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ORDER UNICYCLIC GRAPHS ACCORDING TO SPECTRAL RADIUS OF UNORIENTED LAPLACIAN MATRIX*

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Abstract

The spectral radius of a graph is defined by that of its unoriented Laplacian matrix. In this paper, we determine the unicyclic graphs respectively with the third and the fourth largest spectral radius among all unicyclic graphs of given order.

Keywords: unicyclic graph, Laplacian matrix, spectral radius.

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1. INTRODUCTION

Let $G = (V, E)$ be a *mixed graph* of order n with vertex set $V(G) = \{v_1, v_2, \ldots, v_n\}$ and edge set $E(G) = \{e_1, \ldots, e_m\}$, which is obtained from an undirected graph by orienting some of its edges. Then some edges of G have a special head and tail, while others do not. The *sign* of $e \in E(G)$ is denoted by $\operatorname{sgn} e$ and defined as $\operatorname{sgn} e = 1$ if e is unoriented and $\operatorname{sgn} e = -1$ otherwise. Set $a_{ij} = \operatorname{sgn} v_i v_j$ if $v_i v_j \in E(G)$ and $a_{ij} = 0$ else. Then $A(G) = [a_{ij}]$ is called the *adjacency matrix* of G. The degree of the vertex $v \in V(G)$ is denoted by d_v and is defined to be the number of all (oriented and unoriented) edges incident to v. The *incidence matrix* of G is the $n \times m$ matrix $M = M(G) = [m_{ij}]$ whose entries are given by $m_{ij} = 1$ if e_j is an unoriented edge incident with v_i or e_j is an oriented edge with head v_i, $m_{ij} = -1$ if e_j is an oriented edge with tail v_i, and $m_{ij} = 0$ otherwise. The *Laplacian matrix* of G is defined as $L = L(G) = MM^T$ ([1]), where M^T denotes the transpose of M. One can find that $L(G) = D(G) + A(G)$, where $D(G) = \operatorname{diag}\{d_{v_1}, d_{v_2}, \ldots, d_{v_n}\}$. It is easy to see that $L(G)$ is symmetric and positive semidefinite so that its eigenvalues can be arranged as follows:

$$0 \leq \lambda_n(G) \leq \lambda_{n-1}(G) \leq \cdots \leq \lambda_1(G).$$

We refer $\lambda_1(G)$ the spectral radius of G, and denote it as $\rho(G)$.

A mixed graph G is called *singular* (or *nonsingular*) if $L(G)$ is singular (or nonsingular). Clearly, if G is *all-oriented* (i.e., all edges of G are oriented), then $L(G)$ is a standard Laplacian matrix which is consistent with the Laplacian matrix of a simple graph (see [11]); and there are a lot of results involved with the relations between its spectrum and numerous graph invariants, such as connectivity, diameter, isoperimetric number, and expanding properties of a graph; see, for example, [8, 11, 12]. If G is *all-unoriented* (i.e., all edges of G are unoriented), then $L(G)$ is called the *unoriented Laplacian matrix* ([9]). So the notion of a mixed graph generalizes both the classical approach of orienting all edges and the unoriented approach. For algebraic properties of mixed graphs, one can refer to [1, 3, 4, 5, 6, 14, 15].

A mixed graph G is called *quasi-bipartite* if it does not contain nonsingular cycles, or equivalently, G contains no cycles with an odd number of unoriented edges ([1, Lemma 1]). Denote by $\overrightarrow{G}$ an all-oriented graph obtained from a mixed graph G by assigning to each unoriented edge of G

an arbitrary orientation (of two possible directions). Note that a *signature matrix* is a diagonal matrix with ± 1 along its diagonal.

Lemma 1.1 [14, Lemma 3.2]**.** *A connected mixed graph G is singular if and only if it is quasi-bipartite.*

Theorem 1.2 [1, Theorem 4]**.** *A mixed graph G is quasi-bipartite if and only if there exists a signature matrix D such that $D^T L(G) D = L(\overrightarrow{G})$.*

Suppose G is connected. If G is singular, then by above results the spectrum of $L(G)$ is exactly that of $L(\overrightarrow{G})$, and there are a lot of results on the work of the eigenvalues of $L(\overrightarrow{G})$. One can find that all trees are singular. So we focus on the work of mixed graphs containing cycles; in particular, we discuss the eigenvalues of unicyclic mixed graphs. In the paper [4] Fan determined the unique graph with the largest spectral radius among *all nonsingular unicyclic mixed graph* of given order, and in the paper [6] Fan *et.al.* determined the graphs respectively with the largest, the second largest and the third largest spectral radius among *all unicyclic mixed graphs* of given order. If we restrict our attention to all-unoriented mixed graphs, then by the results of [6] we have found two graphs respectively with the largest and the second largest spectral radius among *all unicyclic all-unoriented mixed graphs* of given order.

Which is (*are*) *the graph*(*s*) *with the third largest* (*or smaller*) *spectral radius among all unicyclic all-unoriented mixed graphs of given order* ?

In this paper, we discuss above problem and determine the graphs respectively with the third and the fourth largest spectral radius among all unicyclic all-unoriented mixed graphs of given order.

Note that the Laplacian matrix of an all-unoriented mixed graph is also called the *unoriented Laplacian matrix* [7, 13], or *signless Laplaican matrix* [2], or quasi-Laplacian matrix (by some Chinese researchers) of the graph, which is received much attention in recent.

2. Preliminaries

We first introduced five all-unoriented unicyclic mixed graphs of order n used in [6]: $G_1(r,s;n)$, $r \geq s$; $G_2(r,s;n), r \geq s$; $G_3(r,s;n)$; $G_4(r,s;n), s \geq 1$; $G_5(r,s;n), r \geq s$. Here r, s are nonnegative integers, which are respectively the number of pendant vertices adjacent to u and v, moreover parameters n, r, s are related by $n = r + s + 3, n = r + s + 4, n = r + s + 5$.

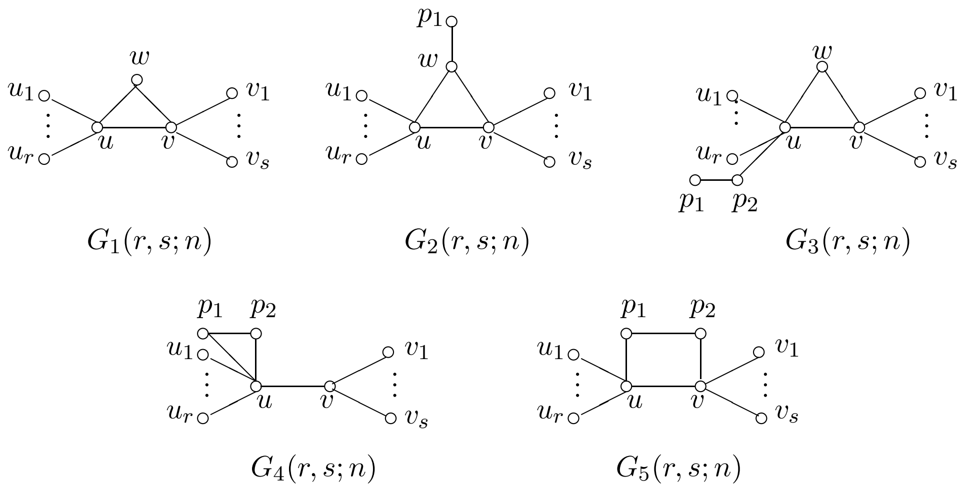

Figure 2.1. Five all-unoriented unicyclic mixed graphs on n vertices.

We next list main results of [6], where two mixed graphs G_1 and G_2 of same order are said *signature isomorphic* if there exist a signature matrix D and a permutation matrix P such that $L(G_1) = (DP)^T L(G_2) DP$.

Theorem 2.1 [6, Theorem 3.3]**.** *For $n \geq 5$, up to signature isomorphisms, $G_1(n-3, 0; n)$ of Figure 2.1 is the unique graph with the largest spectral radius among all unicyclic mixed graphs of order n.*

Theorem 2.2 [6, Theorem 3.5]**.** *For $n \geq 5$, up to signature isomorphisms, $\widehat{G_1}(n-3, 0; n)$ is the unique graph with the second largest spectral radius among all unicyclic mixed graphs of order n, where $\widehat{G_1}(n-3, 0; n)$ is obtained from $G_1(n-3, 0; n)$ by orienting the edge $\{u, v\}$.*

Theorem 2.3 [6, Theorem 3.6]**.** *For $n \geq 5$, up to signature isomorphisms, $G_1(n-4, 1; n)$ of Figure 2.1 is the unique graph with the third largest spectral radius among all unicyclic mixed graphs of order n.*

By Theorems 2.1–2.3, we immediately get the following result.

Corollary 2.4. *For $n \geq 5$, up to isomorphisms, the graphs $G_1(n-3, 0; n)$ and $G_1(n-4, 1; n)$ of Figure* 2.1 *are two graphs respectively with the largest and the second largest spectral radius among all unicyclic all-unoriented mixed graphs of order n.*

We also need some other results which will be used later. Denote by G^c the mixed graph obtained from a mixed graph G by orienting all its unoriented edges and unorienting all its oriented edges, and denote by $\Delta(G)$ the maximum degree among all vertices of G. A graph is called *regular* if all vertices have the same degrees, and is called *semi-regular* if it is bipartite and the vertices in each partition have the same degrees.

Lemma 2.5 ([10, Theorem 3.5(1), Theorem 3.10], [15, Lemma 3.1])**.** *Let G be a mixed graph of order n which contains at least one edge. Then*

$$\Delta(G) + 1 \leq \rho(G) \leq \max\{d(u) + d(v) : \ uv \in E(G)\}.$$

Moreover, if G is connected, then the left equality holds if and only if $\Delta(G) = n - 1$ and G is quasi-bipartite; and the right equality holds if and only if G is regular or semi-regular and G^c is quasi-bipartite.

Lemma 2.6 [3, Lemma 2.4]**.** *Let G be a unicyclic mixed graph on n vertices. Then*

$$s = \max\{d(u) + d(v) : \ uv \in E(G)\} \leq n + 1,$$

with equality if and only if G is one such that $\overline{G}$ is $G_1(r, s; n)$ of Figure 2.1*, and $s = n$ if and only if G is one such that $\overline{G}$ is one of the graphs $G_i(r, s; n)$ of Figure* 2.1 *for $i = 2, 3, 4, 5$, where $\overline{G}$ is one obtained from the mixed graph G by unorienting all its oriented edges.*

3. MAIN RESULTS

For convenience, We simply refer the *first, second, third, fourth graphs* of order n respectively to the graphs with the largest, the second largest, the third largest, the fourth largest spectral radius among all unicyclic all-unoriented mixed graphs of order n. By Corollary 2.4, the first graph and the second graph of order $n \geq 5$ have been determined. In this section, we will determine the third graph(s) and the fourth graph(s). In following we consider only all-unoriented mixed graphs and unoriented Laplacian matrices.

Let G be a connected all-unoriented graph of order n. Then $L(G)$ is (entrywise) nonnegative, irreducible and positive semidefinite symmetric matrix. By the Perron-Frobenius theory, the spectral radius $\rho(G) = \lambda_1(G)$ is a simple eigenvalue of $L(G)$ and there is a unique (up to multiples) corresponding positive eigenvector, usually referred to as its *Perron vector* of $L(G)$. By the theory of a symmetric matrix,

$$\rho(G) = \max_{y,\|y\|=1} y^T L(G) y = \max_{y,\|y\|=1} \sum_{uv \in E(G)} (y_u + y_v)^2, \tag{3.1}$$

with equality if and only if y is an eigenvector corresponding to $\rho(G)$, where y_u denotes the component of y for the entry that corresponds to the vertex u. We also find that $y \neq 0$ is an eigenvector of $L(G)$ corresponding to the eigenvalue λ if and only if for each vertex u of G

$$(\lambda - d_u) y_u = \sum_{v \in N(u)} y_v, \tag{3.2}$$

where $N(u)$ is the neighbour set of u in G, i.e., the set of all vertices in G adjacent to u.

Lemma 3.1 [6, Lemma 3.3]. *Let $G_i(r,s;n)$, $G_i(r+1,s-1;n)$, $G_i(r-1, s+1;n)$ be mixed graphs of Figure* 2.1 *on $n \geq 5$ vertices for $i = 1,\ldots,5$. Then*

(1) *for $i = 1,2,5$ and for $r \geq s \geq 1$, $\rho(G_i(r,s;n)) < \rho(G_i(r+1,s-1;n))$.*
(2) *for $r \geq s-1 \geq 0$, $\rho(G_3(r,s;n)) < \rho(G_3(r+1,s-1;n))$, and for $1 \leq r < s-1$, $\rho(G_3(r,s;n)) < \rho(G_3(r-1,s+1;n))$.*
(3) *for $r \geq s-2 \geq 0$, $\rho(G_4(r,s;n)) < \rho(G_4(r+1,s-1;n))$, and for $1 \leq r < s-2$, $\rho(G_4(r,s;n)) < \rho(G_4(r-1,s+1;n))$.*

By Lemma 3.1 and the fact $G_2(n-4,0;n) \cong G_1(n-4,1;n)$ and $G_3(0, n-5;n) \cong G_4(n-4,1;n)$, we have

$$\begin{aligned} \rho(G_1(n-3,0;n)) &= \max\{\rho(G_1(r,s;n)), \text{ for } r \geq s \geq 0\}; \\ \rho(G_2(n-4,0;n)) &= \max\{\rho(G_2(r,s;n)), \text{ for } r \geq s \geq 0\} \\ &\qquad (= \rho(G_1(n-4,1;n))); \end{aligned}$$

$$\begin{aligned}
\rho(G_3(n-5,0;n)) &= \max\{\rho(G_3(r,s;n)),\ \text{for } r \geq s-1 \geq -1\};\\
\rho(G_3(0,n-5;n)) &= \max\{\rho(G_3(r,s;n)),\ \text{for } 0 \leq r < s-1\};\\
\rho(G_4(n-4,1;n)) &= \max\{\rho(G_4(r,s;n)),\ \text{for } r \geq s-2 \geq -1\}\\
&\quad (= \rho(G_3(n-5,0;n)));\\
\rho(G_4(0,n-4;n)) &= \max\{\rho(G_4(r,s;n)),\ \text{for } 0 \leq r < s-2\};\\
\rho(G_5(n-4,0;n)) &= \max\{\rho(G_5(r,s;n)),\ \text{for } r \geq s \geq 0\}.
\end{aligned}$$

Denote the set

$$\mathcal{S} = \{G_1(n-5,2;n),\ G_2(n-5,1;n),\ G_3(0,n-5;n),\ G_3(n-5,0;n),$$
$$G_4(0,n-4;n),\ G_5(n-4,0;n)\}.$$

Lemma 3.2. *For* $n \geq 7$, $\rho(G_3(n-5,0;n)) > \rho(G_5(n-4,0;n)) > n-1$.

Proof. Let x be the unit Perron vector of $G_5(n-4,0;n)$ corresponding to $\rho(G_5(n-4,0;n)) =: \rho$. Note that $G_3(n-5,0;n)$ is isomorphic to a graph (denoted by $\mathbf{G}$) obtained from $G_5(n-4,0;n)$ by replacing the edge vp_2 by the edge vu_1, and by equation (3.1)

$$\begin{aligned}
x^T L(\mathbf{G})x - x^T L(G_5(n-4,0;n))x &= (x_v + x_{u_1})^2 - (x_v + x_{p_2})^2\\
&= (x_{u_1} - x_{p_2})(x_{p_2} + x_{u_1} + 2x_v).
\end{aligned}$$

If we can show $x_{u_1} > x_{p_2}$, then

$$\begin{aligned}
\rho(G_3(n-5,0;n)) &= \rho(\mathbf{G}) \geq x^T L(\mathbf{G})x > x^T L(G_5(n-4,0;n))x\\
&= \rho(G_5(n-4,0;n)).
\end{aligned}$$

Now we prove $x_{u_1} > x_{p_2}$. Note that there exists an automorphism σ of $G_5(n-4,0;n)$ that interchanges p_1 and v and keeps other vertices invariant. Then we obtain a vector x_σ defined as: $(x_\sigma)_v = x_{\sigma(v)}$ for each vertex v of $G_5(n-4,0;n)$, which is also a unit Perron vector of $L(G_5(n-4,0;n))$ by equation (3.2). As the unit Perron vector of $L(G_5(n-4,0;n))$ is unique, $x_\sigma = x$ so that $x_{p_1} = x_v$. By equation (3.2) and the fact $x_{p_1} = x_v$,

$$(\rho-1)x_{u_1} = x_u,\ (\rho-2)x_v = x_{p_2} + x_u, (\rho-2)x_{p_2} = 2x_v.$$

Thus

$$\left(\frac{1}{2}\rho^2 - 2\rho + 1\right) x_{p_2} = (\rho-1)x_{u_1}.$$

By Lemma 2.6, $\rho(G_5(n-4,0;n)) = \rho > n-1$. If $n \geq 7$ then $\frac{1}{2}\rho^2 - 2\rho + 1 - (\rho - 1) > 0$, and hence $x_{u_1} > x_{p_2}$. The result follows. ■

Lemma 3.3. *The third and the fourth graph(s) of order $n \geq 7$ belong to the set $\mathcal{S}$.*

Proof. By Corollary 2.4, $G_1(n-3,0;n)$ is the unique first graph and $G_1(n-4,1;n) \cong G_2(n-4,0;n)$ is the unique second graph. By Lemma 3.1, except the graphs $G_1(n-3,0;n)$ and $G_1(n-4,1;n)$, the graphs respectively with the largest and the second largest spectral radius among all graphs of Figure 2.1 belong to the set $\mathcal{S}$. By Lemma 3.1, $G_3(n-5,0;n)$ and $G_5(n-4,0;n)$ have different spectral radii both larger than $n-1$. For any unicyclic graph G of order $n \geq 7$ such that G is not one graph of Figure 2.1, then by Lemma 2.5 and Lemma 2.6, $\rho(G) \leq n-1$. The result follows. ■

Lemma 3.4. *For $n \geq 7$, $\rho(G_1(n-5,2;n)) < n-1$.*

Proof. Let λ ($\lambda \neq 1$) be an eigenvalue of $L(G_1(n-5,2;n))$ with the corresponding eigenvector x. Then by euation (3.2), we have

$$x_{u_1} = x_{u_2} = \cdots = x_{u_{n-5}} =: y_1, \; x_{v_1} = x_{v_2} =: y_2$$

and λ is a root of the following equations:

$$\begin{cases} (\lambda-1)y_1 &= x_u, \\ (\lambda-n+3)x_u &= (n-5)y_1 + x_v + x_w, \\ (\lambda-4)x_v &= x_w + x_u + 2y_2, \\ (\lambda-2)x_w &= x_u + x_v, \\ (\lambda-1)y_2 &= x_v. \end{cases}$$

Then λ is a root of the characteristic polynomial $f(\lambda)$ of the coefficient matrix of above homogeneous linear equations, where

$$\begin{aligned} f(\lambda) &= \det \begin{bmatrix} \lambda-1 & -1 & 0 & 0 & 0 \\ -n+5 & \lambda-n+3 & -1 & -1 & 0 \\ 0 & -1 & \lambda-4 & -1 & -2 \\ 0 & -1 & -1 & \lambda-2 & 0 \\ 0 & 0 & -1 & 0 & \lambda-1 \end{bmatrix} \\ &= \lambda^5 - (n+5)\lambda^4 + (7n-3)\lambda^3 - (11n-13)\lambda^2 + (3n+8)\lambda - 4. \end{aligned}$$

If $n \geq 7$, then $f(0) = -4 < 0$, $f(1/3) = (2/81)n - 14/243 > 0$, $f(1) = -2n+10 < 0$, $f(2) = 2n-8 > 0$, $f(5) = -10n-14 < 0$, $f(n-1) = (n-1)^2 [(n-9/2)^2 - 41/4] + (3n-4)(n+3) > 0$. As $\rho(G_1(n-5,2;n)) > n-2 \geq 5$ is the largest root of $f(\lambda)$, $\rho(G_1(n-5,2;n)) < n-1$. ■

Lemma 3.5. *For* $n \geq 7$,

$$\rho(G_1(n-5,2;n)) > \rho(G_2(n-5,1;n)) > \rho(G_3(0,n-5;n)) > \rho(G_4(0,n-4;n)).$$

Proof. (1) $\underline{\rho(G_1(n-5,2;n)) > \rho(G_2(n-5,1;n))}$. Let x be a unit Perron vector of $L(G_2(n-5,1;n))$ corresponding to $\rho(G_2(n-5,1;n))$. Note that $G_1(n-5,2;n)$ is isomorphic to a graph (denoted by $\mathbf{G}$) obtained from $G_2(n-5,1;n)$ by replacing the edge p_1w by p_1v, and

$$x^T L(\mathbf{G})x - x^T L(G_2(n-5,1;n))x = (x_v - x_w)(2x_{p_1} + x_v + x_w).$$

There exists an automorphism σ of $G_2(n-5,1;n)$ such that σ interchanges p_1 and v_1, w and v, and keeps other vertices invariant. Hence $x_v = x_w$, and therefore

$$\begin{aligned}\rho(G_1(n-5,2;n)) &= \rho(\mathbf{G}) \geq x^T L(\mathbf{G})x = x^T L(G_2(n-5,1;n))x \\ &= \rho(G_2(n-5,1;n)).\end{aligned}$$

We assert that the inequality should be strict. Otherwise x is also a Perron vector of $\mathbf{G}$. Then applying Eq. (3.2) to the vertex w of the graph $\mathbf{G}$, we have

$$[\rho(\mathbf{G}) - 2]x_w = x_u + x_v.$$

However, for the graph $G_2(n-5,1;n)$,

$$[\rho(G_2(n-5,1;n)) - 3]x_w = x_{p_1} + x_u + x_v,$$

which yields a contradiction to above equality.

(2) $\underline{\rho(G_2(n-5,1;n)) > \rho(G_3(0,n-5;n))}$. Following the route of above proof, let x be a unit Perron vector of $L(G_3(0,n-5;n))$ corresponding to $\rho(G_3(0,n-5;n)) =: \rho$. Note that $G_2(n-5,1;n)$ is isomorphic to a graph (also denoted by $\mathbf{G}$) obtained from $G_3(0,n-5;n)$ by replacing the edge p_1p_2 by p_1w, and

$$x^T L(\mathbf{G})x - x^T L(G_3(0,n-5;n))x = (x_w - x_{p_2})(2x_{p_1} + x_w + x_{p_21}).$$

Next we will show $x_w > x_{p_2}$ and hence $\rho(G_2(n-5,1;n)) = \rho(\mathbf{G}) > \rho(G_3(0,n-5;n))$. Also by equation (3.2),

$$\left(\rho - 2 - \frac{1}{\rho-1}\right) x_{p_2} = x_u, (\rho-3)x_u = x_{p_2} + x_w + x_v, (\rho-2)x_w = x_u + x_v.$$

Then we have

$$\left[(\rho-2)\left(\rho - 2 - \frac{1}{\rho-1}\right) - 1\right] x_{p_2} = (\rho-1)x_w.$$

As $\rho > n-2$ by Lemma 2.5, if $n \geq 7$ then $(\rho-2)(\rho-2-\frac{1}{\rho-1}) - 1 - (\rho-1) > \rho^2 - 5\rho + 3 > 0$, and hence $x_w > x_{p_2}$, which prove the result.

(3) $\underline{\rho(G_3(0,n-5;n)) > \rho(G_4(0,n-4;n))}$. Let x be a unit Perron vector of $L(G_4(0,n-4;n))$ corresponding to $\rho(G_4(0,n-4;n)) =: \rho$. Note that $G_3(0,n-5;n)$ is isomorphic to a graph (also denoted by $\mathbf{G}$) obtained from $G_4(0,n-4;n)$ by replacing the edge up_1 by uv_1. Thus

$$x^T L(\mathbf{G})x - x^T L(G_4(0,n-4;n))x = (x_{v_1} - x_{p_1})(2x_u + x_{v_1} + +x_{p_1}).$$

It suffices to show $x_{v_1} > x_{p_1}$. Note that there is an automorphism σ of $G_4(0,n-4;n)$ such that σ interchanges p_1 and p_2 and keeps other vertices invariant. Hence $x_{p_1} = x_{p_2}$. By equation (3.2),

$$(\rho-1)x_{v_1} = x_v, (\rho-3)x_u = x_{p_1} + x_{p_2} + x_v, (\rho-2)x_{p_1} = x_{p_2} + x_u.$$

Substituting $x_{p_1} = x_{p_2}$, we have

$$[(\rho-3)^2 - 2]x_{p_1} = (\rho-1)x_{v_1}.$$

If $n \geq 8$, then by Lemma 2.6, $\rho > n-2 \geq 6$, and hence $(\rho-3)^2 - 2 > \rho - 1 > 0$ so that $x_{v_1} > x_{p_1}$, which prove the result. For $n = 7$, by the software MATHEMATICA, $\rho(G_3(0,2;7)) \approx 5.55336 > \rho(G_4(0,3;7)) \approx 5.35386$. The result also follows. ■

Theorem 3.6. *For $n \geq 7$, $G_3(n-5,0;n)$ is the unique third graph.*

Proof. By Lemma 3.3, The third graph(s) of order $n \geq 7$ belong(s) to the set $\mathcal{S}$. By Lemma 3.2, Lemma 3.4 and Lemma 3.5, the result follows. ■

Lemma 3.7. *For* $n \geq 7$, $\rho(G_1(n-5,2;n)) > \max\{\rho(G_3(n-6,1;n)), \rho(G_5(n-5,1;n)\}$.

Proof. We first prove $\rho(G_1(n-5,2;n)) > \rho(G_3(n-6,1;n))$. Let x be the unit Perron vector of $L(G_3(n-6,1;n))$ corresponding to $\rho(G_3(n-6,1;n)) =: \rho$. Note that $G_1(n-5,2;n)$ is isomorphic to a graph (denoted by $\mathbf{G}$) obtained from $G_3(n-6,1;n)$ by replacing the edge p_1p_2 by the edge p_1v, and

$$x^T L(\mathbf{G})x - x^T L(G_3(n-6,1;n))x = (x_v - x_{p_2})(2x_{p_2} + x_v + x_{p_2}).$$

It suffice to show $x_v > x_{p_2}$. By equation (3.2),

$$\left(\rho-2-\frac{1}{\rho-1}\right)x_{p_2} = x_u, \left(\rho-3-\frac{1}{\rho-1}\right)x_v = x_w + x_u, (\rho-2)x_w = x_u + x_v.$$

Then

$$\left[(\rho-2)\left(\rho-3-\frac{1}{\rho-1}\right)-1\right]x_v = (\rho-1)\left(\rho-2-\frac{1}{\rho-1}\right)x_{p_2}.$$

One can easily find that $x_v > x_{p_2}$ and the results follows.

Next we prove $\rho(G_1(n-5,2;n)) > \rho(G_5(n-5,1;n)$. Let x be the unit Perron vector of $L(G_5(n-5,1;n))$ corresponding to $\rho(G_5(n-5,1;n)) =: \rho$. Note that $G_1(n-5,2;n)$ is isomorphic to a graph (also denoted by $\mathbf{G}$) obtained from $G_5(n-5,1;n)$ by replacing the edge p_1p_2 by the edge p_1v, and

$$x^T L(\mathbf{G})x - x^T L(G_5(n-5,1;n))x = (x_v - x_{p_2})(2x_{p_2} + x_v + x_{p_2}).$$

It suffice to show $x_v > x_{p_2}$. By equation (3.2),

$$\left(\rho-3-\frac{1}{\rho-1}\right)x_v = x_{p_2} + x_u, (\rho-2)x_{p_2} = x_{p_1} + x_v, (\rho-2)x_{p_1} = x_{p_2} + x_u.$$

Then

$$(\rho-2)^2 x_{p_2} = \left(2\rho-5-\frac{1}{\rho-1}\right)x_v.$$

So $x_v > x_{p_2}$ and the results follows. ∎

Theorem 3.8. *For* $n \geq 7$, $G_5(n-4,0;n)$ *is the unique fourth graph.*

Proof. By Lemma 3.3, The fourth graph(s) of order $n \geq 7$ belong(s) to the set $\mathcal{S}$. By Lemma 3.7, Lemma 3.4 and Lemma 3.2,

$$\rho(G_3(n-6,1;n)) < \rho(G_1(n-5,2;n)) < n-1 < \rho(G_5(n-4,0;n)).$$

Using Lemma 3.5, we find the result follows. ∎

Remark. $G_1(n-5,2;n)$ is the fifth graph among all graphs of Figure 2.1. The reason is as follows. By Lemma 3.5, $\rho(G_1(n-5,2;n)) > \max\{\rho(G_2(n-5,1;n)), \rho(G_3(0,n-5;n)), \rho(G_4(0,n-4;n))\}$, by Lemma 3.7, $\rho(G_1(n-5,2;n)) > \max\{\rho(G_3(n-6,1;n)), \rho(G_5(n-5,1;n)\}$. However, we do not know whether $G_1(n-5,2;n)$ is the fifth graph among all unicyclic graphs of order n, as $\rho(G_1(n-5,2;n)) < n-1$ by Lemma 3.4 and there maybe exists a graph not in Figure 2.1 but with spectral radius greater than $\rho(G_1(n-5,2;n))$. As a conclusion, we give a partial order of the unicyclic graphs according to spectral radius, where the graphs $G_i(r,s;n)$ are simply written to $G_i(r,s)$.

$G_1(n-3,0)$						1st graph
$G_1(n-4,1)$	$G_2(n-4,0)$					2nd graph
		$G_3(n-5,0)$				3rd graph
					$G_5(n-4,0)$	4th graph
$G_1(n-5,2)$						**unknown**
$G_1(n-6,3)$	$G_2(n-5,1)$	$G_3(n-6,1)$	$G_3(0,n-5)$	$G_4(0,n-5)$	$G_5(n-5,1)$	**order**

Figure 3.1. A partial order of the unicyclic graphs.

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