

CHARACTERIZING PATH-FACTOR DELETED GRAPHS VIA Q -INDEX AND \mathcal{D} -INDEX

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Abstract. A graph G has a $\mathcal{P}_{\geq k}$ -factor if G has a spanning subgraph H such that every component of H is a path of order at least k . A graph G is $\mathcal{P}_{\geq k}$ -factor deleted if $G - e$ has a $\mathcal{P}_{\geq k}$ -factor for each edge $e \in E(G)$. In this paper, we study the $\mathcal{P}_{\geq 2}$ -factor deleted graphs by their Q -index (the largest eigenvalue of the signless Laplacian matrix) and \mathcal{D} -index (the largest eigenvalue of the distance matrix). Sufficient conditions (in terms of Q -index and \mathcal{D} -index) to guarantee that a graph G is a $\mathcal{P}_{\geq 2}$ -factor deleted graph are established.

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1. INTRODUCTION

We say a spanning subgraph F of G is a *path-factor* if each component of F is a path with at least two vertices. A graph G has a $\mathcal{P}_{\geq k}$ -factor if G has a spanning subgraph H such that every component of H is a path of order at least k . A graph G is $\mathcal{P}_{\geq k}$ -factor deleted if $G - e$ has a $\mathcal{P}_{\geq k}$ -factor for each edge e of G . The largest eigenvalues of the adjacency matrix $A(G)$, the signless Laplacian matrix $Q(G)$ and the distance matrix $\mathcal{D}(G)$ are respectively called the A -index, Q -index, and \mathcal{D} -index of G , denoted by $\rho(G)$, $q(G)$ and $\partial(G)$. In the past few years, the study of relationships between the related eigenvalues of a graph G and the existence of path-factors in a graph G has received more and more attention. For example, Miao and Li [14] provided a sufficient condition to ensure that a graph G has a $\mathcal{P}_{\geq 2}$ -factor or is a $\mathcal{P}_{\geq 2}$ -factor covered graph in terms of the A -index. Subsequently, Hao and Li [9] also presented some sufficient conditions to ensure that a graph G has a $\mathcal{P}_{\geq 2}$ -factor or is a $\mathcal{P}_{\geq 2}$ -factor covered graph with respect to the Q -index and \mathcal{D} -index. For more results on path-factors and path-factor covered graphs, we refer the reader to [2, 4–7, 11–13, 17–28]. Very recently, Shen [16] established a lower bound on the A -index to determine whether a graph is $\mathcal{P}_{\geq 2}$ -factor deleted.

Directly motivated by Li and Miao [14], Hao and Li [9] and Shen [16], it is natural and interesting to explore some other sufficient spectral conditions that ensure a graph G is a $\mathcal{P}_{\geq 2}$ -factor deleted graph. Along this line, we first present a sufficient condition involving its Q -index, which ensures that a graph G is a $\mathcal{P}_{\geq 2}$ -factor deleted graph.

Theorem 1.1. *Let G be a connected graph of order n . Then the following holds.*

Keywords. $\mathcal{P}_{\geq 2}$ -factor, $\mathcal{P}_{\geq 2}$ -factor deleted graph, Q -index, \mathcal{D} -index.

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- (i) For $n \geq 4$ and $n \neq 6$, if $q(G) > \hat{\theta}(n)$, then G is a $\mathcal{P}_{\geq 2}$ -factor deleted graph, where $\hat{\theta}(n)$ is the largest root of $x^3 - (3n - 5)x^2 + (2n^2 - 5n)x - 2n^2 + 10n - 12 = 0$.
- (ii) For $n = 6$, if $q(G) > \tilde{\theta}$, then G is a $\mathcal{P}_{\geq 2}$ -factor deleted graph, where $\tilde{\theta}$ is the largest root of $x^5 - 13x^4 + 56x^3 - 100x^2 + 72x - 16 = 0$.

Moreover, we also provide a sufficient condition involving its \mathcal{D} -index to ensure that a connected graph G is a $\mathcal{P}_{\geq 2}$ -factor deleted graph.

Theorem 1.2. *Let G be a connected graph of order n . Then the following holds.*

- (i) For $n \geq 4$ and $n \neq 6$, if $\partial(G) < \hat{\eta}(n)$, then G is a $\mathcal{P}_{\geq 2}$ -factor deleted graph, where $\hat{\eta}(n)$ is the largest root of $x^3 - (n - 3)x^2 - (5n - 9)x - 3n + 5 = 0$.
- (ii) For $n = 6$, if $\partial(G) < \tilde{\eta}_1$, then G is a $\mathcal{P}_{\geq 2}$ -factor deleted graph, where $\tilde{\eta}_1$ is the largest root of $x^4 - 2x^3 - 36x^2 - 74x - 33 = 0$.

The remainder of the paper is organized as follows. In Section 2, we present some preliminary results, which will be used in the subsequent sections. The proof of Theorem 1.1 is given in Section 3. Section 4 provides the proof of Theorem 1.2. In Section 5, we construct extremal graphs to illustrate that all the aforementioned bounds are best possible.

2. PRELIMINARY

In this section, we present some definitions, preliminary results and lemmas which will be used in the subsequent sections.

Let G be a graph with vertex set $V(G)$ and edge set $E(G)$, we use n and m to denote its order and size, respectively. For a subset $S \subseteq V(G)$, we use $G[S]$ and $G - S = G[V(G) \setminus S]$ to denote the subgraphs of G induced by S and $V(G) \setminus S$, respectively. For two disjoint graphs G_1 and G_2 , we use $G_1 \cup G_2$ and $G_1 \nabla G_2$ to denote the *union* and *join* of G_1 and G_2 , respectively. For $u, v \in V(G)$, the *distance* between u and v , denoted by $d(u, v)$, is the length of a shortest path that contains both u and v .

For a graph G with $V(G) = \{v_1, v_2, \dots, v_n\}$, the *adjacency matrix* $A(G) = (a_{ij})$ is an $n \times n$ matrix with $a_{ij} = 1$ if vertices v_i, v_j are adjacent and 0 otherwise. The *signless Laplacian matrix* $Q(G)$ of a graph G is defined as $Q(G) = D(G) + A(G)$, where $D(G) = \text{diag}(d_1, d_2, \dots, d_n)$ denotes the diagonal matrix of vertex degrees. The *distance matrix* $\mathcal{D}(G)$ of a connected graph G is defined as $\mathcal{D}(G) = (d_{i,j})$, where $d_{i,j} = d(i, j)$, i.e., the (i, j) entry is equal to the distance $d(i, j)$ between vertices i and j . Clearly, $A(G)$, $Q(G)$ and $\mathcal{D}(G)$ are real symmetric matrices. The largest eigenvalues of the adjacency matrix $A(G)$, the signless Laplacian matrix $Q(G)$ and the distance matrix $\mathcal{D}(G)$ are respectively called the A -index, Q -index, and \mathcal{D} -index of G , denoted by $\rho(G)$, $q(G)$ and $\partial(G)$.

The eigenvalues of an $n \times n$ real symmetric matrix M are denoted by $\lambda_1(M) \geq \lambda_2(M) \geq \dots \geq \lambda_n(M)$, where we always assume the eigenvalues to be arranged in nonincreasing order. Given a partition $\pi = (X_1, X_2, \dots, X_t)$ of the set $\{1, 2, \dots, n\}$ and a matrix B whose rows and columns are labelled with elements in $\{1, 2, \dots, n\}$, B can be expressed as the following partitioned matrix

$$B = \begin{pmatrix} B_{11} & \cdots & B_{1t} \\ \vdots & \ddots & \vdots \\ B_{t1} & \cdots & B_{tt} \end{pmatrix}$$

with respect to π . The *quotient matrix* B_π of B with respect to π is the t by t matrix (b_{ij}) such that each entry b_{ij} is the average row sum of B_{ij} . If the row sum of each block B_{ij} is a constant, then the partition is *equitable*.

Lemma 2.1 ([3, 8]). *Let M be a real symmetric matrix. If B_π is an equitable quotient matrix of M , then the eigenvalues of B_π are also eigenvalues of M . Furthermore, if M is nonnegative and irreducible, then $\lambda_1(M) = \lambda_1(B_\pi)$.*

Lemma 2.2 ([3]). *Let B be a symmetric $s \times s$ matrix, and let R be a $t \times t$ principal submatrix of B for some $t < s$. If the eigenvalues of B are $\theta_1 \geq \theta_2 \geq \dots \geq \theta_s$, and the eigenvalues of R are $\eta_1 \geq \eta_2 \geq \dots \geq \eta_t$, then $\theta_i \geq \eta_i \geq \theta_{s-t+i}$ for all $1 \leq i \leq t$.*

Lemma 2.3 ([15]). *Let G be a connected graph with two nonadjacent vertices $u, v \in V(G)$. Then $\partial(G + uv) < \partial(G)$.*

Recall that the *Wiener index* of G is defined as $W(G) = \sum_{i < j} d_{ij}$, where d_{ij} is the distance between v_i and v_j . This definition allows us to easily derive the following lemma using the Rayleigh quotient, as detailed in [10].

Lemma 2.4 ([10]). *Let G be a connected graph with order n . Then*

$$\partial(G) = \max_{\mathbf{x} \neq \mathbf{0}} \frac{\mathbf{x}^T \mathcal{D}(G) \mathbf{x}}{\mathbf{x}^T \mathbf{x}} \geq \frac{\mathbf{1}^T \mathcal{D}(G) \mathbf{1}}{\mathbf{1}^T \mathbf{1}} = \frac{2W(G)}{n},$$

where $\mathbf{1} = (1, 1, \dots, 1)^T$.

For any $S \subseteq V(G)$, let $i(G - S)$ denote the number of isolated vertices in the graph $G - S$. An *isolated vertex* is a vertex of degree 0, and an *isolated edge* is an edge which does not have a common endpoint with any other edge in G . A *pendant edge* is an edge with an endpoint of degree 1.

Lemma 2.5 ([1]). *A graph G has a $\mathcal{P}_{\geq 2}$ -factor if and only if $i(G - S) \leq 2|S|$ for all $S \subseteq V(G)$.*

Lemma 2.6 ([16]). *Let G be a connected graph. Then G is a $\mathcal{P}_{\geq 2}$ -factor deleted graph if and only if for all $S \subseteq V(G)$, the following three statements hold:*

- (i) $i(G - S) \leq 2|S|$;
- (ii) *If there exists an isolated edge in $G - S$, then $i(G - S) \leq 2|S| - 2$;*
- (iii) *If there exists a pendant edge in $G - S$, then $i(G - S) \leq 2|S| - 1$.*

Lemma 2.7 ([9]). *Let G be an n -vertex connected graph.*

- (i) *For $n \geq 4$ and $n \neq 7, 8, 10$, if $q(G) > \theta(n)$, where $\theta(n)$ is the largest root of $x^3 - 3(n - 3)x^2 + n(2n - 9)x - 2(n - 4)(n - 5) = 0$, then G has a $\mathcal{P}_{\geq 2}$ -factor.*
- (ii) *For $n = 7$, if $q(G) > \frac{9 + \sqrt{65}}{2}$, then G has a $\mathcal{P}_{\geq 2}$ -factor.*
- (iii) *For $n = 8$, if $q(G) > 5 + \sqrt{21}$, then G has a $\mathcal{P}_{\geq 2}$ -factor.*
- (iv) *For $n = 10$, if $q(G) > 7 + \sqrt{37}$, then G has a $\mathcal{P}_{\geq 2}$ -factor.*

Lemma 2.8 ([9]). *Let G be an n -vertex connected graph.*

- (i) *For $n \geq 4$ and $n \neq 7$, if $\partial(G) < \eta(n)$, where $\eta(n)$ is the largest root of $x^3 - (n - 1)x^2 + (29 - 9n)x - 5n + 17 = 0$, then G has a $\mathcal{P}_{\geq 2}$ -factor.*
- (ii) *For $n = 7$, if $\partial(G) < \frac{9 + \sqrt{89}}{2}$, then G has a $\mathcal{P}_{\geq 2}$ -factor.*

3. PROOF OF THEOREM 1.1

In this section, we give the proof of Theorem 1.1, which presents a sufficient condition to ensure that a connected graph G is a $\mathcal{P}_{\geq 2}$ -factor deleted graph in terms of its Q -index.

Proof of Theorem 1.1. Suppose to the contrary that G is not $\mathcal{P}_{\geq 2}$ -factor deleted. Choose a connected graph G of order n such that its Q -index is as large as possible. Let

$$\hat{h}(x) = x^3 - (3n - 5)x^2 + (2n^2 - 5n)x - 2n^2 + 10n - 12$$

and let $\hat{\theta}(n)$ be the largest root of $\hat{h}(x) = 0$. Denote by $\theta(n)$ the largest zero of $h(x)$, where $h(x) = x^3 - 3(n - 3)x^2 + n(2n - 9)x - 2(n - 4)(n - 5)$ is defined in Lemma 2.7. Then we proceed with the following two cases.

Case 1. G has no $\mathcal{P}_{\geq 2}$ -factor.

By Lemma 2.7, we have $q(G) \leq \theta(n)$ for $n \geq 4$ and $n \neq 7, 8, 10$; $q(G) \leq \frac{9+\sqrt{65}}{2}$ for $n = 7$; $q(G) \leq 5 + \sqrt{21}$ for $n = 8$; $q(G) \leq 7 + \sqrt{37}$ for $n = 10$. In order to obtain a contradiction to the condition in Theorem 1.1, we aim to show that $\theta(n) \leq \hat{\theta}(n)$ for $n \geq 4$ and $n \neq 6$; $\theta(6) \leq \tilde{\theta}$ for $n = 6$; $\frac{9+\sqrt{65}}{2} \leq \hat{\theta}(7)$ for $n = 7$; $5 + \sqrt{21} \leq \hat{\theta}(8)$ for $n = 8$; $7 + \sqrt{37} \leq \hat{\theta}(10)$ for $n = 10$.

By a simple calculation, we obtain that $\theta(4) = 4 < \frac{5+\sqrt{17}}{2} = \hat{\theta}(4)$ for $n = 4$; If $n = 5$, then $\theta(5) = 5 < \frac{7+\sqrt{33}}{2} = \hat{\theta}(5)$; If $n = 6$, then $\theta(6) \approx 6.2015 < 6.4937 \approx \tilde{\theta}$; If $n = 7$, then $\frac{9+\sqrt{65}}{2} < \frac{11+\sqrt{89}}{2} = \hat{\theta}(7)$; If $n = 8$, then $5 + \sqrt{21} < \frac{13+\sqrt{129}}{2} = \hat{\theta}(8)$; If $n = 10$, then $7 + \sqrt{37} < \frac{17+\sqrt{233}}{2} = \hat{\theta}(10)$. Next, we prove that $\theta(n) < \hat{\theta}(n)$ for $n \geq 7$, it suffices to prove that $\hat{h}(\theta(n)) < 0$. According to the proof of Lemma 2.7, we know that $\theta(n) > 2(n-4)$.

$$\hat{h}(x) - h(x) = -4x^2 + 4nx - 8n + 28.$$

It's not difficult to find that $\hat{h}(x) - h(x)$ decreases strictly on $[\frac{n}{2}, +\infty)$. Since $\frac{n}{2} < 2(n-4)$, $\hat{h}(x) - h(x)$ also decreases strictly on $[2(n-4), +\infty)$. By $\theta(n) > 2(n-4)$, we have

$$\hat{h}(\theta(n)) - h(\theta(n)) < \hat{h}(2(n-4)) - h(2(n-4)) = -8n^2 + 88n - 288 \leq -64 < 0.$$

As $h(\theta(n)) = 0$, $\hat{h}(\theta(n)) < 0$ implies that $\theta(n) < \hat{\theta}(n)$, as desired.

Case 2. G has a $\mathcal{P}_{\geq 2}$ -factor.

By Lemma 2.5, we have $i(G - S) \leq 2|S|$ for all subsets $S \subseteq V(G)$. Since G is not $\mathcal{P}_{\geq 2}$ -factor deleted, by Lemma 2.6, there exists a subset $S \subseteq V(G)$ such that one of the following two statements is true.

- (1) There is a pendant edge that is not an isolated edge in $G - S$, and $i(G - S) \geq 2|S|$;
- (2) There is an isolated edge in $G - S$, and $i(G - S) \geq 2|S| - 1$.

Subcase 2.1. Statement (1) holds.

In this subcase, we have $i(G - S) = 2|S|$ and $|S| \geq 0$. As the Q -index of G is as large as possible, by Lemma 2.2, the structure of G has the following properties:

- (1) $G[S]$ is a complete graph;
- (2) There is a non-trivial connected component, say H_1 , in $G - S$. And H_1 is a complete graph to which an edge has been attached;
- (3) G is the join of $G[S]$ and $G - S$, i.e., $G = G[S] \nabla (G - S)$.

Let $\hat{G}(|S|, i(G - S), |V(H_1)|)$ represents the number of vertices in every part of G . Let $s = |S|$. If $s = 0$, we see that $G = G(0, 0, n_1) = H_1$. Let v_1 be a vertex of degree 1 in G and $N_G(v_1) = \{v_2\}$. According to the partition $V(G) = \{v_1\} \cup \{v_2\} \cup V(G \setminus \{v_1, v_2\})$, the quotient matrix of $Q(G)$ is

$$B_0 = \begin{pmatrix} 1 & 1 & 0 \\ 1 & n-1 & n-2 \\ 0 & 1 & 2n-5 \end{pmatrix}.$$

Then the characteristic polynomial of B_0 is

$$\varphi(x) = x^3 - (3n-5)x^2 + (2n^2-5n)x - 2n^2 + 10n - 12.$$

Since $V(G) = \{v_1\} \cup \{v_2\} \cup V(G \setminus \{v_1, v_2\})$ is an equitable partition, by Lemma 2.1, we get that the largest root of $\varphi(x) = 0$ equals the Q -index of G . Since $\varphi(x) = \hat{h}(x)$, we obtain

$$q(G) = \hat{\theta}(n),$$

which contradicts the assumption that $q(G) > \hat{\theta}(n)$.

Now we consider that $s \geq 1$. Let v_1 be a vertex of degree 1 in H_1 and $N_{H_1}(v_1) = \{v_2\}$. Notice that $G = G_s = K_s \nabla ((K_1 \nabla (K_{n-3s-2} \cup K_1)) \cup 2sK_1)$ and $n = 3s + n_1$. According to the partition $V(G) = S \cup \{v_2\} \cup V(H_1 \setminus \{v_1, v_2\}) \cup \{v_1\} \cup I(G - S)$, where $I(G - S)$ is the set of isolated vertices in $G - S$. Then the quotient matrix of $Q(G)$ is

$$B = \begin{pmatrix} n + s - 2 & 1 & n - 3s - 2 & 1 & 2s \\ s & n - 2s - 1 & n - 3s - 2 & 1 & 0 \\ s & 1 & 2n - 5s - 5 & 0 & 0 \\ s & 1 & 0 & s + 1 & 0 \\ s & 0 & 0 & 0 & s \end{pmatrix},$$

whose characteristic polynomial is

$$\begin{aligned} \Phi_s(x) = & x^5 - (4n - 4s - 7)x^4 - (7s^2 + 6ns - 5s - 5n^2 + 16n - 10)x^3 - (22s^3 - 24ns^2 \\ & + 52s^2 + 2n^2s - 22ns + 38s + 2n^3 - 7n^2 + 12)x^2 + (8s^4 + 10ns^3 + 4s^3 - 15n^2s^2 \\ & + 50ns^2 - 32s^2 + 4n^3s - 29n^2s + 68ns - 52s + 2n^3 - 14n^2 + 32n - 24)x + 16s^5 \quad (1) \\ & - 24ns^4 + 72s^4 + 12n^2s^3 - 80ns^3 + 120s^3 - 2n^3s^2 + 26n^2s^2 - 88ns^2 + 88s^2 \\ & - 2n^3s + 14n^2s - 32ns + 24s. \end{aligned}$$

Since the partition $V(G) = S \cup \{v_2\} \cup V(H_1 \setminus \{v_1, v_2\}) \cup \{v_1\} \cup I(G - S)$ is equitable, by Lemma 2.1, the largest root of $\Phi_s(x) = 0$ equals $q(G_s)$.

We first assert that the largest root of $\hat{h}(x) = 0$ is equal to the largest root of $\Phi_0(x)$, where $\Phi_0(x) = x^5 - (4n - 7)x^4 + (5n^2 - 16n + 10)x^3 - (2n^3 - 7n^2 + 12)x^2 + (2n^3 - 14n^2 + 32n - 24)x$. In fact, by a direct computation, we obtain $\hat{\theta}(n) = \frac{1}{2}(2n - 3 + \sqrt{4n^2 - 20n + 33})$ is the largest root of $\hat{h}(x) = 0$. Moreover, we get $\Phi_0(\hat{\theta}(n)) = 0$. Next, if we prove that $\Phi_0(x)$ is monotonically increasing for any $x \geq \hat{\theta}(n)$, then we can demonstrate that $\hat{\theta}(n)$ is also the largest root of $\Phi_0(x) = 0$. The derivative of $\Phi_0(x)$ is $\Phi'_0(x) = 5x^4 - 4(4n - 7)x^3 + 3(5n^2 - 16n + 10)x^2 - 2(2n^3 - 7n^2 + 12)x + 2n^3 - 14n^2 + 32n - 24$ and

$$\begin{aligned} \Phi''_0(x) = & 20x^3 - 12(4n - 7)x^2 + 6(5n^2 - 16n + 10)x - 2(2n^3 - 7n^2 + 12) \\ = & x[20x^2 - 12(4n - 7)x + 6(5n^2 - 16n + 10)] - 2(2n^3 - 7n^2 + 12) \\ \geq & x\left[20(\hat{\theta}(n))^2 - 12(4n - 7)(\hat{\theta}(n)) + 6(5n^2 - 16n + 10)\right] - 2(2n^3 - 7n^2 + 12) \\ = & x\left[22n^2 - 100n + 144 + (12 - 4n)\sqrt{4n^2 - 20n + 33}\right] - 2(2n^3 - 7n^2 + 12) \\ \geq & 12n^3 - 55n^2 + 108n - 42 + (7n^2 - 32n + 54)\sqrt{4n^2 - 20n + 33} \\ > & 0. \end{aligned}$$

So, $\Phi'_0(x)$ is monotonically increasing on $x \geq \hat{\theta}(n)$. Therefore, we have

$$\begin{aligned} \Phi'_0(x) & \geq \Phi'_0(\hat{\theta}(n)) \\ & = \frac{1}{2}\left(4n^4 - 36n^3 + 141n^2 - 272n + 231 + (2n^3 - 11n^2 + 22n - 9)\sqrt{4n^2 - 20n + 33}\right) \\ & > 0. \end{aligned}$$

Hence, $\Phi_0(x)$ is monotonically increasing for any $x \geq \hat{\theta}(n)$, as desired.

Next, we will prove that $\Phi_0(\hat{\theta}(n)) - \Phi_s(\hat{\theta}(n)) < 0$ for $s \geq 1$.

- $s = 1$ and $n_1 = 3$.

Then $G = K_1 \nabla (K_{1,2} \cup 2K_1)$ and $n = 6$. By a direct calculation, we have $q(G) = q(K_1 \nabla (K_{1,2} \cup 2K_1)) = \tilde{\theta}$, where $\tilde{\theta}$ is the largest root of $x^5 - 13x^4 + 56x^3 - 100x^2 + 72x - 16 = 0$, a contradiction.

- $s = 1$ and $n_1 \geq 4$.

Then $G = G_1$ and $n = 3s + n_1 \geq 7$. Recall that $q(G(0, 0, n_1)) = \hat{\theta}(n)$. Since K_{n-1} is a proper subgraph of $G(0, 0, n_1)$, by Lemma 2.2, one has $q(G(0, 0, n_1)) > q(K_{n-1}) = 2(n - 2)$, i.e.,

$$\hat{\theta}(n) > 2(n - 2). \tag{2}$$

We are to show that $\Phi_1(\hat{\theta}(n)) > 0$. In fact,

$$\begin{aligned} \Phi_0(x) - \Phi_1(x) &= -x^2[4x^2 - (6n + 2)x - 2n^2 + 46n - 112] - x(4n^3 - 44n^2 + 128n - 72) \\ &\quad + 4n^3 - 52n^2 + 224n - 320. \end{aligned}$$

Now, we consider the monotonicity of $\Phi_0(x) - \Phi_1(x)$ on $[2(n - 2), +\infty)$. Let $h_1(x) = -x^2[4x^2 - (6n + 2)x - 2n^2 + 46n - 112]$ and $h_2(x) = -x(4n^3 - 44n^2 + 128n - 72)$. We will prove that $h_1(x)$ and $h_2(x)$ decrease monotonically on $[2(n - 2), +\infty)$.

Let $h_1(x) = p_1(x) \cdot p_2(x)$, where $p_1(x) = -x^2$, $p_2(x) = 4x^2 - (6n + 2)x - 2n^2 + 46n - 112$. Notice that $p_2(x)$ increases strictly on $[\frac{3n+1}{4}, +\infty)$. Since $\frac{3n+1}{4} < 2(n - 2)$, $p_2(x)$ also increases strictly on $[2(n - 2), +\infty)$. By $n = 3s + n_1 \geq 7$, we have $p_2(x) > p_2(2(n - 2)) = 2n^2 + 2n - 40 \geq 72 > 0$. Thus, $p_2(x)$ is positive and increases strictly on $[2(n - 2), +\infty)$. Recall that $p_1(x) = -x^2$, then $h_1(x)$ is a strictly decreasing function on $[2(n - 2), +\infty)$.

For $h_2(x)$, let $h_2(x) = -x \cdot t_1(n)$, where $t_1(n) = 4n^3 - 44n^2 + 128n - 72$. As $n = 3s + n_1 \geq 7$, we have $t_1(n) = n(4n^2 - 44n + 128) - 72 \geq 16n - 72 \geq 40 > 0$. Hence, $h_2(x)$ decreases strictly on $[2(n - 2), +\infty)$. Finally, we see that $\Phi_0(x) - \Phi_1(x)$ decreases strictly on $[2(n - 2), +\infty)$. By (2), we have

$$\Phi_0(\hat{\theta}(n)) - \Phi_1(\hat{\theta}(n)) < \Phi_0(2(n - 2)) - \Phi_1(2(n - 2)) = -16n^4 + 132n^3 - 324n^2 + 208n + 32 < 0.$$

As $\Phi_0(\hat{\theta}(n)) = 0$, $\Phi_1(\hat{\theta}(n)) > 0$ implies that $q(G) < \hat{\theta}(n)$, a contradiction.

- $s = 2$ and $n_1 = 3$.

Then $G = K_2 \nabla (K_{1,2} \cup 4K_1)$ and $n = 9$. By a direct calculation, we have $q(G) \approx 10.8824$ and $\Phi_0(q(G)) < 0$, which means that $q(G) < \hat{\theta}(n)$, a contradiction.

- $s = 2$ and $n_1 \geq 4$.

Then $G = G_2$ and $n = 3s + n_1 \geq 10$. We are to show that $\Phi_2(\hat{\theta}(n)) > 0$.

$$\begin{aligned} \Phi_0(x) - \Phi_2(x) &= -x^2[8x^2 - (12n + 18)x - 4n^2 + 140n - 460] - x(8n^3 - 118n^2 + 416n - 72) \\ &\quad + 12n^3 - 228n^2 + 1440n - 3024. \end{aligned}$$

Now, we consider the monotonicity of $\Phi_0(x) - \Phi_2(x)$ on $[2(n - 2), +\infty)$. Let $h_3(x) = -x^2[8x^2 - (12n + 18)x - 4n^2 + 140n - 460]$ and $h_4(x) = -x(8n^3 - 118n^2 + 416n - 72)$. We will prove that $h_3(x)$ and $h_4(x)$ decrease monotonically on $[2(n - 2), +\infty)$.

Let $h_3(x) = p_3(x) \cdot p_4(x)$, where $p_3(x) = -x^2$, $p_4(x) = 8x^2 - (12n + 18)x - 4n^2 + 140n - 460$. Notice that $p_4(x)$ increases strictly on $[\frac{6n+9}{8}, +\infty)$. Since $\frac{6n+9}{8} < 2(n - 2)$, $p_4(x)$ also increases strictly on $[2(n - 2), +\infty)$. By $n = 3s + n_1 \geq 10$, we have $p_4(x) > p_4(2(n - 2)) = 4n^2 + 24n - 260 \geq 380 > 0$. Thus, $p_4(x)$ is positive and increases strictly on $[2(n - 2), +\infty)$. Recall that $p_3(x) = -x^2$, then $h_3(x)$ is a strictly decreasing function on $[2(n - 2), +\infty)$.

For $h_4(x)$, let $h_4(x) = -x \cdot t_2(n)$, where $t_2(n) = 8n^3 - 118n^2 + 416n - 72$. As $n = 3s + n_1 \geq 10$, we have $t_2(n) = n(8n^2 - 118n + 416) - 72 \geq 36n - 72 \geq 288 > 0$. Hence, $h_4(x)$ decreases strictly on $[2(n - 2), +\infty)$. In the end, we see that $\Phi_0(x) - \Phi_2(x)$ decreases strictly on $[2(n - 2), +\infty)$. By (2), we have

$$\Phi_0(\hat{\theta}(n)) - \Phi_2(\hat{\theta}(n)) < \Phi_0(2(n - 2)) - \Phi_2(2(n - 2)) = -32n^4 + 248n^3 - 172n^2 - 1296n + 848 < 0.$$

As $\Phi_0(\hat{\theta}(n)) = 0$, $\Phi_2(\hat{\theta}(n)) > 0$ implies that $q(G) < \hat{\theta}(n)$, a contradiction.

- If $s \geq 3$ and $n_1 \geq 3$.

Then $G = G_s$ and $n = 3s + n_1 \geq 12$. In what follows, we are to show that $\Phi_s(\hat{\theta}(n)) > 0$.

$$\begin{aligned} \Phi_0(x) - \Phi_s(x) &= -s \left[4x^4 - (6n + 7s - 5)x^3 + (24ns - 22s^2 - 52s - 2n^2 + 22n - 38)x^2 \right. \\ &\quad + (4n^3 - (15s + 29)n^2 + (10s^2 + 50s + 68)n + 8s^3 + 4s^2 - 32s - 52)x \\ &\quad + 16s^4 - 24ns^3 + 72s^3 + 12n^2s^2 - 80ns^2 + 120s^2 - 2n^3s + 26n^2s - 88ns \\ &\quad \left. + 88s - 2n^3 + 14n^2 - 32n + 24 \right] \\ &\triangleq -s \cdot [h_5(x) + h_6(x) + f(n, s)], \end{aligned} \tag{3}$$

where $h_5(x) = x^2[4x^2 - (6n + 7s - 5)x + 24ns - 22s^2 - 52s - 2n^2 + 22n - 38]$, $h_6(x) = [4n^3 - (15s + 29)n^2 + (10s^2 + 50s + 68)n + 8s^3 + 4s^2 - 32s - 52]x$ and $f(n, s) = 16s^4 - 24ns^3 + 72s^3 + 12n^2s^2 - 80ns^2 + 120s^2 - 2n^3s + 26n^2s - 88ns + 88s - 2n^3 + 14n^2 - 32n + 24$. Now, we consider the monotonicity of $h_5(x)$ and $h_6(x)$ on $[2(n - 2), +\infty)$, respectively.

Let $h_5(x) = p_5(x) \cdot p_6(x)$, where $p_5(x) = x^2$, $p_6(x) = 4x^2 - (6n + 7s - 5)x + 24ns - 22s^2 - 52s - 2n^2 + 22n - 38$. Notice that $p_6(x)$ increases strictly on $[\frac{6n+7s-5}{8}, +\infty)$. Since $\frac{6n+7s-5}{8} < 2(n - 2)$, $p_6(x)$ also increases strictly on $[2(n - 2), +\infty)$. By $n = 3s + n_1 \geq 3s + 3$, we have $p_6(x) > p_6(2(n - 2)) = 2[n^2 + (5s - 4)n - s(11s + 12) + 3] \geq 2(13s^2 + 9s) > 0$. Thus, $p_6(x)$ is positive and increases strictly on $[2(n - 2), +\infty)$. Hence, $h_5(x)$ is a strictly increasing function on $[2(n - 2), +\infty)$.

Let $h_6(x) = x \cdot t_3(n)$, where $t_3(n) = 4n^3 - (15s + 29)n^2 + (10s^2 + 50s + 68)n + 8s^3 + 4s^2 - 32s - 52$. As $n \geq 3s + 3$, we have $t_3'(n) = 12n^2 - 2(15s + 29)n + 10s^2 + 50s + 68 \geq 2(14s^2 + s + 1) > 0$. It is obvious that $t_3(n)$ is strictly increasing in the interval $[3s + 3, +\infty)$. It follows that $t_3(n) > t_3(3s + 3) = 11s^3 - 23s^2 - 11s - 1 > 0$. Therefore, $h_6(x)$ increases strictly on $[2(n - 2), +\infty)$. Finally, we see that $h_5(x) + h_6(x) + f(n, s)$ increases strictly on $[2(n - 2), +\infty)$. By (2), we have

$$\begin{aligned} &h_5(\hat{\theta}(n)) + h_6(\hat{\theta}(n)) + f(n, s) \\ &> h_5(2(n - 2)) + h_6(2(n - 2)) + f(n, s) \\ &= n[n(16n^2 + (8s - 140)n - 56s^2 - 70s + 450) - 8s^3 + 240s^2 + 192s - 632] + 16s^4 + 40s^3 \\ &\quad - 248s^2 - 168s + 328 \\ &\geq n[n(112s^2 - 178s + 174) - 8s^3 + 240s^2 + 192s - 632] + 16s^4 + 40s^3 - 248s^2 - 168s + 328 \\ &\geq n(328s^3 + 42s^2 + 180s - 110) + 16s^4 + 40s^3 - 248s^2 - 168s + 328 \\ &\geq 1000s^4 + 1150s^3 + 418s^2 + 42s - 2 > 0. \end{aligned}$$

Therefore, $\Phi_0(\hat{\theta}(n)) - \Phi_s(\hat{\theta}(n)) = -s \cdot [h_5(\hat{\theta}(n)) + h_6(\hat{\theta}(n)) + f(n, s)] < 0$. It follows from the fact $\Phi_0(\hat{\theta}(n)) = 0$ that $\Phi_s(\hat{\theta}(n)) > 0$ if $s \geq 3$, as desired.

Subcase 2.2. Statement (2) holds.

In this subcase, we have $|S| \geq 1$ and $2|S| - 1 \leq i(G - S) \leq 2|S|$, i.e., $i(G - S) = 2|S| - 1$ or $i(G - S) = 2|S|$. As the Q -index of G is as large as possible, by Lemma 2.2, the structure of G has the following properties:

- (1) $G[S]$ is a complete graph;
- (2) There are at most two non-trivial connected components in $G - S$, one of which is a complete graph, say H_1 , and the other is a K_2 ;
- (3) G is the join of $G[S]$ and $G - S$, i.e., $G = G[S] \nabla (G - S)$.

We also put $|S| = s \geq 1$ and $|V(H_1)| = n_1$. Then we have $n_1 = 0$ or $n_1 \geq 2$. Next, we distinguish the following two subcases with respect to the value of $i(G - S)$.

Subcase 2.2.1. $i(G - S) = 2s - 1$.

- $n_1 = 0$.

Then $G = K_s \nabla (K_2 \cup (2s - 1)K_1)$ and $n = 3s + 1 \geq 4$. According to the partition $V(G) = V(K_s) \cup V(K_2) \cup V((2s - 1)K_1)$, the quotient matrix of $Q(G)$ is

$$Q_1 = \begin{pmatrix} 4s - 1 & 2 & 2s - 1 \\ s & s + 2 & 0 \\ s & 0 & s \end{pmatrix}.$$

Then the characteristic polynomial of Q_1 is

$$f_1(x) = x^3 - (6s + 1)x^2 + (7s^2 + 7s - 2)x - 2s^3 - 2s^2.$$

Since $V(G) = V(K_s) \cup V(K_2) \cup V((2s - 1)K_1)$ is an equitable partition, together with Lemma 2.1, we obtain that the largest root of $f_1(x) = 0$, say q_1 , equals the Q -index of G .

If $s = 1$, then $n = 4$ and $G = K_1 \nabla (K_2 \cup K_1)$. By a direct calculation, we have $q(G) = \frac{5 + \sqrt{17}}{2} = \hat{\theta}(4)$, which is a contradiction.

We are to show that $f_1(\hat{\theta}(n)) > 0$ for $s \geq 2$. Plugging $n = 3s + 1$ into n of $\hat{h}(x)$ implies $\hat{h}(x) = x^3 - (9s - 2)x^2 + (18s^2 - 3s - 3)x - 18s^2 + 18s - 4$. Then

$$\hat{h}(x) - f_1(x) = -(3s - 3)x^2 + (11s^2 - 10s - 1)x + 2s^3 - 16s^2 + 18s - 4.$$

Clearly, $\frac{11s^2 - 10s - 1}{2(3s - 3)} < 2(3s - 1)$. Hence, $\hat{h}(x) - f_1(x)$ is a strictly decreasing function on $[2(3s - 1), +\infty)$. Then by (2), we obtain

$$\hat{h}(\hat{\theta}(n)) - f_1(\hat{\theta}(n)) < \hat{h}(2(3s - 1)) - f_1(2(3s - 1)) = -40s^3 + 82s^2 - 52s + 10 < 0.$$

As $\hat{h}(\hat{\theta}(n)) = 0$, $f_1(\hat{\theta}(n)) > 0$ implies that $q(G) = q_1 < \hat{\theta}(n)$, a contradiction.

- $n_1 \geq 2$.

Then $G = K_s \nabla (K_{n_1} \cup K_2 \cup (2s - 1)K_1)$ and $n = 3s + n_1 + 1 \geq 3s + 3$. According to the partition $V(G) = V(K_s) \cup V((2s - 1)K_1) \cup V(K_2) \cup V(K_{n_1})$, the quotient matrix of $Q(G)$ is

$$Q_2 = \begin{pmatrix} n + s - 2 & 2s - 1 & 2 & n - 3s - 1 \\ s & s & 0 & 0 \\ s & 0 & s + 2 & 0 \\ s & 0 & 0 & 2n - 5s - 4 \end{pmatrix}.$$

Then the characteristic polynomial of Q_2 is

$$\begin{aligned} f_2(x) = & x^4 - (3n - 2s - 4)x^3 + (2ns - 11s^2 - 12s + 2n^2 - 2n - 4)x^2 + (9ns^2 - 4s^2 - 4n^2s \\ & + 20ns - 24s - 4n^2 + 16n - 16)x + 8s^4 - 8ns^3 + 36s^3 + 2n^2s^2 - 26ns^2 + 32s^2 + 4n^2s \\ & - 12ns + 8s. \end{aligned}$$

Since $V(G) = V(K_s) \cup V((2s - 1)K_1) \cup V(K_2) \cup V(K_{n_1})$ is an equitable partition, together with Lemma 2.1, we obtain that the largest root of $f_2(x) = 0$, say q_2 , equals the Q -index of G .

We are to show that $f_2(\hat{\theta}(n)) > 0$ for $s \geq 1$. By a direct calculation, we have

$$\begin{aligned} x \cdot \hat{h}(x) - f_2(x) &= -(2s - 1)x^3 + (11s^2 - 2ns + 12s - 3n + 4)x^2 - (9ns^2 - 4s^2 - 4n^2s \\ &\quad + 20ns - 24s - 2n^2 + 6n - 4)x - 8s^4 + 8ns^3 - 36s^3 - 2n^2s^2 + 26ns^2 \\ &\quad - 32s^2 - 4n^2s + 12ns - 8s \\ &\triangleq g_1(x). \end{aligned}$$

Now, we consider the monotonicity of $g_1(x)$ on $[2(n - 2), +\infty)$. It's not difficult to find $g'_1(x) = -3(2s - 1)x^2 + 2(11s^2 - 2ns + 12s - 3n + 4)x - 9ns^2 + 4s^2 + 4n^2s - 20ns + 24s + 2n^2 - 6n + 4$. Obviously, $g'_1(x)$ decreases strictly on $[\frac{11s^2 - 2ns + 12s - 3n + 4}{3(2s - 1)}, +\infty)$. Since $\frac{11s^2 - 2ns + 12s - 3n + 4}{3(2s - 1)} < 2(n - 2)$, $g'_1(x)$ also decreases strictly on $[2(n - 2), +\infty)$. Hence, by $n \geq 3s + 3$, we have

$$\begin{aligned} g'_1(x) < g'_1(2(n - 2)) &= -(28s - 2)n^2 + (35s^2 + 140s - 14)n - 84s^2 - 168s + 20 \\ &\leq -147s^3 - 45s^2 - 6s - 4 < 0. \end{aligned}$$

So, $g_1(x)$ decreases strictly on $[2(n - 2), +\infty)$ and

$$\begin{aligned} g_1(x) < g_1(2(n - 2)) &= -n[16sn^2 - (24s^2 + 116s - 4)n - 8s^3 + 106s^2 + 276s - 16] - 8s^4 - 36s^3 \\ &\quad + 128s^2 + 216s - 16 \\ &\leq -n(64s^3 - 26s^2 + 84s - 4) - 8s^4 - 36s^3 + 128s^2 + 216s - 16 \\ &\leq -200s^4 - 150s^3 - 46s^2 - 24s - 4 < 0. \end{aligned}$$

That is, we obtain that $x \cdot \hat{h}(x) - f_2(x)$ is a strictly decreasing function on $[2(n - 2), +\infty)$. By (2), we get

$$\hat{\theta}(n) \cdot \hat{h}(\hat{\theta}(n)) - f_2(\hat{\theta}(n)) < 2(n - 2) \cdot \hat{h}(2(n - 2)) - f_2(2(n - 2)) = g_1(2(n - 2)) < 0.$$

As $\hat{h}(\hat{\theta}(n)) = 0$, $f_2(\hat{\theta}(n)) > 0$ implies that $q(G) = q_2 < \hat{\theta}(n)$, a contradiction.

Subcase 2.2.2. $i(G - S) = 2s$.

- $n_1 = 0$.

Then $G = K_s \nabla (K_2 \cup 2sK_1)$ and $n = 3s + 2 \geq 5$. According to the partition $V(G) = V(K_s) \cup V(2sK_1) \cup V(K_2)$, the quotient matrix of $Q(G)$ is

$$Q_3 = \begin{pmatrix} 4s & 2s & 2 \\ s & s & 0 \\ s & 0 & s + 2 \end{pmatrix}.$$

Then the characteristic polynomial of Q_3 is

$$f_3(x) = x^3 - (6s + 2)x^2 + (7s^2 + 8s)x - 2s^3 - 2s^2.$$

Since $V(G) = V(K_s) \cup V(2sK_1) \cup V(K_2)$ is an equitable partition, together with Lemma 2.1, we obtain that the largest root of $f_3(x) = 0$, say q_3 , equals the Q -index of G .

We will prove $f_3(\hat{\theta}(n)) > 0$ for $s \geq 1$. Plugging $n = 3s + 2$ into n of $\hat{h}(x)$ implies $\hat{h}(x) = x^3 - (9s + 1)x^2 + (18s^2 + 9s - 2)x - 18s^2 + 6s$. Then

$$\hat{h}(x) - f_3(x) = -(3s - 1)x^2 + (11s^2 + s - 2)x + 2s^3 - 16s^2 + 6s.$$

It is obvious that $\hat{h}(x) - f_3(x)$ decreases strictly on $[\frac{11s^2+s-2}{2(3s-1)}, +\infty)$. Since $\frac{11s^2+s-2}{2(3s-1)} < 6s$, $\hat{h}(x) - f_3(x)$ also decreases strictly on $[6s, +\infty)$. Hence, by (2) we have

$$\hat{h}(\hat{\theta}(n)) - f_3(\hat{\theta}(n)) < \hat{h}(6s) - f_3(6s) = -40s^3 + 26s^2 - 6s < 0.$$

As $\hat{h}(\hat{\theta}(n)) = 0$, $f_3(\hat{\theta}(n)) > 0$ implies that $q(G) = q_3 < \hat{\theta}(n)$, a contradiction.

- $n_1 \geq 2$.

Then $G = K_s \nabla (K_{n_1} \cup K_2 \cup 2sK_1)$ and $n = 3s + n_1 + 2 \geq 3s + 4$. According to the partition $V(G) = V(K_s) \cup V(2sK_1) \cup V(K_2) \cup V(K_{n_1})$, the quotient matrix of $Q(G)$ is

$$Q_4 = \begin{pmatrix} n+s-2 & 2s & 2 & n-3s-2 \\ s & s & 0 & 0 \\ s & 0 & s+2 & 0 \\ s & 0 & 0 & 2n-5s-6 \end{pmatrix}.$$

Then the characteristic polynomial of Q_4 is

$$\begin{aligned} f_4(x) = & x^4 - (3n - 2s - 6)x^3 + (2ns - 11s^2 - 18s + 2n^2 - 4n - 4)x^2 + (9ns^2 - 8s^2 - 4n^2s \\ & + 26ns - 32s - 4n^2 + 20n - 24)x + 8s^4 - 8ns^3 + 44s^3 + 2n^2s^2 - 30ns^2 + 60s^2 + 4n^2s \\ & - 20ns + 24s. \end{aligned}$$

Since $V(G) = V(K_s) \cup V(2sK_1) \cup V(K_2) \cup V(K_{n_1})$ is an equitable partition, together with Lemma 2.1, we obtain that the largest root of $f_4(x) = 0$, say q_4 , equals the Q -index of G .

We will prove that $f_4(\hat{\theta}(n)) > 0$ for $s \geq 1$. By a direct calculation, we have

$$\begin{aligned} x \cdot \hat{h}(x) - f_4(x) = & -(2s + 1)x^3 + (11s^2 - 2ns + 18s - n + 4)x^2 - (9ns^2 - 8s^2 - 4n^2s + 26ns \\ & - 32s - 2n^2 + 10n - 12)x - 8s^4 + 8ns^3 - 44s^3 - 2n^2s^2 + 30ns^2 - 60s^2 \\ & - 4n^2s + 20ns - 24s \\ \triangleq & g_2(x). \end{aligned}$$

Now, we consider the monotonicity of $g_2(x)$ on $[2(n - 2), +\infty)$. We have $g_2'(x) = -3(2s + 1)x^2 + 2(11s^2 - 2ns + 18s - n + 4)x - 9ns^2 + 8s^2 + 4n^2s - 26ns + 32s + 2n^2 - 10n + 12$. Obviously, $g_2'(x)$ decreases strictly on $[\frac{11s^2-2ns+18s-n+4}{3(2s+1)}, +\infty)$. Since $\frac{11s^2-2ns+18s-n+4}{3(2s+1)} < 2(n - 2)$, $g_2'(x)$ also decreases strictly on $[2(n - 2), +\infty)$. Then by $n \geq 3s + 4$, we have

$$\begin{aligned} g_2'(x) < g_2'(2(n - 2)) = & -(28s + 14)n^2 + (35s^2 + 158s + 62)n - 80s^2 - 208s - 68 \\ \leq & -147s^3 - 264s^2 - 174s - 44 < 0. \end{aligned}$$

So, $g_2(x)$ decreases strictly on $[2(n - 2), +\infty)$ and

$$\begin{aligned} g_2(x) < g_2(2(n - 2)) = & -n[(16s + 8)n^2 - (24s^2 + 128s + 52)n - 8s^3 + 94s^2 + 324s + 112] \\ & - 8s^4 - 44s^3 + 84s^2 + 264s + 80 \\ \leq & -n(64s^3 + 70s^2 + 104s + 32) - 8s^4 - 44s^3 + 84s^2 + 264s + 80 \\ \leq & -200s^4 - 510s^3 - 508s^2 - 248s - 48 < 0. \end{aligned}$$

Thus, $x \cdot \hat{h}(x) - f_4(x)$ is a strictly decreasing function on $[2(n - 2), +\infty)$. By (2), we obtain

$$\hat{\theta}(n) \cdot \hat{h}(\hat{\theta}(n)) - f_4(\hat{\theta}(n)) < 2(n - 2) \cdot \hat{h}(2(n - 2)) - f_4(2(n - 2)) = g_2(2(n - 2)) < 0.$$

As $\hat{h}(\hat{\theta}(n)) = 0$, $f_4(\hat{\theta}(n)) > 0$ implies that $q(G) = q_4 < \hat{\theta}(n)$, a contradiction. This completes the proof of Theorem 1.1. \square

4. PROOF OF THEOREM 1.2

In this section, we give the proof of Theorem 1.2, which provides a sufficient condition to ensure that a connected graph G to be a $\mathcal{P}_{\geq 2}$ -factor deleted graph in terms of its \mathcal{D} -index.

Proof of Theorem 1.2. Suppose to the contrary that G is not $\mathcal{P}_{\geq 2}$ -factor deleted. Choose such a connected graph G of order n so that its \mathcal{D} -index is as small as possible.

Let

$$\hat{l}(x) = x^3 - (n - 3)x^2 - (5n - 9)x - 3n + 5$$

and let $\hat{\eta}(n)$ be the largest zero of $\hat{l}(x)$. Denote by $\eta(n)$ the largest zero of $l(x)$, where $l(x) = x^3 - (n - 1)x^2 + (29 - 9n)x - 5n + 17$ is defined in Lemma 2.8. We prove our result according to the next two possible cases.

Case 1. G has no $\mathcal{P}_{\geq 2}$ -factor.

In this case, by Lemma 2.8, we have $\partial(G) \geq \eta(n)$ if $n \geq 4$ and $n \neq 7$, $\partial(G) \geq \frac{9+\sqrt{89}}{2}$ if $n = 7$. In what follows we aim to show $\eta(n) \geq \hat{\eta}(n)$ for $n \geq 4$ and $n \neq 6, 7$; $\hat{\eta}_1 \geq \hat{\eta}(6)$ for $n = 6$, where $\hat{\eta}_1$ is the largest root of $x^4 - 2x^3 - 36x^2 - 74x - 33 = 0$; $\frac{9+\sqrt{89}}{2} \geq \hat{\eta}(7)$ for $n = 7$, then we may get a contradiction and thus the result holds.

If $n = 6$, we get $\hat{\eta}_1 \approx 7.8526 > 6.5242 \approx \hat{\eta}(6)$; If $n = 7$, we have $\frac{9+\sqrt{89}}{2} > 7.6646 \approx \hat{\eta}(7)$. In order to complete the proof, it suffices to show $\eta(n) \geq \hat{\eta}(n)$ for $n \geq 4$ and $n \neq 6, 7$. Based on the proof of Lemma 2.8, we know $\eta(n) \geq n + 5 - \frac{18}{n}$. By $n \geq 4$, one has $\eta(n) \geq n + \frac{1}{2}$. Then we have

$$\hat{l}(x) - l(x) = 2x^2 + (4n - 20)x + 2n - 12.$$

Clearly, $5 - n < n + \frac{1}{2}$. So $\hat{l}(x) - l(x)$ is a strictly increasing function in the interval $[n + \frac{1}{2}, +\infty)$. By $\eta(n) \geq n + \frac{1}{2}$, we get

$$\hat{l}(\eta(n)) - l(\eta(n)) > \hat{l}\left(n + \frac{1}{2}\right) - l\left(n + \frac{1}{2}\right) = \frac{1}{2}(12n^2 - 28n - 43) > 0.$$

As $l(\eta(n)) = 0$, $\hat{l}(\eta(n)) > 0$ implies that $\eta(n) > \hat{\eta}(n)$, as desired.

Case 2. G has a $\mathcal{P}_{\geq 2}$ -factor.

In this case, by Lemma 2.5, we have $i(G - S) \leq 2|S|$ for all subsets $S \subseteq V(G)$. Since G is not $\mathcal{P}_{\geq 2}$ -factor deleted, by Lemma 2.6, there exists a subset $S \subseteq V(G)$ such that one of the following two statements is true.

- (1) There is a pendant edge that is not an isolated edge in $G - S$, and $i(G - S) \geq 2|S|$;
- (2) There is an isolated edge in $G - S$, and $i(G - S) \geq 2|S| - 1$.

Subcase 2.1. Statement (1) holds.

In this subcase, we have $i(G - S) = 2|S|$ and $|S| \geq 0$. As the \mathcal{D} -index of G is as small as possible, by Lemma 2.3, the structure of G has the following properties:

- (1) $G[S]$ is a complete graph;
- (2) There is a non-trivial connected component, say H_1 , in $G - S$. And H_1 is a complete graph to which an edge has been attached;
- (3) G is the join of $G[S]$ and $G - S$, i.e., $G = G[S] \nabla (G - S)$.

Let $\hat{G}(|S|, i(G - S), |V(H_1)|)$ be used to specify the number of vertices in every part of G . Let $s = |S|$. If $s = 0$, we see that $G = G(0, 0, n_1) = H_1$. Let v_1 be a vertex of degree 1 in G and $N_G(v_1) = \{v_2\}$. According to the partition $V(G) = \{v_1\} \cup \{v_2\} \cup V(G \setminus \{v_1, v_2\})$, the quotient matrix of $\mathcal{D}(G)$ is

$$D_0 = \begin{pmatrix} 0 & 1 & 2(n - 2) \\ 1 & 0 & n - 2 \\ 2 & 1 & n - 3 \end{pmatrix}.$$

Then the characteristic polynomial of D_0 is

$$\phi(x) = x^3 - (n - 3)x^2 - (5n - 9)x - 3n + 5.$$

Since $V(G) = \{v_1\} \cup \{v_2\} \cup V(G \setminus \{v_1, v_2\})$ is an equitable partition, by Lemma 2.1, we get that the largest root of $\phi(x) = 0$ equals the \mathcal{D} -index of G . Since $\phi(x) = \hat{l}(x)$, we obtain

$$\partial(G) = \hat{\eta}(n),$$

which contradicts the assumption that $\partial(G) < \hat{\eta}(n)$.

Now we consider that $s \geq 1$. Let v_1 be a vertex of degree 1 in H_1 and $N_{H_1}(v_1) = \{v_2\}$. Then $G = G_s = K_s \nabla ((K_1 \nabla (K_{n-3s-2} \cup K_1)) \cup 2sK_1)$ and $n = 3s + n_1 \geq 3s + 3$. According to the partition $V(G) = S \cup \{v_2\} \cup V(H_1 \setminus \{v_1, v_2\}) \cup \{v_1\} \cup I(G - S)$, the quotient matrix of $\mathcal{D}(G)$ is

$$\begin{pmatrix} s-1 & 1 & n-3s-2 & 1 & 2s \\ s & 0 & n-3s-2 & 1 & 4s \\ s & 1 & n-3s-3 & 2 & 4s \\ s & 1 & 2(n-3s-2) & 0 & 4s \\ s & 2 & 2(n-3s-2) & 2 & 2(2s-1) \end{pmatrix}.$$

Its characteristic polynomial is

$$\begin{aligned} \Phi_s(x) = & x^5 - (n + 2s - 6)x^4 - (4ns - 14s^2 - 3s + 8n - 20)x^3 + (2ns^2 - 6s^3 + 51s^2 \\ & - 15ns + 33s - 20n + 38)x^2 + (6ns^2 - 18s^3 + 41s^2 - 13ns + 36s - 19n + 33)x \\ & - 6s^3 + 2ns^2 + 8s^2 - 2ns + 8s - 6n + 10. \end{aligned} \tag{4}$$

Note that the partition $V(G) = S \cup \{v_2\} \cup V(H_1 \setminus \{v_1, v_2\}) \cup \{v_1\} \cup I(G - S)$ is equitable. Hence, by Lemma 2.1, the largest zero of $\Phi_s(x)$ equals $\partial(G_s)$.

If $s \geq 1$ and $n_1 \geq 3$, then $G = G_s$ and $n = 3s + n_1 \geq 3s + 3$. Recall that $\partial(G(0, 0, n_1)) = \hat{\eta}(n)$. By Lemma 2.4, one has

$$\hat{\eta}(n) \geq \frac{\mathbf{1}^T \mathcal{D}(G(0, 0, n_1)) \mathbf{1}}{\mathbf{1}^T \mathbf{1}} = \frac{n^2 + n - 4}{n} = n + 1 - \frac{4}{n}. \tag{5}$$

If $s = 1$, then $G = G_1$ and $n \geq 6$, we have $\partial(G) = \partial(G_1)$ and $\hat{\eta}(n) \geq n + 1 - \frac{4}{6} = n + \frac{1}{3}$, where $\partial(G)$ is the largest root of $\Phi_1(x) = x^5 - (n - 4)x^4 - (12n - 37)x^3 - (33n - 116)x^2 - (26n - 92)x - 6n + 20 = 0$. We will prove that $\Phi_1(\hat{\eta}(n)) < 0$. By a simple computation, we get

$$\begin{aligned} \left(x + \frac{1}{2}\right)^2 \cdot \hat{l}(x) - \Phi_1(x) &= \frac{3}{4} [(8n - 33)x^3 + (33n - 135)x^2 + (29n - 113)x + 7n - 25] \\ &\triangleq \frac{3}{4} \cdot t_1(x). \end{aligned}$$

Now, we consider the monotonicity of $t_1(x)$ on $[n + \frac{1}{3}, +\infty)$, where $t_1(x) = (8n - 33)x^3 + (33n - 135)x^2 + (29n - 113)x + 7n - 25$. Let $t_1(x) = x \cdot g(x) + 7n - 25$, where $g(x) = (8n - 33)x^2 + (33n - 135)x + 29n - 113$. Clearly, $-\frac{33n-135}{2(8n-33)} < n + \frac{1}{3}$. Thus, $g(x)$ increases strictly on $[n + \frac{1}{3}, +\infty)$. Then we have $g(x) > g(n + \frac{1}{3}) = \frac{1}{9}(72n^3 + 48n^2 - 1045n - 1455) > 0$. Hence, $t_1(x)$ increases strictly on $[n + \frac{1}{3}, +\infty)$, and we get

$$\begin{aligned} t_1(x) &> t_1\left(n + \frac{1}{3}\right) = \left(n + \frac{1}{3}\right) \cdot \left(n + \frac{1}{3}\right) + 7n - 25 \\ &= \frac{1}{27}(216n^4 + 216n^3 - 3087n^2 - 5221n - 2130) > 0. \end{aligned}$$

Therefore, $(x + \frac{1}{2})^2 \cdot \hat{l}(x) - \Phi_1(x)$ increases strictly on $[n + \frac{1}{3}, +\infty)$. By $\hat{\eta}(n) \geq n + \frac{1}{3}$, we have

$$\begin{aligned} \left(\hat{\eta}(n) + \frac{1}{2}\right)^2 \cdot \hat{l}(\hat{\eta}(n)) - \Phi_1(\hat{\eta}(n)) &\geq \left(n + \frac{1}{3} + \frac{1}{2}\right)^2 \cdot \hat{l}\left(n + \frac{1}{3}\right) - \Phi_1\left(n + \frac{1}{3}\right) \\ &= \frac{3}{4} \cdot t_1\left(n + \frac{1}{3}\right) > 0. \end{aligned}$$

As $\hat{l}(\hat{\eta}(n)) = 0$, $\Phi_1(\hat{\eta}(n)) < 0$ implies that $\partial(G) > \hat{\eta}(n)$, a contradiction.

If $s \geq 2$. We are to show that $\Phi_s(\hat{\eta}(n)) < 0$. Note that $n = 3s + n_1 \geq 3s + 3 \geq 9$. Then $\hat{\eta}(n) \geq n + 1 - \frac{4}{9} > n + \frac{1}{2}$. By a direct calculation, we get

$$\begin{aligned} x^2 \cdot \hat{l}(x) - \Phi_s(x) &= x[(2s - 3)x^3 - (14s^2 - 4ns + 3s - 3n + 11)x^2 + (6s^3 - 2ns^2 - 51s^2 + 15ns \\ &\quad - 33s + 17n - 33)x + 18s^3 - 6ns^2 - 41s^2 + 13ns - 36s + 19n - 33] + 6s^3 \\ &\quad - 2ns^2 - 8s^2 + 2ns - 8s + 6n - 10 \\ &\triangleq x \cdot f(x) + 6s^3 - 2ns^2 - 8s^2 + 2ns - 8s + 6n - 10. \end{aligned}$$

Now, we consider the monotonicity of $f(x)$ on $[n + \frac{1}{2}, +\infty)$, where

$$\begin{aligned} f(x) &= (2s - 3)x^3 - (14s^2 - 4ns + 3s - 3n + 11)x^2 + (6s^3 - 2ns^2 - 51s^2 + 15ns - 33s + 17n - 33)x \\ &\quad + 18s^3 - 6ns^2 - 41s^2 + 13ns - 36s + 19n - 33. \end{aligned}$$

Then $f'(x) = 3(2s - 3)x^2 - 2(14s^2 - 4ns + 3s - 3n + 11)x + 6s^3 - 2ns^2 - 51s^2 + 15ns - 33s + 17n - 33$. Clearly, $\frac{14s^2 - 4ns + 3s - 3n + 11}{3(2s - 3)} < n + \frac{1}{2}$. Thus, $f'(x)$ increases strictly on $[n + \frac{1}{2}, +\infty)$. Then

$$\begin{aligned} f'(x) &> f'\left(n + \frac{1}{2}\right) \\ &= \frac{1}{4}[(56s - 12)n^2 - (120s^2 - 76s + 44)n + 24s^3 - 260s^2 - 138s - 185] \\ &\geq \frac{1}{4}(168s^3 + 508s^2 + 246s - 425) > 0. \end{aligned}$$

Then $f(x)$ increases strictly on $[n + \frac{1}{2}, +\infty)$. Hence, we get

$$\begin{aligned} f(x) &> f\left(n + \frac{1}{2}\right) \\ &= \frac{n}{8}[48sn^2 - (128s^2 - 152s - 36)n + 48s^3 - 576s^2 - 104s - 144] + \frac{1}{8}(168s^3 - 560s^2 - 424s - 421) \\ &\geq \frac{n}{8}(96s^3 + 360s^2 + 892s - 36) + \frac{1}{8}(168s^3 - 560s^2 - 424s - 421) \\ &\geq \frac{1}{8}(288s^4 + 1536s^3 + 3196s^2 + 2144s - 529) > 0. \end{aligned}$$

Therefore, $x^2 \cdot \hat{l}(x) - \Phi_s(x)$ increases strictly on $[n + \frac{1}{2}, +\infty)$. By $\hat{\eta}(n) > n + \frac{1}{2}$ and $n \geq 3s + 3$, we have

$$\begin{aligned}
 & (\hat{\eta}(n))^2 \cdot \hat{l}(\hat{\eta}(n)) - \Phi_s(\hat{\eta}(n)) \\
 & > \left(n + \frac{1}{2}\right)^2 \cdot \hat{l}\left(n + \frac{1}{2}\right) - \Phi_s\left(n + \frac{1}{2}\right) \\
 & = \left(n + \frac{1}{2}\right) \cdot f\left(n + \frac{1}{2}\right) + 6s^3 - 2ns^2 - 8s^2 + 2ns - 8s + 6n - 10 \\
 & = \frac{n}{16} [n(96sn^2 - (256s^2 - 352s - 72)n + 96s^3 - 1280s^2 - 56s - 252) + 384s^3 - 1728s^2 - 920s - 890] \\
 & \quad + \frac{1}{16} (264s^3 - 688s^2 - 552s - 581) \\
 & \geq \frac{n}{16} [n(192s^3 + 736s^2 + 2080s - 36) + 384s^3 - 1728s^2 - 920s - 890] + \frac{1}{16} (264s^3 - 688s^2 - 552s - 581) \\
 & \geq \frac{n}{16} (576s^4 + 3168s^3 + 6720s^2 + 5212s - 998) + \frac{1}{16} (264s^3 - 688s^2 - 552s - 581) \\
 & \geq \frac{1}{16} (1728s^5 + 11232s^4 + 29928s^3 + 35108s^2 + 12090s - 3575) \\
 & > 0.
 \end{aligned}$$

As $\hat{l}(\hat{\eta}(n)) = 0$, $\Phi_s(\hat{\eta}(n)) < 0$ implies that $\partial(G) > \hat{\eta}(n)$, a contradiction.

Subcase 2.2. Statement (2) holds.

In this subcase, we have $|S| \geq 1$ and $2|S| - 1 \leq i(G - S) \leq 2|S|$, i.e., $i(G - S) = 2|S| - 1$ or $i(G - S) = 2|S|$. As the \mathcal{D} -index of G is as small as possible, by Lemma 2.3, the structure of G has the following properties:

- (1) $G[S]$ is a complete graph;
- (2) There are at most two non-trivial connected components in $G - S$, one of which is a complete graph, say H_1 , and the other is a K_2 ;
- (3) G is the join of $G[S]$ and $G - S$, i.e., $G = G[S] \nabla (G - S)$.

We also put $|S| = s \geq 1$ and $|V(H_1)| = n_1$. Then we have $n_1 = 0$ or $n_1 \geq 2$. Next, we distinguish the following two subcases with respect to the value of $i(G - S)$.

Subcase 2.2.1. $i(G - S) = 2s - 1$.

- $n_1 = 0$.

Then $G = K_s \nabla (K_2 \cup (2s - 1)K_1)$ and $n = 3s + 1 \geq 4$. According to the partition $V(G) = V(K_s) \cup V(K_2) \cup V((2s - 1)K_1)$, the quotient matrix of $\mathcal{D}(G)$ is

$$M_1 = \begin{pmatrix} s - 1 & 2 & 2s - 1 \\ s & 1 & 2(2s - 1) \\ s & 4 & 2(2s - 2) \end{pmatrix}.$$

Then the characteristic polynomial of M_1 is

$$c_1(x) = x^3 - (5s - 4)x^2 + (2s^2 - 20s + 7)x + 6s^2 - 17s + 4.$$

Since $V(G) = V(K_s) \cup V(K_2) \cup V((2s - 1)K_1)$ is an equitable partition, together with Lemma 2.1, we obtain that the largest root of $c_1(x) = 0$, say $\partial(G)$, equals the \mathcal{D} -index of G .

If $s = 1$, then $n = 4$ and $G = K_1 \nabla (K_2 \cup K_1)$. By a direct calculation, we have $\partial(G) \approx 4.1$ and $\hat{l}(\partial(G)) > 0$, which means that $\partial(G) > \hat{\eta}(n)$, a contradiction.

We are to show that $c_1(\hat{\eta}(n)) < 0$ for $s \geq 2$. Note that $n = 3s + 1 \geq 7$. In view of (5), one has

$$\hat{\eta}(n) \geq n + 1 - \frac{4}{n} \geq n + 1 - \frac{4}{7} > n + \frac{1}{3} = 3s + \frac{4}{3}. \tag{6}$$

Plugging $n = 3s + 1$ into n of $\hat{l}(x)$ implies $\hat{l}(x) = x^3 - (3s - 2)x^2 - (15s - 4)x - 9s + 2$. Then

$$\hat{l}(x) - c_1(x) = (2s - 2)x^2 - (2s^2 - 5s + 3)x - 6s^2 + 8s - 2.$$

Now, we consider the monotonicity of $\hat{l}(x) - c_1(x)$ on $[3s + \frac{4}{3}, +\infty)$. Notice that $\frac{2s^2 - 5s + 3}{2(2s - 2)} < 3s + \frac{4}{3}$. Then $\hat{l}(x) - c_1(x)$ increases strictly on $[3s + \frac{4}{3}, +\infty)$. By $\hat{\eta}(n) > 3s + \frac{4}{3}$, we get

$$\hat{l}(\hat{\eta}(n)) - c_1(\hat{\eta}(n)) > \hat{l}\left(3s + \frac{4}{3}\right) - c_1\left(3s + \frac{4}{3}\right) = \frac{1}{9}(108s^3 + 39s^2 - 61s - 86) > 0.$$

As $\hat{l}(\hat{\eta}(n)) = 0$, $c_1(\hat{\eta}(n)) < 0$ implies that $\partial(G) > \hat{\eta}(n)$, a contradiction.

- $n_1 \geq 2$.

Then $G = K_s \nabla (K_{n_1} \cup K_2 \cup (2s - 1)K_1)$ and $n = 3s + 1 + n_1 \geq 3s + 3 \geq 6$. According to the partition $V(G) = V(K_s) \cup V((2s - 1)K_1) \cup V(K_2) \cup V(K_{n_1})$, the quotient matrix of $\mathcal{D}(G)$ is

$$M_2 = \begin{pmatrix} s - 1 & 2s - 1 & 2 & n - 3s - 1 \\ s & 2(2s - 2) & 4 & 2(n - 3s - 1) \\ s & 2(2s - 1) & 1 & 2(n - 3s - 1) \\ s & 2(2s - 1) & 4 & n - 3s - 2 \end{pmatrix}.$$

Then the characteristic polynomial of M_2 is

$$\begin{aligned} c_2(x) = & x^4 - (n + 2s - 6)x^3 - (4ns - 14s^2 - 3s + 8n - 19)x^2 + (2ns^2 - 6s^3 \\ & + 51s^2 - 15ns + 23s - 15n + 26)x - 18s^3 + 6ns^2 + 33s^2 - 11ns \\ & + 18s - 8n + 12. \end{aligned}$$

Since $V(G) = V(K_s) \cup V((2s - 1)K_1) \cup V(K_2) \cup V(K_{n_1})$ is an equitable partition, together with Lemma 2.1, we obtain that the largest root of $c_2(x) = 0$, say $\partial(G)$, equals the \mathcal{D} -index of G .

If $s = 1$ and $n = 6$, then $G = K_1 \nabla (2K_2 \cup K_1)$. By a direct calculation, we have $\partial(G) = \partial(K_1 \nabla (2K_2 \cup K_1)) = \tilde{\eta}_1$, where $\tilde{\eta}_1$ is the largest root of $x^4 - 2x^3 - 36x^2 - 74x - 33 = 0$, a contradiction. If $s = 1$ and $n \geq 7$, then $G = K_1 \nabla (K_{n-2} \cup K_2 \cup K_1)$ and $\hat{\eta}(n) \geq n + 1 - \frac{4}{n} \geq n + 1 - \frac{4}{7} > n + \frac{1}{3}$. We have $\partial(G) = \partial(K_1 \nabla (K_{n-2} \cup K_2 \cup K_1)) = \tilde{\eta}_2$, where $\tilde{\eta}_2$ is the largest root of $\tau_1(x) = x^4 - (n - 4)x^3 - (12n - 36)x^2 - (28n - 94)x - 13n + 45 = 0$. We will prove that $\tau_1(\hat{\eta}(n)) < 0$. By a simple computation, we get

$$(x + 1) \cdot \hat{l}(x) - \tau_1(x) = (6n - 24)x^2 + (20n - 80)x + 10n - 40.$$

Clearly, $-\frac{20n - 80}{2(6n - 24)} < n + \frac{1}{3}$. Thus, $(x + 1) \cdot \hat{l}(x) - \tau_1(x)$ increases strictly on $[n + \frac{1}{3}, +\infty)$. By $\hat{\eta}(n) > n + \frac{1}{3}$, we have

$$\begin{aligned} (\hat{\eta}(n) + 1) \cdot \hat{l}(\hat{\eta}(n)) - \tau_1(\hat{\eta}(n)) &> \left(n + \frac{1}{3} + 1\right) \cdot \hat{l}\left(n + \frac{1}{3}\right) - \tau_1\left(n + \frac{1}{3}\right) \\ &= (6n - 24) \left(n + \frac{1}{3}\right)^2 + (20n - 80) \left(n + \frac{1}{3}\right) + 10n - 40 \\ &= \frac{1}{3}(18n^3 - 236n - 208) > 0. \end{aligned}$$

As $\hat{l}(\hat{\eta}(n)) = 0$, $\tau_1(\hat{\eta}(n)) < 0$ implies that $\partial(G) = \tilde{\eta}_2 > \hat{\eta}(n)$, a contradiction.

Next, we are to show that $c_2(\hat{\eta}(n)) < 0$ for $s \geq 2$. Note that $n = 3s + 1 + n_1 \geq 3s + 3 \geq 9$. In view of (5), one has

$$\hat{\eta}(n) \geq n + 1 - \frac{4}{n} \geq n + 1 - \frac{4}{9} > n + \frac{1}{2}. \tag{7}$$

By a direct calculation, we obtain

$$\begin{aligned} x \cdot \hat{l}(x) - c_2(x) &= (2s - 3)x^3 - (14s^2 - 4ns + 3s - 3n + 10)x^2 + (6s^3 - 2ns^2 - 51s^2 + 15ns - 23s \\ &\quad + 12n - 21)x + 18s^3 - 6ns^2 - 33s^2 + 11ns - 18s + 8n - 12 \\ &\triangleq t_2(x). \end{aligned}$$

Now, we consider the monotonicity of $t_2(x)$ on $[n + \frac{1}{2}, +\infty)$. Notice that $t'_2(x) = 3(2s - 3)x^2 - 2(14s^2 - 4ns + 3s - 3n + 10)x + 6s^3 - 2ns^2 - 51s^2 + 15ns - 23s + 12n - 21$. Clearly, $\frac{14s^2 - 4ns + 3s - 3n + 10}{3(2s - 3)} < n + \frac{1}{2}$. Then $t'_2(x)$ is strictly increasing in the interval $[n + \frac{1}{2}, +\infty)$. By $n \geq 3s + 3$, we have

$$\begin{aligned} t'_2(x) &> t'_2\left(n + \frac{1}{2}\right) = \frac{1}{4}[(56s - 12)n^2 - (120s^2 - 76s + 56)n + 24s^3 - 260s^2 - 98s - 133] \\ &\geq \frac{1}{4}(168s^3 + 508s^2 + 250s - 409) > 0. \end{aligned}$$

Therefore, $t_2(x)$ increases strictly on $[n + \frac{1}{2}, +\infty)$. That is

$$\begin{aligned} t_2(x) &> t_2\left(n + \frac{1}{2}\right) \\ &= \frac{n}{8}[48sn^2 - (128s^2 - 152s - 4)n + 48s^3 - 576s^2 - 40s - 148] + \frac{1}{8}(168s^3 - 496s^2 - 240s - 203) \\ &\geq \frac{n}{8}(96s^3 + 360s^2 + 860s - 136) + \frac{1}{8}(168s^3 - 496s^2 - 240s - 203) \\ &\geq \frac{1}{8}(288s^4 + 1536s^3 + 3164s^2 + 1932s - 611) > 0. \end{aligned}$$

That is, we derive that $x \cdot \hat{l}(x) - c_2(x)$ increases strictly on $[n + \frac{1}{2}, +\infty)$. By $\hat{\eta}(n) > n + \frac{1}{2}$, we have

$$\hat{\eta}(n) \cdot \hat{l}(\hat{\eta}(n)) - c_2(\hat{\eta}(n)) > \left(n + \frac{1}{2}\right) \cdot \hat{l}\left(n + \frac{1}{2}\right) - c_2\left(n + \frac{1}{2}\right) = t_2\left(n + \frac{1}{2}\right) > 0.$$

As $\hat{l}(\hat{\eta}(n)) = 0$, $c_2(\hat{\eta}(n)) < 0$ implies that $\partial(G) > \hat{\eta}(n)$, a contradiction.

Subcase 2.2.2. $i(G - S) = 2s$.

- $n_1 = 0$.

Then $G = K_s \nabla (K_2 \cup 2sK_1)$ and $n = 3s + 2 \geq 5$. Notice that $n \geq 5$. In view of (5), one has

$$\hat{\eta}(n) \geq n + 1 - \frac{4}{n} \geq n + 1 - \frac{4}{5} = n + \frac{1}{5} = 3s + \frac{11}{5}. \tag{8}$$

According to the partition $V(G) = V(K_s) \cup V(K_2) \cup V(2sK_1)$, the quotient matrix of $\mathcal{D}(G)$ is

$$M_3 = \begin{pmatrix} s - 1 & 2 & 2s \\ s & 1 & 4s \\ s & 4 & 2(2s - 1) \end{pmatrix}.$$

Then the characteristic polynomial of M_3 is

$$c_3(x) = x^3 - (5s - 2)x^2 + (2s^2 - 19s - 1)x + 6s^2 - 14s - 2.$$

Since $V(G) = V(K_s) \cup V(K_2) \cup V(2sK_1)$ is an equitable partition, together with Lemma 2.1, we obtain that the largest root of $c_3(x) = 0$, say $\partial(G)$, equals the \mathcal{D} -index of G .

We will prove $c_3(\hat{\eta}(n)) < 0$ for $s \geq 1$. Plugging $n = 3s + 2$ into n of $\hat{l}(x)$ implies $\hat{l}(x) = x^3 - (3s - 1)x^2 - (15s + 1)x - 9s - 1$. Then

$$\hat{l}(x) - c_3(x) = (2s - 1)x^2 - (2s^2 - 4s)x - 6s^2 + 5s + 1.$$

Clearly, $\frac{2s^2 - 4s}{2(2s - 1)} < 3s + \frac{11}{5}$. Then $\hat{l}(x) - c_3(x)$ is strictly increasing in the interval $[3s + \frac{11}{5}, +\infty)$. By $\hat{\eta}(n) \geq 3s + \frac{11}{5}$, we obtain

$$\hat{l}(\hat{\eta}(n)) - c_3(\hat{\eta}(n)) > \hat{l}\left(3s + \frac{11}{5}\right) - c_3\left(3s + \frac{11}{5}\right) = \frac{1}{25}(300s^3 + 475s^2 + 257s - 96) > 0.$$

As $\hat{l}(\hat{\eta}(n)) = 0$, $c_3(\hat{\eta}(n)) < 0$ implies that $\partial(G) > \hat{\eta}(n)$, a contradiction.

- $n_1 \geq 2$.

Then $G = K_s \nabla (K_{n_1} \cup K_2 \cup 2sK_1)$ and $n = 3s + 2 + n_1 \geq 3s + 4 \geq 7$. According to the partition $V(G) = V(K_s) \cup V(K_{n_1}) \cup V(K_2) \cup V(2sK_1)$, the quotient matrix of $\mathcal{D}(G)$ is

$$M_4 = \begin{pmatrix} s - 1 & n - 3s - 2 & 2 & 2s \\ s & n - 3s - 3 & 4 & 4s \\ s & 2(n - 3s - 2) & 1 & 4s \\ s & 2(n - 3s - 2) & 4 & 2(2s - 1) \end{pmatrix}.$$

Then the characteristic polynomial of M_4 is

$$c_4(x) = x^4 - (n + 2s - 5)x^3 - (4ns - 14s^2 - 14s + 10n - 21)x^2 + (2ns^2 - 6s^3 + 46s^2 - 14ns + 64s - 23n + 43)x - 18s^3 + 6ns^2 + 18s^2 - 8ns + 44s - 14n + 26.$$

Since $V(G) = V(K_s) \cup V(K_{n_1}) \cup V(K_2) \cup V(2sK_1)$ is an equitable partition, together with Lemma 2.1, we obtain that the largest root of $c_4(x) = 0$, say $\partial(G)$, equals the \mathcal{D} -index of G .

If $s = 1$ and $n \geq 7$, then $G = K_1 \nabla (K_{n-5} \cup K_2 \cup 2K_1)$ and $\hat{\eta}(n) \geq n + 1 - \frac{4}{n} \geq n + 1 - \frac{4}{7} > n + \frac{1}{3}$. We have $\partial(G) = \partial(K_1 \nabla (K_{n-5} \cup K_2 \cup 2K_1)) = \tilde{\eta}_3$, where $\tilde{\eta}_3$ is the largest root of $\tau_2(x) = x^4 - (n - 3)x^3 - (14n - 49)x^2 - (35n - 147)x - 16n + 70 = 0$. We will prove that $\tau_2(\hat{\eta}(n)) < 0$. By a simple computation, we get

$$x \cdot \hat{l}(x) - \tau_2(x) = (9n - 40)x^2 + (32n - 142)x + 16n - 70.$$

Clearly, $-\frac{32n - 142}{2(9n - 40)} < n + \frac{1}{3}$. Thus, $x \cdot \hat{l}(x) - \tau_2(x)$ increases strictly on $[n + \frac{1}{3}, +\infty)$. By $\hat{\eta}(n) > n + \frac{1}{3}$, we have

$$\begin{aligned} \hat{\eta}(n) \cdot \hat{l}(\hat{\eta}(n)) - \tau_2(\hat{\eta}(n)) &> \left(n + \frac{1}{3}\right) \cdot \hat{l}\left(n + \frac{1}{3}\right) - \tau_2\left(n + \frac{1}{3}\right) \\ &\geq (9n - 40)\left(n + \frac{1}{3}\right)^2 + (32n - 142)\left(n + \frac{1}{3}\right) + 16n - 70 \\ &= \frac{1}{9}(81n^3 - 18n^2 - 1269n - 1096) > 0. \end{aligned}$$

As $\hat{l}(\hat{\eta}(n)) = 0$, $\tau_2(\hat{\eta}(n)) < 0$ implies that $\partial(G) = \tilde{\eta}_3 > \hat{\eta}(n)$, a contradiction.

Next, we will prove that $c_4(\hat{\eta}(n)) < 0$ for $s \geq 2$. Notice that $n \geq 3s + 4 \geq 10$. In view of (5), one has

$$\hat{\eta}(n) \geq n + 1 - \frac{4}{n} \geq n + 1 - \frac{4}{10} = n + \frac{3}{5}. \quad (9)$$

By a direct calculation, we have

$$\begin{aligned} x \cdot \hat{l}(x) - c_4(x) &= (2s - 2)x^3 - (14s^2 - 4ns + 14s - 5n + 12)x^2 + (6s^3 - 2ns^2 - 46s^2 + 14ns \\ &\quad - 64s + 20n - 38)x + 18s^3 - 6ns^2 - 18s^2 + 8ns - 44s + 14n - 26 \\ &\triangleq t_3(x). \end{aligned}$$

Now, we consider the monotonicity of $t_3(x)$ on $[n + \frac{3}{5}, +\infty)$. We have $t'_3(x) = 3(2s - 2)x^2 - 2(14s^2 - 4ns + 14s - 5n + 12)x + 6s^3 - 2ns^2 - 46s^2 + 14ns - 64s + 20n - 38$. Clearly, $\frac{14s^2 - 4ns + 14s - 5n + 12}{3(2s - 2)} < n + \frac{3}{5}$. Then $t'_3(x)$ is strictly increasing in the interval $[n + \frac{3}{5}, +\infty)$. By $n \geq 3s + 4$, we obtain

$$\begin{aligned} t'_3(x) &> t'_3\left(n + \frac{3}{5}\right) \\ &= \frac{1}{25} [(350s + 100)n^2 - (750s^2 + 50s + 130)n + 150s^3 - 1570s^2 - 1966s - 1364] \\ &\geq \frac{1}{25} (1050s^3 + 4580s^2 + 5444s - 284) > 0. \end{aligned}$$

Hence, $t_3(x)$ increases strictly on $[n + \frac{3}{5}, +\infty)$. Then

$$\begin{aligned} t_3(x) &> t_3\left(n + \frac{3}{5}\right) \\ &= \frac{n}{125} [(750s + 375)n^2 - (2000s^2 - 1050s - 1300)n + 750s^3 - 8750s^2 - 7600s - 3345] \\ &\quad + \frac{1}{125} (2700s^3 - 6330s^2 - 10876s - 6694) \\ &\geq \frac{n}{125} (1500s^3 + 7775s^2 + 21500s + 7855) + \frac{1}{125} (2700s^3 - 6330s^2 - 10876s - 6694) \\ &\geq \frac{1}{125} (4500s^4 + 32025s^3 + 89270s^2 + 98689s + 24726) > 0. \end{aligned}$$

That is, $x \cdot \hat{l}(x) - c_4(x)$ is strictly increasing in the interval $[n + \frac{3}{5}, +\infty)$. By $\hat{\eta}(n) \geq n + \frac{3}{5}$, we get

$$\hat{\eta}(n) \cdot \hat{l}(\hat{\eta}(n)) - c_4(\hat{\eta}(n)) > \left(n + \frac{3}{5}\right) \cdot \hat{l}\left(n + \frac{3}{5}\right) - c_4\left(n + \frac{3}{5}\right) = t_3\left(n + \frac{3}{5}\right) > 0.$$

As $\hat{l}(\hat{\eta}(n)) = 0$, $c_4(\hat{\eta}(n)) < 0$ implies that $\partial(G) > \hat{\eta}(n)$, a contradiction.

This completes the proof. □

5. EXTREMAL GRAPHS

In this section, we give the following graphs to show that the conditions established in Theorems 1.1 and 1.2 are best possible. In fact, those extremal graphs can be deduced from the proofs of Theorems 1.1 and 1.2, respectively. Let $\hat{G}(|S|, i(G - S), |V(H_1)|)$ represents the number of vertices in each specified part of G .

Example 5.1. Let n be a positive integer.

- (i) For $n \geq 4$ and $n \neq 6$, we have $q(\hat{G}(0, 0, n)) = \hat{\theta}(n)$ and $\hat{G}(0, 0, n)$ is not a $\mathcal{P}_{\geq 2}$ -factor deleted graph, where $\hat{G}(0, 0, n)$ is a complete graph to which an edge has been attached and $\hat{\theta}(n)$ is the largest root of $x^3 - (3n - 5)x^2 + (2n^2 - 5n)x - 2n^2 + 10n - 12 = 0$.
- (ii) For $n = 6$, we have $q(K_1 \nabla (K_{1,2} \cup 2K_1)) = \tilde{\theta}$ and $K_1 \nabla (K_{1,2} \cup 2K_1)$ is not a $\mathcal{P}_{\geq 2}$ -factor deleted graph, where $\tilde{\theta}$ is the largest root of $x^5 - 13x^4 + 56x^3 - 100x^2 + 72x - 16 = 0$.

Example 5.2. Let n be a positive integer.

- (i) For $n \geq 4$ and $n \neq 6$, we have $\partial(\hat{G}(0, 0, n)) = \hat{\eta}(n)$ and $\hat{G}(0, 0, n)$ is not a $\mathcal{P}_{\geq 2}$ -factor deleted graph, where $\hat{G}(0, 0, n)$ is a complete graph to which an edge has been attached and $\hat{\eta}(n)$ is the largest root of $x^3 - (n - 3)x^2 - (5n - 9)x - 3n + 5 = 0$.
- (ii) For $n = 6$, we have $\partial(K_1 \nabla (2K_2 \cup K_1)) = \tilde{\eta}_1$ and $K_1 \nabla (2K_2 \cup K_1)$ is not a $\mathcal{P}_{\geq 2}$ -factor deleted graph, where $\tilde{\eta}_1$ is the largest root of $x^4 - 2x^3 - 36x^2 - 74x - 33 = 0$.

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CONFLICTS OF INTEREST

The authors have no relevant financial or non-financial interests to disclose.

DATA AVAILABILITY STATEMENT

Data sharing not applicable to this article as no datasets were generated or analysed during the current study.

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