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Order unicyclic mixed graphs by spectral radius*

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Abstract

For a mixed graph, its Laplacian spectral radius is defined by that of its Laplacian matrix. In this paper, we determine respectively the unicyclic mixed graphs with the first, the second and the third largest spectral radii among all unicyclic mixed graphs of given order.

1 Introduction

Let $G = (V, E)$ be a *mixed graph* with vertex set $V = V(G) = \{v_1, v_2, \ldots, v_n\}$ and edge set $E = E(G) = \{e_1, \ldots, e_m\}$, 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. We assume that G has no multi-edges or loops in this paper. 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 $a_{ij} = 0$ otherwise. Then $A(G) = [a_{ij}]$ is called the *adjacency matrix* of G. The degree of the vertex

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$v \in V(G)$ is denoted by $d_G(v) = d(v)$ 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 $D(G) = \text{diag}\{d(v_1), d(v_2), \ldots, d(v_n)\}$. It is easy to see that $L(G)$ is symmetric and positive semidefinite so that its eigenvalues can be arranged as follows: $0 \le \lambda_n(G) \le \lambda_{n-1}(G) \le \cdots \le \lambda_1(G)$. We simply say the eigenvalues and eigenvectors of $L(G)$ are those of G. We also refer to $\lambda_1(G)$ as the spectral radius of G, and denote it by $\rho(G)$.

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, matching number, isoperimetric number, and expanding properties of a graph; see, for example, [6, 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* ([7]). So the notion of a mixed graph generalizes both the classical approach of orienting all edges and the unoriented approach. *It is necessary to stress that even for an unoriented graph G its Laplacian matrix, $L(G) = D(G) + A(G)$, is different from the usual Laplacian matrix* (*which is $L(G) = D(G) - A(G)$*). For algebraic properties of mixed graphs, one can refer to [1, 2, 3, 4, 5, 13, 14].

Denote by $\overrightarrow{G}$ an all-oriented graph obtained from G by assigning to each unoriented edge of G an arbitrary orientation (of two possible directions). G is called *quasi-bipartite* if it does not contain a nonsingular cycle, or equivalently, G contains no cycles with an odd number of unoriented edges ([1, Lemma 1]). Note that a *signature matrix* is a diagonal matrix with ± 1 along its diagonal. Then by the result of [13, Lemma 2.2], *a connected mixed graph G is singular if and only if it is quasi-bipartite*; and by the result of [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 the above results the spectrum of G is exactly that of $\overrightarrow{G}$, and there are lots of results on the work related with the eigenvalues of $\overrightarrow{G}$ ([11, 12]). 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. Note that the first author [4] has determined the graph with the largest spectral radius among all nonsingular unicyclic mixed graphs of given order. In this paper, we extend the above work and determine the unicyclic mixed graphs with the largest, the second largest and the third largest spectral radii among all unicyclic mixed graphs of given order.

2 Preliminaries

Let G be a connected mixed graph. Denote by $\overline{G}$ an all-unoriented graph obtained from G by unorienting each oriented edge of G. Then $L(\overline{G})$ is an unoriented Laplacian matrix, and is also irreducible, nonnegative and symmetric. Let $|A|$ denote $[|a_{ij}|]$ for the matrix $A = [a_{ij}]$. Then $L(\overline{G}) = |L(G)|$.

THEOREM 2.1 *Let G be a connected mixed graph on n vertices $v_1, \ldots, v_n$. Then*

$$\rho(G) \leq \rho(\overline{G})$$

with equality if and only if G has a bipartition (V_1, V_2) such that each edge within V_1 (and within V_2) is unoriented and every edge joining one vertex of V_1 and one vertex of V_2 is oriented, or equivalently, there exists a signature matrix D such that $D^T L(G) D = L(\overline{G})$.

Proof: By the result of nonnegative matrices (see [9, Theorem 8.4.5]), we know that $\rho(G) \leq \rho(\overline{G})$ as $|L(G)| = L(\overline{G})$ with equality if and only if there exists a diagonal matrix $D = [d_{ij}] = \operatorname{diag}\{e^{i\theta_1}, e^{i\theta_2}, \ldots, e^{i\theta_n}\}$ such that $DL(G)D^{-1} = L(\overline{G})$, where $\theta_i \in \mathbb{R}$ for $i = 1, \ldots, n$. Without loss of generality, let $d_{11} = 1$. For any vertex v_j adjacent to v_1, by the above equality we have $d_{11} \operatorname{sgn}\{v_1, v_j\} d_{jj}^{-1} = 1$, and hence $d_{jj} = \operatorname{sgn}\{v_1, v_j\}$. Applying the above discussion to other vertices, we get that each diagonal entry of D is either 1 or -1 since G is connnected. Let $V_1 = \{v_k \mid d_{kk} = 1\}$ and $V_2 = \{v_k \mid d_{kk} = -1\}$ so that they form a bipartition of $V(G)$. For any two vertices v_i, v_j of V_1, if they are adjacent, then the edge joining them is necessarily unoriented because $d_{ii} \operatorname{sgn}\{v_i, v_j\} d_{jj}^{-1} = 1$. Similarly, the edges within V_2 are also unoriented and every edge joining one vertex of V_1 and one vertex of V_2 is oriented. Now we get the necessity of the equality holding.

Conversely, let $D = [d_{ij}]$ be a diagonal matrix such that $d_{ii} = 1$ if $v_i \in V_1$ and $d_{ii} = -1$ if $v_i \in V_2$. One can easily verify that $DL(G)D^{-1} = L(\overline{G})$ and the sufficiency holds. ∎

By the Perron-Frobenius theory, the spectral radius of the connected graph $\overline{G}$ is a simple eigenvalue and there is a unique (up to multiples) corresponding positive eigenvector, usually referred to as its *Perron vector*; see [9]. By the theory of symmetric matrices, $\rho(\overline{G})$ is equal to the maximum value of the quadratic form $x^T L(\overline{G}) x$ as x varies over unit vectors, and also the quadratic form attains its maximum value at a unit vector x if and only if x is an eigenvector corresponding to $\rho(\overline{G})$. So if x is the unit Perron vector of $\overline{G}$, then we have $\rho(\overline{G}) = x^T L(\overline{G}) x$ and $x^T L(\overline{G}) x > y^T L(\overline{G}) y$ for any unit vector y, unless $y = \pm x$. Also we find that

$$x^T L(\overline{G}) x = \sum_{\{u,v\} \in E(\overline{G})} (x_u + x_v)^2, \tag{2.1}$$

and λ is an eigenvalue of $\overline{G}$ with the corresponding eigenvector x if and only if $x \neq 0$ and

$$(\lambda - d(v))x_v = \sum_{\{u,v\} \in E(\overline{G})} x_u, \text{ for all } v \in V(\overline{G}), \tag{2.2}$$

where x_u is the entry of x corresponding to the vertex u.

Let G be a mixed graph. Denote by G^c the mixed graph obtained from G by orienting all of its unorienting edges and unorienting all of its oriented edges (that is, $A(G) = -A(G^c)$), and denote by $\Delta(G)$ the largest degree among all the vertices of G. Note that a graph is called *regular* if all of its vertices have same degrees, and is called *semi-regular* if it is bipartite and the vertices in each partition have same degrees.

THEOREM 2.2 ([10], [14]) *Let G be a mixed graph on n vertices which has at least one edge. Then*

$$\Delta(G) + 1 \leq \rho(G) \leq \max\{d(u) + d(v) : \{u, v\} \in E(G)\}. \tag{2.3}$$

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.

We introduce five all-unoriented unicyclic mixed graphs of order n in Fig. 2.1 which will be used in Section 3: the graphs $G_1(r, s; n), r \geq s$; $G_2(r, s; n), r \geq s$; $G_3(r, s; n)$; $G_4(r, s; n), s \geq 1$; $G_5(r, s; n), r \geq s$. 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 $n = r + s + 3$, $n = r + s + 4$, $n = r + s + 5$.

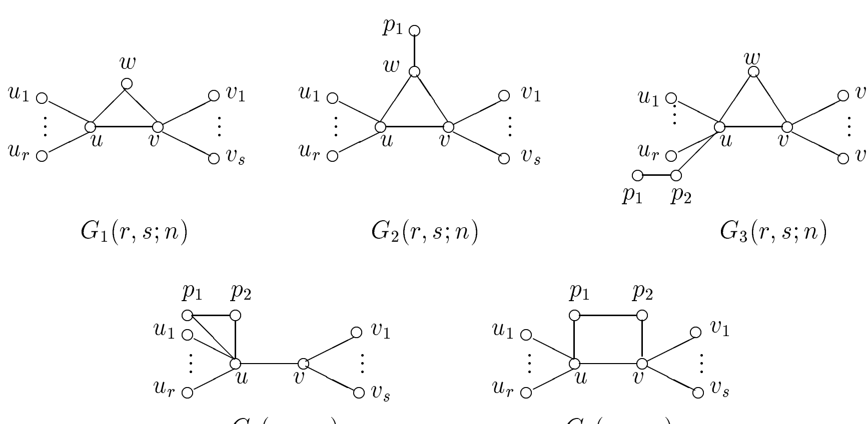

Fig. 2.1. Five all-unoriented unicyclic mixed graphs on n vertices.

Lemma 2.3 [3, Lemma 2.4] *Let G be a unicyclic mixed graph on n vertices. Then*

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

with equality if and only if G is one such that $\overline{G}$ is $G_1(r, s; n)$ of Fig. 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 Fig. 2.1 for $i = 2, 3, 4, 5$.

3 Main results

In this section, we will respectively determine the unicyclic graphs with the largest, the second largest and the third largest spectral radii among all unicyclic mixed graphs on n vertices. For convinence, we simply call them *the first largest graph*, *the second largest graph* and *the third largest graph* on n vertices, respectively.

We need to note that for a signature matrix D and a permutation matrix P both of order n, and for a mixed graph G on n vertices, the graph with the Laplacian matrix $D^T P^T L(G) P D$, denoted by ${}^{DP}G$, differs from the graph ${}^{P}G$ (for $D = I$) only in the orientation of some edges, and has the same spectrum as that of G. We will say that two mixed graphs with the relation of G and ${}^{DP}G$ are *signature isomorphic.*

Let G be a unicyclic mixed graph on n vertices. If $n = 3$, then $\overline{G}$ is $G_1(0, 0; 3)$ of Fig. 2.1. If $n = 4$, then $\overline{G}$ is either the graph $G_1(1, 0; 4)$ or the graph $G_5(0, 0; 4)$ of Fig. 2.1. By Theorem 2.2, $\rho(G_1(1, 0; 4)) > 4 = \rho(G_5(0, 0; 4))$. Then for $n = 4$, by Theorem 2.1, $G_1(1, 0; 4)$ and $G_5(0, 0; 4)$ are respectively the first largest graph and the second largest graph up to a signature isomorphism. In what follows we always assume that $n \geq 5$.

Lemma 3.1 *The first largest graph(s) on n vertices is among the graphs $G_1(r, s; n)$ for $r \geq s \geq 0$ of Fig. 2.1 up to signature isomorphisms, and the second largest graph(s) or its underlying undirected graph(s) on n vertices are among the graphs of Fig. 2.1 up to signature isomorphisms.*

Proof: By Theorem 2.1, the first largest graph is an all-unoriented graph up to a signature matrix. So it suffices to discuss the all-unoriented graphs. Let G be a unicyclic mixed graph on n vertices. By Theorem 2.2 and Lemma 2.3, if $\overline{G}$ is not among the graphs of Fig. 2.1, then $\rho(G) \leq n - 1$, and if $\overline{G}$ is among the graphs $G_i(r, s; n)$ of Fig. 2.1 for $i = 2, 3, 4, 5$, then $\rho(G) \leq n$. However, in Fig. 2.1, the graph $G_1(n-3, 0; n)$ has maximal degree $n-1$, and also by Theorem 2.2, $\rho(G_1(n-3, 0; n)) > n$. So the first largest graph is among the graphs $G_1(r, s; n)$ for all $r \geq s \geq 0$. We also find that graphs $G_2(n - 4, 0; n) = G_1(n - 4, 1; n)$, $G_3(n - 5, 0; n) = G_4(n - 5, 1; n)$, and $G_5(n - 4, 0; n)$ are all of maximal degree $n - 2$. By Theorem 2.2, the spectral radii of these graphs are strictly greater than $n - 1$. So the second largest graph or its underlying graph is among the graphs in Fig. 2.1. ■

LEMMA 3.2 *Let $G_i(r,s;n), G_i(r+1,s-1;n), G_i(r-1,s+1;n)$ be mixed graphs of Fig. 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 $1 \leq r < s-2$, $\rho(G_4(r,s;n)) < \rho(G_4(r-1,s+1;n))$.*

Proof: (1) Note that for $i=1,2,5$, the graphs $G_i(r+1,s-1;n)$ can be obtained from $G_i(r,s;n)$ by deleting the edge $\{v,v_s\}$ and adding the edge $\{u,v_s\}$. We discuss the cases of $i=1$ and $i=5$. The discussion for the case of $i=2$ is similar to that of $i=1$ and we omit the details.

Let x be the unit Perron vector of $L(G_1(r,s;n))$. Then we have

$$\begin{aligned} \rho(G_1(r+1,s-1;n)) &\geq x^T L(G_1(r+1,s-1;n))x, \\ x^T L(G_1(r,s;n))x &= \rho(G_1(r,s;n)) =: \rho, \end{aligned}$$

and

$$\begin{aligned} x^T L(G_1(r+1,s-1;n))x - x^T L(G_1(r,s;n))x &= (x_u + x_{v_s})^2 - (x_v + x_{v_s})^2 \\ &= (x_u - x_v)(x_u + x_v + 2x_{v_s}). \end{aligned}$$

Then $\rho(G_1(r,s;n)) < \rho(G_1(r+1,s-1;n))$ will be true if $x_v < x_u$.

Note that $\rho \geq \Delta(G_1(r,s;n)) + 1 = r+3 \geq 4$ by Theorem 2.2. From the eigenvector equation for the Perron vector x of $L(G_1(r,s;n))$, we can obtain that

$$x_{u_i} = (\rho-1)^{-1}x_u,\ i=1,\cdots,r; \quad x_{v_j} = (\rho-1)^{-1}x_v,\ j=1,\cdots,s;$$

and hence

$$(\rho - (r+2))x_u = \frac{r}{\rho-1}x_u + x_w + x_v. \tag{3.1}$$

$$(\rho - (s+2))x_v = \frac{s}{\rho-1}x_v + x_w + x_u. \tag{3.2}$$

Then we have

$$(\rho - r - 1 - \frac{r}{\rho-1})x_u = (\rho - s - 1 - \frac{s}{\rho-1})x_v. \tag{3.3}$$

The coefficients of x_u and x_v in (3.3) are positive as $\rho \geq r+3$. If $r > s$, then $x_u > x_v$ and the result follows. When $r=s$, the condition $\rho \geq r+3$ gives that $x_u = x_v$ and

$$\rho(G_1(r,s;n)) = x^T L(G_1(r,s;n))x = x^T L(G_1(r+1,s-1;n))x \leq \rho(G_1(r+1,s-1;n)).$$

If this inequality holds as equality, x must be the unit Perron vector of $L(G_1(r+1, s-1;n))$. In this condition, we have

$$(\rho - (r+3))x_u = \frac{r+1}{\rho-1}x_u + x_w + x_v. \tag{3.4}$$

But combining (3.1) and (3.4), we obtain $x_u = -\frac{1}{\rho-1}x_u$, which is a contradiction. So $\rho(G_1(r,s;n)) < \rho(G_1(r+1,s-1;n))$ for all $r \geq s \geq 1$.

Next we discuss the case of $i = 5$. We also let x be the unit Perron vector of $L(G_5(r,s;n))$ corresponding to the eigenvalue $\rho(G_5(r,s;n)) =: \rho$. Note that $\rho \geq \Delta(G_5(r,s;n)) + 1 = r+3$. Then we get

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

and hence

$$(\rho-1)(x_{p_1} - x_{p_2}) = x_u - x_v.$$

Also

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

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

So we have

$$\left(\rho - (r+2) - \frac{r+1}{\rho-1} + 1\right)x_u = \left(\rho - (s+2) - \frac{s+1}{\rho-1} + 1\right)x_v.$$

As $\rho \geq r+3$, the coefficients of x_u and x_v are positive and $x_u > x_v$ if $r > s \geq 1$. If $r = s \geq 1$, then $x_u = x_v$ and $\rho(G_5(r,s;n)) \leq \rho(G_5(r+1,s-1;n))$. Similar to the prior discussion, x cannot be the Perror vector of $L(G_5(r+1,s-1;n))$ so that the strict inequality $\rho(G_5(r,s;n)) < \rho(G_5(r+1,s-1;n))$ holds.

(2) Let x be the unit Perron vector of $L(G_3(r,s;n))$ corresponding to the eigenvalue $\rho(G_3(r,s;n)) =: \rho$. Noting that $\rho \geq \Delta(G_3(r,s;n)) + 1 \geq r+3+1 = r+4$ and using the same method as in the proof of (1), we have

$$\left(\rho - (r+3) - \frac{r}{\rho-1}\right)x_u = x_w + x_v + x_{p_2}, \tag{3.5}$$

$$\left(\rho - (s+2) - \frac{s}{\rho-1}\right)x_v = x_w + x_u, \tag{3.6}$$

$$(\rho - 2 - \frac{1}{\rho-1})x_{p_2} = x_u. \tag{3.7}$$

Then we get

$$\alpha x_u = \beta x_v. \tag{3.8}$$

where

$$\alpha = \left(\rho - (r+3) - \frac{r}{\rho-1} - \frac{1}{\rho - 2 - \frac{1}{\rho-1}} + 1\right) \text{ and } \beta = \left(\rho - (s+2) - \frac{s}{\rho-1} + 1\right).$$

Since $\rho \geq r+4$, the coefficients of x_u and x_v are positive. If $r \geq s-1 \geq 0$,

$$\beta - \alpha = r - s + 1 + \frac{r-s}{\rho-1} + \frac{1}{\rho - 2 - \frac{1}{\rho-1}} > (r-s+1)(1+\frac{1}{\rho-1}) \geq 0.$$

So $x_v < x_u$. Note that the graph $G_3(r+1, s-1; n)$ can be obtained from $G_3(r,s;n)$ by deleting the edge $\{v, v_s\}$ and adding the edge $\{u, v_s\}$, and

$$x^T L(G_3(r+1, s-1; n))x - x^T L(G_3(r,s;n))x = (x_u + x_v + 2x_{v_s})(x_u - x_v) > 0.$$

So the result follows under the condition $r \geq s-1 \geq 0$.

If $1 \leq r \leq s-2$, then

$$\beta - \alpha \leq -1 + \frac{-2}{\rho-1} + 1 < 0$$

so that $x_v > x_u$. Note that the graph $G_3(r-1, s+1; n)$ can be obtained from $G_3(r,s;n)$ by deleting the edge $\{u, u_r\}$ and adding the edge $\{v, u_r\}$, and

$$x^T L(G_3(r-1, s+1; n))x - x^T L(G_3(r,s;n))x = (x_u + x_v + 2x_{u_r})(x_v - x_u) > 0$$

under this condition so that the result also follows.

(3) Letting x be the unit Perron vector of $L(G_4(r,s;n))$ corresponding to the eigenvalue $\rho(G_4(r,s;n)) =: \rho$, and noting that $\rho \geq \Delta(G_4(r,s;n)) + 1 \geq r+4$, we get $x_{p_2} = x_{p_1} = \dfrac{1}{\rho-3}x_u$, and

$$\left(\rho - (r+3) - \frac{r}{\rho-1} - \frac{2}{\rho-3}\right) x_u = x_v.$$

$$\left(\rho - (s+1) - \frac{s}{\rho-1}\right) x_v = x_u.$$

Then we have

$$\left(\rho - (r+3) - \frac{r}{\rho-1} - \frac{2}{\rho-3} + 1\right) x_u = \left(\rho - (s+1) - \frac{s}{\rho-1} + 1\right) x_v$$

As $\rho \geq r+4$, the coefficients of x_u and x_v are positive. If $r \geq s-2 \geq 0$, $x_v < x_u$, and if $1 \leq r \leq s-3$, $x_u < x_v$. The result follows by a similar discussion to the proof of (2). ■

THEOREM 3.3 *For $n \geq 5$, $G_1(n-3, 0; n)$ of Fig. 2.1 is the unique largest graph on n vertices up to signature isomorphisms.*

Proof: By Lemma 3.1, the largest graph is among the graphs among the graphs $G_1(r, s; n)$ for all $r \geq s \geq 0$ of Fig. 2.1. The result follows from Lemma 3.2 (1). ■

LEMMA 3.4 *The second largest graph on n vertices is among the graphs $G_1(n-4, 1; n)$, $G_3(n-5, 0; n)$, $G_3(0, n-5; n)$, $G_4(0, n-4; n)$, $G_5(n-4, 0; n)$ of Fig. 2.1, and $\widehat{G_1}(n-3, 0; n)$ obtained from $G_1(n-3, 0; n)$ by orienting the edge $\{u, v\}$, up to signature isomorphisms.*

Proof: By Theorem 3.3, we find that the first largest graph $G_1(n-3, 0; n)$ is non-singular as it contains odd number of unoriented edges. Hence by Lemma 3.1 and Lemma 3.2, up to signature isomorphisms, the second largest graph is among of following graphs $G_1(n-4, 1; n) = G_2(n-4, 0; n)$, $G_3(n-5, 0; n) = G_4(n-5, 1; n)$, $G_3(0, n-5; n)$, $G_4(0, n-4; n)$, $G_5(n-4, 0; n)$, and the singular graph, denoted by H, which has the same underlying graph as $G_1(n-3, 0; n)$. Since H is singular, by the result in paragraph 3 of Section 1, there exists a signature matrix D such that ${}^D H = \widehat{G_1}(n-3, 0; n)$. The result follows. ■

THEOREM 3.5 *For $n \geq 5$, $\widehat{G_1}(n-3, 0; n)$ with the underlying graph $G_1(n-3, 0; n)$ of Fig. 2.1 is the unique second largest graph on n vertices up to signature isomorphisms.*

Proof: We divide our discussion into four assertions.

Assertion 1: *For $n \geq 5$, $\rho(G_1(n-4, 1; n)) > \rho(G_3(n-5, 0; n)) \geq \rho(G_3(0, n-5; n))$; and for $n \geq 6$, the second inequality is strict.*

Now, we begin to prove the first inequality. Note that if we replace the edge $\{p_1, p_2\}$ of $G_3(n-5, 0; n)$ by the edge $\{p_1, v\}$, then the graph $G_1(n-4, 1; n)$ is obtained. Let x be the unit Perron vector of $L(G_3(n-5, 0; n))$ corresponding to the largest eigenvalue $\rho(G_3(n-5, 0; n)) =: \rho_1$. It suffices to prove $x_{p_2} < x_v$. From the eigenvector equation for the Perron vector of $L(G_3(n-5, 0; n))$ we have

$$\left(\rho_1 - 2 - \frac{1}{\rho_1 - 1}\right) x_{p_2} = x_u, \ (\rho_1 - 2)x_v = x_u + x_w, \ (\rho_1 - 2)x_w = x_u + x_v.$$

By calculation, we have

$$\left(\rho_1 - 2 - \frac{1}{\rho_1 - 1}\right) x_{p_2} = (\rho_1 - 3)x_v.$$

Moreover $\rho_1 > \Delta(G_3(n-5, 0; n)) + 1 = n - 1 \geq 4$, so the desired result holds.

Then we prove the second inequality. Note that the graph $G_3(n-5, 0; n)$ can be obtained from $G_3(0, n-5; n)$ by deleting the edge $\{u, p_2\}$ and adding the edge $\{v, p_2\}$. Let x be the unit Perron vector of $G_3(0, n-5; n)$ corresponding to the largest eigenvalue $\rho(G_3(0, n-5; n)) =: \rho_2$. It is sufficient to prove $x_u < x_v$. By a similar discussion, we get

$$\left(\rho_2 - 2 - \frac{1}{\rho_2 - 1}\right) x_{p_2} = x_u, \ (\rho_2 - 2)x_w = x_u + x_v, \ (\rho_2 - 3)x_u = x_w + x_v + x_{p_2},$$

and hence

$$\left(\rho_2 - 3 - \frac{1}{\rho_2 - 2 - \frac{1}{\rho_2 - 1}} - \frac{1}{\rho_2 - 2}\right) x_u = \left(1 + \frac{1}{\rho_2 - 2}\right) x_v.$$

If $n \geq 7$, then $\rho_2 \geq \Delta(G_3(0, n-5; n)) + 1 = n - 2 \geq 5$, and

$$\rho_2 - 3 - \frac{1}{\rho_2 - 2 - \frac{1}{\rho_2 - 1}} - \frac{1}{\rho_2 - 2} - (1 + \frac{1}{\rho_2 - 2}) > 0.$$

In this conditon, we get $x_u < x_v$ and the result follows. If $n = 6$, by Lemma 3.2(2), $\rho(G_3(0,1;6)) < \rho(G_3(1,0;6))$. Note that for the case of $n = 5$, the graphs $G_3(n-5, 0; n)$ and $G_3(0, n-5; n)$ are same and the result follows.

Assertion 2: *For* $n \geq 5$, $\rho(G_1(n-4, 1; n)) > \rho(G_4(0, n-4; n))$.

If $n = 5$, then $G_4(0,1;5) = G_3(0,0;5)$ and the result in this case is proved by Assertion 1. If $n = 6$, then by Lemma 3.2(3), $\rho(G_4(0,2;6)) < \rho(G_4(1,1;6)) = \rho(G_3(1,0;6))$ as $G_4(1,1;6)) = G_3(1,0;6)$. The result also follows by Assertion 1. So we assume that $n \geq 7$ in below.

Note that the graph $G_1(n-4, 1; n)$ can be obtained from $G_4(0, n-4; n)$ by deleting the edge $\{p_2, p_1\}$ and adding the edge $\{p_2, v\}$. Let x be the unit Perron vector of $L(G_4(0, n-4; n))$ corresponding to the eigenvalue $\rho(G_4(0, n-4; n)) =: \rho$. It suffices to show $x_{p_1} < x_v$. From the eigenvector equation, we have $x_{p_1} = x_{p_2}$ and $(\rho-2)x_{p_1} = x_{p_2} + x_u$ so that $(\rho - 3)x_{p_1} = x_u$. In addition, $(\rho - 3)x_u = 2x_{p_2} + x_v = 2x_{p_1} + x_v$. Then

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

Then by Theorem 2.2, $\rho \geq \Delta(G_4(0, n-4; n)) + 1 = n - 2 \geq 5$ and the result follows.

Assertion 3: *For* $n \geq 5$, $\rho(G_1(n-4, 1; n)) > \rho(G_5(n-4, 0; n))$.

Note that the graph $G_1(n-4, 1; n)$ can be obtained from $G_5(n-4, 0; n)$ by deleting the edge $\{p_1, p_2\}$ and adding the edge joining $\{p_1, v\}$. Let x be the unit Perron vector of $G_5(n-4, 0; n)$ corresponding to the eigenvalue $\rho(G_5(n-4, 0; n)) =: \rho$. Then we suffice to show $x_{p_2} < x_v$. We have

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

It is obvious that $x_{p_1} = x_v$ as $\rho > \Delta(G_5(n-4, 0; n)) + 1 = n - 1 \geq 4$ by Theorem 2.2, and hence

$$(\rho - 2)x_{p_2} = x_v + x_{p_1} = 2x_v,$$

which implies that $x_{p_2} < x_v$. The result follows.

Assertion 4: *For* $n \geq 5$, $\rho(G_1(n-4, 1; n)) < \rho(\widehat{G_1}(n-3, 0; n))$.

By Theorem 2.2, we have $\rho(\widehat{G_1}(n-3, 0; n)) = n$. Let $\lambda \neq 1$ be an eigenvalue of $G_1(n-4, 1; n)$ with the corresponding eigenvector x. Then by the eigenvector equation of x,

$$x_{u_1} = x_{u_2} = \cdots = x_{u_{n-4}} =: y_1,$$

and λ is a root of the following equations:

$$\begin{cases} (\lambda-1)y_1 & = & x_u, \\ (\lambda-n+2)x_u & = & (n-4)y_1+x_v+x_w, \\ (\lambda-3)x_v & = & x_w+x_u+x_{v_1}, \\ (\lambda-2)x_w & = & x_u+x_v, \\ (\lambda-1)x_{v_1} & = & x_v. \end{cases}$$

Therefore λ is a root of following polynomial $f(\lambda)$:

$$f(\lambda)=\det\begin{bmatrix} \lambda-1 & -1 & 0 & 0 & 0 \\ -n+4 & \lambda-n+2 & -1 & -1 & 0 \\ 0 & -1 & \lambda-3 & -1 & -1 \\ 0 & -1 & -1 & \lambda-2 & 0 \\ 0 & 0 & -1 & 0 & \lambda-1 \end{bmatrix}.$$

From a little calculation,

$$f(\lambda)=-4+8\lambda+3n\lambda+\lambda^2-9n\lambda^2+3\lambda^3+6n\lambda^3-5\lambda^4-n\lambda^4+\lambda^5.$$

If $n\geq 5$, we have $f(0)<0$, $f(1/2)=(11-2n)/32>0$ if $n=5$, $f(1/3)=(51n-284)/243>0$ if $n\geq 6$, $f(1)=4-n<0$, $f(2)=-8+2n>0$, $f(4)=-20-4n<0$ and $f(n)=-4+8n+4n^2-6n^3+n^4>0$, which implies that $\rho(G_1(n-4,1;n))<n$. The result follows. ■

By Lemma 3.4 and the Assertions 1–3 in the proof of Theorem 3.5, we determine the third largest graph on n vertices.

THEOREM 3.6 *For $n\geq 5$, $G_1(n-4,1;n)$ of Fig. 2.1 is the unique third largest graph on n vertices up to signature isomorphisms.*

References

[1] R.B. Bapat, J.W. Grossman and D.M. Kulkarni, Generalized matrix tree theorem for mixed graphs, *Linear and Multilinear Algebra* 46 (1999), 299–312.

[2] R.B. Bapat, J.W. Grossman and D.M. Kulkarni, Edge version of the matrix tree theorem for trees, *Linear and Multilinear Algebra* 47 (2000), 217–229.

[3] Y.-Z. Fan, On spectral integral variations of mixed graph, *Linear Algebra Appl.* 374 (2003), 307–316.

[4] Y.-Z. Fan, Largest eigenvalue of a unicyclic mixed graph, *App. Math. J. Chinese Univ. Ser. B* 19(2) (2004), 140–148.

[5] Y.-Z. Fan, On the least eigenvalue of a unicyclic mixed graph, *Linear and Multilinear Algebra* 53(2) (2005), 97–113.

[6] M. Fiedler, Algebraic connectivity of graphs, *Czechoslovak Math. J.* 23 (1973), 298–305.

[7] J. W. Grossman, D. M. Kulkarni and I. E. Schochetman, Algebraic graph theory without orientation, *Linear Algebra Appl.* 212/213 (1994), 289–307.

[8] Guo Jiming and Tan Shangwang, A relation between the matching number and the Laplacian spectrum of a graph. *Linear Algebra Appl.* 325 (2001), 71–74.

[9] R. A. Horn and C. R. Johnson, *Matrix Analysis*, Cambridge Univ. Press, Cambridge, 1985.

[10] Y.-P. Hou, J.-S. Li and Y.-L. Pan, On the Laplacian eigenvalues of signed graphs, *Linear and Multilinear Algebra* 51 (2003), 21–30.

[11] R. Merris, Laplacian matrices of graphs: a survey, *Linear Algebra Appl.* 197/198 (1998), 143–176.

[12] B. Mohar, Some applications of Laplacian eigenvalues of graphs, in: *Graph Symmetry* (G. Hahn and G. Sabidussi Eds.), Kluwer Academic Publishers, Dordrecht, 1997, pp. 225–275.

[13] X.-D. Zhang and J.-S. Li , The Laplacian spectrum of a mixed graph, *Linear Algebra Appl.* 353 (2002), 11–20.

[14] X.-D. Zhang and Rong Luo, The Laplacian eigenvalues of mixed graphs, *Linear Algebra Appl.* 362 (2003), 109–119.

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