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Research article

Sharp bounds for the general Randić index of graphs with fixed number of vertices and cyclomatic number

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Abstract: The cyclomatic number, denoted by γ, of a graph G is the minimum number of edges of G whose removal makes G acyclic. Let $\mathscr{G}_n^\gamma$ be the class of all connected graphs with order n and cyclomatic number γ. In this paper, we characterized the graphs in $\mathscr{G}_n^\gamma$ with minimum general Randić index for $\gamma \geq 3$ and $1 \leq \alpha \leq \frac{39}{25}$. These extend the main result proved by A. Ali, K. C. Das and S. Akhter in 2022. The elements of $\mathscr{G}_n^\gamma$ with maximum general Randić index were also completely determined for $\gamma \geq 3$ and $\alpha \geq 1$.

Keywords: extremal graphs; the general Randić index; cyclomatic number; sharp bounds
Mathematics Subject Classification: 05C92, 05C76, 05C35

1. Introduction

We only consider finite and undirected graphs throughout this paper. Let $G = (V(G), E(G))$ be a graph with $n = |V(G)|$ vertices and $m = |E(G)|$ edges. For any vertex $u \in V(G)$, we use $d_G(u)$ (or d_u when no confusion can arise) to denote the degree of u in G, which is the number of edges incident to u. Such a maximal number (resp. minimal number) is called the maximal degree $\Delta(G)$ (resp. minimal degree $\delta(G)$). For any vertex u in G, we use $N_G(u)$ to denote the set of all vertices adjacent with u, and the elements of $N_G(u)$ are called neighbors of u. A sequence of positive integers $\pi = (d_1, d_2, \ldots, d_n)$ is called the degree sequence of G if $d_i = d_{v_i}$ for any vertex $v_i \in V(G)$, where $i = 1, 2, \ldots, n$.

The join of two graphs G_1 and G_2, denoted by $G_1 + G_2$, is the graph with the vertex set $V(G_1) \cup V(G_2)$ and edge set $E(G_1) \cup E(G_2) \cup \{xy | x \in V(G_1), y \in V(G_2)\}$. The cyclomatic number of G is the minimum number of edges in it whose removal makes it acyclic, denoted by $\gamma = \gamma(G)$. Let $\mathscr{G}_n^\gamma$ be the set of n-vertex graphs with cyclomatic number γ. We use K_n and P_n to denote the complete graph and path of n vertices, respectively. As usual, we use the symbol $\ell(P_n)$ to denote the length of the path P_n, which equals to the number of edges in P_n. The cyclomatic number, denoted by γ, of a graph G

is the minimum number of edges of G whose removal makes G acyclic. Let $\mathscr{G}_n^\gamma$ be the class of all connected graphs with order n and cyclomatic number γ. We use [4] for terminology and notation not defined here.

The topological index is a real number that can be used to characterize the properties of the molecule graph. Nowadays, hundreds of topological indices have been considered and used in quantitative structure-activity and quantitative structure-property relationships. One of the well-known topological indices is the general Randić index, which was defined by Bollobás and Erdös [5] and Amic [1] independently:

$$R_\alpha(G) = \sum_{uv\in E(G)} [d_u d_v]^\alpha ,$$

where α is a nonzero real number. This topological index has been extensively investigated. We encourage interested readers to consult [3, 6, 7, 10, 11, 13] for more mathematical properties and their applications.

Even though the mathematical and chemical theory of the general Randić index has been well considered, some extremal graph-theoretical problems concerning this graph invariant are still open. In this paper, we focus on exploring the extremal graphs in $\mathscr{G}_n^\gamma$ with respect to the general Randić index.

2. Graphs in $\mathscr{G}_n^\gamma$ with minimum general Randić index

It is interesting to explore the extremal graphs for some topological indices in the class of graphs with a given cyclomatic number. In this section, we focus on determining the extremal graphs in $\mathscr{G}_n^\gamma$ with the minimum general Randić index. Before proceeding, we shall prove or list several facts as preliminaries.

Lemma 2.1. *The function* $P(x,\alpha) = 2^\alpha x^{\alpha+1} - (x-1)^\alpha [2^\alpha(x-2) + 3^\alpha] + x^\alpha (2^\alpha - 3^\alpha) - 6^\alpha > 0$ *for* $x \geq 4$ *and* $1 \leq \alpha \leq \frac{39}{25}$.

Proof. It is routine to check that

$$\begin{aligned}
P(x,\alpha) =& 2^\alpha x^{\alpha+1} - (x-1)^\alpha [2^\alpha(x-2) + 3^\alpha] + x^\alpha (2^\alpha - 3^\alpha) - 6^\alpha \\
=& 2^\alpha x^{\alpha+1} - (x-1)^\alpha [2^\alpha(x-1) - 2^\alpha + 3^\alpha] + x^\alpha (2^\alpha - 3^\alpha) - 6^\alpha \\
=& 2^\alpha \left[x^{\alpha+1} - (x-1)^{\alpha+1}\right] + (2^\alpha - 3^\alpha)(x-1)^\alpha + (2^\alpha - 3^\alpha) x^\alpha - 6^\alpha \\
=& 2^\alpha \left[x^{\alpha+1} - (x-1)^{\alpha+1}\right] + (2^\alpha - 3^\alpha)[x^\alpha + (x-1)^\alpha] - 6^\alpha \\
=& 2^\alpha [x^\alpha + (x-1)^\alpha] + 2^\alpha x(x-1)\left[x^{\alpha-1} - (x-1)^{\alpha-1}\right] \\
&+ (2^\alpha - 3^\alpha)[x^\alpha + (x-1)^\alpha] - 6^\alpha \\
=& (2\cdot 2^\alpha - 3^\alpha)[x^\alpha - (x-1)^\alpha] + 2^\alpha x(x-1)\left[x^{\alpha-1} - (x-1)^{\alpha-1}\right] - 6^\alpha.
\end{aligned}$$

Note that $\rho(t) = t^\alpha - (t-1)^\alpha$ is an increasing function for $t \in [4, +\infty)$, and $2\cdot 2^\alpha > 3^\alpha$ if, and only if, $\alpha < \frac{\ln 2}{\ln 3 - \ln 2} \approx 1.709$, then we have

$$\begin{aligned}
P(x,\alpha) =& (2\cdot 2^\alpha - 3^\alpha)[x^\alpha - (x-1)^\alpha] + 2^\alpha x(x-1)\left[x^{\alpha-1} - (x-1)^{\alpha-1}\right] - 6^\alpha \\
\geq& (2\cdot 2^\alpha - 3^\alpha)(4^\alpha + 3^\alpha) + 2^\alpha \cdot 12 \cdot \left(4^{\alpha-1} - 3^{\alpha-1}\right) - 6^\alpha \\
=& 5\cdot 8^\alpha - 3\cdot 6^\alpha - 9^\alpha - 12^\alpha.
\end{aligned}$$

For simplicity, let $H(\alpha) = 5 \cdot 8^\alpha - 3 \cdot 6^\alpha - 9^\alpha - 12^\alpha$. To continue our proof, we first verify the following fact. □

Claim 1. *The function $\varrho(t) = k_1 a^t - k_2 b^t - k_3 c^t$ has a unique zero point in the interval $[0, +\infty)$ for any positive real numbers k_1, k_2, k_3, a, b, c such that $k_1 - k_2 - k_3 > 0$ and $1 < a < b < c$.*

Proof of Claim 1. It is routine to check that $\varrho'(t) = k_1 \ln a \cdot a^t - k_2 \ln b \cdot b^t - k_3 \ln c \cdot c^t$. Note that $\varrho(0) = k_1 - k_2 - k_3 > 0$ and $\varrho(M) = a^t \left[k_1 - k_2 \left(\frac{b}{a}\right)^t - k_3 \left(\frac{c}{a}\right)^t\right]_{t=M} \to -\infty$, and it follows that $\varrho(t)$ has zero points in the interval $[0, +\infty)$. Without loss of generality, we assume that $t_1, t_2 = t_1 + h \in [0, +\infty)$ are the two distinct zero points of $\varrho(t)$ for $h > 0$, which is equivalent to $k_1 a^{t_1} - k_2 b^{t_1} - k_3 c^{t_1} = 0$ and $k_1 a^{t_2} - k_2 b^{t_2} - k_3 c^{t_2} = 0$. Besides, we know that $\varrho'(t) = k_1 \ln a \cdot a^t - k_2 \ln b \cdot b^t - k_3 \ln c \cdot c^t$, which implies that

$$\begin{aligned}\varrho'(t_1) =& k_1 \ln a \cdot a^{t_1} - k_2 \ln b \cdot b^{t_1} - k_3 \ln c \cdot c^{t_1} \\ <& \ln a \left(k_1 a^{t_1} - k_2 b^{t_1} - k_3 c^{t_1}\right) \\ =& 0.\end{aligned}$$

In addition, we have

$$\begin{aligned}\varrho(t_2) = \varrho(t_1 + h) =& k_1 a^{t_1} a^h - k_2 b^{t_1} b^h - k_3 c^{t_1} c^h \\ =& \left(k_2 b^{t_1} + k_3 c^{t_1}\right) a^h - k_2 b^{t_1} b^h - k_3 c^{t_1} c^h \\ <& \left(k_2 b^{t_1} + k_3 c^{t_1}\right) a^h - \left(k_2 b^{t_1} + k_3 c^{t_1}\right) b^h \\ =& \left(k_2 b^{t_1} + k_3 c^{t_1}\right) \left(a^h - b^h\right) \\ <& 0,\end{aligned}$$

which contradicts to the fact that $\varrho(t_2) = 0$. Hence, there must exist a unique number $t_0 \in [0, +\infty)$ such that $\varrho(t_0) = 0$. As desired, we have completed the proof of Claim 1. □

Claim 2. *The function $H(\alpha) = 5 \cdot 8^\alpha - 3 \cdot 6^\alpha - 9^\alpha - 12^\alpha$ has a unique zero point in the interval $(1, 2)$.*

Proof of Claim 2. It is routine to check that $H'(\alpha) = 5 \ln 8 \cdot 8^\alpha - 3 \ln 6 \cdot 6^\alpha - \ln 9 \cdot 9^\alpha - \ln 12 \cdot 12^\alpha$. Note that $H(1) = 1 > 0$ and $H(2) = -13 < 0$, and it follows that $H(\alpha)$ has zero points in the interval $(1, 2)$. Without loss of generality, we assume that $\alpha_0, \alpha_1, \ldots, \alpha_l$ are the zero points of $H(\alpha)$ such that $1 < \alpha_0 < \alpha_1 < \ldots < \alpha_l$. Hence, $H(\alpha_0) = 5 \cdot 8^{\alpha_0} - 3 \cdot 6^{\alpha_0} - 9^{\alpha_0} - 12^{\alpha_0} = 0$. Furthermore,

$$\begin{aligned}H'(\alpha_0) =& 5 \ln 8 \cdot 8^{\alpha_0} - 3 \ln 6 \cdot 6^{\alpha_0} - \ln 9 \cdot 9^{\alpha_0} - \ln 12 \cdot 12^{\alpha_0} \\ =& \ln 8 \left(3 \cdot 6^{\alpha_0} + 9^{\alpha_0} + 12^{\alpha_0}\right) - 3 \ln 6 \cdot 6^{\alpha_0} - \ln 9 \cdot 9^{\alpha_0} - \ln 12 \cdot 12^{\alpha_0} \\ =& \underbrace{3 (\ln 8 - \ln 6)}_{k_1} 6^{\alpha_0} - \underbrace{(\ln 9 - \ln 8)}_{k_2} 9^{\alpha_0} - \underbrace{(\ln 12 - \ln 8)}_{k_3} 12^{\alpha_0}.\end{aligned}$$

It follows from Claim 1 that $\varrho(t)|_{a=6,b=9,c=12}$ has a unique zero point in the interval $t_0 \in [0, +\infty)$. Consequently, we know that the unique zero point of $\varrho(t)|_{a=6,b=9,c=12}$ must lie in the interval $(0, 1)$ since $\varrho(0)|_{a=6,b=9,c=12} > 0$ and $\varrho(1)|_{a=6,b=9,c=12} = -0.7473 < 0$. Hence, $\varrho(t)|_{a=6,b=9,c=12} < 0$ always holds for any real number $t \geq 1$. This implies that $H'(\alpha_i) = \varrho(\alpha_i)|_{a=6,b=9,c=12} < 0$ for $\alpha_i > 1$ and $i = 0, 1, \ldots, l$, which contradicts to the continuity of the function $H(\alpha)$. As desired, we have completed the proof of Claim 2. □

Now, we continue to our proof. Note that $H(\frac{39}{25}) = 5 \cdot 8^{\frac{39}{25}} - 3 \cdot 6^{\frac{39}{25}} - 9^{\frac{39}{25}} - 12^{\frac{39}{25}} \approx 0.01857 > 0$ and $H(1.57) = 5 \cdot 8^{1.57} - 3 \cdot 6^{1.57} - 9^{1.57} - 12^{1.57} \approx -0.07428 < 0$. Hence, $P(x, \alpha) \geq H(\alpha) > 0$ for $\alpha \in [1, \frac{39}{25}]$. As desired, we have completed the proof of Lemma 2.1.

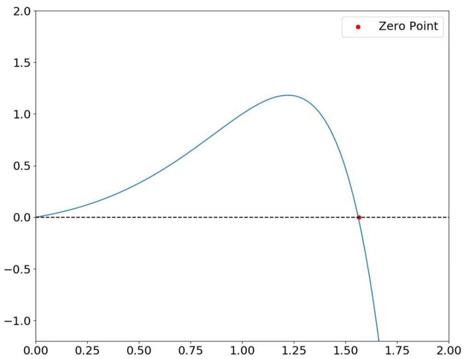

Figure 1. The graph of the function $H(\alpha) = 5 \cdot 8^\alpha - 3 \cdot 6^\alpha - 9^\alpha - 12^\alpha$ for $\alpha \in [0, \frac{39}{25})$, where α and $H(\alpha)$ denote the horizontal and vertical axes, respectively.

Lemma 2.2. *The function* $Q(x, \alpha) = 3^\alpha(x^{\alpha+1} - (x-1)^{\alpha+1}) - 9^\alpha + 2x^\alpha(2^\alpha - 3^\alpha) > 0$ *for* $x \geq 4$ *and* $\alpha \geq 1$.

Proof. For simplicity, we distinguish the following two cases.

Case 1. $\alpha \in [1, 3)$.

Note that $h(t) = t^\alpha$ is an increasing function in the interval $[1 - \frac{1}{x}, 1]$ for $\alpha \geq 1$, and it follows from Lagrange's mean value formula that $h(1) - h\left(1 - \frac{1}{x}\right) = \left[1 - \left(1 - \frac{1}{x}\right)\right] h'(\xi) = \frac{1}{x} h'(\xi) = \frac{1}{x}\alpha\xi^{\alpha-1} > 0$, where $\xi \in (1 - \frac{1}{x}, 1)$. Hence, $x\left[1 - \left(1 - \frac{1}{x}\right)^\alpha\right] = x\left[h(1) - h\left(1 - \frac{1}{x}\right)\right] = \alpha\xi^{\alpha-1}$. Thus, we have

$$\begin{aligned}
Q_x(x, \alpha) =& 3^\alpha(\alpha + 1)\left[x^\alpha - (x-1)^\alpha\right] + 2\alpha x^{\alpha-1}(2^\alpha - 3^\alpha) \\
=& x^{\alpha-1}\left\{3^\alpha(\alpha+1)x\left[1 - \left(1 - \frac{1}{x}\right)^\alpha\right] + 2\alpha(2^\alpha - 3^\alpha)\right\} \\
=& x^{\alpha-1}\left[3^\alpha\alpha(\alpha+1)\xi^{\alpha-1} + 2\alpha(2^\alpha - 3^\alpha)\right] \\
=& \alpha x^{\alpha-1}\left[3^\alpha(\alpha+1)\xi^{\alpha-1} + 2(2^\alpha - 3^\alpha)\right].
\end{aligned}$$

By our initial hypothesis, it is routine to check that $\xi^{\alpha-1} > (1 - \frac{1}{x})^{\alpha-1}$, then we have

$$\begin{aligned}
Q_x(x, \alpha) >& \alpha x^{\alpha-1}\left[3^\alpha(\alpha+1)\left(1 - \frac{1}{x}\right)^{\alpha-1} + 2(2^\alpha - 3^\alpha)\right] \\
>& \alpha x^{\alpha-1}\left[3^\alpha(\alpha+1)\left(\frac{3}{4}\right)^{\alpha-1} + 2(2^\alpha - 3^\alpha)\right] \quad \left(\text{because } 1 - \frac{1}{x} > \frac{3}{4}\right) \\
=& 2\alpha 3^\alpha x^{\alpha-1}\left[\frac{1}{2}(\alpha+1)\left(\frac{3}{4}\right)^{\alpha-1} + \left(\frac{2}{3}\right)^\alpha - 1\right] \\
>& 2\alpha 3^\alpha x^{\alpha-1}\left[\frac{9}{32}(\alpha+1) + \left(\frac{2}{3}\right)^\alpha - 1\right] \quad \left(\text{because } \left(\frac{3}{4}\right)^{\alpha-1} > \left(\frac{3}{4}\right)^2\right).
\end{aligned}$$

Let $p(\alpha) = \frac{9}{32}(\alpha+1) + \left(\frac{2}{3}\right)^{\alpha} - 1$, then we have $p'(\alpha) = \frac{9}{32} + \left(\frac{2}{3}\right)^{\alpha} \ln\frac{2}{3}$ and $p''(\alpha) = \left(\frac{2}{3}\right)^{\alpha}\left(\ln\frac{2}{3}\right)^{2} > 0$. Hence, $p'(\alpha) \geq p'(1) = \frac{9}{32} + \frac{2}{3}\ln\left(\frac{2}{3}\right) \geq \frac{1}{100} > 0$, which implies that $p(\alpha)$ is increasing in the interval $[1, +\infty)$. Hence, $p(\alpha) \geq p(1) = \frac{11}{48} > 0$. It immediately yields that $Q_x(x,\alpha) > 2\alpha 3^{\alpha} x^{\alpha-1} p(\alpha) > 0$. Therefore, we have

$$\begin{aligned} Q(x,\alpha) \geq & f(4,\alpha) = 3^{\alpha}(4^{\alpha+1} - 3^{\alpha+1}) - 9^{\alpha} + 2\cdot 4^{\alpha}(2^{\alpha} - 3^{\alpha}) \\ =& 2\cdot 9^{\alpha}\left[\left(\frac{12}{9}\right)^{\alpha} + \left(\frac{8}{9}\right)^{\alpha} - 2\right] \\ >& 0, \end{aligned}$$

as desired, and we have completed the proof.

Case 2. $\alpha \in [3, +\infty)$.

Note that

$$\begin{aligned} Q_x(x,\alpha) =& 3^{\alpha}(\alpha+1)\left[x^{\alpha} - (x-1)^{\alpha}\right] + 2\alpha x^{\alpha-1}(2^{\alpha} - 3^{\alpha}) \\ =& x^{\alpha-1}\left\{3^{\alpha}(\alpha+1)x\left[1 - \left(1 - \frac{1}{x}\right)^{\alpha}\right] + 2\alpha(2^{\alpha} - 3^{\alpha})\right\}. \end{aligned}$$

Let $g(\alpha) = 1 - \frac{2}{x} - \left(1 - \frac{1}{x}\right)^{\alpha}$ be a function defined in the interval $[3, +\infty)$, then we have $g'(\alpha) = \left(1 - \frac{1}{x}\right)^{\alpha} \ln\left(1 + \frac{1}{x-1}\right) > 0$. Hence, $g(\alpha) \geq g(3) = 1 - \frac{2}{x} - \left(1 - \frac{1}{x}\right)^{3} = \frac{x^2-3x+1}{x^3} > 0$, implying that $1 - \left(1 - \frac{1}{x}\right)^{\alpha} > \frac{2}{x}$. Thus, we have

$$\begin{aligned} Q_x(x,\alpha) =& x^{\alpha-1}\left\{3^{\alpha}(\alpha+1)x\left[1 - \left(1 - \frac{1}{x}\right)^{\alpha}\right] + 2\alpha(2^{\alpha} - 3^{\alpha})\right\} \\ >& 2\alpha x^{\alpha-1}\left[3^{\alpha}\frac{\alpha+1}{\alpha} - (3^{\alpha} - 2^{\alpha})\right] \quad \left(\text{because } \frac{\alpha+1}{\alpha} > 1\right) \\ >& 0. \end{aligned}$$

Let $l(\alpha) = \left(\frac{12}{9}\right)^{\alpha} + \left(\frac{8}{9}\right)^{\alpha} - 2$. It is routine to check that $l'(\alpha) = \left(\frac{8}{9}\right)^{\alpha}\left[\left(\frac{12}{8}\right)^{\alpha}\ln\left(\frac{12}{9}\right) + \ln\left(\frac{8}{9}\right)\right] > \left(\frac{8}{9}\right)^{\alpha}\left[\ln\left(\frac{12}{9}\right) + \ln\left(\frac{8}{9}\right)\right] = \left(\frac{8}{9}\right)^{\alpha}\ln 15 > 0$. Hence, $l(\alpha) \geq l(3) = \frac{782}{729} > 0$. It then follows that

$$\begin{aligned} Q(x,\alpha) \geq & f(4,\alpha) = 3^{\alpha}(4^{\alpha+1} - 3^{\alpha+1}) - 9^{\alpha} + 2\cdot 4^{\alpha}(2^{\alpha} - 3^{\alpha}) \\ =& 2\cdot 9^{\alpha}\left[\left(\frac{12}{9}\right)^{\alpha} + \left(\frac{8}{9}\right)^{\alpha} - 2\right] \\ >& 0, \end{aligned}$$

as desired, and we have completed the proof. □

Proposition 2.3. *Let $G \in \mathscr{G}_n^{\gamma}$ be a graph with $\gamma \geq 3$ and $n \geq 2(\gamma - 1)$, then there is no pendent vertex in G if it has a minimum general Randić index for $\alpha \geq 1$.*

Proof. Suppose to the contrary that there exists a pendent vertex in G. Let u be a vertex of degree at least three and $N_G(u) = \{u_1, u_2, \ldots, u_k\}$. In what follows, we use $P = uu_1\widehat{u_2}\ldots\widehat{u_r}$ to denote a pendent path in G. Assume that $u_2 \neq u_1$ is another neighbor of u with $d_{u_2} \geq 2$. We consider the graph $\widehat{G_1} = G - uu_2 + u_2\widehat{u_r}$ (depicted in Figure 2), which is an element of $\mathscr{G}_n^\gamma$. Let $l-2$ be the number of vertices in $\{u_3, u_4, \ldots, u_k\}$, whose degree is greater than or equal to two. Clearly, $l \geq 2$ and $\sum_{i=3}^{k} d_{u_i}^\alpha \geq 2^\alpha(l-2)$. For simplicity, we distinguish the following two cases:

Case 1. $\ell(P) = 1$.

Direct calculations show that

$$\begin{aligned}
R_\alpha(G) - R_\alpha(\widehat{G_1}) =& d_u^\alpha d_{u_2}^\alpha + d_u^\alpha - 2^\alpha (d_u - 1)^\alpha - 2^\alpha d_{u_2}^\alpha + [d_u^\alpha - (d_u - 1)^\alpha] \sum_{i=3}^{k} d_{u_i}^\alpha \\
\geq& d_u^\alpha d_{u_2}^\alpha + d_u^\alpha - 2^\alpha (d_u - 1)^\alpha - 2^\alpha d_{u_2}^\alpha + 2^\alpha (l-2) [d_u^\alpha - (d_u - 1)^\alpha] \\
=& \underbrace{\left[(d_{u_2}^\alpha - 2^\alpha + 1)(d_u^\alpha - 2^\alpha)\right]}_{\mathscr{A}_1} + \underbrace{2^\alpha \{(l-1)[d_u^\alpha - (d_u - 1)^\alpha] + (1 - 2^\alpha)\}}_{\mathscr{A}_2}.
\end{aligned}$$

It is not difficult to find the first term of the previous equality $\mathscr{A}_1 = \left[(d_{u_2}^\alpha - 2^\alpha + 1)(d_u^\alpha - 2^\alpha)\right] > 0$ for $\alpha \geq 1$, $d_u \geq 3$ and $d_{u_2} \geq 2$. To continue the proof, it remains to verify that $\mathscr{A}_2 > 0$. For simplicity, we let $H(x) = (l-1)[x^\alpha - (x-1)^\alpha] - (2^\alpha - 1)$ for $\alpha \geq 1$ and $x \geq 3$. It is routine to check that $H(x) > [(x^\alpha - (x-1)^\alpha) - (3^\alpha - 2^\alpha)] + [(3^\alpha - 2^\alpha) - (2^\alpha - 1)]$ since $l \geq 3$. Note that $f_1(x) = x^\alpha - (x-1)^\alpha$ is increasing in the interval $[3, \triangle]$, then we have $x^\alpha - (x-1)^\alpha \geq 3^\alpha - 2^\alpha$. In addition, we know that $3^\alpha - 2^\alpha \geq 2^\alpha - 1$ always holds for $\alpha \geq 1$. Hence, $H(x) > 0$ and, consequently, we have $\mathscr{A}_2 > 0$. It then immediately deduces that $R_\alpha(G) - R_\alpha(\widehat{G_1}) > 0$, a contradiction. This implies that there is no pendent vertex in G.

Case 2. $\ell(P) \geq 2$.

Direct calculations show that

$$\begin{aligned}
R_\alpha(G) - R_\alpha(\widehat{G_1}) =& d_u^\alpha d_{u_2}^\alpha - (d_u - 1)^\alpha 2^\alpha + 2^\alpha d_u^\alpha - 2^\alpha (d_u - 1)^\alpha \\
&+ 2^\alpha (1 - 2^\alpha) - 2^\alpha d_{u_2}^\alpha + [d_u^\alpha - (d_u - 1)^\alpha] \sum_{i=3}^{k} d_{u_i}^\alpha \\
\geq& d_u^\alpha d_{u_2}^\alpha - (d_u - 1)^\alpha 2^\alpha + 2^\alpha d_u^\alpha - 2^\alpha (d_u - 1)^\alpha \\
&+ 2^\alpha (l-2) [d_u^\alpha - (d_u - 1)^\alpha] + 2^\alpha (1 - 2^\alpha) - 2^\alpha d_{u_2}^\alpha \\
=& \underbrace{d_{u_2}^\alpha (d_u^\alpha - 2^\alpha)}_{\mathscr{A}_3} + \underbrace{2^\alpha (l-1) [d_u^\alpha - (d_u - 1)^\alpha]}_{\mathscr{A}_4} \\
&+ \underbrace{2^\alpha [d_u^\alpha - (d_u - 1)^\alpha + 1 - 2^\alpha]}_{\mathscr{A}_5}.
\end{aligned}$$

Note that $\mathscr{A}_3 > 0$ and $\mathscr{A}_4 > 0$, and it is also not difficult to find that $\mathscr{A}_5 = \frac{1}{l-1}\mathscr{A}_2$ is positive under the initial assumptions. Hence, $R_\alpha(G) - R_\alpha(\widehat{G_1}) > 0$. Again a contradiction. This implies that there is no pendent vertex in G.

As desired, we complete the proof of Proposition 2.3. □

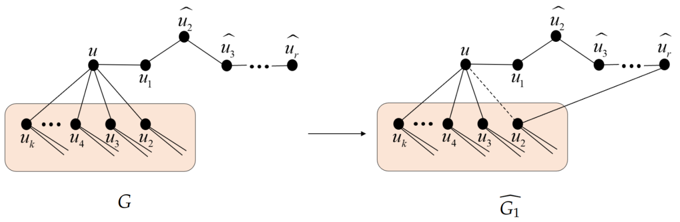

Figure 2. The transformation $G \Rightarrow \widehat{G_1}$.

Proposition 2.4. *Let $G \in \mathscr{G}_n^{\gamma}$ be a graph with $\gamma \geq 3$ and $n \geq 2(\gamma-1)$, then the maximum vertex degree is three in G if it has minimum general Randić index for $1 \leq \alpha \leq \frac{39}{25}$.*

Proof. It follows from Proposition 2.3 that G contains at least one cycle as its induced subgraph, and the n-vertex cycle is the only connected graph for the which minimum and maximum vertex degree is two. Hence, in conjunction with the assumption $\gamma \geq 3$, we have $\Delta = \Delta(G) \geq 3$. To complete the proof, it suffices to show that $\Delta = 3$. If $\Delta > 3$, then it is routine to check that

$$n = \sum_{2\leq i\leq\Delta} n_i \geq 2(\gamma-1) = 2(m-n) = 2\left(\sum_{2\leq i\leq\Delta}\frac{in_i}{2} - \sum_{2\leq i\leq\Delta} n_i\right),$$

which is equivalent to

$$n_2 \geq \sum_{4\leq i\leq\Delta}(i-3)n_i > \sum_{4\leq i\leq\Delta}(4-3)n_i > 0.$$

Hence, there at least exists a vertex of degree two. For simplicity, we suppose that u is the vertex in G with maximum degree and $N_G(u) = \{u_1, u_2, \ldots, u_\Delta\}$. We distinguish the following two cases.
Case 1. $\exists i \in \{1, 2, \ldots, \Delta\}$ such that $d_{u_i} = 2$.

For convenience, we suppose that u_1 is the neighbor of u with degree two and $d_{u_2} \geq d_{u_3} \geq \ldots \geq 2$.
Subcase 1.1. $d_{u_2} = 2$ and u_1 is not adjacent to u_2.

Let $\widehat{G_2} = G - uu_2 + u_1u_2 \in \mathscr{G}_n^{\gamma}$. t is the neighbor of u_1, different from u, depicted in Figure 3. Hence, we have

$$\begin{aligned}
R_\alpha(G) - R_\alpha(\widehat{G_2}) =& d_u^\alpha 2^{\alpha+1} - (d_u-1)^\alpha\, 3^\alpha - 6^\alpha + d_t^\alpha\,(2^\alpha - 3^\alpha) + \left[d_u^\alpha - (d_u-1)^\alpha\right]\sum_{i=3}^{\Delta} d_{u_i}^\alpha \\
=& d_u^\alpha 2^{\alpha+1} - (d_u-1)^\alpha\, 3^\alpha - 6^\alpha + d_t^\alpha\,(2^\alpha - 3^\alpha) + 2^\alpha\,(d_u-2)\left[d_u^\alpha - (d_u-1)^\alpha\right] \\
=& 2^\alpha d_u^{\alpha+1} - (d_u-1)^\alpha\left[2^\alpha(d_u-2) + 3^\alpha\right] + d_t^\alpha\,(2^\alpha - 3^\alpha) - 6^\alpha \\
\geq& 2^\alpha d_u^{\alpha+1} - (d_u-1)^\alpha\left[2^\alpha(d_u-2) + 3^\alpha\right] + d_u^\alpha\,(2^\alpha - 3^\alpha) - 6^\alpha.
\end{aligned}$$

For simplicity, we let $f_2(x) = 2^\alpha x^{\alpha+1} - (x-1)^\alpha\left[2^\alpha(x-2) + 3^\alpha\right] + x^\alpha\,(2^\alpha - 3^\alpha) - 6^\alpha$. It follows from Lemma 2.1 that $f_2(x) = P(x, \alpha) > 0$ for $x \geq 4$ and $1 \leq \alpha \leq \frac{39}{25}$. Hence, $R_\alpha(G) - R_\alpha(\widehat{G_2}) > 0$, which contradicts to the choice of G. Hence, the maximum vertex degree of G is three.

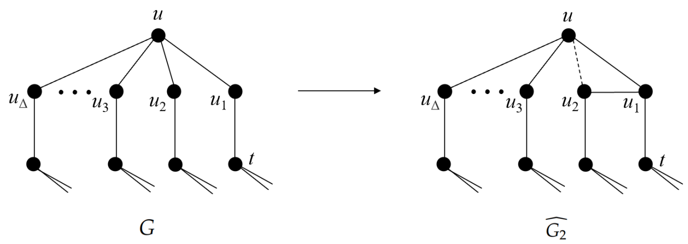

Figure 3. The transformation $G \Rightarrow \widehat{G_2}$.

Subcase 1.2. $d_{u_2} = 2$ and u_1 is adjacent to u_2.

Let $\widehat{G_3} = G - uu_3 + u_1u_3 \in \mathscr{G}_n^{\gamma}$, depicted in Figure 4. Hence, we have

$$\begin{aligned} R_\alpha(G) - R_\alpha(\widehat{G_3}) =& 3 \times d_u^\alpha 2^\alpha + 4^\alpha - (d_u - 1)^\alpha\, 3^\alpha - 2 \times 6^\alpha - 2^\alpha (d_u - 1)^\alpha + \left[d_u^\alpha - (d_u - 1)^\alpha\right] \sum_{i=4}^{\Delta} d_{u_i}^\alpha \\ =& 3 \times d_u^\alpha 2^\alpha + 4^\alpha - (d_u - 1)^\alpha\, 3^\alpha - 2 \times 6^\alpha - 2^\alpha (d_u - 1)^\alpha + 2^\alpha\,(d_u - 3)\left[d_u^\alpha - (d_u - 1)^\alpha\right] \\ =& 2^\alpha d_u^{\alpha+1} + 4^\alpha - (d_u - 1)^\alpha\,[2^\alpha (d_u - 2) + 3^\alpha] - 2 \times 6^\alpha. \end{aligned}$$

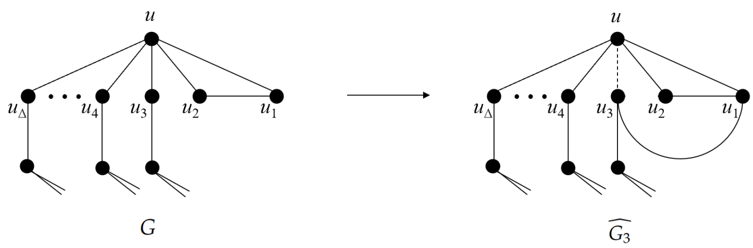

Figure 4. The transformation $G \Rightarrow \widehat{G_3}$.

Let $f_3(x) = 2^\alpha x^{\alpha+1} + 4^\alpha - (x - 1)^\alpha\,[2^\alpha(x - 2) + 3^\alpha] - 2 \times 6^\alpha$, and then we have $f_3(x) = f_2(x) + (3^\alpha - 2^\alpha)(x^\alpha - 2^\alpha) > 0$. Hence, $R_\alpha(G) - R_\alpha(\widehat{G_3}) > 0$ for $x \geq 4$ and $1 \leq \alpha \leq \frac{39}{25}$, which contradicts to the choice of G. Hence, the maximum vertex degree of G is three.

Subcase 1.3. $d_{u_2} > 2$ and u_1 is adjacent to u_2 and $d_{u_3} > 2$.

Let $\widehat{G_4} = G - uu_3 + u_1u_3 \in \mathscr{G}_n^{\gamma}$, depicted in Figure 5. Hence, we have

$$\begin{aligned} R_\alpha(G) - R_\alpha(\widehat{G_4}) =& d_u^\alpha 2^\alpha + 2^\alpha d_{u_2}^\alpha + d_u^\alpha d_{u_2}^\alpha + d_u^\alpha d_{u_3}^\alpha - (d_u - 1)^\alpha\, 3^\alpha - 3^\alpha d_{u_2}^\alpha \\ & - d_{u_2}^\alpha (d_u - 1)^\alpha - 3^\alpha d_{u_3}^\alpha + \left[d_u^\alpha - (d_u - 1)^\alpha\right] \sum_{i=4}^{\Delta} d_{u_i}^\alpha \\ \geq& d_u^\alpha 2^\alpha + d_{u_2}^\alpha (2^\alpha - 3^\alpha) + d_{u_3}^\alpha (d_u^\alpha - 3^\alpha) - (d_u - 1)^\alpha\, 3^\alpha \\ & + d_{u_2}^\alpha (d_{u_3}^\alpha - 3^\alpha) - (d_u - 1)^\alpha\, 3^\alpha + 2^\alpha\,(d_u - 3)[d_u^\alpha - (d_u - 1)^\alpha] \\ >& 2^\alpha d_u^{\alpha+1} - (d_u - 1)^\alpha\,[2^\alpha (d_u - 2) + 3^\alpha] + d_u^\alpha\,(2^\alpha - 3^\alpha) - 6^\alpha \\ >& 0, \end{aligned}$$

and the last inequality holds because $f_2(x) > 0$ for $x \geq 4$ and $1 \leq \alpha \leq \frac{39}{25}$. Hence, $R_\alpha(G) - R_\alpha(\widehat{G_4}) > 0$. Again, a contradiction. Hence, the maximum vertex degree of G is three.

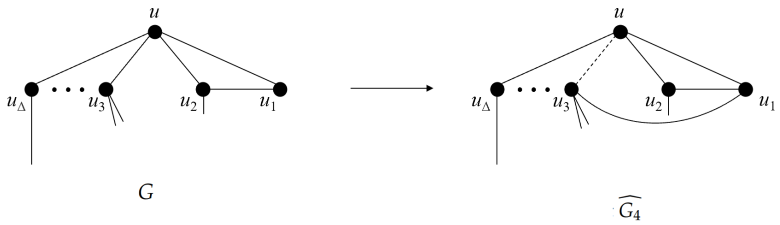

Figure 5. The transformation $G \Rightarrow \widehat{G_4}$.

Subcase 1.4. $d_{u_2} > 2$, u_1 is adjacent to u_2 and $d_{u_3} = 2$.

Let $\widehat{G_5} = G - uu_3 + u_1u_3 \in \mathscr{G}_n^\gamma$, depicted in Figure 6. Hence, we have

$$\begin{aligned}
R_\alpha(G) - R_\alpha(\widehat{G_5}) =& d_u^\alpha 2^{\alpha+1} + 2^\alpha d_{u_2}^\alpha + d_u^\alpha d_{u_2}^\alpha - 6^\alpha - (d_u - 1)^\alpha\, 3^\alpha - d_{u_2}^\alpha 3^\alpha \\
& - (d_u - 1)^\alpha\, d_{u_2}^\alpha + [d_u^\alpha - (d_u - 1)^\alpha] \sum_{i=4}^{\Delta} d_{u_i}^\alpha \\
\geq& d_u^\alpha 2^{\alpha+1} - 6^\alpha - (d_u - 1)^\alpha\, 3^\alpha + d_{u_2}^\alpha \left[(2^\alpha - 3^\alpha + d_u^\alpha - (d_u - 1)^\alpha)\right] \\
& + 2^\alpha\, (d_u - 3)\left[d_u^\alpha - (d_u - 1)^\alpha\right] \\
>& 2^\alpha d_u^{\alpha+1} - (d_u - 1)^\alpha\, [2^\alpha (d_u - 2) + 3^\alpha] + 4^\alpha - 2 \times 6^\alpha \\
>& 0,
\end{aligned}$$

and the last inequality holds because $f_3(x) > 0$ for $x \geq 4$ and $1 \leq \alpha \leq \frac{39}{25}$. Hence, $R_\alpha(G) - R_\alpha(\widehat{G_5}) > 0$. Again, a contradiction. Thus, we have completed that the maximum vertex degree of G is three.

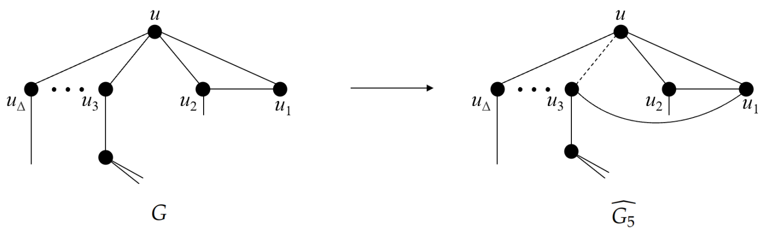

Figure 6. The transformation $G \Rightarrow \widehat{G_5}$.

Subcase 1.5. $d_{u_2} > 2$, u_1 is not adjacent to u_2.

Let $\widehat{G_6} = G - uu_2 + u_1u_2 \in \mathscr{G}_n^\gamma$, depicted in Figure 7. Hence, we have

$$\begin{aligned}
R_\alpha(G) - R_\alpha(\widehat{G_6}) =& d_u^\alpha 2^\alpha + 2^\alpha d_t^\alpha + d_u^\alpha d_{u_2}^\alpha - (d_u - 1)^\alpha\, 3^\alpha - 3^\alpha d_t^\alpha - 3^\alpha d_{u_2}^\alpha + [d_u^\alpha - (d_u - 1)^\alpha] \sum_{i=3}^{\Delta} d_{u_i}^\alpha \\
\geq& d_u^\alpha 2^\alpha + d_u^\alpha (2^\alpha - 3^\alpha) + 2^\alpha\, (d_u^\alpha - 3^\alpha) - (d_u - 1)^\alpha\, 3^\alpha + 2^\alpha\, (d_u - 2)\left[d_u^\alpha - (d_u - 1)^\alpha\right] \\
=& 2^\alpha d_u^{\alpha+1} - (d_u - 1)^\alpha\, [2^\alpha (d_u - 2) + 3^\alpha] + d_u^\alpha\, (2^\alpha - 3^\alpha) - 6^\alpha > 0,
\end{aligned}$$

and the last inequality holds because $f_2(x) > 0$ for $x \geq 4$ and $1 \leq \alpha \leq \frac{39}{25}$. Hence, $R_\alpha(G) - R_\alpha(\widehat{G_6}) > 0$, a contradiction to the choice of G. Hence, the maximum vertex degree of G is three.

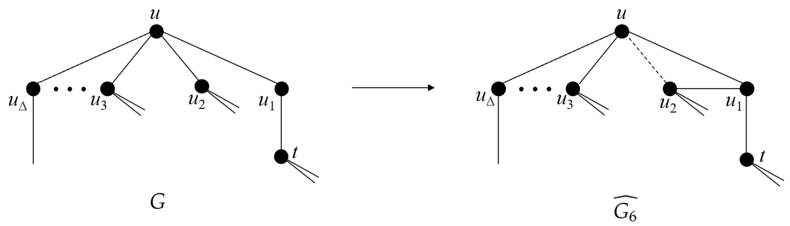

Figure 7. The transformation $G \Rightarrow \widehat{G_6}$.

Case 2. $\forall i \in \{1, 2, \ldots, \Delta\}$ such that $d_{u_i} > 2$.

Note that there is a vertex $u_0 \in V(G) \setminus N_G(u)$ of degree two, which is not adjacent to at least one neighbor, say u_1, of u. Let $\widehat{G_7} = G - uu_1 + u_0u_1 \in \mathscr{G}_n^\gamma$ (depicted in Figure 8). Hence,

$$\begin{aligned} R_\alpha(G) - R_\alpha(\widehat{G_7}) =& d_{u_1}^\alpha \left(d_u^\alpha - 3^\alpha\right) + \left(2^\alpha - 3^\alpha\right) \sum_{z \in N_G(u_0)} d_z^\alpha + \left[d_u^\alpha - (d_u - 1)^\alpha\right] \sum_{i=2}^{\Delta} d_{u_i}^\alpha \\ \geq& 3^\alpha \left(d_u^\alpha - 3^\alpha\right) + 2 \times d_u^\alpha \left(2^\alpha - 3^\alpha\right) + 3^\alpha \left(d_u - 1\right) \left[d_u^\alpha - (d_u - 1)^\alpha\right] \\ =& 3^\alpha \left[d_u^{\alpha+1} - (d_u - 1)^{\alpha+1}\right] - 9^\alpha + 2 \times d_u^\alpha (2^\alpha - 3^\alpha). \end{aligned}$$

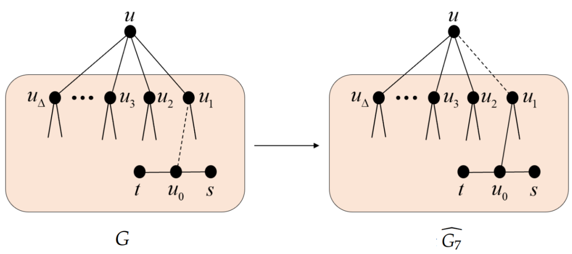

Figure 8. The transformation $G \Rightarrow \widehat{G_7}$.

For simplicity, we let $f_4(x) = 3^\alpha[x^{\alpha+1} - (x-1)^{\alpha+1}] - 9^\alpha + 2x^\alpha(2^\alpha - 3^\alpha) = Q(x, \alpha)$, which is positive for $x \geq 4$ and $\alpha \geq 1$ by Lemma 2.2. Hence, we have $R_\alpha(G) - R_\alpha(\widehat{G_7}) > 0$. Thus, there would be a contradiction to the choice of G, and the maximum vertex degree of G is three.

This completes the proof of Proposition 2.4. □

Let φ_{ij} be the number of edges in G joining the vertices of degree i and j, and we use n_i and n_j to denote the number of vertices of degree i and j, respectively.

Proposition 2.5. *([2]) Let $G \in \mathscr{G}_n^\gamma$, $\gamma \geq 3$, be a graph such that it contains only vertices of degrees two and three, then the following holds:*

(i) at least two vertices of degree two are adjacent if $n > 5(\gamma - 1)$.

(ii) $\varphi_{22} = 0$ implies $\varphi_{33} = 0$ (or $\varphi_{33} = 0$ implies $\varphi_{22} = 0$) if $n = 5(\gamma - 1)$.

(iii) at least two vertices of degree three are adjacent if $2(\gamma - 1) \leq n \leq 5(\gamma - 1)$.

Proposition 2.6. *Let $G \in \mathscr{G}_n^{\gamma}$ be a graph with $\gamma \geq 3$ and $n > 5(\gamma - 1)$, then at least one of the vertices x and y for any edge $e = xy$ has the degree two in G if it has a minimum general Randić index for $1 \leq \alpha \leq \frac{39}{25}$.*

Proof. By Proposition 2.3 and Proposition 2.4, we know $2 \leq d_u \leq 3$ holds for any vertex u in G. Simultaneously, it follows from Proposition 2.5 that there at least exist two vertices, say u_1 and u_2, such that $\varphi_{22} > 0$. Suppose to the contrary that there exists two adjacent vertices v_1 and v_2 of degree three (i.e., $\varphi_{33} > 0$). Let $u_0 \neq u_1$ be the vertex adjacent with u_2, which may coincide with v_1 or v_2. For convenience, we distinguish the following two cases.

Case 1. $N_G(u_1) \cap N_G(u_2) = \emptyset$.

Let $\widehat{G_8} = G - \{u_1u_2, u_2u_0, v_1v_2\} + \{u_1u_0, v_1u_2, v_2u_2\}$ (depicted in Figure 9), which is an element in $\mathscr{G}_n^{\gamma}$. By direct calculations, we have $R_\alpha(G) - R_\alpha(\widehat{G_8}) = 4^\alpha + 9^\alpha - 2 \times 6^\alpha > 0$. This contradicts to the assumption of G. Hence, $\varphi_{33} = 0$. As desired, we have completed the proof.

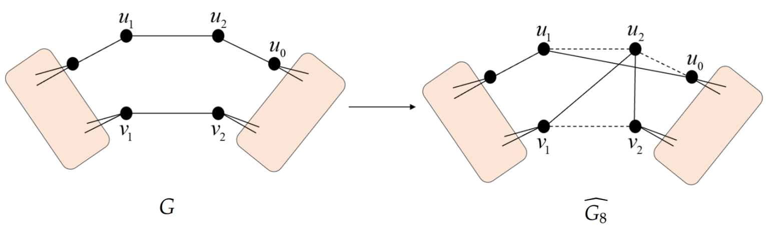

Figure 9. The transformation $G \Rightarrow \widehat{G_8}$.

Case 2. $N_G(u_1) \cap N_G(u_2) \neq \emptyset$.

Without loss of generality, we let $u_0 \in N_G(u_1) \cap N_G(u_2) \neq \emptyset$. In what follows, we consider the following three subcases.

If $u_0 \neq \{v_1, v_2\}$ and u_0 is not adjacent to v_1 and v_2, we let $\widehat{G_9} = G - \{u_2u_0, v_1v_2\} + \{u_2v_2, v_1u_0\}$ (depicted in Figure 10), which is an element in $\mathscr{G}_n^{\gamma}$. By direct calculations, we have $R_\alpha(G) - R_\alpha(\widehat{G_9}) = 0$. Note that $N_{\widehat{G_9}}(u_1) \cap N_{\widehat{G_9}}(u_2) = \emptyset$, by the analogous method as in Case 1, and there exists a new graph $\widetilde{G_1}$ such that $R_\alpha(G) - R_\alpha(\widetilde{G_1}) = R_\alpha(\widehat{G_9}) - R_\alpha(\widetilde{G_1}) > 0$. This contradicts to the assumption of G. As desired, we have completed the proof.

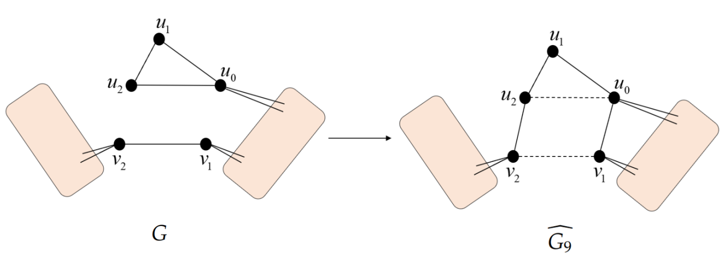

Figure 10. The transformation $G \Rightarrow \widehat{G_9}$.

If $u_0 \neq \{v_1, v_2\}$ and u_0 is adjacent to v_1, we let $\widehat{G_{10}} = G - \{u_1u_2, v_1v_2\} + \{u_1v_1, u_2v_2\}$, which is an element in $\mathscr{G}_n^\gamma$. By direct calculations, we have $R_\alpha(G)-R_\alpha(\widehat{G_{10}}) = 4^\alpha+9^\alpha-2\cdot 6^\alpha > 0$. This contradicts to the assumption of G. As desired, we have completed the proof.

If $u_0 = v_2$, then we consider a neighbor $\widetilde{v}$ of v_1 different from v_2. Let $\widehat{G_{11}} = G - \{u_2v_2, \widetilde{v}v_1\} + \{v_1u_2, \widetilde{v}v_2\} \in \mathscr{G}_n^\gamma$, and again we obtain that $R_\alpha(G) - R_\alpha(\widehat{G_{11}}) = 0$. Note that $N_{\widehat{G_{11}}}(u_1) \cap N_{\widehat{G_{11}}}(u_2) = \emptyset$, by the analogous method as in Case 1, and there exists a new graph $\widetilde{G_2}$ such that $R_\alpha(G) - R_\alpha(\widetilde{G_2}) = R_\alpha(\widehat{G_{11}}) - R_\alpha(\widetilde{G_2}) > 0$. This contradicts to the assumption of G. We have completed the proof. □

Proposition 2.7. *Let $G \in \mathscr{G}_n^\gamma$ be a graph with $\gamma \geq 3$ and $n = 5(\gamma-1)$, then one of the vertices x and y for any edge $e = xy$ has the degree two and the other has the degree three in G if it has the minimum general Randić index for $1 \leq \alpha \leq \frac{39}{25}$.*

Proof. It follows from Propositions 2.3 and 2.4 that $2 \leq d_u \leq 3$ holds for any vertex u in G. If $\varphi_{22} = 0$ and $\varphi_{33} \neq 0$, then one can find that $\varphi_{23} = 0$ by Proposition 2.5, a contradiction. If $\varphi_{22} \neq 0$ and $\varphi_{33} \neq 0$, then from the proof of Proposition 2.6 we conclude that there exists a graph $\widehat{G_{12}} \in \mathscr{G}_n^\gamma$ such that $R_\alpha(G) - R_\alpha(\widehat{G_{12}}) > 0$. This contradicts to the initial assumption of G. Hence, $\varphi_{22} = \varphi_{33} = 0$. As desired, we complete the proof of Proposition 2.7. □

In a similar way, we obtain the following fact.

Proposition 2.8. *Let $G \in \mathscr{G}_n^\gamma$ be a graph with $\gamma \geq 3$ and $2(\gamma-1) < n < 5(\gamma-1)$, then G does not contain any edge connecting the vertices of degree two if it has a minimum general Randić index for $1 \leq \alpha \leq \frac{39}{25}$.*

Denote by $\overline{G_{ij}[\varphi_{ij} \neq 0]}$ that the graphs contain only vertices of degree i and j, such that for every edge in a one end-vertex has the degree i and the other end-vertex has the degree j, and we use $\overline{G_{ij}[\varphi_{ii} = 0]}$ (resp. $\overline{G_{ij}[\varphi_{jj} = 0]}$) to denote the graphs containing only vertices of degree i and j, such that no vertices of degree i (resp. j) are adjacent.

Theorem 2.9. *Let $G \in \mathscr{G}_n^\gamma$ be a graph with $\gamma \geq 3$ and n vertices, then the following holds for $1 \leq \alpha \leq \frac{39}{25}$:*

(i) $R_\alpha(G) \geq 9^\alpha(n+\gamma-1)$ for $n = 2(\gamma-1)$, with equality if, and only if, G is isomophic to cubic graphs.

(ii) $R_\alpha(G) \geq 6^\alpha(2n-4\gamma+4) - 9^\alpha(n-5\gamma+5)$ for $2(\gamma-1) < n < 5(\gamma-1)$, with equality if, and only if, G is isomophic to $\overline{G_{23}[\varphi_{22} = 0]}$.

(iii) $R_\alpha(G) \geq 6^\alpha(n+\gamma-1)$ for $n = 5(\gamma-1)$, with equality if, and only if, G is isomophic to $\overline{G_{23}[\varphi_{23} \neq 0]}$.

(iv) $R_\alpha(G) \geq 4^\alpha(n-5\gamma+5)+6^\alpha(6\gamma-6)$ for $n > 5(\gamma-1)$, with equality if, and only if, G is isomophic to $\overline{G_{23}[\varphi_{33} = 0]}$.

Proof. Let $\widehat{G_{13}} \in \mathscr{G}_n^\gamma$ be a graph that achieves the minimum general Randić index. We only give the proof of (ii); the rest could be proved in a similar way. It follows from Propositions 2.3 and 2.4 that $2 \leq d_u \leq 3$ holds for any vertex u in $\widehat{G_{13}}$. Hence, we have $n_2 + n_3 = n$ and $2n_2 + 3n_3 = 2(n+\gamma-1)$ by the Handshaking Theorem. Besides, by Proposition 2.8, it is easily seen that $\varphi_{22} = 0$. Hence, $\varphi_{23} = 2n_2$ and $\varphi_{23} + 2\varphi_{33} = 3n_3$. Direct calculations show that $\varphi_{23} = 2n-4\gamma+4$ and $\varphi_{33} = 5\gamma-n-5$. Thus, $R_\alpha(G) \geq R_\alpha(\widehat{G_{13}}) = 6^\alpha(2n-4\gamma+4) - 9^\alpha(n-5\gamma+5)$. The corresponding extremal graph is $\overline{G_{23}[\varphi_{22} = 0]}$. □

The second Zagreb index is another well-known vertex degree-based graph invariant in chemical graph theory, which was introduced in 1972 by Gutman and Trinajstić [8]. We encourage the interested reader to consult [9,12] for more information for this graph invariant. Undoubtedly, the second Zagreb index is the special case of the general Randić index when $\alpha = 1$. It is easily seen that Theorem 2.9 extends one of the main results proved by Ali et al. [2].

3. Graphs in $\mathscr{G}_n^\gamma$ with maximum general Randić index

We begin with the following auxiliary result, which plays an important part in our proofs.

Proposition 3.1. *Let $G \in \mathscr{G}_n^\gamma$ be a graph with a maximum general Randić index for $\alpha \geq 1$, then $\Delta(G) = n - 1$.*

Proof. Suppose to the contrary that there exists a vertex u in G with $\Delta(G) = d_u < n - 1$. Note that there exists $v \in V(G)$ such that $u \neq v$, $d_u \geq d_v$ and $N_G(v)\backslash N_G(u) = \{v_1, v_2, \ldots, v_p\} \neq \emptyset$. We can construct a new graph $\widehat{G_{14}}$ the following way

$$\widehat{G_{14}} = G - \{vv_1, vv_2, \ldots, vv_p\} + \{uv_1, uv_2, \ldots, uv_p\} \in \mathscr{G}_n^\gamma.$$

It is routine to check that

$$\begin{aligned} R_\alpha(\widehat{G_{14}}) - R_\alpha(G) = &\sum_{x \in N_G(u)\backslash N_G(v)} \left[(d_u + p)^\alpha - d_u^\alpha\right] d_x^\alpha + \sum_{i=1}^{p} \left[(d_u + p)^\alpha - d_v^\alpha\right] d_{v_i}^\alpha \\ &+ \sum_{y \in N_G(u)\cap N_G(v)} \left[(d_u + p)^\alpha + (d_v - p)^\alpha - d_u^\alpha - d_v^\alpha\right] d_y^\alpha. \end{aligned}$$

Note that $H(t) = t^\alpha$ is an increasing function for $\alpha \geq 1$, and the first and second terms of the previous equality are nonnegative. By the Lagrange mean value theorem, we have $(d_u + p)^\alpha - d_u^\alpha = \alpha p \xi^{\alpha-1}$ (resp. $d_v^\alpha - (d_v - p)^\alpha = \alpha p \eta^{\alpha-1}$) for $\xi \in (d_u, d_u + p)$ (resp. $\eta \in (d_v - p, d_v)$). Hence, $\mathscr{A}_6 = (d_u + p)^\alpha + (d_v - p)^\alpha - d_u^\alpha - d_v^\alpha > 0$, and, consequently, we have $R_\alpha(\widehat{G_{14}}) > R_\alpha(G)$, a contradiction. This completes the proof. □

Proposition 3.2. *([14]) Let $x_1, x_2, \ldots, x_n, p, t \geq 1$ be integers, α be any real number such that $\alpha \notin \{0, 1\}$ and $x_1 + x_2 + \ldots + x_n = p$.*

(1) The function $f(x_1, x_2, \ldots, x_n) = \sum_{i=1}^n x_i^\alpha$ is the minimum for $\alpha < 0$ or $\alpha > 1$ (maximum for $0 < \alpha < 1$, respectively) if, and only if, $x_1, x_2, \ldots, x_n$ are almost equal, or $|x_i - x_j| \leq 1$ for every $i, j = 1, 2, \ldots, n$.

(2) If $x_1 \geq x_2 \geq t$, the maximum of the function $f(x_1, x_2, \ldots, x_n)$ is reached for $\alpha < 0$ or $\alpha > 1$ (minimum for $0 < \alpha < 1$, respectively) only for $x_1 = p - t - n + 2, x_2 = t, x_3 = x_4 = \ldots = x_n = 1$. The second maximum (the second minimum, respectively) is attained only for $x_1 = p - t - n + 1, x_2 = t + 1, x_3 = x_4 = \ldots = x_n = 1$.

Theorem 3.3. *Let $G \in \mathscr{G}_n^\gamma$ be a graph with $\gamma = \binom{k-1}{2}$ and $k \geq 4$, then for $\alpha \geq 1$ we have*

$$R_\alpha(G) \leq \binom{k-1}{2}(k^2 - 2k + 3)^{2\alpha} + (n-1)^\alpha(k^2 - 2k + 3)^\alpha + (n-2)(n-1)^\alpha,$$

with equality if, and only if, $G \cong (K_1^\gamma \cup (n-2)K_1) + K_1 \cong K_n^\gamma$, depicted in Figure 11.

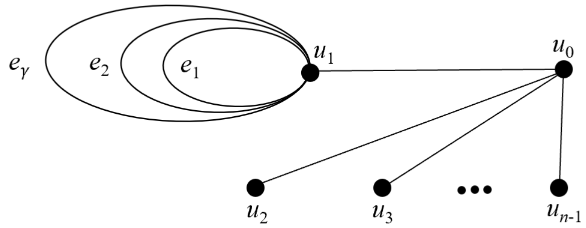

Figure 11. The graph $G \cong (K_1^\gamma \cup (n-2)K_1) + K_1 \cong K_n^\gamma$ with degree sequence $(n-1, 2\gamma + 1, 1, 1, \ldots, 1)$.

Proof. It follows from Proposition 3.1 that there at least exists one vertex with a maximum degree $n-1$. Hence, we have $G = \widehat{G_{15}} + K_1$, which contains $|V(\widehat{G_{15}})| = n-1$ vertices and $m(\widehat{G_{15}}) = \binom{k-1}{2}$ edges. For simplicity, let $\pi = (d_1, d_2, \ldots, d_n)$ and $\widehat{\pi} = (\widehat{d_1}, \widehat{d_2}, \ldots, \widehat{d_{n-1}})$ be the nonincreasing degree sequence of G and $\widehat{G_{15}}$, respectively. Hence, $d_i = \widehat{d_{i-1}} + 1$ for $i = 2, 3, \ldots, n$ and $d_1 = n-1$. Thus, we have

$$\begin{aligned}R_\alpha(G) =& \sum_{v_1v_j \in E(G)} \left[d_1 d_j\right]^\alpha + \sum_{v_iv_j \in E(G), 2\le i<j\le n} \left[d_i d_j\right]^\alpha \\ =&(n-1)^\alpha \sum_{i=2}^{n} d_i^\alpha + \sum_{v_iv_j \in E(\widehat{G_{15}})} \left[\left(\widehat{d_i}+1\right)\left(\widehat{d_j}+1\right)\right]^\alpha .\end{aligned}$$

By Proposition 3.2 for $\alpha \ge 1$, we have

$$\begin{aligned}\mathscr{A}_7 =& \sum_{i=1}^{n} d_i^\alpha - d_1^\alpha \\ \le& 1\cdot(n-1)^\alpha + 1\cdot t^\alpha + (n-2)\cdot 1^\alpha - 1\cdot(n-1)^\alpha \\ =&(n-1)^\alpha + (k^2-3k+3)^\alpha + (n-2) - (n-1)^\alpha \\ =&(k^2-3k+3)^\alpha + (n-2),\end{aligned}$$

where $d_1 = n-1 = 2m - t - n + 2, d_2 = t = 2\gamma + 1$ and $d_3 = d_4 = \ldots = d_n = 1$. In addition, we find the maximum value of

$$\begin{aligned}\mathscr{A}_8 =& \sum_{v_iv_j \in E(\widehat{G_{15}})} \left[\left(\widehat{d_i}+1\right)\left(\widehat{d_j}+1\right)\right]^\alpha \\ \le& \binom{k-1}{2}\left[\left(k^2-3k+3\right)\left(k^2-3k+3\right)\right]^\alpha,\end{aligned}$$

with equality if, and only if, $\widehat{G_{15}} \cong K_1^\gamma \cup (n-2)K_1$.

It follows from the previous that

$$\begin{aligned}R_\alpha(G) =&(n-1)^\alpha \mathscr{A}_7 + \mathscr{A}_8 \\ \le& \binom{k-1}{2}(k^2-2k+3)^{2\alpha} + (n-1)^\alpha(k^2-2k+3)^\alpha + (n-2)(n-1)^\alpha,\end{aligned}$$

Hence, $G = (K_1^\gamma \cup (n-2)K_1) + K_1 \cong K_n^\gamma$. This completes the proof of Theorem 3.3. □

Use of AI tools declaration

The authors declare they have not used Artificial Intelligence(AI) tools in the creation of this article.

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Conflict of interest

The authors declare that they have no conflicts of interest.

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