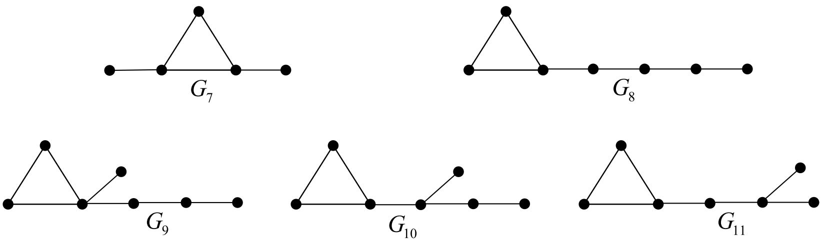

Fig. 8. Unicyclic graphs, G_i $(7 \leqslant i \leqslant 11)$.

Let $v \in V(G)$. $L_v(G)$ is defined as the principal submatrix of $L(G)$ formed by deleting the row and column corresponding to vertex v.

Lemma 3.4 [9]. *Let uv be a cut edge of a graph G. Let $G - uv = G_1 + G_2$ and let $u \in V(G_1)$ and $v \in V(G_2)$. Then*

$$\Phi(L(G)) = \Phi(L(G_1))\Phi(L(G_2)) - \Phi(L(G_1))\Phi(L_v(G_2)) - \Phi(L_u(G_1))\Phi(L(G_2)).$$

By Lemma 3.4, we get that $\Phi(L(T(k,k)); x) = x(x-1)^{2k-4}(x-k)[x^2 - (k+2)x + 2]$. Then $\mu_1(T(k,k)) = \frac{k+2+\sqrt{(k+2)^2-8}}{2}$. Here $T(a,b)$ is defined in Lemma 2.5.

Lemma 3.5 [23]. *Let $U \in \mathscr{U}_n$. Then for any positive integer a $(2 \leqslant a \leqslant \lfloor \frac{n}{2} \rfloor)$, there is an $(a-1)$-vertex subset V' of U such that all components $U_1, U_2, \ldots, U_t$ of $U - V'$ satisfy one of the following three conditions*:

1. *Each U_i $(i = 1, 2, \ldots, t)$ is a tree of order at most $\lfloor \frac{n}{2} \rfloor$.*
2. *There exists a unicyclic graph U_p of order at most $\lfloor \frac{n}{2} \rfloor$, and other components U_i $(i = 1, 2, \ldots, t, i \neq p)$ are trees of order at most $\lfloor \frac{n}{2} \rfloor$.*
3. *There exists U_q of order at most $2\lfloor \frac{n}{2} \rfloor$, which is obtained from joining two trees of orders at most $\lfloor \frac{n}{2} \rfloor$ with an edge, and other components $U_i (i = 1, 2, \ldots, t, i \neq q)$ are trees of order at most $\lfloor \frac{n}{2} \rfloor$.*

Lemma 3.6 [5,17]. *For each $v \in V(G)$ and each $i \in \{1, 2, \ldots, n-1\}$, $\mu_{i+1}(G) - 1 \leqslant \mu_i(G - v) \leqslant \mu_i(G)$.*

Thus, in particular, $\mu_2(G) \leqslant \mu_1(G - v) + 1$ and $\mu_2(G - v) \leqslant \mu_2(G)$.

Theorem 3.7. *If $U \in \mathscr{U}_n$, then $\mu_2(U) \leqslant \frac{k+4+\sqrt{(k+2)^2-8}}{2}$, where $k = \lfloor \frac{n}{2} \rfloor$.*

Proof. Let $k = \lfloor \frac{n}{2} \rfloor$. By taking $a = 2$ in Lemma 3.5, there exists a vertex $v_0 \in V(U)$ such that all the components $U_1, U_2, \ldots, U_t$ of $U - v_0$ satisfy one of the cases in Lemma 3.5. We consider the following two cases.

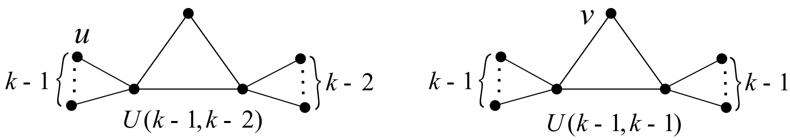

Fig. 9. Unicyclic graphs $U(k-1,k-2)$ and $U(k-1,k-1)$.

Case 1. All the components $U_1, U_2, \ldots, U_t$ of $U - v_0$ satisfy the first or second case in Lemma 3.5. It is well-known that $\mu_1(G) \leqslant n$, and equality holds if and only if the complement of G is disconnected [4]. By Lemma 3.6 and Corollary 2.12, since $|U_i| \leqslant k$ for $i = 1, 2, \ldots, t$, we have

$$\mu_2(U) \leqslant \mu_1(U_1 + U_2 + \cdots + U_t) + 1 \leqslant k + 1.$$

Case 2. There exists a graph U_q of order at most $2k$, which is obtained from joining two trees of order at most k with an edge, and other components U_i $(i = 1, 2, \ldots, t, i \neq q)$ are trees with order at most $\lfloor \frac{n}{2} \rfloor$. In this case, for each components U_i $(i = 1, 2, \ldots, t, i \neq q)$ of $U - v_0$, we have $\mu_1(U_i) \leqslant k$. So, by Lemma 2.5, Lemma 3.6 and Lemma 2.1, we have

$$\mu_2(U) \leqslant \mu_1(U_1 + U_2 + \cdots + U_t) + 1 \leqslant \mu_1(T(k,k)) + 1 = \frac{k + 4 + \sqrt{(k+2)^2 - 8}}{2}.$$

The proof is completed. $\square$

Remark. For the cases $n = 2k$ and $n = 2k + 1$, we have, respectively, two unicyclic graphs $U(k-1, k-2)$ and $U(k-1, k-1)$ as shown in Fig. 9. In the former case, since $U(k-1, k-2) - u \cong U(k-2, k-2)$, $\mu_2(U(k-1, k-2)) \geqslant \mu_2(U(k-2, k-2)) \geqslant \frac{k+1+\sqrt{(k+1)^2-8}}{2}$. In the latter case, we have $\mu_2(U(k-1, k-1)) \geqslant \mu_2(U(k-1, k-1) - v) = \frac{k+2+\sqrt{(k+2)^2-8}}{2}$. With the upper bound obtained in Theorem 3.7, we have

$$\frac{k + 1 + \sqrt{(k+1)^2 - 8}}{2} \leqslant \mu_2(U(k-1, k-2)) \leqslant \frac{k + 4 + \sqrt{(k+2)^2 - 8}}{2} \quad \text{and}$$
$$\frac{k + 2 + \sqrt{(k+2)^2 - 8}}{2} \leqslant \mu_2(U(k-1, k-1)) \leqslant \frac{k + 4 + \sqrt{(k+2)^2 - 8}}{2}.$$

The differences between two bounds are $\frac{3}{2} + \frac{2k+3}{2(\sqrt{(k+2)^2-8}+\sqrt{(k+1)^2-8})}$ and 1, respectively.

Since $\lim_{k\to\infty} \frac{3}{2} + \frac{2k+3}{2(\sqrt{(k+2)^2-8}+\sqrt{(k+1)^2-8})} = 2$, the upper bound obtained in Theorem 3.7 is "asymptotically good".

4. Maximum (Laplacian) separator

The *separator* $S_A(G)$ of a graph G is the difference between its largest and second largest eigenvalues, i.e., $S_A(G) = \lambda_1(G) - \lambda_2(G)$. Similarly, the *Laplacian separator* $S_L(G)$ of G is the difference between its largest and second largest Laplacian eigenvalues, i.e., $S_L(G) = \mu_1(G) - \mu_2(G)$.

Theorem 4.1. *If G is a regular graph of order n, then $S_A(G) = \mu_{n-1}(G)$. In particular, if G is a regular bipartite graph, then $S_A(G) = S_L(G)$.*

Proof. If G is r-regular, then $L(G) = rI - A(G)$, we have

$$\mu_{n-i+1}(G) = r - \lambda_i(G) \text{ or equivalent to}$$
$$\lambda_i(G) = r - \mu_{n-i+1}(G) \quad \text{for } i = 1, 2, \ldots, n.$$

In particular, $\lambda_1(G) = r$, $\lambda_2(G) = r - \mu_{n-1}(G)$. Hence we have $S_A(G) = \mu_{n-1}(G)$.

If G is an r-regular bipartite graph, then $\lambda_i(G) = -\lambda_{n-i+1}(G) = \mu_i(G) - r$, $i = 1, \ldots, n$. So $S_L(G) = \mu_1(G) - \mu_2(G) = (\lambda_1(G) + r) - (\lambda_2(G) + r) = \lambda_1(G) - \lambda_2(G) = S_A(G)$. $\square$

Let n, m be the numbers of vertices and edges of a graph G, respectively. Also let $M(G)$ be the incidence matrix of G. We can see their relations as follows:

$$M(G)M^T(G) = D(G) + A(G), \quad M^T(G)M(G) = A(G^L) + 2I,$$

where $A(G^L)$ is the adjacency matrix of the line graph G^L of G.

Since we have the same set of non-zero eigenvalues of $M(G)M^T(G)$ and $M^T(G)M(G)$, so

$$\Phi(A(G^L); x) = (x+2)^{m-n}\Phi(Q(G); (x+2)), \tag{4.1}$$

where $Q(G) = D(G) + A(G)$.

By Eq. (4.1), assume the eigenvalues of the $Q(G)$ are $\theta_1 \geqslant \theta_2 \geqslant \cdots \geqslant \theta_n \geqslant 0$, then the eigenvalues of $A(G^L)$ must be $\lambda_i(G^L) = \theta_i - 2$ $(1 \leqslant i \leqslant n)$ for $m \geqslant n$. If $m > n$, we further have $\lambda_{n+1}(G^L) = \lambda_{n+2}(G^L) = \cdots = \lambda_m(G^L) = -2$.

Lemma 4.2 [13]. *Let G be a bipartite graph. Then $Q(G) = D(G) + A(G)$ and $L(G) = D(G) - A(G)$ are unitary similar, i.e., there exists an orthogonal matrix U such that $Q(G) = U^{-1}L(G)U$.*

Theorem 4.3. *The Laplacian separator of a bipartite graph G is the same as the separator of G^L, i.e., $S_L(G) = S_A(G^L)$.*

Proof. By Lemma 4.2, the matrix $Q(G) = M(G)M^T(G) = D(G) + A(G)$ is unitary similar to $L(G) = D(G) - A(G)$. Thus they have the same eigenvalues. Hence,

$$\begin{aligned} S_A(G^L) &= \lambda_1(G^L) - \lambda_2(G^L) = (\theta_1 - 2) - (\theta_2 - 2) \\ &= \theta_1 - \theta_2 = \mu_1(G) - \mu_2(G) = S_L(G). \quad \square \end{aligned}$$

In the following, we will show that $K_{1,n-1}$ and U_n^2 are the unique tree and the unique unicyclic graph with maximum separator and Laplacian separator among all trees and unicyclic graphs of order n, respectively.

4.1. Trees with maximal (Laplacian) separator

Lemma 4.4 [14]. *Let $T \in \mathscr{T}_n$ with $n \geqslant 4$. If T is neither $K_{1,n-1}$ nor T_n^2, then $\lambda_2(T) \geqslant 1$.*

Theorem 4.5. *If $T \in \mathscr{T}_n$ with $n \geqslant 4$, then $S_A(T) \leqslant \sqrt{n-1}$. The equality holds if and only if $T = K_{1,n-1}$.*

Proof. It is known that for each $T \in \mathscr{T}_n$, $\lambda_1(T) \leqslant \sqrt{n-1}$ (see [20]).

Since $\lambda_2(G) \leqslant 0$ if and only if G is a complete multipartite graph (see [4]), $\lambda_2(T) > 0$ if T is not isomorphic to $K_{1,n-1}$. Hence $S_A(T) < \sqrt{n-1}$ if T is not isomorphic to $K_{1,n-1}$.

Actually $S_A(K_{1,n-1}) = \sqrt{n-1}$. Hence the proof is complete. $\square$

Theorem 4.6 [9]. *If $T \in \mathscr{T}_n$ $(n \geqslant 3)$, then $\mu_2(T) \geqslant 1$. The equality holds if and only if $T = K_{1,n-1}$.*

Theorem 4.7 [9]. *Let $T \in \mathscr{T}_n$ $(n \geqslant 4)$. If $T \neq K_{1,n-1}$, then $\mu_2(T) \geqslant r$, where r is the second largest root of the equation $x^3 - (n+2)x^2 + (3n-2)x - n = 0$, and the equality holds if and only if $T = T_n^2$. Moreover, for $r \geqslant 2$, $\mu_2(T) = r$ if and only if $n = 4$. Also r is a strictly increasing function of n, and converges to $\frac{3+\sqrt{5}}{2}$ as $n \to \infty$.*

Theorem 4.8 [9]. *Let $T \in \mathscr{T}_n$ $n \geqslant 5)$. If T is neither $K_{1,n-1}$ nor T_n^2, then $\mu_2(T) \geqslant \frac{3+\sqrt{5}}{2}$, and the equality holds if and only if $T \cong T_n^i$ $(i \geqslant 3)$.*

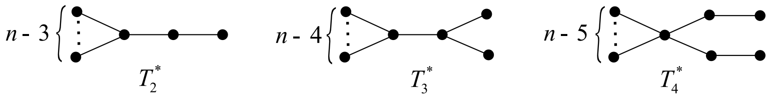

Fig. 10. Trees T_i^* $(2 \leqslant i \leqslant 4)$.

It is known that $\mu_1(G) \leqslant n$ (see [4]), and the equality holds if and only if the complement of G is disconnected. Thus, if $T \in \mathscr{T}_n$, then $\mu_1(T) \leqslant n$, and the equality holds if and only if $T = K_{1,n-1}$. By Theorem 4.6, it is easy to get that for each $T \in \mathscr{T}_n$ $(n \geqslant 3)$, $S_L(T) \leqslant n-1$, and the equality holds if and only if $T = K_{1,n-1}$.

Consider the characteristic polynomial of $L(T_n^2)$ which is

$$\Phi(L(T_n^2); x) = x(x-1)^{n-4}[x^3 - (n+2)x^2 + (3n-2)x - n].$$

Let $f(x) = x^3 - (n+2)x^2 + (3n-2)x - n$. We have

$$\begin{aligned} &f(n) = n^2 - 3n > 0 \quad (n \geqslant 4),\\ &f(n-1) = -1 < 0,\\ &f\left(\frac{3+\sqrt{5}}{2}\right) = -1 < 0,\\ &f(1) = n-3 > 0 \quad (n \geqslant 4),\\ &f(0) = -n < 0. \end{aligned}$$

Hence, $n > \mu_1(T_n^2) > n-1$ and $\frac{3+\sqrt{5}}{2} > \mu_2(T_n^2) > 1$. Therefore, $n-1 > S_L(T_n^2) > n-1-\frac{3+\sqrt{5}}{2} = n - \frac{5+\sqrt{5}}{2}$.

Guo [10] gave the first four trees $T_1^*, T_2^*, T_3^*, T_4^*$ in $\mathscr{T}_n$ $(n \geqslant 6)$ ordered according to their Laplacian spectral radii. Namely, $T_1^* = K_{1,n-1}$, $T_2^* = T_n^2$, T_3^* and T_4^* are shown in Fig. 10.

Lemma 4.9. *For any $T \in \mathscr{T}_n$ with $n \geqslant 6$, if T is neither $K_{1,n-1}$ nor T_n^2, then $\mu_1(T) < n-1$.*

Proof. By the discussion above, we only need to prove that $\mu_1(T_3^*) < n-1$. In fact, the characteristic polynomial of $L(T_3^*)$ is

$$\Phi(L(T_3^*); x) = x(x-1)^{n-4}[x^3 - (n+2)x^2 + (4n-7)x - n].$$

Let $f(x) = x^3 - (n+2)x^2 + (4n-7)x - n$. We have

$$\begin{aligned} &f(n-1) = n^2 - 6n + 4 > 0 \quad (n \geqslant 6),\\ &f(n-2) = -2 < 0,\\ &f(1) = 2n-8 > 0 \quad (n \geqslant 6),\\ &f(0) = -n < 0. \end{aligned}$$

The three roots of the equation $f(x) = 0$ lie in $(0,1)$, $(1, n-2)$ and $(n-2, n-1)$, respectively. Then $\mu_1(T_3^*) < n-1$. $\square$

Theorem 4.10. *For any $T \in \mathscr{T}_n$ with $n \geqslant 6$, if T is neither $K_{1,n-1}$ nor T_n^2, then $S_L(T) < n - \frac{5+\sqrt{5}}{2}$.*

Proof. If T is neither $K_{1,n-1}$ nor T_n^2, by Theorem 4.8 and Lemma 4.9, we have

$$S_L(T) = \mu_1(T) - \mu_2(T) < n-1-\frac{3+\sqrt{5}}{2} = n - \frac{5+\sqrt{5}}{2}. \qquad \square$$

4.2. Unicyclic graphs with maximal (Laplacian) separator

Lemma 4.11 [24]. *If $U \in \mathscr{U}_n$ with $n \geqslant 8$, then $\lambda_2(U) \geqslant r_2$, where r_2 is the second largest root of the equation $x^4 - nx^2 - 2x + (n-3) = 0$, and the equality holds if and only if $U = U_n^2$.*

It is known that for each $U \in \mathscr{U}_n$, $\lambda_1(U) \leqslant r_1$, where r_1 is the first largest root of the equation $x^4 - nx^2 - 2x + (n-3) = 0$ (see [23]), and the equality holds if and only if $U = U_n^2$. By Lemma 4.11, we have the following result.

Theorem 4.12. *If $U \in \mathscr{U}_n$ with $n \geqslant 8$, then $S_A(U) \leqslant r_1 - r_2$, where r_1 and r_2 are the first and second largest roots of the equation $x^4 - nx^2 - 2x + (n-3) = 0$, respectively. Moreover, the equality holds if and only if $U = U_n^2$.*

By Corollary 2.12 and the conclusion after Theorem 3.3, we have the following theorem.

Theorem 4.13. *If $U \in \mathscr{U}_n$ for $n \geqslant 6$, then $S_L(U) \leqslant n-3$, and the equality if and only if $U \cong U_n^2$.*

5. Maximum Laplacian spread of unicyclic graphs

The *spread* of the graph G is defined as

$$\mathscr{L}_A(G) = \lambda_1(G) - \lambda_n(G).$$

If G is a bipartite graph, then $\lambda_1(G) = -\lambda_n(G)$, hence $\mathscr{L}_A(G) = 2\lambda_1(G)$. Moreover, since $\lambda_1(P_n) \leqslant \lambda_1(T) \leqslant \lambda_1(K_{1,n-1})$, we have $\mathscr{L}_A(P_n) \leqslant \mathscr{L}_A(T) \leqslant \mathscr{L}_A(K_{1,n-1})$ for all $T \in \mathscr{T}_n$.

Shu et al. [21] investigated the spread of unicyclic graphs, and got that for any $U \in \mathscr{U}_n$ $(n \geqslant 6)$, $\mathscr{L}_A(C_n) \leqslant \mathscr{L}_A(U) \leqslant \mathscr{L}_A(U_n^2)$.

Recently, Fan et al. [7] defined the Laplacian spread of the graph G as

$$\mathscr{L}_L(G) = \mu_1(G) - \mu_{n-1}(G).$$

They investigated the Laplacian spread of trees and got that for any tree $T \in \mathscr{T}_n$ $(n \geqslant 5)$,

$$\mathscr{L}_L(P_n) \leqslant \mathscr{L}_L(T) \leqslant \mathscr{L}_L(K_{1,n-1}).$$

The first equality holds only if $T \cong P_n$, and the second equality holds only if $T \cong K_{1,n-1}$.

For regular graph G, by the same with the proof of Theorem 4.1, we have the following result.

Theorem 5.1. *If G is a regular graph, then $\mathscr{L}_A(G) = \mu_1(G)$. In particular, if G is a regular bipartite graph, then $\mathscr{L}_L(G) = \lambda_1(G) + \lambda_2(G)$.*

We now consider the maximal Laplacian spread of unicyclic graphs. It is known that for any unicyclic graph $U \in \mathscr{U}_n$ $(n > 6)$,

$$\mu_1(U) \leqslant \mu_1(U_n^2) = n \quad \text{(see [11])}, \tag{5.1}$$

$$\mu_{n-1}(U) \leqslant \mu_{n-1}(U_n^2) = 1 \quad \text{(see [6])}. \tag{5.2}$$

The equalities hold if and only if $U = U_n^2$. With inequalities (5.1) and (5.2), we cannot directly tell that U_n^2 is the one with maximum Laplacian spread among all graphs in $\mathscr{U}_n$. In the following, we shall show that U_n^2 is the unique unicyclic graph with maximum Laplacian spread among all graphs in $\mathscr{U}_n$.

Lemma 5.2 [11,16]. *For $n \geqslant 10$, $U_1^*, U_2^*, U_3^*, U_4^*, U_5^*, U_6^*, U_7^*, U_8^*, U_9^*$ and U_{10}^* are the first ten unicyclic graphs in descendent order according to the largest Laplacian eigenvalue, where $U_1^* = U_n^2$, U_i^*, $2 \leqslant i \leqslant 10$ are shown in Fig. 11.*

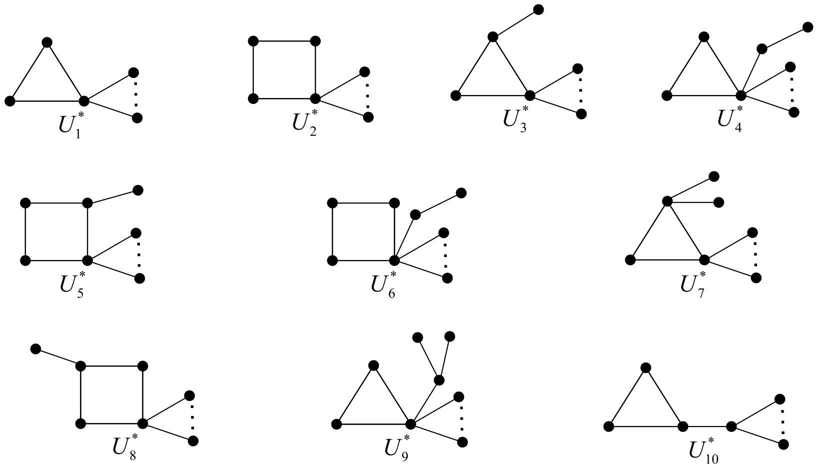

Fig. 11. Unicyclic graphs U_i^* $(1 \leqslant i \leqslant 10)$.

Lemma 5.3. *If $U \in \mathscr{U}_n$ for $n \geqslant 10$, then $\mu_1(U) < \mu_1(U_5^*) < n-1$, for any $U \notin \{U_1^*, U_2^*, U_3^*, U_4^*, U_5^*\}$.*

Proof. By Lemma 5.2, we only need to prove that $\mu_1(U_5^*) < n-1$. In fact, the characteristic polynomial of $L(U_5^*)$ is

$$\Phi(L(U_5^*); x) = x(x-1)^{n-5}[x^4 - (n+5)x^3 + (7n-1)x^2 - (13n-19)x + 4n].$$

Let $f_5(x) = x^4 - (n+5)x^3 + (7n-1)x^2 - (13n-19)x + 4n$. Since $n \geqslant 10$, we have

$$f_5(n-1) = (n-1)\left[\left(n - \frac{9}{2}\right)^2 - \frac{25}{4}\right] + 4n > 0,$$

$$f_5(4) = -4 < 0,$$

$$f_5(3) = n - 6 > 0,$$

$$f_5(1) = -3n + 14 < 0,$$

$$f_5(0) = 4n > 0.$$

The four roots of the equation $f_5(x) = 0$ lie in $(0,1)$, $(1,3)$, $(3,4)$ and $(4, n-1)$, respectively. Hence, $\mu_1(U_5^*) < n-1$. $\square$

By Lemma 5.3, we know that for any $U \in \mathscr{U}_n$ $(n \geqslant 10)$, if $\mu_1(U) > n-1$, then $U \in \{U_1^*, U_2^*, U_3^*, U_4^*\}$.

Theorem 5.4. *For any $U \in \mathscr{U}_n$ for $n \geqslant 10$, $\mathscr{L}_L(U) \leqslant n-1$, with equality holds if and only if $U \cong U_1^* = U_n^2$.*

Proof. The characteristics polynomial of $L(U_1^*)$ is

$$\Phi(L(U_1^*); x) = x(x-3)(x-n)(x-1)^{n-3}.$$

Then $\mathscr{L}_L(U_1^*) = n-1$.

For any $U \in \mathscr{U}_n \setminus \{U_1^*, U_2^*, U_3^*, U_4^*\}$ $(n \geqslant 10)$, by Lemma 5.3, we have $\mathscr{L}_L(U) < \mu_1(U) < n-1$. So we only need to consider U_1^*, U_2^*, U_3^*, and U_4^*.

The characteristics polynomial of $L(U_2^*)$ is

$$\Phi(L(U_2^*); x) = x(x-2)(x-1)^{n-5}[x^3 - (n+3)x^2 + 2(2n-1)x - 2n].$$

Let $f_2(x) = x^3 - (n+3)x^2 + 2(2n-1)x - 2n$. Since $n \geqslant 10$, we have

$$f_2\left(n - \frac{2}{3}\right) = \frac{(3n-8)^2 - 72}{27} > 0,$$
$$f_2(4) = -2(n-4) < 0,$$
$$f_2(1) = n - 4 > 0,$$
$$f_2\left(\frac{1}{3}\right) = -\frac{21n+26}{27} < 0.$$

The three roots of the equation $f_2(x) = 0$ lie in $\left(\frac{1}{3}, 1\right)$, $(1,4)$ and $\left(4, n - \frac{2}{3}\right)$, respectively.

So $\mu_1(U_2^*) \in \left(4, n - \frac{2}{3}\right)$ and $\mu_{n-1}(U_2^*) \in \left(\frac{1}{3}, 1\right)$. Hence $\mathscr{L}_L(U_2^*) < \left(n - \frac{2}{3}\right) - \frac{1}{3} < n - 1$.

The characteristics polynomial of $L(U_3^*)$ is

$$\Phi(L(U_3^*); x) = x(x-1)^{n-5}[x^4 - (n+5)x^3 + 3(2n+1)x^2 - (9n-5)x + 3n].$$

Let $f_3(x) = x^4 - (n+5)x^3 + 3(2n+1)x^2 - (9n-5)x + 3n$. Since $n \geqslant 10$, we have

$$f_3\left(n - \frac{2}{3}\right) = \frac{n^3}{3} - \frac{8n^2}{3} + \frac{138n}{27} - \frac{26}{81} > 0,$$
$$f_3(4) = -(n-4) < 0,$$
$$f_3(2) = n - 2 > 0,$$
$$f_3(1) = -n + 4 < 0,$$
$$f_3\left(\frac{1}{3}\right) = \frac{51n+148}{81} > 0.$$

The four roots of the equation $f_3(x) = 0$ lie in $\left(\frac{1}{3}, 1\right)$, $(1,2)$, $(2,4)$ and $\left(4, n - \frac{2}{3}\right)$, respectively. So $\mu_1(U_3^*) \in \left(4, n - \frac{2}{3}\right)$ and $\mu_{n-1}(U_3^*) \in \left(\frac{1}{3}, 1\right)$. Hence $\mathscr{L}_L(U_3^*) < \left(n - \frac{2}{3}\right) - \frac{1}{3} < n - 1$.

The characteristics polynomial of $L(U_4^*)$ is

$$\Phi(L(U_4^*); x) = x(x-3)(x-1)^{n-5}[x^3 - (n+2)x^2 + (3n-2)x - n].$$

Let $f_4(x) = x^3 - (n+2)x^2 + (3n-2)x - n$. Since $n \geqslant 10$, we have

$$f_4\left(n - \frac{2}{3}\right) = \frac{9n^2 - 39n + 4}{27} > 0,$$
$$f_4(3) = 3 - n < 0,$$
$$f_4(1) = n - 3 > 0,$$
$$f_4\left(\frac{1}{3}\right) = -\frac{3n+23}{27} < 0.$$

The three roots of the equation $f_4(x) = 0$ lie in $\left(\frac{1}{3}, 1\right)$, $(1,3)$ and $\left(3, n - \frac{2}{3}\right)$, respectively.

So $\mu_1(U_4^*) \in \left(3, n - \frac{2}{3}\right)$ and $\mu_{n-1}(U_4^*) \in \left(\frac{1}{3}, 1\right)$. Hence $\mathscr{L}_L(U_4^*) < \left(n - \frac{2}{3}\right) - \frac{1}{3} < n - 1$.

From the discussions above, we have $\mathscr{L}_L(U) < n - 1$ for each $U \in \mathscr{U}_n \setminus \{U_1^*\}$. This completes the proof. □

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