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A Lower Bound for the First Zagreb Index and Its Application

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Abstract

For a graph G, the first Zagreb index is defined as the sum of the squares of the vertices degrees. By investigating the connection between the first Zagreb index and the first three coefficients of the Laplacian characteristic polynomial, we give a lower bound for the first Zagreb index, and we determine all corresponding extremal graphs. By doing so, we generalize some known results, and, as an application, we use these results to study the Laplacian spectral determination of graphs with small first Zagreb index.

1 Introduction

All graphs considered here are simple, undirected and finite. Let $G = G(V(G), E(G))$ be a graph with order $n = n(G) = |V(G)|$, size $m = m(G) = |E(G)|$ and $d_i = d_G(v_i)$ being the degree of vertex v_i of G $(1 \leq i \leq n)$. Let $M = M(G)$ be a *graph matrix* defined in a prescribed way. The *M-polynomial* of G is defined as $\det(\lambda I - M)$, where I is the identity matrix. The *M-spectrum* of G is a multiset consisting of the eigenvalues of $M(G)$. The largest eigenvalue of $M(G)$ is called the *M-spectral radius* of G. Usually the graph matrices considered are the adjacency matrix $A(G)$, the Laplacian matrix $L(G) = D(G) - A(G)$, the signless Laplacian matrix $Q(G) = D(G) + A(G)$, where $D(G) = \mathrm{diag}(d_1, d_2, \ldots, d_n)$. Graphs sharing the spectrum of a graph matrix M are called *M-cospectral graphs*. A graph G is said to be *determined by its M-spectrum* if the M-cospectral graphs to G are also isomorphic to G. For some basic results on graph spectra, we refer the reader to [8].

For other notation and graphs used throughout this paper, we refer the reader to see the appendix.

Among graph topological indices, one of the most studied is surely the *first Zagreb index* [25], here denoted by $M_1(G)$, that is defined as

$$M_1(G) = \sum_{i=1}^{n} d_i^2.$$

In more than forty years after its first appearance, a significant number of papers have appeared in various scientific journals, including those specialized in mathematics and/or chemistry. For some recent results, we refer the reader to see, for example, [1, 3, 7, 14, 15, 34]; for less recent results, those most relevant are surveyed in the papers [24, 35]. Regarding the bounds on the M_1-index, our impression is that the results about the lower bounds of general graphs are less numerous than to those about the upper bounds. Let us recall some known lower bounds for M_1-index for a graph G of order n and size m. By $\lfloor x \rfloor$ (resp., $\lceil x \rceil$), we denote the largest integer not greater (resp., not less) than x.

(A) Das [13] and Gutman [23]:

$$M_1(G) \geq 2m(2p+1) - pn(1+p),$$

with equality if and only if the difference of the degrees of any two vertices of graph G is at most one, where $p = \lfloor \frac{2m}{n} \rfloor$;

(B) Das [13]:

$$M_1(G) \geq d_1^2 + d_n^2 + \frac{(2m - d_1 - d_n)^2}{n-2},$$

with equality if and only if $d_2 = d_3 = \cdots = d_{n-1}$;

(C) Yoon and Kim [59]:

$$M_1(G) \geq \frac{4m^2}{n},$$

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

(D) Cheng et al. [6]: If G is bipartite of order $n \geq 2$ and size $0 \leq m \leq \lfloor \frac{n}{2} \rfloor \lceil \frac{n}{2} \rceil$, then the minimum possible value of $M_1(G)$ is

$$\begin{cases} (4m - n - nt)t + 2m & \text{if } n \text{ is even; or } nt + t \leq 2m \leq nt + n - t - 1; \\ (4m + 1 - nt)t, & \text{if } n \text{ is odd and } nt \leq 2m < nt + t; \\ (4m - n + 1 - nt)(t+1) & \text{if } n \text{ is odd and } nt + n - t + 1 \leq 2m < nt + n, \end{cases}$$

where $t = \lfloor \frac{2m}{n} \rfloor$.

Investigating the relations among the graph parameters is a well-studied research field due to many relevant applications. For example, Gutman and Das [24] have showed that the M_1-index is related to various quantities of interest in Chemical Graph Theory. Furthermore, they have pointed out some of its general mathematical properties, including the relations between the M_1-index and other invariants as the number of pairs of independent edges, the second Laplacian spectral moment, the coefficients of characteristic polynomial, the variance of vertex degrees, etc. It is worth to mention that in the literature [3, 19, 30, 31, 57, 58, 61] we find relations involving the M_1-index with the Wiener index, the hyper-Wiener index, the diameter, the connectivity, the number of pendent vertices, and the clique number.

In this paper, for a given graph, we consider the relation between the M_1-index and the first three coefficients of its L-polynomial. By doing so, we deduce a lower bound for M_1-index and we identify the corresponding extremal graphs. From the connections among these extremal graphs, we give a construction to characterize all the connected graphs with a given M_1-index. The readers will see that some known results can be deduced as special cases of the results presented here. Finally, we make use of such results to investigate the Laplacian spectral determination of graphs with small M_1-index.

The paper is organized as follows. In Section 2, we investigate the relation between the M_1-index and the first three coefficients of the Laplacian polynomial, and we determine a lower bound for the M_1-index with the corresponding extremal graphs. In Section 3, we make use of the M_1-index to study the Laplacian spectral determination problem of graphs. Finally, Section 4 is an appendix where the graphs considered through this paper are depicted.

2 Lower bounds for $M_1(G)$

Let the L-polynomial of a graph G be

$$\psi(G,\lambda) = \det(\lambda I - L(G)) = \sum_{i=0}^{n} q_i(G)\lambda^{n-i}.$$

Lemma 2.1. [36] *Let G be a graph with order n, size m and degree sequence $d = (d_1, d_2, \cdots, d_n)$. Then*

$$q_0(G) = 1 \quad q_1(G) = -2m \quad q_2(G) = 2m^2 - m - \frac{1}{2}\sum_{i=1}^{n} d_i^2.$$

The authors of [43] used these three coefficients in Lemma 2.1 to define the following invariant

$$I_1(G) = \begin{cases} 0 & \text{if } q_1(G) = 0; \\ -q_2(G) + \binom{-q_1(G)-1}{2} - q_0(G) & \text{if } q_1(G) \neq 0, \end{cases} \tag{1}$$

which is a quantity evidently determined by the L-spectrum. Here, our interest is the relation between $I_1(G)$ and the M_1-index. Clearly, if G has at least one edge, then by (1) and Lemma 2.1 we have $I_1(G) = \frac{1}{2}\sum_{i=1}^{n} d_i^2 - 2m(G)$. Note, $M_1(G) = \sum_{i=1}^{n} d_i^2$. Hence, $I_1(G)$ is the difference $\frac{1}{2}M_1(G) - 2m(G)$. From this point of view, $I_1(G)$ is the algebraic transformation of $M_1(G)$. In order to keep the notation consistent, we adopt $\mathcal{M}_1(G)$ instead of $I_1(G)$ and rewrite the above difference as

$$\mathcal{M}_1(G) = \frac{1}{2}M_1(G) - 2m(G). \tag{2}$$

Observe that if G has no edges (so G consists of isolated vertices), by (2) we have $\mathcal{M}_1(G) = 0$, and thus it is more convenient than (1). We next show that, in order to study of $M_1(G)$, investigating $\mathcal{M}_1(G)$ instead of $M_1(G)$ gives some advantages.

We now present a lower bound for $\mathcal{M}_1(G)$ and we identify the corresponding extremal graphs. Before that, we consider some algebraic properties of $\mathcal{M}_1(G)$. The first one is that $\mathcal{M}_1(G)$ is an integer, due to the well-known fact that the number of vertices of odd degree is even.

For a graph G and $e = uv \in E(G)$, the neighbor set and the degree of edge e are respectively defined as $N_G(e) = N_G(u) \cup N_G(v) - \{u, v\}$ and $d_G(e) = |N_G(e)| = d(u) + d(v) - 2$, where $N_G(u)$ is the neighbor set of vertex u.

Lemma 2.2. *Let G be a non-empty connected graph with size m and $e = uv \in E(G)$. Then*

$$\mathcal{M}_1(G) = \mathcal{M}_1(G - e) + d_G(e) - 1.$$

Proof. From (2) we have that

$$\begin{aligned} \mathcal{M}_1(G - e) &= \frac{1}{2}\Big(\sum_{w \in G\setminus\{u,v\}} d_G^2(w) + \big(d_G(u) - 1\big)^2 + \big(d_G(v) - 1\big)^2\Big) - 2(m - 1) \\ &= \frac{1}{2}\sum_{w \in G} d_G^2(w) - 2m - d_G(u) - d_G(v) + 3 \\ &= \mathcal{M}_1(G) - d_G(e) + 1. \end{aligned}$$

This completes the proof. ■

If G is connected graph with no edges, then $G = P_1$ and $\mathcal{M}_1(P_1) = 0$. If $G = P_2$ and $e \in E(G)$, then $\mathcal{M}_1(P_2) = -1 < \mathcal{M}_1(P_2 - e) = 0$. If $G \notin \{P_1, P_2\}$, then $d_G(e) \geq 1$ for any edge $e \in E(G)$. Hence, the following corollary immediately follows from (2) and Lemma 2.2.

Corollary 2.3. *Let G be a connected graph with $G \notin \{P_1, P_2\}$. Then*

(i) *if H is a subgraph of G, then $\mathcal{M}_1(G) \geq \mathcal{M}_1(H)$ with equality iff $H = G$.*

(ii) $M_1(G) = M_1(G - e) + d_G(e) + 2$.

Lemma 2.4. [46] *Let $(d_1, d_2, \cdots, d_n)$ be the degree sequence of a graph G of order n and size m, and $\overline{d}$ the average degree. Then $\sum_{i=1}^{n} d_i^2$ is minimal if and only if*

$$d_1 = \cdots = d_{t(G)} = \lfloor \overline{d} \rfloor + 1 \quad \text{and} \quad d_{t(G)+1} = \cdots = d_n = \lfloor \overline{d} \rfloor,$$

that is, G is an almost regular graph, where $t(G) = \sum_{i=1}^{n} d_i - n\lfloor \overline{d} \rfloor$. Further, G is a $\overline{d}$-regular graph for $t = 0$, and G is a $(\lfloor \overline{d} \rfloor, \lfloor \overline{d} + 1 \rfloor)$-almost regular graph for $t \neq 0$.

We now are in position to find some lower bounds of $\mathcal{M}_1(G)$ and to characterize the corresponding extremal graphs. The following lemma is a part of Theorem 2.2 in [42], but we provide a straightforward proof in this paper.

Let $\mathscr{G}_i = \{G \mid G \text{ is connected}, \mathcal{M}_1(G) = i, i \geq -1 \text{is an integer}\}$.

Lemma 2.5. *Let G be a connected graph with order n and size m. Then, under the notation reported in Section 4, we have:*

(i) *$\mathcal{M}_1(G) \geq -1$, the equality holds if and only if $G \in \mathscr{G}_{-1} = \{P_n \big| n \geq 2\}$;*

(ii) *$\mathcal{M}_1(G) = 0$ if and only if $G \in \mathscr{G}_0 = \{P_1, C_n \mid n \geq 3\} \cup \{T_{l_1,l_2,l_3} \mid n \geq 4\}$;*

(iii) *$\mathcal{M}_1(G) = 1$ if and only if $G \in \mathscr{G}_1 = \{L_{g,l} \mid n \geq 4\} \cup \{P^{a_1,a_2}_{z_1,z_2,l} \mid n \geq 6\}$;*

(iv) *$\mathcal{M}_1(G) = 2$ if and only if $G \in \mathscr{G}_2 = \{C^{a_1,a_2}_{z_1,z_2,g}, T_{l_1,l_2,l_3,l_4} \mid n \geq 5\} \cup \{M^{g}_{l_1,l_2,l_3} \mid n \geq 6\} \cup \{P^{a_1,a_2,a_3}_{z_1,z_2,z_3,l} \mid n \geq 8\}$;*

Proof. If $G \in \{P_1, P_2\}$, then $\mathcal{M}_1(P_1) = 0$ and $\mathcal{M}_1(P_2) = -1$. Now suppose that G is a connected graph with at least two edges. A straightforward calculation shows $\mathcal{M}(P_n) = -1$ by (2). From Lemma 2.4 we get that $\sum_{i=1}^{n} d_i^2$ reaches the minimum if and only if $|d_i - d_j| \leq 1$ for $1 \leq i, j \leq n$. In other words,

$$\max\{\mathcal{M}_1(T) \mid T \text{ is a tree of order } n\} \geq \mathcal{M}_1(P_n) = -1. \tag{3}$$

Since G is connected, G contains a spanning tree T. By Corollary 2.3(i) and (3) we have

$$\mathcal{M}_1(G) \geq \mathcal{M}_1(T) \geq \mathcal{M}_1(P_n) = -1,$$

and so the lower bound of $\mathcal{M}_1(G)$ follows.

Let $m = n + \delta$. For connected graphs $\delta \geq -1$, note that $\delta + 1$ is the cyclomatic number. By (2) we obtain

$$\sum_{i=1}^{n} d_i^2 = 4m + 2\mathcal{M}_1(G).$$

Substituting $2m = \sum_{i=1}^{n} d_i$ into the above equality we arrive at

$$\sum_{i=1}^{n} d_i(d_i - 2) = 2\mathcal{M}_1(G). \tag{4}$$

In view of $\sum_{i=1}^{n} d_i = 2n + 2\delta$, thus

$$\sum_{i=1}^{n} (d_i - 2) = 2\delta. \tag{5}$$

From (4) and (5) it follows that

$$\sum_{i=1}^{n} (d_i - 1)(d_i - 2) = 2\mathcal{M}_1(G) - 2\delta. \tag{6}$$

Note that the vertices of degree 1, degree 2, degree 3 and degree 4 in G contribute, respectively, 0, 0, 2 and 6 to $\sum_{i=1}^{n}(d_i - 1)(d_i - 2)$. Furthermore, $\sum_{i=1}^{n}(d_i - 1)(d_i - 2) \geq 0$. By the values of δ we distinguish the following cases.

Case 1. $\delta = -1$. Thus, G is a tree. Recall that $\mathcal{M}_1(G) \geq -1$ is an integer.

Subcase 1.1. $\mathcal{M}_1(G) = -1$. By (6) we get $\sum_{i=1}^{n}(d_i - 1)(d_i - 2) = 0$ implying $G \cong P_n$.

Subcase 1.2. $\mathcal{M}_1(G) = 0$. By (6) we have $\sum_{i=1}^{n}(d_i - 1)(d_i - 2) = 2$. So, G has exactly one vertex of degree 3 and $n - 1$ vertices of degree 1 or 2. Hence, $G \cong T_{l_1,l_2,l_3}$.

Subcase 1.3. $\mathcal{M}_1(G) = 1$. By (6) we get $\sum_{i=1}^{n}(d_i - 1)(d_i - 2) = 4$, which implies that G only has two vertices of degree 3 and $n-2$ vertices of degree 1 or 2. Therefore, $G \cong P_{z_1,z_2,l}^{a_1,a_2}$.

Subcase 1.4. $\mathcal{M}_1(G) = 2$. Thus, $\sum_{i=1}^{n}(d_i - 1)(d_i - 2) = 6$. The latter implies that G has either one vertex of degree 4 and the others are degree of 1 or 2, or G has exactly three vertices of degree 3 and $n - 3$ vertices of 1 or 2. Consequently, $G \cong T_{l_1,l_2,l_3,l_4}$ or $G \cong P_{z_1,z_2,z_3,l}^{a_1,a_2,a_3}$.

Case 2. $\delta = 0$. In this case, G is a unicyclic graph.

Subcase 2.1. $\mathcal{M}_1(G) = -1$. Then, $\sum_{i=1}^{n}(d_i - 1)(d_i - 2) = -2$, a contradiction. That is to say, there exists no graph such that $\delta = 0$ and $\mathcal{M}_1(G) = 1$. In Table 1, we use the word "none" to express such a case.

Subcase 2.2. $\mathcal{M}_1(G) = 0$. Thus, $\sum_{i=1}^{n}(d_i - 1)(d_i - 2) = 0$ showing $G \cong C_n$.

Subcase 2.3. $\mathcal{M}_1(G) = 1$. So, $\sum_{i=1}^{n}(d_i - 1)(d_i - 2) = 2$, hence G has one vertex of degree 3 and $n - 1$ vertices of degree 1 or 2. Therefore, $G \cong L_{g,l}$.

Subcase 2.4. $\mathcal{M}_1(G) = 2$. Thereby, $\sum_{i=1}^{n}(d_i - 1)(d_i - 2) = 4$. This implies that G has exactly two vertices of degree 3 and $n-2$ vertices of degree of 1 or 2. If the two vertices of degree 3 lie in the cycle of G, then $G \cong C_{z_1,z_2,g}^{a_1,a_2}$. Otherwise, $G \cong M_{l_1,l_2,l_3}^{g}$.

Case 3. $\delta = 1$. In this case, G is a bicyclic graph.

Subcase 3.1. $\mathcal{M}_1(G) = -1$. Then, $\sum_{i=1}^{n}(d_i - 1)(d_i - 2) = -4$, a contradiction.

Subcase 3.2. $\mathcal{M}_1(G) = 0$. Then, $\sum_{i=1}^{n}(d_i - 1)(d_i - 2) = -2$, a contradiction.

Subcase 3.3. $\mathcal{M}_1(G) = 1$. Thus, $\sum_{i=1}^{n}(d_i - 1)(d_i - 2) = 0$, so that the maximum degree of G is 2, which is impossible.

Subcase 3.4. $\mathcal{M}_1(G) = 2$. Thus, $\sum_{i=1}^{n}(d_i - 1)(d_i - 2) = 2$. Therefore, G contains exactly one vertex of degree 3 and $n-1$ vertices of degree 1 or 2 which is again impossible, since connected bicyclic graphs either have at least two vertices of degree 3, or they have a vertex of degree 4.

Additionally, if there are no graphs with $\mathcal{M}_1(G) = k$ and $m = n + \delta$, then, in view of Corollary 2.3(i), the same applies for graphs with $\mathcal{M}_1(G) = k$ and $m = n+\delta+1$. Namely, if a slot in Table 1 is filled with "none" , then all the right blank slots in the same row must be written as "none", as well.

This completes the proof. ■

$\mathcal{M}_1(G)$ \ δ	-1	0	1	≥ 2
-1	$P_n (n \geq 2)$	none		
0	P_1, T_{l_1,l_2,l_3}	C_n	none	
1	$P_{z_1,z_2,l}^{a_1,a_2}$	$L_{g,l}$	none	
2	$T_{l_1,l_2,l_3,l_4}, P_{z_1,z_2,z_3,l}^{a_1,a_2,a_3}$	$C_{z_1,z_2,g}^{a_1,a_2}$, M_{l_1,l_2,l_3}^{g}	none	

Table 1: Graphs with $-1 \leq \mathcal{M}_1(G) \leq 2$.

From the above results, we deduce the following theorem which gives the lowest bounds for the M_1-index together with the corresponding extremal graphs.

Theorem 2.6. *Let G be a connected graph with order n and size m. Then, under the notation reported in Lemma 2.5, we have:*

(i) *$M_1(G) \geq 4m - 2$, the equality holds iff $G \in \mathscr{G}_{-1}$;*

(ii) *if $G \notin \mathscr{G}_{-1}$, then $M_1(G) \geq 4m$ with equality iff $G \in \mathscr{G}_0$;*

(iii) *if $G \notin \mathscr{G}_{-1} \cup \mathscr{G}_0$, then $M_1(G) \geq 4m + 2$ with equality iff $G \in \mathscr{G}_1$;*

(iv) *if $G \notin \mathscr{G}_{-1} \cup \mathscr{G}_0 \cup \mathscr{G}_1$, then $M_1(G) \geq 4m + 4$ with equality iff $G \in \mathscr{G}_2$.*

Proof. In view of (2) we have the following expression of $M_1(G)$:

$$M_1(G) = 4m(G) + 2\mathcal{M}_1(G). \tag{7}$$

From Lemma 2.5(i) it follows that $M_1(G) \geq 4m(G) - 2$ with equality iff $G \in \mathscr{G}_{-1}$, and thus (i) follows.

For (ii), since $G \notin \mathscr{G}_{-1}$, by Lemma 2.5(i) and (ii) we obtain $\mathcal{M}_1(G) \geq 0$, and therefore $M_1(G) \geq 4m$ with equality iff $G \in \mathscr{G}_0$.

For (iii), due to $G \notin \mathscr{G}_{-1} \cup \mathscr{G}_0$, by Lemma 2.5(i)–(iii) we have $\mathcal{M}_1(G) \geq 1$, and consequently $M_1(G) \geq 4m + 2$ with equality iff $G \in \mathscr{G}_1$.

Finally, (iv) similarly holds. This completes the proof. ■

Remark 2.7. *The above theorem contains information about $M_1(G)$ that includes or extends some known results.*

(i) *Gutman and Das in [24] showed that among n-vertex tree, the path P_n minimizes the M_1-index; Li et al. in [32] extended this result to all graphs. Actually, their results are a special cases of Theorem 2.6, since it characterizes the graphs (or trees) with the first four smallest M_1-indices.*

(ii) *Deng in [16] determined the unicylic graph with the smallest M_1-index; Xia and Chen in [56] identified the unicyclic graphs with the first two smallest M_1-indices. As a matter of fact, Theorem 2.6(ii)-(iv) identifies the unicyclic graphs with the first three smallest M_1-indices but it is extended to all graphs.*

The method used to prove Lemma 2.5 is quite effective when $\mathcal{M}_1(G)$ is a small number. Inspired by the essential relationships among the graphs in families $\mathscr{G}_{-1} - \mathscr{G}_2$, we will offer a construction to find all the connected graphs with larger $\mathcal{M}_1(G)$, which will certainly provide a more general lower bound for the M_1-index. In the sequel, we proceed to further investigate the algebraic properties of $\mathcal{M}_1(G)$.

Lemma 2.8. *Let G be a graph with k connected components $G_1, G_2, \cdots, G_k$. Then*

$$\mathcal{M}_1(G) = \sum_{i=1}^{k} \mathcal{M}_1(G_i).$$

Proof. Let G and G_i have sizes m and m_i $(1 \leq i \leq k)$ respectively. So, $m = \sum_{i=1}^{k} m_i$.

From (2) it follows that

$$\begin{aligned}\sum_{i=1}^{k}\mathcal{M}_1(G_i) &= \sum_{i=1}^{k}\Big(\frac{1}{2}\sum_{v\in V(G_i)} d_{G_i}^2(v) - 2m_i\Big)\\ &= \frac{1}{2}\sum_{i=1}^{k}\sum_{v\in V(G_i)} d_{G_i}^2(v) - 2\sum_{i=1}^{k} m_i\\ &= \frac{1}{2}\sum_{v\in V(G)} d_G^2(v) - 2m\\ &= \mathcal{M}_1(G).\end{aligned}$$

This completes the proof. ■

Let $[G]_E$ be the edge-induced subgraph of a graph G, where $E = E(G)$. Note that if G is a connected graph having at least one edge, then there exists an edge $e \in E(G)$ such that $[G-e]_E$ is also connected. It can be realized by taking the edge e which is one of pendent edges of some spanning tree of G.

Lemma 2.9. *Let G be a graph. Then $\mathcal{M}_1(G) = \mathcal{M}_1([G]_E)$.*

Proof. It is easy to see that $[G]_E$ is the graph obtained from G by deleting the isolated vertices (if any). Without loss of generality, suppose G has k isolated vertices. So, $G = [G]_E \cup kP_1$. By Lemma 2.8 and Theorem 2.5(ii) we get $\mathcal{M}_1(G) = \mathcal{M}_1([G]_E) + \mathcal{M}_1(kP_1) = \mathcal{M}_1([G]_E)$. ■

Lemma 2.10. *Let $G \in \mathscr{G}_k$, $e \in E(G)$ and $[G-e]_E$ be connected. Then*

(i) $d_G(e) \leq k+2$.

(ii) *If $d_G(e) = j$, then $[G-e]_E \in \mathscr{G}_{k-j+1}$.*

Proof. Assume that $d_G(e) > k+2$. By Lemma 2.2 we get

$$\mathcal{M}_1(G-e) = \mathcal{M}_1(G) - d_G(e) + 1 < k - k - 2 + 1 = -1,$$

a contradiction by Lemma 2.5(i).

For (ii), from Lemma 2.9 we obtain

$$\mathcal{M}_1([G-e]_E) = \mathcal{M}_1(G-e) = \mathcal{M}_1(G) - d_G(e) + 1 = k - j + 1,$$

and so $[G-e]_E \in \mathscr{G}_{k-j+1}$ by the condition that $[G-e]_E$ is connected. ■

Set $\mathscr{G}_k^0 = \{G \in \mathscr{G}_k \mid$ there exists no edge $e \in E(G)$ such that $d_G(e) = 1\}$. Evidently, any graph belonging to $\mathscr{G}_k$ can be obtained from the graph in $\mathscr{G}_k^0$ by adding edge e of degree 1. Let $G \in \mathscr{G}_k^0$, $e \in E(G)$ and $[G - e]_E$ be connected. By the definition of $\mathscr{G}_k^0$ we know $d_G(e) = j \geq 2$. From Lemma 2.10(ii) it follows that $[G - e]_E \in \mathscr{G}_{k-j+1}^0 = \mathscr{G}_t^0$, where $t \leq k - 1$ (by $t = k - j + 1$ we get $j = k + 1 - t \geq 2$ and so $t \leq k - 1$).

On the basis of the above discussion, we obtain the following facts.

Fact. Under the above notation, we have:

(i) Set $G \in \mathscr{G}_t$ $(t < k)$. If $e \notin E(G)$ and $d_{G+e}(e) = k - t + 1$, then $G + e \in \mathscr{G}_k$.

(ii) For any graph $G \in \mathscr{G}_k^0$, there exists $t < k$, $G' \in \mathscr{G}_t$ and $e \notin E(G')$ such that $G = G' + e$ (here, $d_G(e) = k - t + 1$).

Now we give the following construction which can characterize all the connected graphs in $\mathscr{G}_k$.

Construction: Suppose that $\mathscr{G}_{-1}, \mathscr{G}_0, \cdots, \mathscr{G}_{k-1}$ have been defined. For each graph $G \in \mathscr{G}_t$ $(-1 \leq t \leq k - 1)$, we search for all the possible edges e such that $e \notin E(G)$ and $d_{G+e}(e) = k - t + 1$ to construct the graph $G + e$ (add some vertices where necessary). Collect these new graphs $G + e$ in $\mathscr{G}_k'$. By adding all the possible edges of degree 1 to the graphs in $\mathscr{G}_k'$, we obtain all the graphs belonging to $\mathscr{G}_k$.

Proof. Note that $\mathscr{G}_k^0 \subseteq \mathscr{G}_k' \subseteq \mathscr{G}_k$. Then Facts (i) and (ii) guarantee that the construction of $\mathscr{G}_k$ is valid. ■

As an example to the above described construction, we characterize all the connected graphs with $\mathcal{M}_1(G) = 3$; in fact, $\mathcal{M}_1(G) = 3$ if and only if

$$G \in \mathscr{G}_3 = \{P_{z_1,z_2,z_3,z_4,l}^{a_1,a_2,a_3,a_4}, C_{z_1,z_2,z_3,g}^{a_1,a_2,a_3}, F_n, D_{l,g_1,g_2}, J_{g,l_1,l_2}, \theta_{i,j,k}, F_{l_1,l_2,l_3}^{g,l}, S_{h_1,h_2,h_3}^{l,l_1,l_2}, K_{l,z_1,z_2}^{g,a_1,a_2}\},$$

where the graphs are shown in Subsection 4.2. At the same time, we give the following result as an extra case of Theorem 2.6.

Theorem 2.6. (v) if $G \notin \mathscr{G}_{-1} \cup \mathscr{G}_0 \cup \mathscr{G}_1 \cup \mathscr{G}_2$, then $M_1(G) \geq 4m + 6$ with equality if and only if $G \in \mathscr{G}_3$.

Remark 2.11. *Deng [16] determined the bicyclic graphs with smallest M_1-index, which are the graphs D_{l,g_1,g_2} and $\theta_{i,j,k}$ (see Subsection 4.2). It is, however, a special case of Theorem 2.6(v). Furthermore, for a fixed number k, by Construction we can get all k-cyclic graphs with smallest M_1-index.*

By (7), Theorem 2.6 and Construction, a basic property of the M_1-index is summarized below.

Theorem 2.12. *For a fixed connected graph G with order n and size m, its M_1-index is equal to an even number $4m+2k$; Moreover, all the connected graphs with the same M_1-index as G belong to the family $\mathscr{G}_k$, where $k \geq -1$ and $\mathscr{G}_k$ is defined in Construction.*

The following theorem generalizes Theorem 2.6.

Theorem 2.13. *Let G be a connected graph with order n and size m. Then*

(i) *$M_1(G) \geq 4m-2$ with equality if and only if $G \in \mathscr{G}_{-1}$.*

(ii) *if $G \notin \mathscr{G}_{-1} \cup \mathscr{G}_0 \cup \cdots \cup \mathscr{G}_{k-1}$ $(k \geq 0)$, then*

$$M_1(G) \geq 4m+2k$$

with equality if and only if $G \in \mathscr{G}_k$.

Proof. We only need to show (ii). Since $G \notin \mathscr{G}_{-1} \cup \mathscr{G}_0 \cup \cdots \cup \mathscr{G}_{k-1}$, then G belongs to some $\mathscr{G}_x$ with $\mathcal{M}_1(G) = x \geq k$. Hence, by (7) we get $M_1(G) = 4m+2x \geq 4m+2k$. Obviously, the equality holds if and only $\mathcal{M}_1(G) = k$ if and only if $G \in \mathscr{G}_k$, and Construction makes $\mathscr{G}_k$ valid. ■

It is worth to observe that the minimum value of e in each item of Theorems 2.6 and 2.13 should make the graphs meaningful (take the cycle C_e as an example, e is at least 3). Otherwise, the graphs may not exist, for example, there is no a cycle with less than three edges. More precisely, let $e(G,k) = \min\{e(G) | G \in \mathscr{G}_k\}$ with $k \geq -1$, then this minimum value is just $e(G,k)$. By the graphs shown in Subsection 3.2, it is easy to obtain $e(G,-1) = 1$, $e(G,0) = 3$, $e(G,1) = 4$, $e(G,2) = 4$ and $e(G,3) = 5$.

Recall, $M_1(G) = 4e(G) + 2k$ is an even number. All such numbers consist of $S_1 = \{4e-2 \mid e \text{ is an integer}\}$ and $S_2 = \{4e \mid e \text{ is an integer}\}$. Obviously, 4 and 8 belong to S_2 and the corresponding e's are $e=1$ and $e=2$, respectively. By Theorem 2.6(ii) we know that the number of edges of graphs with $M_1(G) = 3$ is at least 3 (i.e., $e(G,0)$=3). Therefore, there is no graph with $M_1(G) = 4$ or 8. On the other hand, with the exception of 4 and 8, we can always use Construction to find all graphs with $M_1(G)$ being any even number. In fact, let $\alpha \neq 4$ or 8 be an even number. Clearly, it can be decomposed into $\alpha = 4e+2k$. In order to find all the connected graphs with $M_1(G) = \alpha = 4e+2k$, we need to solve the valid solutions (e,k) of the following equations with the below given conditions:

$$\begin{aligned}
&\alpha = 4e+2k,\\
&e \geq 0\text{: the number of edges of } G,\\
&k \geq -1\text{: } \mathcal{M}(G) = k \text{ is an integer.}
\end{aligned}$$

By the theory of indeterminate equations, the above equation always has integral solutions. After picking up all valid solutions (e, k), for each k we employ Construction to obtain the family $\mathscr{G}_k$, and therefore all graphs are obtained.

As a consequence of the above discussion, we get the following theorem.

Theorem 2.14. *For any given even number $\alpha \neq 4$ or 8, all the connected graphs with $M_1(G) = \alpha$ can be determined.*

Remark 2.15. *The above theorem generalizes a result due to Li et al, which said that "for any given even number $m_1 \neq 4$ or 8, there exists a tree T such that $M_1(T) = m_1$" (see [32], Theorem 5.3).*

In the end of this section, we use the example of $\alpha = 20$ to illustrate the application of Theorem 2.14. Solving the indeterminate equation $4e + 2k = 20$, we get $e = 5 + t$ and $k = -2t$, where t is an integer. Note that $e \geq 0$ and $k \geq -1$. Hence, $-5 \leq t \leq 0$, and thus the integer solutions

$$(e, k) \in \{(5, 0), (4, 2), (3, 4), (2, 6), (1, 8), (0, 10)\}.$$

For $e = 0, 1, 2$, the corresponding graphs are the paths P_1, P_2 and P_3 with $\mathcal{M}(P_1) = 0$ and $\mathcal{M}(P_2) = \mathcal{M}(P_3) = -1$ by Theorem 2.5(i) and (ii). Thereby, the solutions (2,6),(1,8) and (0,10) are invalid. For $e = 3$, the corresponding graphs are the path P_4, the cycle C_3 and the T-shape tree $T_{1,1,1}$; while $\mathcal{M}(P_4) = -1$ and $\mathcal{M}(C_3) = \mathcal{M}(T_{1,1,1}) = 0$. Thus, $(3, 4)$ is also invalid. Then the valid solutions are

$$(e, k) \in \{(5, 0), (4, 2)\}.$$

For $(e, k) = (5, 0)$ we get $G \in \mathscr{G}_0$ with $e(G) = 5$, and consequently G is the cycle C_5 and the T-shape trees $T_{1,1,3}$ and $T_{1,2,2}$ by Lemma 2.5(ii). For $(e, k) = (4, 2)$, we get $G \in \mathscr{G}_2$ with $e(G) = 4$, and thus G is star $T_{1,1,1,1}$ by Lemma 2.5(vi). Finally, all the connected graphs with $M_1(G) = 20$ are collected into the following set

$$\{C_5, T_{1,1,3}, T_{1,2,2}, T_{1,1,1,1}\}.$$

3 The spectral characterization of extremal graphs

The spectral characterization (or, determination) problem of graphs consists in the detection of all cospectral graphs to a given graph with respect to some graph matrix. The latter problem was considered in 1956 by Günthard and Primas [21] in the context of

Hückel's theory. Under the motivation of [11], many researchers have devoted their attention to study the spectral determination of families of graphs. For more details on this topic and basic results, we refer the reader to [11, 12]. In general, we can consider two categories of graphs so far studied. The first category is about those graphs with rather good algebraic properties, such as the distance regular graphs [2, 10], the strongly regular graphs [11], the graphs with A-least eigenvalue at least -2 [11, 50], and so on. The second one consists of graphs with simple structures. For the latter, several covered families of graphs include some extremal graphs described in Subsection 4.2.

In particular, for the graphs with $-1 \leq \mathcal{M}_1(G) \leq 1$, the above question was trivial for the *path* P_n, the *cycle* C_n and the *isolated vertices* nK_1 (but not for their disjoint unions, cf. [9, 52]), while it was not trivial for the T*-shape tree* T_{l_1,l_2,l_3} [37, 53]. Also *lollipop graphs* $L_{g,l}$ were considered in [26, 28, 60]. Thus, it remains only the so-called H*-shape tree* $P^{a_1,a_2}_{z_1,z_2,l}$. For $\mathcal{M}_1(G) = 2, 3$, the jellyfish graph $J^g_{l_1,l_2}$[33], the starlike tree T_{l_1,l_2,l_3,l_4} [38], the *dumbbell graph* D_{l,g_1,g_2} [46, 48] and the θ*-graph* $\theta_{i,j,k}$ [39, 47] were discussed. For the larger $\mathcal{M}_1(G)$, only the line graphs of lollipop graphs [51] and the ∞-graphs [49] appear to be studied. In fact, even for the graphs with simple structures, it is pretty complicated to study their spectral characterization, and the reasons is that there are not many effective methods. Nevertheless, Theorem 2.6 is helpful for this topic with respect to the L-spectrum, since many graph structures can be discarded at once.

As an example to the above discussion, we now study the spectral determination problem for a subfamily of the H-shape trees. In fact, we consider the H-shape trees without internal vertices of degree 2 and we prove that they are determined by the spectrum of their Laplacian matrix. Let $H(a, b, c, d)$ be such a tree (cf. Fig. 1) and without loss of generality we may assume that $1 \leq a \leq b$, $c \leq d$ and $a \leq c$.

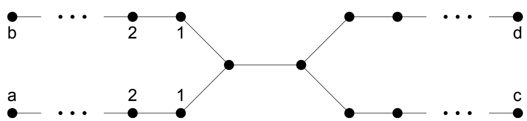


Figure 1: The graph $H(a, b, c, d)$.

Note, if G and H are L-cospectral graphs, then they have the same order, size, M_1-index, and number of components [11, 44]. Thus, by (2) we obtain

$$\mathcal{M}_1(G) = \mathcal{M}_1(H),$$

that is $\mathcal{M}_1(G)$ is determined by L-spectrum. In our case, the connected graphs G with $\mathcal{M}_1(G) = 1$ are the H-shape trees and the lollipop graphs. Since the lollipop graphs are known to be determined by their spectra, then the Laplacian cospectral mate of $H(a, b, c, d)$ must be another (possibly nonisomorphic) H-shape tree. We first show that a cospectral mate of $H(a, b, c, d)$ can be only another $H(a', b', c', d')$. In order to do prove this, we need the three following lemmas.

Lemma 3.1. *Let G be a graph and $\mu_1(G) \geq \mu_2(G) \geq \cdots \geq \mu_n(G) \geq 0$ be its Laplacian eigenvalues. For any edge $e \in G$ we have*

$$\mu_1(G) \geq \mu_1(G-e) \geq \mu_2(G) \geq \mu_2(G-e) \geq \cdots \geq \mu_n(G) \geq \mu_n(G-e).$$

Hoffman and Smith [29] defined an *internal path* as a walk $v_0, v_1, \ldots, v_k$, with $(k \geq 1)$, where the vertices $v_1, \ldots, v_k$ are distinct (v_0, v_k need not be distinct), $d(v_0) > 2$, $d(v_k) > 2$ and $d(v_i) = 2$ whenever $0 < i < k$, with $d(v)$ as the degree of vertex v in G. The lemma below is a (reduced) Laplacian variant of a well-known result for internal paths (see Theorem 2.1 in [45]).

Lemma 3.2. *Let T be a tree, T_{uv} be obtained from T by subdividing its edge uv, and $\mu(G)$ be the Laplacian spectral radius of G. Hence, we have that*

(i) *if uv is not in an internal path of T, then $\mu(T_{uv}) > \mu(T)$;*

(ii) *if uv belongs to an internal path of T, then $\mu(T_{uv}) < \mu(T)$.*

Let $H_k(a, b, c, d)$ be obtained from $H(a, b, c, d)$ by inserting k vertices of degree 2 between the two vertices of degree 3.

Lemma 3.3. *Let $\mu(G)$ be the Laplacian spectral radius of a graph G. Then,*

i) $\mu(H_1(a, b, c, d)) < 4.66$, $\mu(H_1(1, t, 1, t)) < 4.56$ *and* $\mu(H_1(1, 1, t, t)) < 4.58$.

ii) $\mu(H_k(a, b, c, d)) < 4.59$, *for* $k \geq 2$.

Proof. Let $H = H_k(a, b, c, d)$ be a H-shape tree. Assume first that $k \geq 2$ and let $t = \max\{a, b, c, d\}$. In view of Lemma 3.2 we have that $\mu(H) \leq \mu(H_2(t, t, t, t)) = \mu$. So we now compute the limit for the spectral radius when t tends to infinity. Since trees are bipartite graphs, we can consider, instead of the Laplacian matrix, the the signless Laplacian matrix $Q = D + A$ and the corresponding Perron eigenvector $\mathbf{x} = (x_1, x_2, \ldots, x_n)$. The eigenvalue equation now reads

$$(\mu - d(v))x_v = \sum_{u \sim v} x_u.$$

By symmetry, for the graph $H_2(t, t, t, t)$ we have that the vertices at the same distance from the center of the tree do get the same Perron component. Let us naturally label the vertices of the paths such that the vertex of degree 3 correspond to v_0. So the eigenvalue equation (in each pendant path) is $(\mu-2)x_i = x_{i+1} + x_{i-1}$ $(1 \le i \le t-1)$. By solving the latter recurrence equations and by letting t tending to infinity, we obtain that $x_1 = \frac{1}{2}(\mu - 2 - \sqrt{\mu^2 - 4\mu})x_0$. By computing the eigenvalue equations at the vertices of degree 3, at the central vertices of degree 2, and by combining the equations, we arrive at the following polynomial whose largest root is an upper bound for μ:

$$\mu^4 - 10\mu^3 + 32\mu^2 - 32\mu - 4 = 0,$$

and the largest root is approximately $\mu \cong 4.58155$. For the other bounds, similar routine works, for example, the upper bound for $\mu(H_1(t,t,t,t))$ comes from the polynomial $\mu^3 - 8\mu^2 + 19\mu - 16 = 0$. The details are left to the reader. This completes the proof. ■

Lemma 3.4. *Let* $H = H_k(a', b', c', d')$ *be Laplacian cospectral with* $H(a,b,c,d)$. *Then* $k = 0$.

Proof. Let $\mu(G)$ be the Laplacian spectral radius of G. First assume that $k \ge 2$, then by Lemmas 3.1 and 3.3 we have $\mu(H_k(a', b', c', d')) < 4.59 < 4.62 < \mu(H(1,1,1,2))$, and the two graphs cannot be cospectral. So assume in the remainder that $k = 1$. Similarly, we have that

$$\mu(H_1(a', b', c', d')) < 4.66 < 4.68 < \min\{\mu(H(1,2,1,2)), \mu(H(1,1,2,2))\},$$

so $k = 0$ if two pendant paths in $H(a,b,c,d)$ have length at least 2. It remains to consider $H_1(a', b', c', d')$ and $H(1,1,1,t)$. Since $\mu(H(1,1,1,2)) > 4.62$, in view of Lemma 3.3, we have that both $H_1(1,b,1,d)$ and $H_1(1,1,c,d)$ have spectral radius too small and must be discarded. So $H_1(a', b', c', d')$ contains the graph $H_1(1,2,2,2)$. But $\mu_2(H_1(1,2,2,2)) > 4$ and by interlacing the same applies to $H_1(a', b', c', d')$, while $\mu_2(H(1,1,1,t)) < 4$, again by interlacing $4 > \mu_1(P_{t+2}) \ge \mu_2(H(1,1,1,t))$. So also $k = 1$ is not allowed. This completes the proof. ■

Now we just need to compare the polynomial of any two $H(a,b,c,d)$'s and check whether they can be the same. This will be done by decomposing the L-polynomial and by using a transformation on the variable which facilitates this comparison.

The formulas in the lemma below have a natural use in the context of the adjacency matrix. However, they can be used for the Laplacian or signless Laplacian of graphs by mapping the Laplacian matrix of a signed graph as the adjacency matrix of a weighted multigraph. Note that the degrees in the main diagonal are interpreted as weighted loops.

Lemma 3.5 ([4]). *Let $A = (a_{ij})$ be the adjacency matrix of a weighted graph G and $\phi(G, x) = \phi(G)$ be the characteristic polynomial of A. Then we have*

$$\begin{aligned}\phi(G) &= (x - a_{vv})\phi(G - v) - \sum_{u\sim v} a_{uv}^2 \phi(G - u - v) - 2\sum_{C\in\mathcal{C}_v} \omega(C)\phi(G \setminus V(C)),\\ \phi(G) &= \phi(G - uv) - a_{uv}^2\phi(G - u - v) - 2\sum_{C\in\mathcal{C}_{uv}} \omega(C)\phi(G \setminus V(C)),\end{aligned}$$

where $\mathcal{C}_a$ is the set of cycles passing through a and $\omega(C) = \prod_{uw\in C} a_{uw}$.

Let B_n be the matrix of order n obtained from $L(P_{n+1})$ by deleting the row and column corresponding to some end-vertex of P_{n+1}. The first of the following items is given by Guo in [22], the second is proved in [42].

Lemma 3.6. *Let P_n be the path of order n and H_n, B_n defined as above. Then*

(i) $x\,\psi(B_n) = \psi(P_{n+1}) + \psi(P_n)$,

(ii) $\psi(P_n) = (x - 2)\psi(P_{n-1}) - \psi(P_{n-2})$.

Now we are able to prove the main result of this section.

Theorem 3.7. *The tree $H(a, b, c, d)$ is determined by its L-spectrum.*

Proof. By Lemma 3.5 stepwise applied to the degree 3 vertices of $H = H(a, b, c, d)$, we obtain

$$\begin{aligned}\psi(H) &= [(x - 3)\psi(B_a)\psi(B_b) - \psi(B_{a-1})\psi(B_b) - \psi(B_a)\psi(B_{b-1})][(x - 3)\psi(B_c)\psi(B_d)\\ &\quad -\psi(B_{c-1})\psi(B_d) - \psi(B_c)\psi(B_{d-1})] - \psi(B_a)\psi(B_b)\psi(B_c)\psi(B_d).\end{aligned}$$

Consider Lemma 3.6 (ii), the formula $\psi(P_n) = (x - 2)\psi(P_{n-1}) - \psi(P_{n-2})$ can be seen as a second order recurrence equation $p_n = (x - 2)p_{n-1} - p_{n-2}$, with $p_0 = 0$ and $p_1 = x$ as boundary conditions. It is a matter of computation (cf. [42] for the details) to check that the solution is

$$p_n = \frac{(y^{2n} - 1)(y + 1)}{y^n(y - 1)},$$

where y is the solution of the characteristic equation $y^2 - (x - 2)y + 1 = 0$. In view of Lemma 3.6 (i) and by the latter transformation, we get

$$\psi(B_n) = \frac{y^{2n+1} - 1}{y^n(y - 1)}.$$

Let $\Phi(H) = \dfrac{y^{2n}(y+1)}{(y-1)^3}\,\psi(H) - (y^{2n+2} - 2y^{2n+1} - y^{2n} + y^2 + 2y - 1)$, we have

$$\begin{aligned}\Phi(H) \;=\; & +y^{2a+2b+2c+4} + y^{2a+2b+2d+4} + y^{2a+2c+2d+4} + y^{2b+2c+2d+4} \\ & -y^{2a+2b+4} + y^{2a+2b+2} - y^{2c+2d+4} + y^{2c+2d+2} - y^{2a+2} \\ & -y^{2b+2} - y^{2c+2} - y^{2d+2}.\end{aligned}$$

It is routine to check that two cospectral $H(a,b,c,d)$'s must be isomorphic as well. This completes the proof. ■

To conclude, let us mention that in order to spectrally characterize all graphs in $\mathscr{G}_1$, then it remains to consider all the H-shape trees, denoted in Section 4 by $P^{a_1,a_2}_{z_1,z_2,l}$. This problem might be solved using the tools shown so far, but we will not attempt to do it within this paper. So we pose the following conjecture.

Conjecture 1. *No two non-isomorphic H-shape trees are L-cospectral.*

4 Appendix

4.1 Notations

(i) Let P_n, C_n, K_n and $K_{1,n-1}$ denote the *path*, the *cycle*, the *complete graph* and the *star* of order n respectively.

(ii) $L_{g,l}$ denotes the *lollipop graph* obtained from C_g and P_l by identifying a vertex of C_g with an end-vertex of P_l, where $g \geq 3$, $l \geq 2$ and $n = g + l - 1$.

(iii) $T_{l_1,l_2,\ldots,l_k}$ stands for the *starlike tree* with a vertex u of degree k satisfying $T_{l_1,l_2,\ldots,l_k} - u = P_{l_1} \cup P_{l_2} \cup \ldots \cup P_{l_k}$, where $l_k \geq \ldots l_2 \geq l_1 \geq 1$ and $n = \sum_{i=1}^{k} l_i + 1$. T_{l_1,l_2,l_3} is also named as T-shape tree.

(iv) The *centipede graph* $P^{a_1,a_2,\ldots,a_t}_{z_1,z_2,\ldots,z_t,l}$ is defined as a path of l vertices $(1 \sim 2 \sim \ldots \sim l)$ with pendant paths of z_i edges joining at vertex a_i for $i = 1, 2, \ldots, t$, where $\{a_1, a_2, \ldots, a_t\} \subseteq \{2, \ldots, l-1\}$, $z_i \geq 1 (1 \leq i \leq t)$ and $n = l + \sum_{i=1}^{t} z_i$.

(v) The *sun-like graph* $C^{a_1,a_2,\ldots,a_t}_{z_1,z_2,\ldots,z_t,g}$ is defined as a cycle with grith g $(1 \sim 2 \sim \ldots \sim g \sim 1)$ with pendant paths of z_i edges joining at vertex a_i for $i = 1, 2, \ldots, t$, where $\{a_1, a_2, \ldots, a_t\} \subseteq \{1, \ldots, g\}$, $z_i \geq 1 (1 \leq i \leq t)$ and $n = g + \sum_{i=1}^{t} z_i$.

(vi) The *dumbbell graph* D_{l,g_1,g_2} is obtained by joining two cycles C_{g_1} and C_{g_2} with a path of length l, where $g_1, g_2 \geq 3$, $k \geq 1$ and $n = g_1 + g_2 + l - 1$.

(vii) $M^{g}_{l_1,l_2,l_3}$ stands for the *mirror graph* obtained from C_g and T_{l_1,l_2,l_3} by identifying a vertex of C_g with an end-vertex of T_{l_1,l_2,l_3}, where $l_i \geq 1 (1 \leq i \leq 3)$, $g \geq 3$ and $n = g + \sum_{i=1}^{3} l_1$.

(viii) The *θ-graph* $\theta_{i,j,k}$ consists of two vertices joined by three disjoint paths whose order are i, j and k, respectively, where $n = i + j + k - 4$.

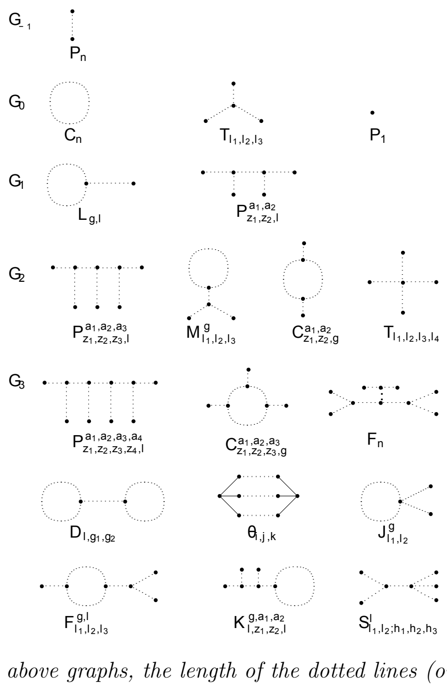
(ix) Let $J^{g}_{l_1,l_2,\ldots,l_k}$ be the *jellyfish graph* obtained from C_g and $T_{l_1,l_2,\ldots,l_k}$ by identifying a vertex of C_g with the center of $T_{l_1,l_2,\ldots,l_k}$, where $g \geq 3$, $l_i \geq 1 (1 \leq i \leq k)$.

(x) The *fish graph* $F^{g,l}_{l_1,l_2,l_3}$ is obtained from P_l and $M^{g}_{l_1,l_2,l_3}$ by identifying an end-vertex of P_l with a vertex of degree 2 which lies in the cycle of $M^{g}_{l_1,l_2,l_3}$, where $g \geq 3$, $l, l_1, l_2, l_3 \geq 1$.

(xi) The *key graph* $K^{g,a_1,a_2}_{l,z_1,z_2}$ is obtained from C_g and $P^{a_1,a_2}_{z_1,z_2,l}$ by overlapping a vertex of C_g with an end-vertex of $P^{a_1,a_2}_{z_1,z_2,l}$, where $g \geq 3$ and $z_1, z_2 \geq 1$.

(xii) The *double-starlike tree* $S^{l}_{l_1,l_2,\ldots,l_k;h_1,h_2,\ldots,h_s}$ is obtained by joining the centers of $T_{l_1,l_2,\ldots,l_k}$ and $T_{h_1,h_2,\ldots,h_s}$ with a path P_l, where $l_i, h_j \geq 1$.

4.2 The family $\mathscr{G}_i = \{G \mid G$ is a connected graph$, \mathcal{M}(G) = i, i \geq -1\}$



Remark 4.1. *In the above graphs, the length of the dotted lines (or the dotted cycles) is at least* 1 *(or* 3*).*

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