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On Graphs with c_2-c_3 Successive Minimal Laplacian Coefficients

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Abstract: Let G be a graph of order n and $L(G)$ be its Laplacian matrix. The Laplacian polynomial of G is defined as $P(G;\lambda) = \det(\lambda I - L(G)) = \sum_{i=0}^{n}(-1)^i c_i(G)\lambda^{n-i}$, where $c_i(G)$ is called the i-th Laplacian coefficient of G. Denoted by $\mathcal{G}_{n,m}$ the set of all (n,m)-graphs, in which each of them contains n vertices and m edges. The graph G is called *uniformly minimal* if, for each $i(i = 0, 1, \ldots, n)$, H is $c_i(G)$-minimal in $\mathcal{G}_{n,m}$. The Laplacian matrix and eigenvalues of graphs have numerous applications in various interdisciplinary fields, such as chemistry and physics. Specifically, these matrices and eigenvalues are widely utilized to calculate the energy of molecular energy and analyze the physical properties of materials. The Laplacian-like energy shares a number of properties with the usual graph energy. In this paper, we investigate the existence of uniformly minimal graphs in $\mathcal{G}_{n,m}$ because such graphs have minimal Laplacian-like energy. We determine that the $c_2(G)$-$c_3(G)$ successive minimal graph is exactly one of the four classes of threshold graphs.

Keywords: Laplacian coefficient; uniformly minimal graphs; threshold graph

1. Introduction

The Laplacian matrices and eigenvalues of graphs have been employed in various fields, including chemistry and physics. In the realm of chemistry, molecular graphs are frequently used to represent molecules. The Laplacian matrices of these graphs enable the calculation of numerous properties of molecules including their energies and vibrational spectra [1]. Additionally, the Laplacian matrices and eigenvalues of graphs can be utilized to investigate chemical bonding between atoms in a molecule, enabling the determination of bond strength and prediction of molecular reactivity [2]. In the field of materials science, the Laplacian matrices and eigenvalues of graphs are useful in studying physical properties such as the electrical conductivity of metals and the thermal conductivity of insulators [3]. In physics, the Laplacian matrices and eigenvalues of graphs play a prominent role in network analysis. They aid in investigating the flow of information in complex networks [4]. Lastly, the Laplacian matrices and eigenvalues of graphs have applications in quantum mechanics, where they are utilized to study electron behavior in materials and calculate electronic structures of atoms and molecules [5].

Furthermore, the Laplacian-like energy shares a number of properties with the usual graph energy. Stevanović has proved that the graph with uniformly minimum Laplacian coefficients is the graph with the minimal Laplacian-like energy [6], so it is crucial to determine whether a graph with uniformly minimum Laplacian coefficients exists. But this is extremely difficult. So far, only some small dimensional special graph classes with uniformly minimum Laplacian coefficients have been determined.

Many interesting results have been drawn on uniformly minimal graphs with small dimensions. For instance, Mohar [7] proved that the star is the unique uniformly minimal graph among all trees of order n. Then Stevanović and Ilić [8], He and Shan [9] and Pai, Liu and Guo [10] determined, respectively, the unique uniformly minimal graph among all

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unicyclic graphs, bicyclic graphs and tricyclic graphs of order n. For more results on the Laplacian coefficients of graphs, one can see [11–19].

A graph G is said to be a *threshold* graph if G is $\{2K_2, C_4, P_4\}$-free. Threshold graphs have beautiful structures and possess many important mathematical properties such as the extreme cases of certain graph properties, see [20–23]. For more information on threshold graphs, one can see the monograph [22].

In reference [24], Gong, Zou and Zhang gave a characterization of c_i-minimal graphs as follows.

Theorem 1 ([24], Theorem 1)**.** *Let $n \geq 3$ and $n-1 \leq m \leq \binom{n}{2}$. Then, for each i, $2 \leq i \leq n-2$, c_i-minimal (n,m)-graph is a threshold graph.*

In reference [24], Gong et al., proved additionally that there does not exist uniformly minimal graphs in $\mathcal{G}_{n,n+3}$, $n \geq 6$; see [24] (Theorem 6). Therefore, a natural question is proposed.

Question ([24], Question 7) For two positive integers n and m with $n \geq 5$ and $n+3 \leq m \leq n(n-1)/2$, determine all pairs (n,m) such that the uniformly minimal graphs in $\mathcal{G}_{n,m}$ exist.

In this paper, we investigate the above Question. The rest of the paper is organized as follows. In Section 2, we will introduce the notations and terminologies. In Section 3, we determine that the c_2-minimal graphs in $\mathcal{G}_{n,m}$ are six classes of threshold graphs. Then, in Section 4, we give a characterization of c_2-c_3 successive minimal graphs in $\mathcal{G}_{n,m}$, determine that each c_2-c_3 successive minimal graph is exactly one of the four classes of threshold graphs. In Section 5, we give the main results of this paper and a flow diagram of the idea of proof. Finally, in Section 6, we draw some conclusions and describe the further development of this work.

2. Preliminaries

In this section, we will introduce the notations and terminologies, which will be utilized in the subsequent discussion.

Throughout the paper, graphs are simple, finite and undirected. Let G be a graph of order n. Denote by $A(G)$ and $D(G)$ the adjacency matrix and the degree diagonal matrix of G, respectively. The Laplacian characteristic polynomial $P(G;\lambda)$ of G is defined by

$$P(G;\lambda) = \det(\lambda I - L(G)) = \sum_{i=0}^{n} (-1)^i c_i(G) \lambda^{n-i}, \tag{1}$$

where $c_i(G)$ is referred to as the i-th Laplacian coefficient of G. Because the Laplacian matrix $L(G)$ is positive semi-defined, $c_i(G) \geq 0$ holds for each i. Without causing confusion, we abbreviate $c_i(G)$ to c_i.

A graph G having n vertices and m edges is called a (n,m)-graph. Denote by $\mathcal{G}_{n,m}$ the set of all (n,m)-graphs. Let $H \in \mathcal{G}_{n,m}$. The graph H is called

- c_i*-minimal* if $c_i(H) \leq c_i(G)$ holds for any graph G in $\mathcal{G}_{n,m}$;
- c_2-c_3 *successive minimal* if H is c_3-minimal among all c_2-minimal graphs;
- *uniformly minimal* if, for each $i (i = 0, 1, \ldots, n)$, H is c_i-minimal in $\mathcal{G}_{n,m}$.

Let $G \in \mathcal{G}_{n,m}$ with vertex set V. The degree of the vertex i of G is the number of edges incident with i, denoted by d_i. Denote by $D(G) = (d_1, d_2, \ldots, d_n)$ the degree sequence of G and $\triangle(G)$ the number of triangles contained in G.

Let A and B be two disjoint graphs. Denote by $A \cup B$ the *sum* of A and B, where $V(A \cup B) = V(A) \cup V(B)$ and $E(A \cup B) = E(A) \cup E(B)$, and by $A \vee B$, the *product* of A and B, the graph obtained from $A \cup B$ by adding all the edges (u,h) with $u \in V(A)$ and $h \in V(B)$.

Let (n, m) be an integer pair with $n \geq 5$ and $n-1 \leq m \leq n(n-1)/2$. Suppose that the integers k, j, r and s satisfy

$$m = \binom{k+1}{2} - j,\ 1 \leq j \leq k, \tag{2}$$

$$m = \binom{n}{2} - \binom{r+1}{2} + s,\ 1 \leq s \leq r. \tag{3}$$

We introduce six special threshold graphs as follows (see Figures 1–3):

- $C_{n,m} := (K_{k-j} \vee (K_1 \cup K_j)) \cup (n-k-1)K_1$;
- $R_{n,m} := (K_1 \vee (K_{k-1} \cup (k-j)K_1)) \cup (n-2k+j)K_1$, where $k+1 \leq 2k-j-1 \leq n-1$;
- $T_{n,m} := (K_{k-2} \vee 3K_1) \cup (n-k-1)K_1$, where $j = 3$;
- $S_{n,m} := K_{n-r-1} \vee ((K_1 \vee sK_1) \cup (r-s)K_1)$;
- $Q_{n,m} := K_{n-2r+s} \vee ((K_{r-s} \vee (r-1)K_1) \cup K_1)$, where $r+1 \leq 2r-s-1 \leq n-1$;
- $P_{n,m} := K_{n-r-1} \vee (K_3 \cup (r-2)K_1)$, where $s = 3$.

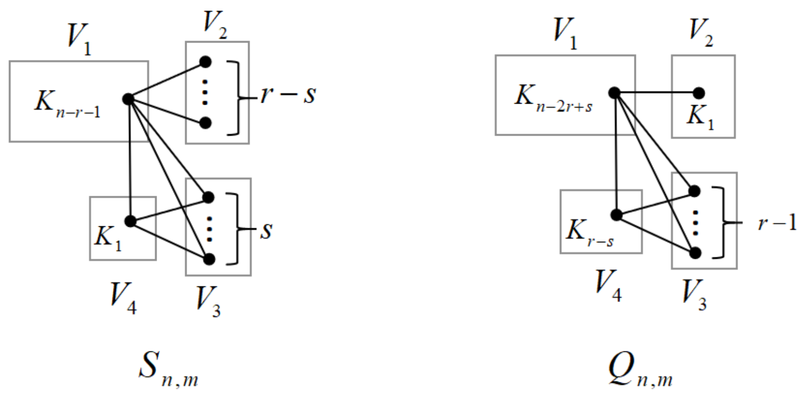

Figure 1. $S_{n,m} := K_{n-r-1} \vee ((sK_1 \vee K_1) \cup (r-s)K_1)$, $Q_{n,m} := K_{n-2r+s} \vee ((K_{r-s} \vee (r-1)K_1) \cup K_1)$.

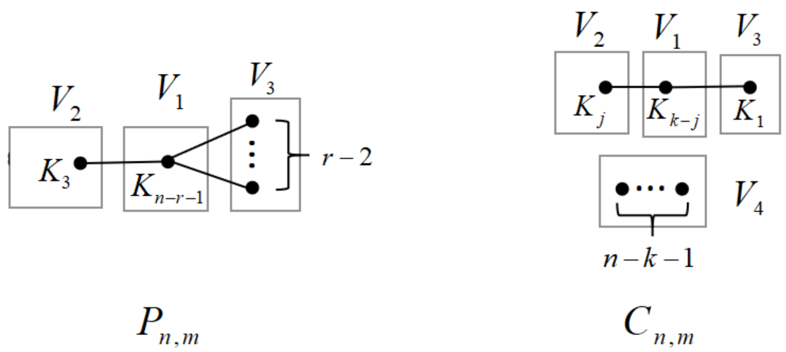

Figure 2. $P_{n,m} := K_{n-r-1} \vee (K_3 \cup (r-2)K_1)$, $C_{n,m} := (K_{k-j} \vee (K_1 \cup K_j)) \cup (n-k-1)K_1$.

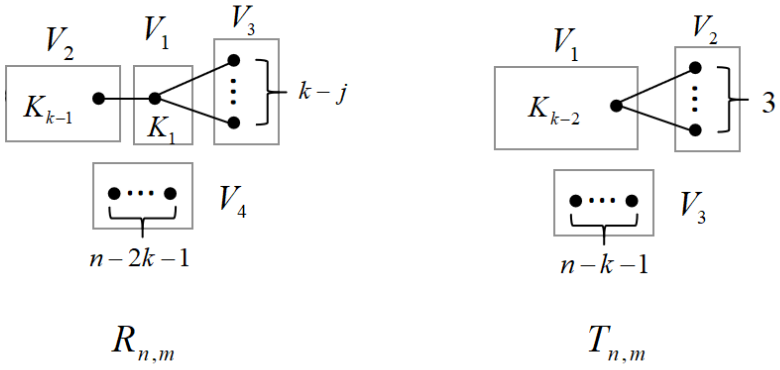

Figure 3. $R_{n,m} := (K_1 \vee (K_{k-1} \cup (k-j)K_1)) \cup (n-2k+j)K_1$, $T_{n,m} := (K_{k-2} \vee 3K_1) \cup (n-k-1)K_1$.

Moreover, we refer $S_{n,m}$ as the *quasi-star* graph and refer $C_{n,m}$ as the *quasi-complete* graph.

In the final of this section, we need to introduce some terminology results, which will be used in the subsequent discussion.

Let G be a graph with order n and degree sequence $D(G) = (d_1, d_2, \ldots, d_n)$. The problem of characterizing the graphs having maximum invariant

$$\sum_{i=1}^{n} d_i^2$$

in $\mathcal{G}_{n,m}$ was first investigated by Katz [25] in 1971 and by R. Ahlswede and G.O.H. Katona [20] in 1978. Then the invariant $\sum_{i=1}^{n} d_i^2$ is named as the *first Zagreb index*, denoted by $M(G)$; see [26,27]. For convenience, a graph G is referred to as *optimal* if $M(G)$ is maximal among all graphs in $\mathcal{G}_{n,m}$.

3. On c_2-Minimal Graphs in $\mathcal{G}_{n,m}$

For any given graph G, the following results provide combinatorial expressions on the Laplacian coefficients $c_2(G)$ and $c_3(G)$ in terms of their degree sequence and the trace of A^3.

Lemma 1 ([28], Theorem 3.1)**.** *Let $G \in \mathcal{G}_{n,m}$ be a graph with degree sequence $(d_1, \ldots, d_n)$. Then*

$$c_2(G) = 2m^2 - m - \frac{1}{2}\sum_{i=1}^{n} {d_i}^2. \tag{4}$$

Lemma 2 ([28], Theorem 3.2)**.** *Let $G \in \mathcal{G}_{n,m}$ be a graph with adjacency matrix A and degree sequence $(d_1, \ldots, d_n)$. Then*

$$c_3(G) = \frac{1}{3}(4m^3 - 6m^2 - 3m\sum_{i=1}^{n} {d_i}^2 + \sum_{i=1}^{n} {d_i}^3 - tr(A^3)). \tag{5}$$

From Lemma 1, it can be seen that the graph with the largest sum of degree squares, i.e., the optimal graph, is a graph of c_2-minimal.

In 1999, Peled, Petreschi and Sterbini [29], and Byer [30], independently showed that all optimal graphs, which may not necessarily be connected, belong to one of the six classes of threshold graphs defined above.

Lemma 3 ([31], Theorems 2.4, 2.6, 2.7)**.** *Let n and m be two integers such that $0 \le m \le \binom{n}{2}$. Let also k, r, j and s satisfy Equations (1) and (2). Then the set of optimal graphs are contained in*

$$\{S_{n,m},\ Q_{n,m},\ P_{n,m},\ C_{n,m},\ R_{n,m},\ T_{n,m}\}.$$

Moreover,

(1). *at least one of $S_{n,m}$ and $C_{n,m}$ is optimal;*

(2). *if $Q_{n,m}$ or $P_{n,m}$ is optimal, then $S_{n,m}$ must be optimal;*

(3). *if $R_{n,m}$ or $T_{n,m}$ is optimal, then $C_{n,m}$ must be optimal;*

(4). *if $Q_{n,m}$ and $C_{n,m}$ are both optimal, then $j = k$, $r = k+1$, $s = 2k - n + 2$, $n > 5$ and k are positive integers that satisfy Pell's equation $(2n-3)^2 - 2(2k-1)^2 = -1$;*

(5). *if $P_{n,m}$ and $C_{n,m}$ are both optimal, then $j = s$, $k = r$, $n > 9$ and k are positive integers that satisfy Pell's equation $(2n-1)^2 - 2(2k+1)^2 = -49$;*

(6). *if $Q_{n,m}$ and $P_{n,m}$ are both optimal, then $(n,m) = (7,9)$ or $(9,18)$, and $C_{n,m}$ also exists.*

The following theorem indicates that there are few integer pairs (n,m) that satisfy $M(S_{n,m}) = M(C_{n,m})$ for $n \geq 5$ and $n+3 \leq m \leq n(n-1)/2$.

Let $k_0 = k_0(n)$ be an integer such that

$$\binom{k_0}{2} \leq \frac{1}{2}\binom{n-1}{2} < \binom{k_0+1}{2}$$

and define the quadratic function

$$q_0 = \frac{1 - 2(2k_0-3)^2 + 2(n-5)^2}{4}, \quad R_0 = \frac{4(\binom{n}{2} - 2\binom{k_0}{2})(k_0-2)}{-1 - 2(2k_0-4)^2 + (2n-5)^2}.$$

Theorem 2 ([31], Theorem 2.8)**.** *Let n be a positive integer.*
(1). *If $q_0(n) > 0$, then*

$$M(S_{n,m}) \geq M(C_{n,m}) \text{ for } 0 \leq m \leq \tfrac{1}{2}\tbinom{n}{2},$$

$$M(C_{n,m}) \geq M(S_{n,m}) \text{ for } \tfrac{1}{2}\tbinom{n}{2} \leq m \leq \tbinom{n}{2}.$$

$M(S_{n,m}) = M(C_{n,m})$ if and only if $m \in \{0,1,2,3,\frac{1}{2}\binom{n}{2}\}$, or $m = \binom{k_0}{2}$ and $(2n-3)^2 - 2(2k_0-3)^2 = -1,7$.
(2). *If $q_0(n) < 0$, then*

$$M(S_{n,m}) \geq M(C_{n,m}) \text{ for } 0 \leq m \leq \tfrac{1}{2}\tbinom{n}{2} - R_0 \text{ or } \tfrac{1}{2}\tbinom{n}{2} \leq m \leq \tfrac{1}{2}\tbinom{n}{2} + R_0;$$

$$M(C_{n,m}) \geq M(S_{n,m}) \text{ for } \tfrac{1}{2}\tbinom{n}{2} - R_0 \leq m \leq \tfrac{1}{2}\tbinom{n}{2} \text{ or } \tfrac{1}{2}\tbinom{n}{2} + R_0 \leq m \leq \tbinom{n}{2}.$$

$M(C_{n,m}) = M(S_{n,m})$ if and only if $m \in \{0,1,2,3,\frac{1}{2}\binom{n}{2} - R_0, \frac{1}{2}\binom{n}{2}\}$.
(3). *If $q_0(n) = 0$, then*

$$M(S_{n,m}) \geq M(C_{n,m}) \text{ for } 0 \leq m \leq \tfrac{1}{2}\tbinom{n}{2},$$

$$M(C_{n,m}) \geq M(S_{n,m}) \text{ for } \tfrac{1}{2}\tbinom{n}{2} \leq m \leq \tbinom{n}{2}.$$

$M(S_{n,m}) = M(C_{n,m})$ if and only if $m \in \{0,1,2,3,\binom{k_0}{2},\ldots,\frac{1}{2}\binom{n}{2}\}$.

From Theorem 2, there are few integer pairs (n,m) that satisfy $M(S_{n,m}) = M(C_{n,m})$ for $n \geq 5$ and $n+3 \leq m \leq n(n-1)/2$.

Below, Figure 4 ([31] Figures 2.5–2.8) shows the value $M(S_{n,m}) - M(C_{n,m})$ for $n = 25, 15, 17$, and 23, respectively. It is easy to see that $S_{n,m}$ and $C_{n,m}$ are rarely both optimal.

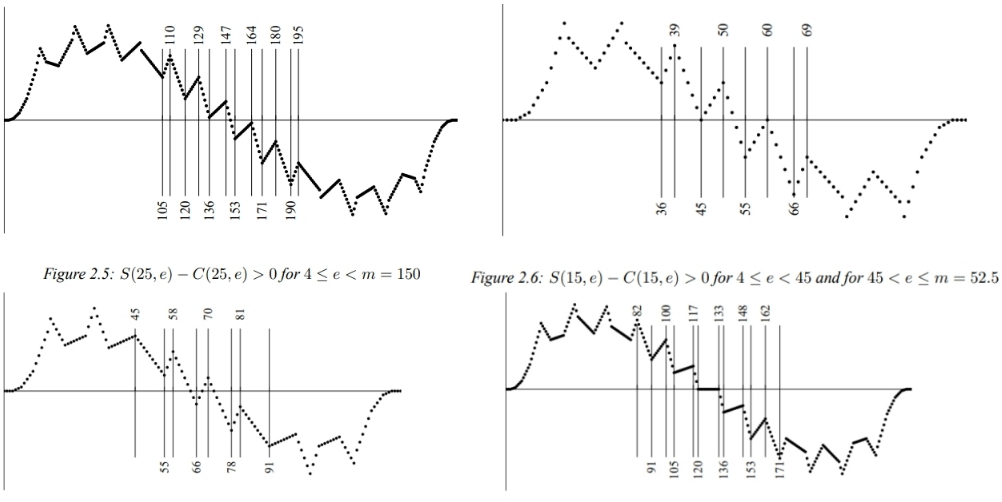

Figure 2.5: $S(25,e) - C(25,e) > 0$ *for* $4 \le e < m = 150$

Figure 2.6: $S(15,e) - C(15,e) > 0$ *for* $4 \le e < 45$ *and for* $45 < e \le m = 52.5$

Figure 2.7: $S(17,e) - C(17,e) > 0$ *for* $4 \le e \le 63.$

Figure 2.8: $S(23,e) - C(23,e) > 0$ *for* $4 \le e \le 119$, $S(23,e) = C(23,e)$ *for* $120 \le e < m = 126.5$

Figure 4. In reference [31], $m = \frac{1}{2}\binom{n}{2}$. $S(25,e)$ and e denote the sum of squares of degrees and the number of edges of the quasi-star graph.

4. On c_2-c_3 Successive Minimal Graphs in $\mathcal{G}_{n,m}$

Combining with Lemma 3 and the definition of the c_2-c_3 successive minimal graphs, we have the following result immediately.

Corollary 1. *Let G be a c_2-c_3 successive minimal graph in $\mathcal{G}_{n,m}$. Then*

$$G \in \{S_{n,m},\ Q_{n,m},\ P_{n,m},\ C_{n,m},\ R_{n,m},\ T_{n,m}\}.$$

Let G be a graph with an adjacency matrix A. The following result is well known.

Lemma 4 ([32], Proposition 2)**.** *Let $G \in \mathcal{G}_{n,m}$ be a graph with adjacency matrix A. Then*

$$tr(A^3) = 6\triangle(G). \tag{6}$$

Set

$$\alpha(G) = \sum_{i=1}^{n} {d_i}^3 - 6\triangle(G). \tag{7}$$

As a consequence of Lemma 3 and Corollary 1, we have

Proposition 1. *Let $G \in \mathcal{G}_{n,m}$ be a graph with adjacency matrix A. Then G is a c_2-c_3 successive minimal graph if and only if G has minimal value $\alpha(G)$ among all graphs in*

$$\{S_{n,m},\ Q_{n,m},\ P_{n,m},\ C_{n,m},\ R_{n,m},\ T_{n,m}\}.$$

Therefore, to determine the c_2-c_3 successive minimal graph, we need to compare the values $\alpha(G)$ among all graphs in $\{S_{n,m},\ Q_{n,m},\ P_{n,m},\ C_{n,m},\ R_{n,m},\ T_{n,m}\}$.

Firstly, by the structures of those special threshold graphs, we can easily list the degree sequences of all graphs above as follows.

$$(1).\ D(S_{n,m}) = (\overbrace{n-1,\ldots,n-1}^{n-r-1},\ n-r+s-1,\ \overbrace{n-r,\ldots,n-r}^{s});$$
$$(2).\ D(Q_{n,m}) = (\overbrace{n-1,\ldots,n-1}^{n-2r+s},\ \overbrace{n-2,\ldots,n-2}^{r-s},\ \overbrace{n-r,\ldots,n-r}^{r-1},\ n-2r+s);$$
$$(3).\ D(P_{n,m}) = (\overbrace{n-1,\ldots,n-1}^{n-r-1},\ \overbrace{n-r+1,\ldots,n-r+1}^{3},\ \overbrace{n-r-1,\ldots,n-r-1}^{r-2});$$
$$(4).\ D(C_{n,m}) = (\overbrace{k,\ldots,k}^{k-j},\ \overbrace{k-1,\ldots,k-1}^{j},\ k-j,\ \overbrace{0,\ldots,0}^{n-k-1});$$
$$(5).\ D(R_{n,m}) = (2k-j-1,\ \overbrace{k-1,\ldots,k-1}^{k-1},\ \overbrace{1,\ldots,1}^{k-j},\ \overbrace{0,\ldots,0}^{n-2k+j});$$
$$(6).\ D(T_{n,m}) = (\overbrace{k,\ldots,k}^{k-2},\ k-2,\ k-2,\ k-2,\ \overbrace{0,\ldots,0}^{n-k-1}).$$

By the structures of those special threshold graphs, we have

Proposition 2. *Let (n,m) be a given integer pair with $n-1 \le m \le n(n-1)/2$. Then*

$$(1).\ \triangle(S_{n,m}) = \binom{n-r+1}{3} + (s-1)\binom{n-r}{2} + (r-s)\binom{n-r-1}{2};$$
$$(2).\ \triangle(Q_{n,m}) = \binom{n-r+1}{3} + (r-2)\binom{n-r}{2} + \binom{n-2r+s}{2};$$
$$(3).\ \triangle(P_{n,m}) = \binom{n-r+2}{3} + (r-2)\binom{n-r-1}{2};$$
$$(4).\ \triangle(C_{n,m}) = \binom{k}{3} + \binom{k-j}{2};$$
$$(5).\ \triangle(R_{n,m}) = \binom{k}{3};$$
$$(6).\ \triangle(T_{n,m}) = \binom{k-1}{3} + 2\binom{k-2}{2}.$$

Proof. (1). We divide all vertices of $S_{n,m}$ into four parts:
V_1: the vertices that are contained in the complete graph K_{n-r+1};
V_2: the vertices that are contained in the isolated vertices $(r-s)K_1$;
V_3: the vertices that are contained in the isolated vertices sK_1;
V_4: the unique isolated vertex (see Figure 1).

The number of triangles each of whose all vertices are contained in V_1 is $\binom{n-r-1}{3}$, the number of triangles each of whose two vertices are contained in V_1 and one vertex is contained in V_2 is $(r-s)\binom{n-r-1}{2}$, the number of triangles each of whose two vertices are contained in $V_1 \vee V_4$ and one vertex is contained in V_3 is $s\binom{n-r}{2}$, and the number of triangles each of whose two vertices are contained in V_1 and one vertex is contained in V_4 is $\binom{n-r-1}{2}$. Besides, by a simple calculation, it can be seen that $\binom{n-r-1}{3} + s\binom{n-r}{2} + \binom{n-r-1}{2} = \binom{n-r+1}{3} + (s-1)\binom{n-r}{2}$.

(2). We divide all vertices of $Q_{n,m}$ into four parts:
V_1: the vertices that are contained in the complete graph K_{n-2r+1};
V_2: the unique isolated vertex K_1;
V_3: the vertices that are contained in the isolated vertices $(r-1)K_1$;
V_4: the vertices that are contained in the complete graph K_{r-s} (see Figure 1).

The number of triangles each of whose all vertices are contained in $V_1 \vee V_4$ is $\binom{n-r}{3}$, the number of triangles each of whose two vertices are contained in V_1 and one vertex is contained in V_2 is $\binom{n-2r+s}{2}$, the number of triangles each of whose two vertices are contained in $V_1 \vee V_4$ and one vertex is contained in V_3 is $(r-1)\binom{n-r}{2}$. Besides, by a simple calculation, it can be seen that $\triangle(Q_{n,m}) = \binom{n-r}{3} + (r-1)\binom{n-r}{2} = \binom{n-r+1}{3} + (r-2)\binom{n-r}{2}$.

(3). We divide all vertices of $P_{n,m}$ into three parts:
V_1: the vertices that are contained in the complete graph K_{n-r-1};
V_2: the vertices that are contained in the complete graph K_3;
V_3: the vertices that are contained in the isolated vertices $(r-2)K_1$ (see Figure 2).

The number of triangles each of whose all vertices are contained in $V_1 \vee V_2$ is $\binom{n-r+2}{3}$, the number of triangles each of whose two vertices are contained in V_1 and one vertex is contained in V_3 is $(r-2)\binom{n-r-1}{2}$. So $\triangle(P_{n,m}) = \binom{n-r+2}{3} + (r-2)\binom{n-r-1}{2}$.

(4). We divide all vertices of $C_{n,m}$ into four parts:
V_1: the vertices that are contained in the complete graph K_{k-j};
V_2: the vertices that are contained in the complete graph K_j;
V_3: the isolated vertex K_1;
V_4: some isolated vertices $(n-k-1)K_1$ (see Figure 2).

The number of triangles each of whose all vertices are contained in V_1 is $\binom{k-j}{3}$, the number of triangles each of whose two vertices are contained in V_1 and one vertex is contained in V_2 is $j\binom{k-j}{2}$. The number of triangles each of whose all vertices are contained in V_2 is $\binom{j}{3}$, the number of triangles each of whose two vertices are contained in V_2 and one vertex is contained in V_1 is $(k-j)\binom{j}{2}$. The number of triangles each of whose two vertices are contained in V_1 and one vertex is contained in V_3 is $\binom{k-j}{2}$. Besides, by a simple calculation, it can be seen that $\binom{k-j}{3} + j\binom{k-j}{2} + \binom{j}{3} + (k-j)\binom{j}{2} = \binom{k}{3}$. So $\triangle(C_{n,m}) = \binom{k}{3} + \binom{k-j}{2}$.

(5). We divide all vertices of $R_{n,m}$ into four parts:
V_1: one vertex K_1;
V_2: the vertices that are contained in the complete graph K_{k-1};
V_3: some isolated vertices $(k-j)K_1$;
V_4: some isolated vertices $(n-2k-1)K_1$ (see Figure 3).

The number of triangles each of whose all vertices are contained in V_2 is $\binom{k-1}{3}$, the number of triangles each of whose two vertices are contained in V_2 and one vertex is contained in V_1 is $\binom{k-1}{2}$. Besides, by a simple calculation, it can be seen that $\binom{k-1}{3} + \binom{k-1}{2} = \binom{k}{3}$. So $\triangle(R_{n,m}) = \binom{k}{3}$.

(6). We divide all vertices of $T_{n,m}$ into three parts:
V_1: the vertices that are contained in the complete graph K_{k-2};
V_2: three isolated vertices $3K_1$;
V_3: some isolated vertices $(n-k-1)K_1$ (see Figure 3).

The number of triangles each of whose all vertices are contained in V_1 is $\binom{k-2}{3}$, the number of triangles each of whose two vertices are contained in V_1 and one vertex is contained in V_2 is $3\binom{k-2}{2}$. Besides, by a simple calculation, it can be seen that $\binom{k-2}{3} + 3\binom{k-2}{2} = \binom{k-1}{3} + 2\binom{k-2}{2}$. So $\triangle(T_{n,m}) = \binom{k}{3}$.

Therefore, the proof is complete. □

Now we establish two main theorems as follows. These theorems can help us better identify the candidate graphs of c_2-c_3 minimal successive graphs in $\mathcal{G}_{n,m}$.

Theorem 3. *Let (n,m) be a given integer pair with $n-1 \le m \le n(n-1)/2$. Then*

(1). *$\alpha(P_{n,m}) < \alpha(S_{n,m})$ if $P_{n,m}$ and $S_{n,m}$ are c_2-minimal;*

(2). *$\alpha(C_{n,m}) < \alpha(T_{n,m})$ if $C_{n,m}$ and $T_{n,m}$ are c_2-minimal;*

(3). *$\alpha(Q_{n,m}) < \alpha(S_{n,m})$ if $Q_{n,m}$ and $S_{n,m}$ are c_2-minimal;*

(4). *$\alpha(C_{n,m}) < \alpha(R_{n,m})$ if $C_{n,m}$ and $R_{n,m}$ are c_2-minimal.*

Proof. Combining with the degree sequences above and Lemma 2, we have

$$\begin{aligned}\alpha(S_{n,m}) &= (n-r-1)(n-1)^3 + (n-r+s-1)^3 + s(n-r)^3 + (r-s)(n-r-1)^3 \\ &\quad - 6(\binom{n-r+1}{3} + (s-1)\binom{n-r}{2} + (r-s)\binom{n-r-1}{2}); \\ \alpha(Q_{n,m}) &= (n-2r+s)(n-1)^3 + (r-s)(n-2)^3 + (r-1)(n-r)^3 + (n-2r+s)^3 \\ &\quad - 6(\binom{n-r+1}{3} + (r-2)\binom{n-r}{2} + \binom{n-2r+s}{2});\end{aligned}$$

$$\begin{aligned}\alpha(P_{n,m}) &= (n-r-1)(n-1)^3 + 3(n-r+1)^3 + (r-2)(n-r-1)^3 \\ &\quad - 6(\binom{n-r+2}{3} + (r-2)\binom{n-r-1}{2}); \\ \alpha(C_{n,m}) &= (k-j)k^3 + j(k-1)^3 + (k-j)^3 - 6(\binom{k}{3} + \binom{k-j}{2}); \\ \alpha(R_{n,m}) &= (2k-j-1)^3 + (k-1)^4 + k - j - 6\binom{k}{3}; \\ \alpha(T_{n,m}) &= (k-2)k^3 + 3(k-2)^3 + (k-3)^3 - 6(\binom{k-1}{3} + 2\binom{k-2}{2}).\end{aligned}$$

(1). By a direct calculation, $\alpha(S_{n,m}) - \alpha(P_{n,m}) = 12 > 0$ as $s = 3$.
(2). $\alpha(C_{n,m}) - \alpha(T_{n,m}) = -12 < 0$ as $j = 3$. So (1) and (2) are trivial.
(3). Note that $\alpha(S_{n,m}) - \alpha(Q_{n,m}) = 3r^3 - (6s+3)r^2 + (3s^2+3s)r$, we define

$$f(r) = \alpha(S_{n,m}) - \alpha(Q_{n,m}) = 3r^3 - (6s+3)r^2 + (3s^2+3s)r.$$

Recall that $r+1 \le 2r-s-1 \le n-1$, then $r \ge s+2$ and thus the derivative $f'(r)$ satisfies $f'(r) = 9r^2 - 2(6s+3)r + 3s^2 + 3s \ge f'(s+2) = 3s + 24 > 0$, which implies that $f(r)$ is an increasing function on r. Consequently, $\alpha(S_{n,m}) - \alpha(Q_{n,m}) \ge f(3) = 18 > 0$. Thus (3) follows.
(4). Note that $\alpha(C_{n,m}) - \alpha(R_{n,m}) = -7k^3 + (6j+10)k^2 - (3j^2 - 3j + 10)k - 3j^2 - 4j + 2$, we define

$$g(k) = \alpha(C_{n,m}) - \alpha(R_{n,m}) = -7k^3 + (6j+10)k^2 - (3j^2 - 3j + 10)k - 3j^2 - 4j + 2,$$

a function on k. Recall that $k+1 \le 2k-j-1 \le n-1$, then $k \ge j+2$ and thus the derivative $g'(k)$ satisfies $g'(k) = -108j^2 + 228j - 440 < 0$, which implies that $g(k)$ is a decreasing function on k. Consequently, $\alpha(C_{n,m}) - \alpha(R_{n,m}) \le g(3) = -80 < 0$. Thus 4) follows. □

In the following theorem, we exclude the rare case of $M(S_{n,m}) = M(C_{n,m})$, $r+1 \le 2r-s-1 \le n-1$ and $s = 3$.

Theorem 4. *Let (n, m) be a given integer pair with $n-1 \le m \le \frac{n(n-1)}{2}$. Then*

(1). $\alpha(C_{n,m}) < \alpha(Q_{n,m})$ if $C_{n,m}$ and $Q_{n,m}$ are c_2-minimal;

(2). $\alpha(C_{n,m}) < \alpha(P_{n,m})$ if $C_{n,m}$ and $P_{n,m}$ are c_2-minimal;

(3). $\alpha(C_{n,m}) < \alpha(Q_{n,m})$ and $\alpha(C_{n,m}) < \alpha(P_{n,m})$ if $Q_{n,m}$ and $P_{n,m}$ are c_2-minimal.

Proof. (1). Note that $\alpha(Q_{n,m}) - \alpha(C_{n,m}) = n^4 - (k+7)n^3 + (3k+21)n^2 + (6k^2 - 9k - 28)n - k^4 - 15k^2 + 13k + 15$, we define

$$F(n) = \alpha(Q_{n,m}) - \alpha(C_{n,m}) = n^4 - (k+7)n^3 + (3k+21)n^2 + (6k^2 - 9k - 28)n - k^4 - 15k^2 + 13k + 15,$$

a function on n. Recall that $n > 5$ and thus the derivative $F'(n)$ satisfies $F'(n) = 4n^3 - 3(k+7)n^2 + 2(3k+21)n + 6k^2 - 9k - 28 = 6k^2 - (3n^2 - 6n + 9)k + 4n^3 - 21n^2 + 42n - 28$. We define $G(k) = 6k^2 - (3n^2 - 6n + 9)k + 4n^3 - 21n^2 + 42n - 28$. Recall that $r + 1 \le 2r - s - 1 \le n - 1$ and $r = k + 1$, $s = 2k - n + 2$, then $k \le n - 3$ and thus the first derivative $G'(k)$ satisfies $G'(k) = 12k - 2n^2 + 6n - 9 \le G'(n-3) = -3n^2 + 18n - 45 < 0$, which implies that $G(k)$ is a decreasing function on k. $F'(n) = G(k) \ge G(n-3) = n^3 - 21 + 53 > 168 > 0$, which implies that $F(n)$ is an increasing function on n. If $n = 5$, then $k = 2$. Consequently, $\alpha(Q_{n,m}) - \alpha(C_{n,m}) > F(5) = 30 > 0$. Thus 1) follows.

(2). Since integer $n > 9$ satisfies the Pell's equation $(2n-1)^2 - 2(2k+1)^2 = -49$, integer n is at least 12, and at the same time $n = 12$, $k = 8$. Note that $\alpha(P_{n,m}) - \alpha(C_{n,m}) = n^4 - 4n^3 - (3k^2 + 3k - 24)n^2 + (3k^3 + 12k^2 - 27k - 21)n - 2k^4 - 6k^3 + 24k^2 - 44k + 84$, we define

$$H(n) = n^4 - 4n^3 - (3k^2 + 3k - 24)n^2 + (3k^3 + 12k^2 - 27k - 21)n - 2k^4 - 6k^3 + 24k^2 - 44k + 84.$$

The derivative $H'(n)$ satisfies

$$H'(n) = 4n^3 - 12n^2 - (6k^2 + 6k - 48)n + 3k^3 + 12k^2 + 27k - 21.$$

The second derivative $H''(n)$ satisfies

$$H''(n) = 12n^2 - 24n - (6k^2 + 6k - 48).$$

The third derivative $H'''(n)$ satisfies

$$H'''(n) = 24n - 24 > 0,$$

which implies that $H''(n)$ is an increasing function on n. $H''(n) \ge H''(12) = 1056 > 0$, which implies that $H'(n)$ is an increasing function on n. $H'(n) \ge H'(12) = 3075 > 0$, which implies that $H(n)$ is an increasing function on n. Consequently, $\alpha(P_{n,m}) - \alpha(C_{n,m}) \ge H(12) = 7204 > 0$. Thus 2) follows.

(3). By Lemma 3 (6), if $Q_{n,m}$ and $P_{n,m}$ are all optimal, then $(n,m) = (7,9)$ or $(9,18)$, and $C_{n,m}$ also exists. Substituting $(n,m) = (7,9)$ into Equations (1) and (2) yields $k = 4$, $j = 1$, $r = 5$, and $s = 3$. By further direct calculation, $\alpha(Q_{n,m}) = 258$, $\alpha(P_{n,m}) = 276$ and $\alpha(C_{n,m}) = 204$. Similarly, substituting $(n,m) = (9,18)$ into Equations (1) and (2) yields $k = r = 6$ and $j = s = 3$. By further direct calculation, $\alpha(Q_{n,m}) = 1068$, $\alpha(P_{n,m}) = 1164$ and $\alpha(C_{n,m}) = 912$. It is not difficult to see that $\alpha(C_{n,m})$ is always the smallest. $\square$

5. Results

By Theorem 4 and Lemma 3 (6), if $Q_{n,m}$ and $P_{n,m}$ are c_2-minimal, then $C_{n,m}$ also exists, and $C_{n,m}$ is c_2-c_3 successive minimal.

By Lemma 3, Proposition 1 and Theorem 3, at least one of $S_{n,m}$ and $C_{n,m}$ be a c_2-c_3 successive minimal graph in $\mathcal{G}_{n,m}$. $Q_{n,m}$ or $P_{n,m}$ can only be a c_2-c_3 successive minimal graph if certain conditions are satisfied, while $R_{n,m}$ or $T_{n,m}$ cannot be c_2-c_3 successive minimal graph. Therefore, we have the main results of the paper as follows.

Theorem 5. *Let $G \in \mathcal{G}_{n,m}$. If $M(S_{n,m}) < M(C_{n,m})$, or $M(S_{n,m}) = M(C_{n,m})$ with $r + 1 \le 2r - s - 1 \le n - 1$ or $M(S_{n,m}) = M(C_{n,m})$ with $s = 3$, the c_2-c_3 successive minimal graph is $C_{n,m}$.*

Theorem 6. *Let $G \in \mathcal{G}_{n,m}$. If $M(S_{n,m}) \ne M(C_{n,m})$, or $M(S_{n,m}) = M(C_{n,m})$ with $r + 1 \le 2r - s - 1 \le n - 1$, or $M(S_{n,m}) = M(C_{n,m})$ with $s = 3$, each Laplacian coefficient c_2-c_3 successive minimal graph is exactly one of the four classes of threshold graphs $S_{n,m}$, $Q_{n,m}$, $P_{n,m}$ and $C_{n,m}$.*

The Figure 5 describes the logical progression of our proofs.

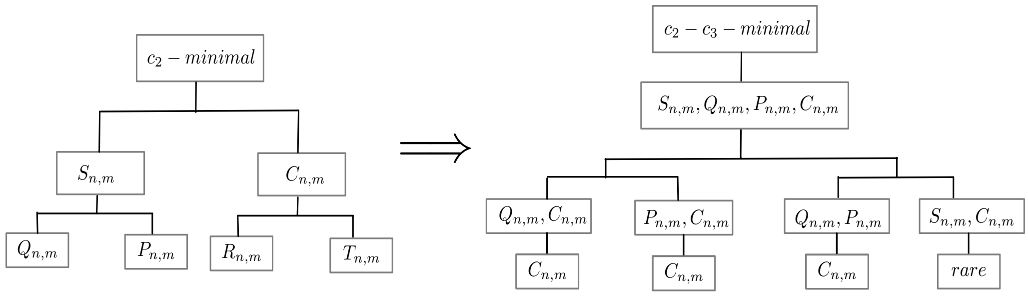

Figure 5. Only when $S_{n,m}$ is c_2-minimal graph, $P_{n,m}$ and $Q_{n,m}$ can be c_2-minimal graphs. Similarly, only when $C_{n,m}$ is c_2-minimal graph, $R_{n,m}$ and $T_{n,m}$ can be c_2-minimal graphs. The application of Theorem 3 enables us to reduce the set of candidate graphs for c_2-c_3 successive minimal graphs to four types of threshold graphs, namely: $S_{n,m}$, $Q_{n,m}$, $P_{n,m}$ and $C_{n,m}$. Besides, Theorem 4 indicates that, if $M(S_{n,m}) = M(C_{n,m})$ with $r+1 \leq 2r-s-1 \leq n-1$ $M(S_{n,m}) = M(C_{n,m})$ with $s=3$, the c_2-c_3 successive minimal graph is $C_{n,m}$.

Lemma 1 declares that the uniqueness of c_2-minimal graphs cannot be guaranteed in $\mathcal{G}_{n,m}$. For instance, Theorem 2.5 in [31] demonstrates six c_2-minimal graphs existing in $\mathcal{G}_{9,18}$. Theorems 3 and 4 further state that the c_2-c_3 minimal successive graph in $\mathcal{G}_{n,m}$ must be one of the four threshold graphs, that is, $S_{n,m}$, $Q_{n,m}$, $P_{n,m}$, and $C_{n,m}$, with the exception that only $S_{n,m}$ and $C_{n,m}$ can be c_2-minimal. Bearing in mind that for most integer pairs (n,m) with $n+3 \leq m \leq n(n-1)-3$, where the corresponding optimal (n,m)-graph is unique, the c_2-minimal graph is also unique. This being said, the cases where solely $S_{n,m}$ and $C_{n,m}$ are c_2-minimal are infrequent and encompassed in Theorem 2.

After excluding the case where solely $S_{n,m}$ and $C_{n,m}$ are c_2-minimal, we have successfully demonstrated the uniqueness of the c_2-c_3 minimal successive graph in $\mathcal{G}_{n,m}$. However, it must be noted that this scenario is rarely encountered (as noted in Theorem 2, where the possibility of $S_{n,m}$ and $C_{n,m}$ both being c_2-minimal is already uncommon). In light of this, we propose the conjecture that the c_2-c_3 minimal successive graph in $\mathcal{G}_{n,m}$ is indeed unique.

6. Conclusions

The research on the Laplacian matrix and its eigenvalues of graphs in the fields of physics and chemistry is notable. The coefficients of Laplacian matrix are directly linked to the eigenvalues and they serve as a reflection of the graph structure. In this paper, we extend Ábrego et al.'s work [31] and conduct a study of the c_2-c_3 successive minimal graphs. Our research aims to gain a better understanding of the structural properties of molecular graphs.

Our next step is to map the threshold graph to the Ferrers matrix (the adjacency matrix of a threshold graph such that the upper-triangular part is left justified and the number of zeros in each row of the upper-triangular part does not decrease. We demonstrate Ferrers matrices using "+" for the main diagonal, an empty circle "∘" for the zero entries, and a black dot, "•" for the entries equal to one), attach weights corresponding to Laplacian coefficients to each element in the Ferrers matrix, and use a special perturbation of the threshold graph to minimize some Laplacian coefficients.

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