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A Unified Approach to Extremal Cacti for Different Indices

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Abstract

Many chemical indices have been invented in theoretical chemistry, such as Wiener index, Merrifield-Simmons index, Hosoya index, spectral radius and Randić index, etc. The extremal trees and unicyclic graphs for these chemical indices are interested in existing literature. Let G be a molecular graph (called a cacti), which all of blocks of G are either edges or cycles. Denote $\mathscr{G}(n,r)$ the set of cacti of order n and with r cycles. Obviously, $\mathscr{G}(n,0)$ is the set of all trees and $\mathscr{G}(n,1)$ is the set of all unicyclic graphs. In this paper, we present a unified approach to the extremal cactus, which have the same or very similar structures, for Wiener index, Merrifield-Simmons index, Hosoya index and spectral radius. From our results, we can derive some known results.

1. Introduction

Mathematical descriptors of molecular structure, such as various topological indices, have been widely used in structure-property-activity studies (see [10, 11, 16]). Among the numerous topological indices considered in chemical graph theory, only a few have been found noteworthy in practical application (see [15]). The Wiener index is the first chemical index introduced in 1947 by Harold Wiener. It was shown

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that there are excellent correlations between the Wiener index of the molecular graph of an organic compound and a variety of physical and chemical properties of the organic compound (see [20], [21]). M. Randić [18] showed that if alkanes are ordered so that their Randić-index decrease then the extent of their branching should increase. The Hosoya index of a graph was introduced by Hosoya in 1971 [9] and was applied to correlations with boiling points, entropies, calculated bond orders, as well as for coding of chemical structures (see [14, 17]). Merrifield and Simmons [14] developed a topological approach to structural chemistry. The cardinality of the topological space in their theory turns out to be equal to Merrifield-Simmons index of the respective molecular graph G. There have been many publications on these chemical indices (see [4]-[7], [12], [13], [20]-[24]). In [12], Li and Zheng put forward a problem, which *asked for a more unified approach that can cover extremal result for as many as chemical indices as possible*. Here, we present a unified and simple approach to extremal cactus for the Wiener index, Merrifield-Simmons index, Hosoya index and spectral radius.

In order to discuss our results, we first introduced some terminologies and notations of graphs. Other undefined notations may refer to [1, 2]. Let $G = (V, E)$ be a simple undirected graph of order n. For a vertex u of G, we denote the neighborhood and the degree of u by $N_G(u)$ and $d_G(u)$, respectively. For two vertices u and v $(u \neq v)$ of G, the distance between u and v, denoted by $d_G(u, v)$, is the number of edges in a shortest path joining u and v in G. For $H \subseteq V(G)$, we let $N_H(u) = N_G(u) \cap H$. Denote $N_H[u] = N_H(u) \cup \{u\}$. We will use $G - x$ or $G - xy$ to denote the graph that arises from G by deleting the vertex $x \in V(G)$ or the edge $xy \in E(G)$. Similarly, $G + xy$ is a graph that arises from G by adding an edge $xy \notin E(G)$, where $x,\ y \in V(G)$.

We list the definitions of some topological indices as follows.

(i) The Wiener index of G, is defined as

$$W(G) = \sum_{u,v} d_G(u, v),$$

where $d_G(u, v)$ is the distance between u and v in G and the sum goes over all the pairs of vertices.

(ii) The *Merrifield-Simmons index*, is defined as

$$\sigma(G) = \sum_{k \geq 0} i(G; k),$$

where $i(G; k)$ is the number of k-independent vertex sets of G. Note that $i(G; 0) = 1$.

(iii) The *Hosoya index*, is defined as

$$z(G)=\sum_{k\geq 0} m(G;k),$$

where $m(G;k)$ is the number of k-independent edge sets of G. Note that $m(G;0)=1$.

(iv) The *Randić index* of G is defined (see [18]) as

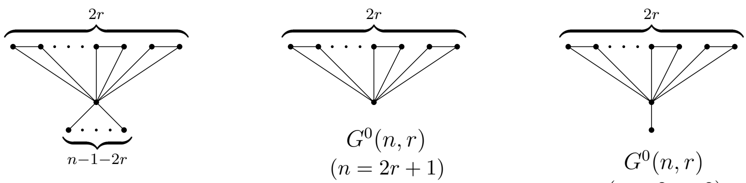
$$R(G)=\sum_{u,v}(d(u)d(v))^{-\frac{1}{2}},$$

where $d(u)$ denotes the degree of the vertex u of the molecular graph G, the summation goes over all pairs of adjacent vertices of G.

(v) The *spectral radius*, $\rho(G)$, of G is the largest eigenvalue of $A(G)$, where $A(G)$ be the adjacency matrix of a graph G. When G is connected, $A(G)$ is irreducible and by the Perron-Frobenius Theorem, the spectral radius is simple and has a unique positive eigenvector. We will refer to such an eigenvector as the Perron vector of G.

Let G be a connected graph. We call G a cactus if all of blocks of G are either edges or cycles. Denote $\mathscr{G}(n,r)$ the set of cacti of order n and with r cycles. Obviously, $\mathscr{G}(n,0)$ is the set of all trees and $\mathscr{G}(n,1)$ is the set of all unicyclic graphs.

We use $G^0(n,r)$ to denote the cactus obtained from the n-vertex star by adding r mutually independent edges (see Fig. 1).



$G^0(n,r)$ $\qquad$ $G^0(n,r)$ $(n=2r+1)$ $\qquad$ $G^0(n,r)$ $(n=2r+2)$

Fig. 1

2. Lemmas

Denote the characteristic polynomial of a graph G by $\phi(G;\lambda)$.

Lemma 2.1 (see [19]). *Let v be a vertex of a graph G, and let $\mathscr{C}(v)$ be the set of all cycles containing v. Then*

$$\phi(G;\lambda)=\lambda\phi(G-v;\lambda)-\sum_{vw\in E(G)}\phi(G-v-w;\lambda)-2\sum_{Z\in\mathscr{C}(v)}\phi(G-V(Z);\lambda).$$

Lemma 2.2 (see [22]). *Let G be a connected graph, and let $u, v \in V(G)$. Suppose $v_1, v_2, \ldots, v_s \in N(v) \setminus N(u)$ $(1 \le s \le d_G(v))$ and $x = (x_1, x_2, \ldots, x_n)^t$ is the Perron vector of $A(G)$, where x_i corresponds to the vertex v_i $(1 \le i \le n)$. Let G^* be the graph obtained from G by deleting the edges vv_i and adding the edges uv_i, $1 \le i \le s$. If $x_u \ge x_v$, then*

$$\rho(G) < \rho(G^*).$$

Lemma 2.3 (see [8]). *Let G be a graph and $v \in V(G)$. Then*

(i) $\sigma(G) = \sigma(G - v) + \sigma(G - N_G[v])$;

(ii) $z(G) = z(G - v) + \sum_{u \in N_G(v)} z(G - \{u, v\})$;

(iii) Moreover, if $G_1, G_2, \cdots, G_\omega$ are the components of a graph G, then $\sigma(G) = \prod_{j=1}^{\omega} \sigma(G_j)$ and $z(G) = \prod_{j=1}^{\omega} z(G_j)$.

From Lemma 2.3, if v is a vertex of G, then $\sigma(G) > \sigma(G - v)$. Moreover, if G is a graph with at least one edge, then $z(G) > z(G - v)$.

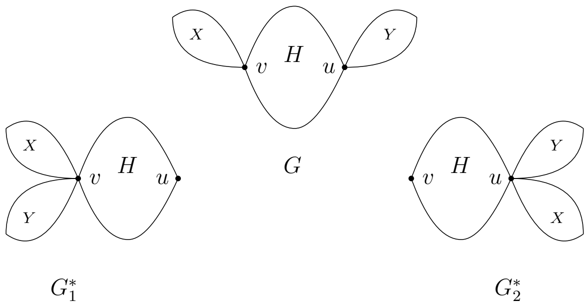


Fig. 2

Lemma 2.4. *Let H, X, Y be three connected graphs disjoint in pair. Suppose that u, v are two vertices of H, v' is a vertex of X, u' is a vertex of Y. Let G be the graph obtained from H, X, Y by identifying v with v' and u with u', respectively. Let G_1^* be the graph obtained from H, X, Y by identifying vertices v, v', u', and let G_2^* be the graph obtained from H, X, Y by identifying vertices u, v', u' (see Fig. 2). Then*

(i) $\sigma(G_1^*) > \sigma(G)$ *or* $\sigma(G_2^*) > \sigma(G)$;

(ii) $z(G_1^*) < z(G)$ *or* $z(G_2^*) < z(G)$;

(iii) $W(G_1^*) < W(G)$ *or* $W(G_2^*) < W(G)$;

(iv) $\rho(G_1^*) > \rho(G)$ *or* $\rho(G_2^*) > \rho(G)$.

Proof. (i) Denote $a = \sigma(X - v)$, $a' = \sigma(X - N_X[v])$, $b = \sigma(Y - u)$ and $b' = \sigma(Y - N_Y[u])$. Then $a > a' > 0$ and $b > b' > 0$. Let $i_{u,v}$ be the number of independent vertex subsets in H containing both u and v. Then $i_{u,v} = 0$ if $uv \in E(G)$, $i_{u,v} = \sigma(H - N_H[u] - N_H[v])$ if $uv \in E(G)$. By Lemma 2.3, we have

$$\begin{aligned}\sigma(G) &= \sigma(G - v) + \sigma(G - N_G[v]) \\ &= ab\sigma(H - v - u) + ab'\sigma(H - v - N_H[u]) + a'b\sigma(H - u - N_H[v]) + a'b'i_{u,v}.\end{aligned}$$

Similarly, we have

$$\begin{aligned}\sigma(G_1^*) &= ab[\sigma(H - v - u) + \sigma(H - v - N_H[u])] + a'b'[\sigma(H - u - N_H[v]) + i_{u,v}], \\ \sigma(G_2^*) &= ab[\sigma(H - v - u) + \sigma(H - u - N_H[v])] + a'b'[\sigma(H - v - N_H[u]) + i_{u,v}].\end{aligned}$$

Therefore

$$\begin{aligned}\sigma(G) - \sigma(G_1^*) &= a'(b - b')\sigma(H - u - N_H[v]) - a(b - b')\sigma(H - v - N_H[u]), \\ \sigma(G) - \sigma(G_2^*) &= b'(a - a')\sigma(H - v - N_H[u]) - b(a - a')\sigma(H - u - N_H[v]).\end{aligned}$$

If $\sigma(G) - \sigma(G_1^*) \geq 0$, then $(b - b')[a'\sigma(H - u - N_H[v]) - a\sigma(H - v - N_H[u])] \geq 0$. Since $a > a'$ and $b > b'$, we have $\sigma(H - u - N_H[v]) > \sigma(H - v - N_H[u])$. So

$$\begin{aligned}\sigma(G) - \sigma(G_2^*) &= (a - a')[b'\sigma(H - v - N_H[u]) - b\sigma(H - u - N_H[v])] \\ &< (a - a')[b'\sigma(H - v - N_H[u]) - b\sigma(H - v - N_H[u])] \\ &= (a - a')(b' - b)\sigma(H - v - N_H[u]) < 0.\end{aligned}$$

(ii) Let $\delta = 0$ if $uv \notin E(G)$ and $\delta = 1$ if $uv \in E(G)$. Let $e_0 = 1$ if $uv \notin E(G)$; and $e_0 = 2$ if $uv \in E(G)$. Denote $p = z(X - v)$, $q = z(Y - u)$, $p' = \sum\limits_{x \in N_X(v)} \frac{z(X-v-x)}{z(X-v)}$, $q' = \sum\limits_{y \in N_Y(u)} \frac{z(Y-u-y)}{z(Y-u)}$, $r_u = \sum\limits_{u' \in N_{H-v}(u)} z(H-v-u-u')$, $r_v = \sum\limits_{v' \in N_H(v)-u} z(H-v-u-v')$, $r_0 = \sum\limits_{v' \in N_H(v)-u} \sum\limits_{u' \in N_{H-v-v'}(u)} z(H - v - u - v' - u')$.

By Lemma 2.3, we have

$$\begin{aligned}z(G) &= z(G - v) + \sum_{v' \in N_G(v)-u} z(G - v - v') + \delta z(G - v - u) \\ &= e_0 z(G - v - u) + \sum_{u' \in N_{G-v}(u)} z(G - v - u - u') \\ &\quad + \sum_{v' \in N_G(v)-u} z(G - v - v' - u) + \sum_{v' \in N_G(v)-u} \sum_{u' \in N_{G-v-v'}(u)} z(G - v - v' - u - u')\end{aligned}$$

$$\begin{aligned}
&= e_0 z(G-v-u) + \sum_{u'\in N_{H-v}(u)} z(G-v-u-u') + \sum_{u'\in N_Y(u)} z(G-v-u-u') \\
&\quad + \sum_{u'\in N_Y(u)} \sum_{v'\in N_X(v)} z(G-v-u-v'-u') + \sum_{v'\in N_H(v)-u} z(G-v-u-v') \\
&\quad + \sum_{v'\in N_X(v)} z(G-v-u-v') + \sum_{v'\in N_X(v)} \sum_{u'\in N_{H-v}(u)} z(G-v-u-v'-u') \\
&\quad + \sum_{v'\in N_H(v)-u} \sum_{u'\in N_Y(u)} z(G-v-u-v'-u') \\
&\quad + \sum_{v'\in N_H(v)-u} \sum_{u'\in N_{H-v-v'}(u)} z(G-v-u-v'-u') \\
&= pq\cdot[e_0 z(H-v-u) + q'z(H-v-u) + r_u + p'q'z(H-v-u) + r_v \\
&\quad + p'z(H-v-u) + r_u p' + r_v q' + r_0] \\
&= pq[z(H-v-u)(e_0+q'+p'+p'q') + r_v(1+q') + r_u(1+p') + r_0].
\end{aligned}$$

Similarly, we get

$$\begin{aligned}
z(G_1^*) &= pq[z(H-v-u)(e_0+q'+p') + r_u(1+p'+q') + r_v + r_0], \\
z(G_2^*) &= pq[z(H-v-u)(e_0+q'+p') + r_v(1+p'+q') + r_u + r_0].
\end{aligned}$$

Thus

$$\begin{aligned}
z(G) - z(G_1^*) &= pqq'[z(H-v-u)p' + r_v - r_u], \\
z(G) - z(G_2^*) &= pqp'[z(H-v-u)q' + r_u - r_v].
\end{aligned}$$

If $z(G) - z(G_1^*) \leq 0$, then $pqq'[z(H-v-u)p' + r_v - r_u] \leq 0$, that is, $r_u - r_v \geq z(H-v-u)p'$. So

$$\begin{aligned}
z(H-v-u)q' + r_u - r_v &\geq z(H-v-u)q' + z(H-v-u)p' \\
&= z(H-v-u)(q'+p') > 0.
\end{aligned}$$

Note that $pqp' > 0$, and hence $z(G_2^*) < z(G)$.

(iii) We have

$$\begin{aligned}
W(G) &= \sum_{x,y\in V(X)} d_G(x,y) + \sum_{x,y\in V(Y)} d_G(x,y) + \sum_{x\in V(X-v), y\in V(Y-u)} d_G(x,y) \\
&\quad + \sum_{x,y\in V(H)} d_G(x,y) + \sum_{x\in V(H), y\in V(Y-u)} d_G(x,y) + \sum_{x\in V(H), y\in V(X-v)} d_G(x,y) \\
&= \sum_{x,y\in V(X)} d_X(x,y) + \sum_{x,y\in V(Y-u)} d_Y(x,y) + \sum_{x\in V(X-v), y\in V(Y-u)} d_G(x,y)
\end{aligned}$$

$$+ \sum_{x,y \in V(H)} d_H(x,y) + \sum_{x \in V(H), y \in V(Y-u)} d_G(x,y) + \sum_{x \in V(H), y \in V(X-v)} d_G(x,y).$$

Thus

$$\begin{aligned}
& W(G) - W(G_1^*) \\
= & \sum_{x \in V(X-v), y \in V(Y-u)} [d_G(x,y) - d_{G_1^*}(x,y)] + \sum_{x \in V(H), y \in V(Y-u)} [d_G(x,y) - d_{G_1^*}(x,y)], \\
> & \sum_{x \in V(H), y \in V(Y)} [d_G(x,y) - d_{G_1^*}(x,y)] = \sum_{x \in V(H-u-v)} [d_H(x,u) - d_H(x,v)], \qquad (1) \\
& W(G) - W(G_2^*) \\
= & \sum_{x \in V(X), y \in V(Y)} [d_G(x,y) - d_{G_2^*}(x,y)] + \sum_{x \in V(X-v), y \in V(H)} [d_G(x,y) - d_{G_2^*}(x,y)] \\
> & \sum_{x \in V(H-u-v)} [d_H(x,v) - d_H(x,u)]. \qquad (2)
\end{aligned}$$

If $W(G) - W(G_1^*) \leq 0$, then by (1), $\sum_{x \in V(H-u-v)} [d_H(x,u) - d_H(x,v)] < 0$. Thus by (2), $W(G) - W(G_2^*) > 0$.

(iv) Let $x = (x_{v_1}, x_{v_2}, \ldots, x_{v_n})$ is the Perron vector of $A(G)$, where x_{v_i} corresponds to the vertex v_i $(1 \leq i \leq n)$. If $x_v \geq x_u$, then $\rho(G_1^*) > \rho(G)$, and if $x_v < x_u$, then $\rho(G_2^*) > \rho(G)$ by Lemma 2.2. ■

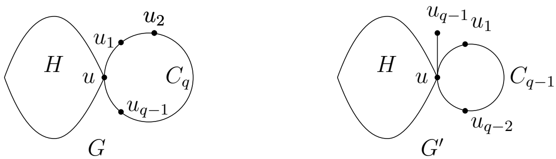


Fig. 3

Let F_n be the nth Fibonacci number, i.e., $F_0 = F_1 = 1$, $F_n = F_{n-1} + F_{n-2}$. Note that $\sigma(P_n) = F_{n+1}$, $z(P_n) = F_n$.

Lemma 2.5. *Suppose that G be a graph of order $n \geq 7$ obtained from a connected graph $H \ncong P_1$ and a cycle $C_q = u_0u_1 \cdots u_{q-1}u_0$ $(q \geq 4)$ by identifying u_0 with a vertex u of the graph H (see Fig. 3). Let $G' = G - u_{q-1}u_{q-2} + uu_{q-2}$. Then*

(i) $\sigma(G') > \sigma(G)$;
(ii) $z(G') < z(G)$;
(iii) $W(G') < W(G)$;
(iv) $\rho(G') > \rho(G)$.

Proof. (i) By Lemma 2.3, we have

$$\begin{aligned}\sigma(G) &= \sigma(G-u)+\sigma(G-N_G[u]) = F_q\sigma(H-u)+F_{q-2}\sigma(H-N_H[u]),\\ \sigma(G') &= \sigma(G'-u)+\sigma(G'-N_{G'}[u]) = 2F_{q-1}\sigma(H-u)+F_{q-3}\sigma(H-N_H[u]).\end{aligned}$$

Therefore $\sigma(G')-\sigma(G) = F_{q-3}\sigma(H-u)-F_{q-4}\sigma(H-N_H[u])>0$.

(ii) By Lemma 2.3, we have

$$\begin{aligned}z(G) &= z(G-u)+\sum_{u'\in N_G(u)} z(G-u-u')\\ &= (F_{q-1}+2F_{q-2})z(H-u)+\sum_{u'\in N_H(u)} z(H-u-u'),\\ z(G') &= z(G'-u)+\sum_{u'\in N_{G'}(u)} z(G-u-u')\\ &= (2F_{q-2}+2F_{q-3})z(H-u)+\sum_{u'\in N_H(u)} z(H-u-u').\end{aligned}$$

Therefore $z(G')-z(G) = -F_{q-4}z(H-u)<0$.

(iii) By the definition of Wiener index, $W(C_q)=\begin{cases} q^3/8 & \text{if } q \text{ is even,}\\ (q^3-q)/8 & \text{if } q \text{ is odd.}\end{cases}$

Note that if $q\geq 4$ is even, then $\sum_{j=0}^{q-2} d_{G'}(u_{q-1},u_j) = 1+2(2+3+\cdots+q/2) = (q^2+2q-4)/4$, thus

$$\begin{aligned}& W(G)-W(G')\\ =& \sum_{x\in V(H)-u_0}\sum_{i=0}^{q-1}[d_G(x,u_i)-d_{G'}(x,u_i)]+\sum_{0\leq i<j\leq q-1}[d_G(u_i,u_j)-d_{G'}(u_i,u_j)]\\ =& \frac{q-2}{2}\sum_{x\in V(H)-u_0} d_H(x,u_0)+\frac{q^3}{8}-\frac{(q-1)^3-(q-1)}{8}-\frac{q^2+2q-4}{4}\\ \geq& \frac{q-2}{2}+\frac{q^3}{8}-\frac{(q-1)^3-(q-1)}{8}-\frac{q^2+2q-4}{4}\\ =& \frac{q^2-2q}{8}>0.\end{aligned}$$

Note that if $q\geq 5$ is odd, then $\sum_{j=0}^{q-2} d_{G'}(u_{q-1},u_j) = 1+2(2+3+\cdots+(q-1)/2)+(q+1)/2 = (q^2+2q-3)/4$, thus

$$\begin{aligned}& W(G)-W(G')\\ =& \sum_{x\in V(H)-u_0}\sum_{i=0}^{q-1}[d_G(x,u_i)-d_{G'}(x,u_i)]+\sum_{0\leq i<j\leq q-1}[d_G(u_i,u_j)-d_{G'}(u_i,u_j)]\end{aligned}$$

$$
\begin{aligned}
&= \frac{q-3}{2}\sum_{x\in V(H)-u_0} d_H(x,u_0) + \frac{q^3-q}{8} - \frac{(q-1)^3}{8} - \frac{q^2+2q-3}{4} \\
&\geq \frac{q-3}{2} + \frac{q^3-q}{8} - \frac{(q-1)^3}{8} - \frac{q^2+2q-3}{4} \qquad (3) \\
&= \frac{q^2-4q-5}{8}. \qquad (4)
\end{aligned}
$$

If $q \geq 6$, then $W(G) - W(G') > 0$ by (4); and if $q = 5$, then $|V(H)| \geq 3$ by $n \geq 7$, and hence the inequality in (3) should be strictly. Therefore $W(G) - W(G') > 0$.

(iv) Let $x = (x_{u_0}, x_{u_1}, \ldots, x_{u_{n-1}})$ is the Perron vector of $A(G)$, where x_{u_i} corresponds to the vertex u_i $(0 \leq i \leq n-1,\ u_0 = u)$. If $x_u \geq x_{u_{q-1}}$, then let $G^* = G - u_{q-1}u_{q-2} + uu_{q-2}$. If $x_u < x_{u_{q-1}}$, then let

$$G^* = G - uu_1 - uw_1 - \cdots - uw_s + u_{q-1}u_1 + u_{q-1}w_1 + \cdots + u_{q-1}w_s,$$

where $N_H(u) = \{w_1, \ldots, w_s\}$. Then in either case, $G^* \cong G'$. Thus, by Lemma 2.2, $\rho(G') > \rho(G)$. ■

Lemma 2.6. *(i)* $\sigma(G^0(n,r)) = 3^r 2^{n-2r-1} + 1$*;*
(ii) $z(G^0(n,r)) = 2^r(n-r)$*;*
(iii) $W(G^0(n,r)) = (n-1)^2 - r$*;*
(iv) $\rho(G^0(n,r))$ *is the root of* $\lambda^4 - n\lambda^2 - 2r\lambda + (n-2r-1) = 0$.

Proof. (i) By Lemma 2.3, we get
$\sigma(G^0(n,r)) = \sigma(G^0(n,r) - u) + \sigma(G^0(n,r) - N_{G^0(n,r)}[u]) = 3^r 2^{n-2r-1} + 1$.
(ii) By Lemma 2.3, we get

$$
\begin{aligned}
z(G^0(n,r)) &= z(G^0(n,r) - u) + \sum_{uu'\in E} z(G^0(n,r) - u - u') \\
&= 2^r + (n-2r-1)2^r + 2r2^{r-1} = 2^r(n-r).
\end{aligned}
$$

(iii) Note that $W(K_{1,n}) = (n-1)^2$, and hence $W(G^0(n,r)) = (n-1)^2 - r$.
(iv) By Lemma 2.1, we have

$$
\begin{aligned}
\phi(G^0(n,r);\lambda) &= \lambda^{n-2r}(\lambda^2-1)^r - (n-2r-1)\lambda^{n-2r-2}(\lambda^2-1)^r \\
&\quad -2r\lambda^{n-2r}(\lambda^2-1)^{r-1} - 2r\lambda^{n-2r-1}(\lambda^2-1)^{r-1} \\
&= \lambda^{n-2r-2}(\lambda^2-1)^{r-1}(\lambda^4 - n\lambda^2 - 2r\lambda + (n-2r-1)).
\end{aligned}
$$

Since $\rho(G^0(n,r)) > 1$, $\rho(G^0(n,r))$ is the root of $\lambda^4 - n\lambda^2 - 2r\lambda + (n-2r-1) = 0$.■

Let $C(a_1, a_2, \ldots, a_r; k)$ be a graph obtained from r cycles $C_{a_i}, 1 \leq i \leq r$ and k edges by taking one vertex of each cycle and each edge, and combining them as one vertex. Denote $\mathscr{C}^0(n,r) = \{C(a_1, a_2, \ldots, a_r; k) : a_i \geq 3, 1 \leq i \leq r, \sum_{i=1}^{r}(a_i - 1) + k + 1 = n\}$. Then $\mathscr{C}^0(n,r) \subseteq \mathscr{C}(n,r)$ and $G^0(n,r) = C(\underbrace{3, \ldots, 3}_{r}; n - 2r - 1)$.

3. Results

In this section, we derive the extremal cacti for the Wiener index, Merrifield-Simmons index, Hosoya index and spectral radius by a unified approach.

In [3], Borovicanin and Petrovic show that $G^0(n,r)$ is the maximal spectral radius in the set $\mathscr{G}(n,r)$. Here, in order to discover the unification of our approach, we still consider the spectral radius.

Denote $f(G) \in \{\sigma(G), \rho(G), -z(G), -W(G)\}$.

Theorem 3.1. *Let $G \in \mathscr{G}(n,r)$, $n \geq 7$. Then*

$$f(G) \leq f(G^0(n,r))$$

with equality holds if and only if $G \cong G^0(n,r)$.

Proof. We have to prove that if $G \in \mathscr{G}(n,r)$, then $f(G) \leq f(G^0(n,r))$ with equality only if $G \cong G^0(n,r)$.

Let $V_c = \{v \in V(G) : v$ is a cutvertex of $G\}$.

Choose $G \in \mathscr{G}(n,r)$ such that $f(G)$ is as large as possible. In the following, we will show some facts.

Fact 1. $G \in \mathscr{G}^0(n,r)$, *i.e.*, $|V_c| = 1$.

Proof of Fact 1. Suppose that $|V_c| > 1$. Let $u, v \in V_c$ and H be a component containing u, v with $N_G(u) \setminus N_H(u), N_G(v) \setminus N_H(v) \neq \emptyset$. Denote $N_G(u) \setminus N_H(u) = \{w_1, w_2, \ldots, w_s\}$ and $N_G(v) \setminus N_H(v) = \{v_1, v_2, \ldots, v_t\}$. Then $s, t \geq 1$. Let $G_1^* = G - \{uw_1, \ldots, uw_s\} + \{vw_1, \ldots, vw_s\}$ and $G_2^* = G - \{vv_1, \ldots, vv_t\} + \{uv_1, \ldots, uv_t\}$. Then $G_1^*, G_2^* \in \mathscr{G}(n,r)$. But, by Lemma 2.4, either $f(G_1^*) > f(G)$ or $f(G_2^*) > f(G)$, a contradiction. Therefore $|V_c| = 1$. ∎

By Fact 1, we let u denote the only cut-vertex of G.

Fact 2. $G \cong G^0(n,r)$.

Proof of Fact 2. Assume that $G \not\cong G^0(n,r)$. Then there exists a cycle $C_q = uu_1 \cdots u_{q-1}u$ with $q \geq 4$. Let $G' = G - u_1u_2 + uu_2$. Then $G' \in \mathscr{G}(n,r)$. By Lemma 2.5, $f(G') > f(G)$, a contradiction. ∎

Therefore the proof of Theorem 3.1 is complete. ∎

In [13], Lu, Zhang and Tian prove that $G^0(n,r)$ is the minimal Randić index in the set $\mathscr{G}(n,r)$. Combining to Theorem 3.1, we have the following result.

Theorem 3.2. *The maximal spectral radius [3], the maximal Merrifield-Simmons index, the minimal Hosoya index, the minimal Wiener index and the minimal Randić index [13] in the set* $\mathscr{G}(n,r)$ $(n \geq 7)$ *are obtained uniquely at* $G^0(n,r)$.

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