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Extremal Graphs with Respect to Vertex–Degree–Based Topological Indices for c-Cyclic Graphs

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Abstract

Let G be a simple connected graph with vertex set $V(G)$ and edge set $E(G)$. A formal definition of a vertex-degree-based topological index (VDB topological index) of G is

$$\mathcal{TI}_f(G) = \sum_{uv \in E} f(d_G(u), d_G(v)),$$

where $f(x, y) > 0$ is a symmetric real function with $x \geq 1$ and $y \geq 1$, and $d_G(u)$ is the degree of vertex u in G.

In this paper, we give some conditions related to the function $f(x, y)$, and show that if a VDB topological index satisfies these conditions, then the extremal graphs must be almost regular. From this conclusion, we obtained the minimum/maximum values of such VDB topological indices among c-cyclic graphs, and characterize the extremal c-cyclic graphs that achieve the minimum/maximum values. As an application, we show that there are many VDB topological indices that satisfy the conditions given in this paper. These VDB topological indices include the second Zagreb index, reciprocal Randić index, first hyper-Zagreb index, first Gourava index, second Gourava index, product-connectivity Gourava index, exponential reciprocal sum-connectivity index, exponential inverse degree index, first Zagreb index, forgotten index, inverse degree index, Sombor index, reduced Sombor index, third Sombor index, fourth Sombor index, and so on.

1 Introduction

All graphs considered are assumed to be simple and connected. Let $G = (V(G), E(G))$ be a such graph with $|V(G)| = n$ and $|E(G)| = m$. If $m = n+c-1$, then G is called a c-cyclic graph. Specially, if $c = 0, 1, 2, 3, 4$, then G is called a tree, a unicyclic graph, a bicyclic graph, a tricyclic graph and a tetracyclic graph, respectively. Let $N(v)$ denote the neighbor set of vertex v in G. Then $|N(v)|$ is the degree of v in G, denoted by $d_G(v)$. Let $\Delta(G)$ and $\delta(G)$ be the maximum degree and minimum degree of G, respectively. If $\Delta(G) - \delta(G) \leq 1$, then we say that G is said to be almost regular. If $\Delta(G) \leq 4$, then G is called a chemical graph. Denote by $\mathcal{G}_{n,c}$ (resp. $\mathcal{CG}_{n,c}$) the set of all c-cyclic graphs (resp. c-cyclic chemical graphs) of order n.

In mathematical chemistry, there is a large number of topological indices. We are mostly interested in vertex-degree-based topological indices, which are defined as a sum, over all edges of a graph, of certain numbers that depend on the degrees of the end-vertices of each edge. A formal definition of a vertex-degree-based topological index (VDB topological index) of G is as follows

$$\mathcal{TI}_f = \mathcal{TI}_f(G) = \sum_{uv \in E} f(d_G(u), d_G(v)), \tag{1}$$

where $f(x, y) > 0$ is a pertinently chosen symmetric real function with $x \geq 1$ and $y \geq 1$.

Let n_i be the number of vertices of G with degree i, and $m_{i,j}$ the number of edges of G joining a vertex of degree i and a vertex of degree j. Then

$$\mathcal{TI}_f(G) = \sum_{\delta(G) \leq i \leq j \leq \Delta(G)} m_{i,j} f(i, j). \tag{2}$$

The problem of characterizing extremal graphs with respect to VDB topological indices among all c-cyclic graphs is one of the most studied problems in chemical graph theory. In many cases, the extremal graphs for different VDB topological indices are same or have some common properties. Yao et al. [16] presented a uniform method to some extremal results together with its corresponding extremal graphs for VDB topological indices among the class of trees, unicyclic graphs and bicyclic graphs with fixed number of independence number and/or matching number, respectively. Ghalavand and Ashrafi [8] ordered the connected graphs and connected chemical graphs with cyclomatic number c with respect to total irregularity. Liu et al. [12] ordered the minimal Sombor indices of chemical trees, chemical unicyclic graphs, chemical bicyclic graphs and chemical tricyclic graphs, respectively. Other related results can be found in [1–7, 9, 10, 13–15, 17] and/or related references listed therein.

The main purpose of this paper is to attack the above problem for general VDB topological indices. In Section 2, we give some conditions related to the function $f(x, y)$, and show that if a VDB topological index satisfies these conditions, then the extremal graphs must be almost regular. From this conclusion, in Sections 3 and 4, we obtained the minimum/maximum values of such VDB topological indices among $\mathcal{G}_{n,c}$ ($\mathcal{CG}_{n,c}$), and characterize the extremal graphs that achieve the minimum/maximum values, respectively. In Section 5, as an application, we show that there are many VDB topological indices that satisfy the conditions given in this paper. These VDB topological indices include the second Zagreb index, reciprocal Randić index, first hyper-Zagreb index, first Gourava index, second Gourava index, product-connectivity Gourava index, exponential reciprocal sum-connectivity index, exponential inverse degree index, first Zagreb index, forgotten index, inverse degree index, Sombor index, reduced Sombor index, third Sombor index, fourth Sombor index, and so on.

2 Extremal graphs of VDB topological indices over graphs

Let $f(x, y) > 0$ be a symmetric real function with $x \geq 1$ and $y \geq 1$. We define the following four functions, where a and b are given numbers and $b > a > 0$.

$$\begin{cases} \quad g(y) = f(b,y) - f(a,y), \\ A(x,y) = yf(x+1,y) - (x+y-1)f(x+1,y-1) \\ \qquad\quad -f(x+1,x+1) + xf(x,y-1), \\ B(x,y) = yf(y,y) - f(x+1,y) - (y-1)f(y-1,y) \\ \qquad\quad -x\left[f(x,x+1) - f(x,x)\right], \\ C(x,y) = (x+y-1)f(x,y) - f(x+1,y-1) - f(x,x+1) \\ \qquad\quad -(y-2)f(x,y-1) - (x-1)f(x+1,y), \\ D(x,y) = f(x,y) - f(x+1,y-1) + (y-1)f(y,y) \\ \qquad\quad -f(x+1,y) - (y-2)f(y-1,y) \\ \qquad\quad -(x-1)\left[f(x,x+1) - f(x,x)\right]. \end{cases} \tag{3}$$

We also give the following four conditions, where c and d are any positive integers with $d \geq c+2$.

(C1) $g(y)$ is increasing on $y \geq 1$, $A(c,d) > 0$ and $C(c,d) > 0$.

(C2) $g(y)$ is increasing on $y \geq 1$, $B(c,d) < 0$ and $D(c,d) < 0$.

(C3) $g(y)$ is decreasing on $y \geq 1$, $B(c,d) > 0$ and $D(c,d) > 0$.

(C4) $g(y)$ is decreasing on $y \geq 1$, $A(c,d) < 0$ and $C(c,d) < 0$.

Let G be a graph, $\Delta(G) = \Delta$, $\delta(G) = \delta$, and $\Delta - \delta \geq 2$. Let u, v be a closest pair of vertices in G such that $d_G(u) = \Delta$ and $d_G(v) = \delta$. Take $G' = G - uu_1 + vu_1$, where $u_1 \in N(u) \setminus (N(v) \cup \{v\})$.

Lemma 2.1. *(1) If the condition (C1) holds, then $\mathcal{TI}_f(G) > \mathcal{TI}_f(G')$.*

(2) If the condition (C2) holds, then $\mathcal{TI}_f(G) < \mathcal{TI}_f(G')$.

Proof. Suppose that the function $g(y)$ is increasing on $y \geq 1$.

Case 1. $uv \notin E(G)$.

Denote $N(u) = \{u_1, u_2, \ldots, u_\Delta\}$ and $N(v) = \{v_1, v_2, \ldots, v_\delta\}$. Note that $d_{G'}(u) = \Delta - 1$, $d_{G'}(v) = \delta + 1$, $d_{G'}(u_i) = d_G(u_i)$ for $i = 1, \ldots, \Delta$, and $d_{G'}(v_j) = d_G(v_j)$ for $j = 1, \ldots, \delta$. Then

$$\begin{aligned} &\mathcal{TI}_f(G) - \mathcal{TI}_f(G') \\ =& \sum_{i=1}^{\Delta} f(d_G(u), d_G(u_i)) + \sum_{j=1}^{\delta} f(d_G(v), d_G(v_j)) - f(d_{G'}(v), d_{G'}(u_1)) \end{aligned}$$

$$
\begin{aligned}
&-\sum_{i=2}^{\Delta} f(d_{G'}(u), d_{G'}(u_i)) - \sum_{j=1}^{\delta} f(d_{G'}(v), d_{G'}(v_j)) \\
=&\sum_{i=1}^{\Delta} f(\Delta, d_G(u_i)) + \sum_{j=1}^{\delta} f(\delta, d_G(v_j)) - f(\delta+1, d_G(u_1)) \\
&-\sum_{i=2}^{\Delta} f(\Delta-1, d_G(u_i)) - \sum_{j=1}^{\delta} f(\delta+1, d_G(v_j)) \\
=&f(\Delta, d_G(u_1)) + \sum_{i=2}^{\Delta} \left[f(\Delta, d_G(u_i)) - f(\Delta-1, d_G(u_i))\right] \\
&- f(\delta+1, d_G(u_1)) - \sum_{j=1}^{\delta} \left[f(\delta+1, d_G(v_j)) - f(\delta, d_G(v_j))\right]. \qquad (4)
\end{aligned}
$$

Note that $uv \notin E(G)$, and u, v is a closest pair of vertices in G such that $d_G(u) = \Delta$ and $d_G(v) = \delta$. We have $\delta + 1 \leq d_G(u_i) \leq \Delta$ for $i = 1, \ldots, \Delta$, and $\delta \leq d_G(v_j) \leq \Delta - 1$ for $j = 1, \ldots, \delta$. Since $g(y)$ is increasing on $y \geq 1$, we have

$$
\begin{aligned}
f(\Delta, \Delta) - f(\delta+1, \Delta) &\geq f(\Delta, d_G(u_1)) - f(\delta+1, d_G(u_1)) \\
&\geq f(\Delta, \delta+1) - f(\delta+1, \delta+1),
\end{aligned}
$$

and for $i = 2, \ldots, \Delta$ and $j = 1, \ldots, \delta$,

$$
\begin{aligned}
f(\Delta, \Delta) - f(\Delta-1, \Delta) &\geq f(\Delta, d_G(u_i)) - f(\Delta-1, d_G(u_i)) \\
&\geq f(\Delta, \delta+1) - f(\Delta-1, \delta+1), \\
f(\delta+1, \Delta-1) - f(\delta, \Delta-1) &\geq f(\delta+1, d_G(v_j)) - f(\delta, d_G(v_j)) \\
&\geq f(\delta+1, \delta) - f(\delta, \delta).
\end{aligned}
$$

So by Eq. (4),

$$
\begin{aligned}
&\mathcal{TI}_f(G) - \mathcal{TI}_f(G') \\
\geq& f(\Delta, \delta+1) - f(\delta+1, \delta+1) + (\Delta-1)\left[f(\Delta, \delta+1) - f(\Delta-1, \delta+1)\right] \\
&- \delta\left[f(\delta+1, \Delta-1) - f(\delta, \Delta-1)\right] \\
=&\Delta f(\Delta, \delta+1) - (\Delta+\delta-1) f(\Delta-1, \delta+1)
\end{aligned}
$$

$$- f(\delta+1,\delta+1) + \delta f(\delta,\Delta-1) = A(\delta,\Delta),$$

and

$$\begin{aligned}
&\mathcal{TI}_f(G) - \mathcal{TI}_f(G') \\
\leq& f(\Delta,\Delta) - f(\delta+1,\Delta) + (\Delta-1)\left[f(\Delta,\Delta) - f(\Delta-1,\Delta)\right] \\
&- \delta\left[f(\delta+1,\delta) - f(\delta,\delta)\right] \\
=&\Delta f(\Delta,\Delta) - f(\delta+1,\Delta) - (\Delta-1)f(\Delta-1,\Delta) - \delta\left[f(\delta+1,\delta) - f(\delta,\delta)\right] \\
=&B(\delta,\Delta).
\end{aligned}$$

Thus for Case 1, if the condition (C1) holds, then $\mathcal{TI}_f(G) > \mathcal{TI}_f(G')$; and if the condition (C2) holds, then $\mathcal{TI}_f(G) < \mathcal{TI}_f(G')$.

Case 2. $uv \in E(G)$.

Denote $N(u) = \{v, u_1, u_2, \ldots, u_{\Delta-1}\}$ and $N(v) = \{u, v_1, v_2, \ldots, v_{\delta-1}\}$. Note that $d_{G'}(u) = \Delta - 1$, $d_{G'}(v) = \delta + 1$, $d_{G'}(u_i) = d_G(u_i)$ for $i = 1, \ldots, \Delta-1$, and $d_{G'}(v_j) = d_G(v_j)$ for $j = 1, \ldots, \delta-1$. Then

$$\begin{aligned}
&\mathcal{TI}_f(G) - \mathcal{TI}_f(G') \\
=&f(d_G(u), d_G(v)) + \sum_{i=1}^{\Delta-1} f(d_G(u), d_G(u_i)) + \sum_{j=1}^{\delta-1} f(d_G(v), d_G(v_j)) \\
&- f(d_{G'}(u), d_{G'}(v)) - f(d_{G'}(v), d_{G'}(u_1)) - \sum_{i=2}^{\Delta-1} f(d_{G'}(u), d_{G'}(u_i)) \\
&- \sum_{j=1}^{\delta-1} f(d_{G'}(v), d_{G'}(v_j)) \\
=&f(\Delta,\delta) + \sum_{i=1}^{\Delta-1} f(\Delta, d_G(u_i)) + \sum_{j=1}^{\delta-1} f(\delta, d_G(v_j)) \\
&- f(\Delta-1,\delta+1) - f(\delta+1, d_G(u_1)) - \sum_{i=2}^{\Delta-1} f(\Delta-1, d_G(u_i)) \\
&- \sum_{j=1}^{\delta-1} f(\delta+1, d_G(v_j)) \\
=&f(\Delta,\delta) - f(\Delta-1,\delta+1) + f(\Delta, d_G(u_1)) - f(\delta+1, d_G(u_1))
\end{aligned}$$

$$+\sum_{i=2}^{\Delta-1}\left[f(\Delta,d_G(u_i))-f(\Delta-1,d_G(u_i))\right]$$
$$-\sum_{j=1}^{\delta-1}\left[f(\delta+1,d_G(v_j))-f(\delta,d_G(v_j))\right]. \qquad (5)$$

Note that $\delta \leq d_G(u_i) \leq \Delta$ for $i = 1,\ldots,\Delta$, and $\delta \leq d_G(v_j) \leq \Delta$ for $j = 1,\ldots,\delta$. Since $g(y)$ is increasing on the interval $y \geq 1$, we have

$$f(\Delta,\Delta)-f(\delta+1,\Delta) \geq f(\Delta,d_G(u_1))-f(\delta+1,d_G(u_1)) \geq f(\Delta,\delta)-f(\delta+1,\delta),$$

and for $i = 2,\ldots,\Delta-1$ and $j = 1,\ldots,\delta-1$,

$$f(\Delta,\Delta)-f(\Delta-1,\Delta) \geq f(\Delta,d_G(u_i))-f(\Delta-1,d_G(u_i)) \geq f(\Delta,\delta)-f(\Delta-1,\delta),$$

$$f(\delta+1,\Delta)-f(\delta,\Delta) \geq f(\delta+1,d_G(v_j))-f(\delta,d_G(v_j)) \geq f(\delta+1,\delta)-f(\delta,\delta).$$

So by Eq. (5),

$$\begin{aligned}
&\mathcal{TI}_f(G)-\mathcal{TI}_f(G')\\
\geq& f(\Delta,\delta)-f(\Delta-1,\delta+1)+f(\Delta,\delta)-f(\delta+1,\delta)\\
&+(\Delta-2)\left[f(\Delta,\delta)-f(\Delta-1,\delta)\right]-(\delta-1)\left[f(\delta+1,\Delta)-f(\delta,\Delta)\right]\\
=&(\Delta+\delta-1)f(\delta,\Delta)-f(\Delta-1,\delta+1)-f(\delta+1,\delta)\\
&-(\Delta-2)f(\Delta-1,\delta)-(\delta-1)f(\delta+1,\Delta)\\
=&C(\delta,\Delta),
\end{aligned}$$

and

$$\begin{aligned}
&\mathcal{TI}_f(G)-\mathcal{TI}_f(G')\\
\leq& f(\Delta,\delta)-f(\Delta-1,\delta+1)+f(\Delta,\Delta)-f(\delta+1,\Delta)\\
&+(\Delta-2)\left[f(\Delta,\Delta)-f(\Delta-1,\Delta)\right]-(\delta-1)\left[f(\delta+1,\delta)-f(\delta,\delta)\right]\\
=&f(\Delta,\delta)-f(\Delta-1,\delta+1)+(\Delta-1)f(\Delta,\Delta)-f(\delta+1,\Delta)\\
&-(\Delta-2)f(\Delta-1,\Delta)-(\delta-1)\left[f(\delta+1,\delta)-f(\delta,\delta)\right]\\
=&D(\delta,\Delta).
\end{aligned}$$

Thus for Case 2, if the condition (C1) holds, then $\mathcal{TI}_f(G) > \mathcal{TI}_f(G')$; and if the condition (C2) holds, then $\mathcal{TI}_f(G) < \mathcal{TI}_f(G')$.

The lemma now follows. ■

Similar the proof of Lemma 2.1, we also have the following lemma.

Lemma 2.2. *(1) If the condition (C3) holds, then* $\mathcal{TI}_f(G) > \mathcal{TI}_f(G')$.

(2) If the condition (C4) holds, then $\mathcal{TI}_f(G) < \mathcal{TI}_f(G')$.

The following two theorems are easily derived from Lemmas 2.1 and 2.2.

Theorem 2.3. *Suppose the condition (C1) or (C3) holds. If a graph G minimizes $\mathcal{TI}_f$ index among all graphs of order n, then G is almost regular.*

Theorem 2.4. *Suppose the condition (C2) or (C4) holds. If a graph G maximizes $\mathcal{TI}_f$ index among all graphs of order n, then G is almost regular.*

3 Minimum values of VDB topological indices over $\mathcal{G}_{n,c}$ ($\mathcal{CG}_{n,c}$)

In this section, we determine the minimum values of VDB topological indices satisfying the condition (C1) or (C3) over $\mathcal{G}_{n,c}$ ($\mathcal{CG}_{n,c}$), and characterize those graphs that achieve the minimum values. In order to obtain the main results, we establish three useful lemmas on c-cyclic almost regular graphs.

Lemma 3.1. *Let $n \geq 3$ and $G \in \mathcal{G}_{n,c}$ be almost regular.*

(1) If $c = 0$, then $G \cong P_n$.

(1) If $c = 1$, then $G \cong C_n$.

Proof. Since G is almost regular, $\Delta(G) - \delta(G) \leq 1$.

(1) If $c = 0$, then $\delta(G) = 1$. So $\Delta(G) \leq 2$. Thus $G \cong P_n$.

(2) If $c = 1$ and G isn't a cycle, then $\delta(G) = 1$, and $\Delta(G) \geq 3$. It is a contradiction. ■

Lemma 3.2. *Let $n \geq 6$ and $G \in \mathcal{G}_{n,2}$ be almost regular. Then $\delta(G) = 2$, $\Delta(G) = 3$, and $(m_{2,2}, m_{2,3}, m_{3,3}) = (n-4, 4, 1)$ or $(n-5, 6, 0)$.*

Proof. Let $n \geq 6$ and $G \in \mathcal{G}_{n,2}$ be almost regular. It is easy to see that $\Delta(G) \geq 3$ and there is at least one vertex with degree 2. So $\Delta(G) = 3$ and $\delta(G) = 2$. It implies that two cycles in G cannot have exactly one common vertex. Then $G \cong G_1$ or G_2, where G_1 and G_2 are showed in Figure 3.1, $s \geq t \geq 3$, $r \geq 2$, $s + t + r - 2 = n$, $m \geq 2$, $2m \leq t + 2$, and $s + t - m = n$.

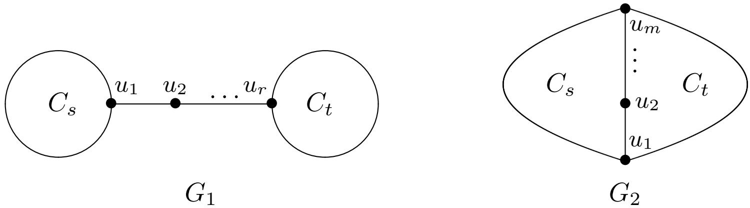

Figure 3.1 Graphs G_1 and G_2

If $G \cong G_1$, then

$$(m_{2,2}, m_{2,3}, m_{3,3}) = \begin{cases} (n-4, 4, 1), & \text{if } r = 2, \\ (n-5, 6, 0), & \text{if } r \geq 3. \end{cases}$$

If $G \cong G_2$, then

$$(m_{2,2}, m_{2,3}, m_{3,3}) = \begin{cases} (n-4, 4, 1), & \text{if } m = 2, \\ (n-5, 6, 0), & \text{if } m \geq 3. \end{cases}$$

The lemma holds. ■

Lemma 3.3. *Let $c \geq 3$, $n \geq 5(c-1)$, and $G \in \mathcal{G}_{n,c}$ be almost regular. Then*

(1) $\delta(G) = 2$ and $\Delta(G) = 3$.

(2) $n_2 = n - 2(c-1)$, $n_3 = 2(c-1)$, $m_{2,2} = n - 5(c-1) + m_{3,3}$, and $m_{2,3} = 6(c-1) - 2m_{3,3}$.

(3) $0 \leq m_{3,3} \leq 3c - 4$.

Proof. (1) Since $c \geq 3$ and G is almost regular, we have $\Delta(G) \geq 3$, and

$\delta(G) \geq \Delta(G) - 1 \geq 2$. If $\delta(G) \geq 3$, then

$$\sum_{i\geq 3} n_i = n, \quad \sum_{i\geq 3} i n_i = 2(n+c-1).$$

We get

$$2n + 2c - 2 \geq 3 \sum_{i\geq 3} n_i = 3n.$$

Thus $n \leq 2c-2$, which is a contradiction with $c \geq 3$ and $n \geq 5(c-1)$. Therefore, $\delta(G) = 2$ and $\Delta(G) = 3$.

(2) By the claim (1), $n_1 = 0$ and $n_i = 0$ for $i \geq 4$. Then

$$\begin{cases} n_2 + n_3 = n, \\ 2n_2 + 3n_3 = 2(n+c-1), \\ 2m_{2,2} + m_{2,3} = 2n_2, \\ m_{2,3} + 2m_{3,3} = 3n_3. \end{cases} \tag{6}$$

Solving the system (6) with unknowns $n_2, n_3, m_{2,2}, m_{2,3}$, we can obtain $n_2 = n - 2(c-1)$, $n_3 = 2(c-1)$, $m_{2,2} = n - 5(c-1) + m_{3,3}$, and $m_{2,3} = 6(c-1) - 2m_{3,3}$.

(3) Since G is a connected graph with $\delta(G) = 2$ and $\Delta(G) = 3$, we have $m_{2,3} \neq 0$. Then by the last equation in (6), $m_{3,3} = \frac{3n_3 - m_{2,3}}{2} = 3c - 3 - \frac{m_{2,3}}{2}$. So $0 \leq m_{3,3} \leq 3c-4$. ■

The following theorem can be deduced directly from Theorem 2.3 and Lemma 3.1.

Theorem 3.4. *Let $G \in \mathcal{G}_{n,c}$ (or $G \in \mathcal{CG}_{n,c}$) with $n \geq 3$, and the condition (C1) or (C3) hold.*

(1) If $c = 0$, then

$$\mathcal{TI}_f(G) \geq \mathcal{TI}_f(P_n) = 2f(1,2) + (n-3)f(2,2),$$

and the equality holds if and only if $G \cong P_n$.

(2) If $c = 1$, then

$$\mathcal{TI}_f(G) \geq \mathcal{TI}_f(C_n) = nf(2,2),$$

and the equality holds if and only if $G \cong C_n$.

Theorem 3.5. *Let* $G \in \mathcal{G}_{n,2}$ *(or* $G \in \mathcal{CG}_{n,2}$*) with* $n \geq 6$*, and the condition (C1) or (C3) hold.*

(1) If $f(2,2)+f(3,3)-2f(2,3) > 0$*, then*

$$\mathcal{TI}_f(G) \geq (n-5)f(2,2)+6f(2,3),$$

and the equality holds if and only if $m_{2,2}=n-5$*,* $m_{2,3}=6$*, and* $m_{3,3}=0$.

(2) If $f(2,2)+f(3,3)-2f(2,3) < 0$*, then*

$$\mathcal{TI}_f(G) \geq (n-4)f(2,2)+4f(2,3)+f(3,3),$$

and the equality holds if and only if $m_{2,2}=n-4$*,* $m_{2,3}=4$*, and* $m_{3,3}=1$.

(3) If $f(2,2)+f(3,3)-2f(2,3) = 0$*, then*

$$\mathcal{TI}_f(G) \geq (n-5)f(2,2)+6f(2,3),$$

and the equality holds if and only if $G \in \mathcal{G}'_{n,2}$*, where* $\mathcal{G}'_{n,2} = \{H \in \mathcal{G}_{n,2} \mid \delta(H)=2, \Delta(H)=3, (m_{2,2},m_{2,3},m_{3,3}) = (n-4,4,1)$ *or* $(n-5,6,0)\}$.

Proof. Let $\mathcal{G}'_{n,2} = \{H \in \mathcal{G}_{n,2} \mid \delta(H)=2, \Delta(H)=3, (m_{2,2},m_{2,3},m_{3,3}) = (n-5,6,0)$ or $(n-4,4,1)\}$. By Eq. (2), for any $H \in \mathcal{G}'_{n,2}$,

$$\begin{aligned} &\mathcal{TI}_f(H) = m_{2,2}f(2,2)+m_{2,3}f(2,3)+m_{3,3}f(3,3) \\ &= \begin{cases} (n-4)f(2,2)+4f(2,3)+f(3,3), & \text{if } (m_{2,2},m_{2,3},m_{3,3})=(n-4,4,1), \\ (n-5)f(2,2)+6f(2,3), & \text{if } (m_{2,2},m_{2,3},m_{3,3})=(n-5,6,0). \end{cases} \end{aligned}$$

Since the condition (C1) or (C3) holds, by Theorem 2.3 and Lemma 3.2, we have for any $G \in \mathcal{G}_{n,2}$ or $\mathcal{CG}_{n,2}$,

$$\mathcal{TI}_f(G) \geq \min_{H \in \mathcal{G}'_{n,2}} \mathcal{TI}_f(H).$$

Then it is easy to see that the theorem follows. ■

Theorem 3.6. *Let* $G \in \mathcal{G}_{n,c}$ *(or* $G \in \mathcal{CG}_{n,c}$*) with* $c \geq 3$ *and* $n \geq 5(c-1)$*, and the condition (C1) or (C3) hold.*

(1) If $f(2,2)+f(3,3)-2f(2,3)>0$, *then*

$$\mathcal{TI}_f(G) \geq (n-5(c-1))f(2,2)+6(c-1)f(2,3),$$

and the equality holds if and only if $m_{3,3}=0$, $m_{2,2}=n-5(c-1)$, *and* $m_{2,3}=6(c-1)$.

(2) If $f(2,2)+f(3,3)-2f(2,3)<0$, *then*

$$\mathcal{TI}_f(G) \geq (n-2c+1)f(2,2)+2f(2,3)+(3c-4)f(3,3),$$

and the equality holds if and only if $m_{3,3}=3c-4$, $m_{2,2}=n-2c+1$, *and* $m_{2,3}=2$.

(3) If $f(2,2)+f(3,3)-2f(2,3)=0$, *then*

$$\mathcal{TI}_f(G) \geq (n-5(c-1))f(2,2)+6(c-1)f(2,3),$$

and the equality holds if and only if $G \in \mathcal{G}'_{n,c}$, *where* $\mathcal{G}'_{n,c}=\{H \in \mathcal{G}_{n,c} \mid \delta(H)=2, \Delta(H)=3, m_{2,2}=n-5(c-1)+m_{3,3}, m_{2,3}=6(c-1)-2m_{3,3}, 0 \leq m_{3,3} \leq 3c-4\}$.

Proof. Let $\mathcal{G}'_{n,c}=\{H \in \mathcal{G}_{n,c} \mid \delta(H)=2, \Delta(H)=3, m_{2,2}=n-5(c-1)+m_{3,3}, m_{2,3}=6(c-1)-2m_{3,3}, 0 \leq m_{3,3} \leq 3c-4\}$. By Eq. (2), we have for any $H \in \mathcal{G}'_{n,c}$,

$$\begin{aligned}
&\mathcal{TI}_f(H)=m_{2,2}f(2,2)+m_{2,3}f(2,3)+m_{3,3}f(3,3)\\
&=(n-5(c-1)+m_{3,3})f(2,2)+(6(c-1)-2m_{3,3})f(2,3)+m_{3,3}f(3,3)\\
&=(n-5(c-1))f(2,2)+6(c-1)f(2,3)+m_{3,3}(f(2,2)-2f(2,3)+f(3,3)).
\end{aligned}$$

Since the condition (C1) or (C3) holds, by Theorem 2.3 and Lemma 3.3, we have for any $G \in \mathcal{G}_{n,c}$ or $\mathcal{CG}_{n,c}$,

$$\mathcal{TI}_f(G) \geq \min_{H \in \mathcal{G}'_{n,c}} \mathcal{TI}_f(H).$$

Then it is easy to see that the theorem follows. ■

4 Maximum values of VDB topological indices over $\mathcal{G}_{n,c}$ ($\mathcal{CG}_{n,c}$)

In this section, we determine the maximum values of VDB topological indices satisfying the condition (C2) or (C4) over $\mathcal{G}_{n,c}$ ($\mathcal{CG}_{n,c}$), and characterize those graphs that achieve the maximum values. The proofs of the following theorems are similar to the proofs of Theorems 3.4, 3.5 and 3.6, and we ignore all proofs.

Theorem 4.1. *Let $G \in \mathcal{G}_{n,c}$ (or $G \in \mathcal{CG}_{n,c}$) with $n \geq 3$, and the condition (C2) or (C4) hold.*

(1) If $c = 0$, then

$$\mathcal{TI}_f(G) \leq \mathcal{TI}_f(P_n) = 2f(1,2) + (n-3)f(2,2),$$

and the equality holds if and only if $G \cong P_n$.

(2) If $c = 1$, then

$$\mathcal{TI}_f(G) \leq \mathcal{TI}_f(C_n) = nf(2,2),$$

and the equality holds if and only if $G \cong C_n$.

Theorem 4.2. *Let $G \in \mathcal{G}_{n,2}$ (or $G \in \mathcal{CG}_{n,2}$) with $n \geq 6$, and the condition (C2) or (C4) hold.*

(1) If $f(2,2) + f(3,3) - 2f(2,3) < 0$, then

$$\mathcal{TI}_f(G) \leq (n-5)f(2,2) + 6f(2,3),$$

and the equality holds if and only if $m_{2,2} = n-5$, $m_{2,3} = 6$, and $m_{3,3} = 0$.

(2) If $f(2,2) + f(3,3) - 2f(2,3) > 0$, then

$$\mathcal{TI}_f(G) \leq (n-4)f(2,2) + 4f(2,3) + f(3,3),$$

and the equality holds if and only if $m_{2,2} = n-4$, $m_{2,3} = 4$, and $m_{3,3} = 1$.

(3) If $f(2,2) + f(3,3) - 2f(2,3) = 0$, then

$$\mathcal{TI}_f(G) \leq (n-5)f(2,2) + 6f(2,3),$$

and the equality holds if and only if $G \in \mathcal{G}'_{n,2}$, *where* $\mathcal{G}'_{n,2} = \{H \in \mathcal{G}_{n,2} \mid \delta(H) = 2, \Delta(H) = 3, (m_{2,2}, m_{2,3}, m_{3,3}) = (n-5, 6, 0)$ *or* $(n-4, 4, 1)\}$.

Theorem 4.3. *Let* $G \in \mathcal{G}_{n,c}$ *(or* $G \in \mathcal{CG}_{n,c}$*) with* $c \geq 3$ *and* $n \geq 5(c-1)$*, and the condition (C2) or (C4) hold.*

(1) If $f(2,2) + f(3,3) - 2f(2,3) < 0$*, then*

$$\mathcal{TI}_f(G) \leq (n - 5(c-1))f(2,2) + 6(c-1)f(2,3),$$

and the equality holds if and only if $m_{3,3} = 0$, $m_{2,2} = n - 5(c-1)$*, and* $m_{2,3} = 6(c-1)$.

(2) If $f(2,2) + f(3,3) - 2f(2,3) > 0$*, then*

$$\mathcal{TI}_f(G) \leq (n - 2c + 1)f(2,2) + 2f(2,3) + (3c-4)f(3,3),$$

and the equality holds if and only if $m_{3,3} = 3c - 4$, $m_{2,2} = n - 2c + 1$*, and* $m_{2,3} = 2$.

(3) If $f(2,2) + f(3,3) - 2f(2,3) = 0$*, then*

$$\mathcal{TI}_f(G) \leq (n - 5(c-1))f(2,2) + 6(c-1)f(2,3),$$

and the equality holds if and only if $G \in \mathcal{G}'_{n,c}$*, where* $\mathcal{G}'_{n,c} = \{H \in \mathcal{G}_{n,c} \mid \delta(H) = 2, \Delta(H) = 3, m_{2,2} = n - 5(c-1) + m_{3,3}, m_{2,3} = 6(c-1) - 2m_{3,3}, 0 \leq m_{3,3} \leq 3c - 4\}$.

5 Applications

In this section, we consider the VDB topological indices in Table 5.1. It is not difficult to verify that

- the VDB topological indices from No.1 to No.8 in Table 5.1 satisfy the condition (C1), and $f(2,2) + f(3,3) - 2f(2,3) > 0$;
- the VDB topological indices from No.9 to No.11 in Table 5.1 satisfy the condition (C1), and $f(2,2) + f(3,3) - 2f(2,3) = 0$; and
- the VDB topological indices from No.12 to No.15 in Table 5.1 satisfy the condition (C3), and $f(2,2) + f(3,3) - 2f(2,3) < 0$.

Table 5.1 Some VDB topological indices

No.	Function $f(x,y)$	Eq. (1) corresponds to
1	xy	Second Zagreb index
2	$\sqrt{xy}$	Reciprocal Randić index
3	$(x+y)^2$	First hyper-Zagreb index
4	$x+y+xy$	First Gourava index
5	$(x+y)xy$	Second Gourava index
6	$\sqrt{(x+y)xy}$	Product-connectivity Gourava index
7	$e^{\sqrt{x+y}}$	Exponential reciprocal sum-connectivity index
8	$e^{\frac{1}{x^2}+\frac{1}{y^2}}$	Exponential inverse degree index
9	$x+y$	First Zagreb index
10	x^2+y^2	Forgotten index
11	$\frac{1}{x^2}+\frac{1}{y^2}$	Inverse degree index
12	$\sqrt{x^2+y^2}$	Sombor index
13	$\sqrt{(x-1)^2+(y-1)^2}$	Reduced Sombor index
14	$\sqrt{2}\pi\frac{x^2+y^2}{x+y}$	Third Sombor index
15	$\frac{\pi}{2}\left(\frac{x^2+y^2}{x+y}\right)^2$	Fourth Sombor index

By Theorems 3.4, 3.5 and 3.6, we have the following theorems.

Theorem 5.1. *Let $G \in \mathcal{G}_{n,c}$ (or $G \in \mathcal{CG}_{n,c}$) with $n \geq 3$. For all VDB topological indices in Table 5.1,*

(1) if $c = 0$, then

$$\mathcal{TI}_f(G) \geq \mathcal{TI}_f(P_n) = 2f(1,2) + (n-3)f(2,2),$$

and the equality holds if and only if $G \cong P_n$; and

(2) if $c = 1$, then

$$\mathcal{TI}_f(G) \geq \mathcal{TI}_f(C_n) = nf(2,2),$$

and the equality holds if and only if $G \cong C_n$.

Theorem 5.2. *Let $G \in \mathcal{G}_{n,2}$ (or $G \in \mathcal{CG}_{n,2}$) with $n \geq 6$.*

(1) For VDB topological indices from No.1 to No.8 in Table 5.1,

$$\mathcal{TI}_f(G) \geq (n-5)f(2,2) + 6f(2,3),$$

and the equality holds if and only if $m_{2,2} = n-5$, $m_{2,3} = 6$, *and* $m_{3,3} = 0$.

(3) For VDB topological indices from No.9 to No.11 in Table 5.1,

$$\mathcal{TI}_f(G) \geq (n-5)f(2,2) + 6f(2,3),$$

and the equality holds if and only if $G \in \mathcal{G}'_{n,2}$, *where* $\mathcal{G}'_{n,2} = \{H \in \mathcal{G}_{n,2} \mid \delta(H) = 2, \Delta(H) = 3, (m_{2,2}, m_{2,3}, m_{3,3}) = (n-5, 6, 0)$ *or* $(n-4, 4, 1)\}$.

(3) For VDB topological indices from No.12 to No.15 in Table 5.1,

$$\mathcal{TI}_f(G) \geq (n-4)f(2,2) + 4f(2,3) + f(3,3),$$

and the equality holds if and only if $m_{2,2} = n-4$, $m_{2,3} = 4$, *and* $m_{3,3} = 1$.

Theorem 5.3. *Let* $G \in \mathcal{G}_{n,c}$ *(or* $G \in \mathcal{CG}_{n,c}$*) with* $c \geq 3$ *and* $n \geq 5(c-1)$.

(1) For VDB topological indices from No.1 to No.8 in Table 5.1,

$$\mathcal{TI}_f(G) \geq (n-5(c-1))f(2,2) + 6(c-1)f(2,3),$$

and the equality holds if and only if $m_{3,3} = 0$, $m_{2,2} = n-5(c-1)$, *and* $m_{2,3} = 6(c-1)$.

(2) For VDB topological indices from No.9 to No.11 in Table 5.1,

$$\mathcal{TI}_f(G) \geq (n-5(c-1))f(2,2) + 6(c-1)f(2,3),$$

and the equality holds if and only if $G \in \mathcal{G}'_{n,c}$, *where* $\mathcal{G}'_{n,c} = \{H \in \mathcal{G}_{n,c} \mid \delta(H) = 2, \Delta(H) = 3, m_{2,2} = n-5(c-1)+m_{3,3}, m_{2,3} = 6(c-1)-2m_{3,3}, 0 \leq m_{3,3} \leq 3c-4\}$.

(3) For VDB topological indices from No.12 to No.15 in Table 5.1,

$$\mathcal{TI}_f(G) \geq (n-2c+1)f(2,2) + 2f(2,3) + (3c-4)f(3,3),$$

and the equality holds if and only if $m_{3,3} = 3c-4$, $m_{2,2} = n-2c+1$, *and* $m_{2,3} = 2$.

6 Conclusions

In this paper, we try to unify the solution for extremal graphs with respect to vertex-degree-based topological indices for c-cyclic graphs. We give some conditions, and show that if a VDB topological index satisfies these conditions, then the extremal graphs with respect to the VDB topological index (under consideration) must be almost regular. Applying this conclusion, we describe extremal graphs with respect to some vertex-degree-based topological indices for c-cyclic graphs. These VDB topological indices include the second Zagreb index, reciprocal Randić index, first hyper-Zagreb index, first Gourava index, second Gourava index, product-connectivity Gourava index, exponential reciprocal sum-connectivity index, exponential inverse degree index, first Zagreb index, forgotten index, inverse degree index, Sombor index, reduced Sombor index, third Sombor index, fourth Sombor index, and so on.

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References

[1] A. Ali, D. Dimitrov, Z. Du, F. Ishfaq, On the extremal graphs for general sum-connectivity index (χ_α) with given cyclomatic number when $\alpha > 1$, *Discr. Appl. Math.* **257** (2019) 19–30.

[2] S. Balachandran, H. Deng, S. Elumalai, T. Mansour, Extremal graphs on geometric-arithmetic index of tetracyclic chemical graphs, *Int. J. Quantum Chem.* **121** (2021) #e26516.

[3] G. Caporossi, P. Hansen, D. Vukičević, Comparing Zagreb indices of cyclic graphs, *MATCH Commun. Math. Comput. Chem.* **63** (2010) 441–451.

[4] R. Cruz, J. Rada, W. Sanchez, Extremal unicyclic graphs with respect to vertex-degree-based topological indices, *MATCH Commun. Math. Comput. Chem.* **88** (2022) 481–503.

[5] K. C. Das, A. Ghalavand, A. R. Ashraf, On a conjecture about the Sombor index of graphs, *Symmetry* **13** (2021) #1830.

[6] H. Deng, A unified approach to the extremal Zagreb indices for trees, unicyclic graphs and bicyclic graphs, *MATCH Commun. Math. Comput. Chem.* **57** (2007) 597–616.

[7] H. Deng, S. Elumalai, S. Balachandran, Maximum and second maximum of geometric-arithmetic index of tricyclic graphs, *MATCH Commun. Math. Comput. Chem.* **79** (2018) 467–475.

[8] A. Ghalavand, A. R. Ashrafi, Ordering of c-cyclic graphs with respect to total irregularity, *J. Appl. Math. Comput.* **63** (2020) 707–715.

[9] I. Gutman, A. Ghalavand, T. Dehghan-Zadeh, A. R. Ashraf, Graphs with smallest forgotten index, *Iranian J. Math. Chem.* **8** (2017) 259–273.

[10] H. Liu, Extremal (n, m)-graphs with respect to VDB topological indices, *Open J. Discr. Appl. Math.* **6** (2023) 16–20.

[11] H. Liu, Z. Du, Y. Huang, H. Chen, S. Elumalai, Note on the minimum bond incident degree indices of k-cyclic graphs, *MATCH Commun. Math. Comput. Chem.* **91** (2024) 255–266.

[12] H. Liu, L. You, Y. Huang, Ordering chemical graphs by Sombor indices and its applications, *MATCH Commun. Math. Comput. Chem.* **87** (2022) 5–22.

[13] H. Liu, L. You, Y. Huang, Extremal Sombor indices of tetracyclic (chemical) graphs, *MATCH Commun. Math. Comput. Chem.* **88** (2022) 573–581.

[14] H. Liu, L. You, Y. Huang, Sombor index of c-cyclic chemical graphs, *MATCH Commun. Math. Comput. Chem.* **90** (2023) 495–504.

[15] J. Rada, Exponential vertex-degree-based topological indices and discrimination, *MATCH Commun. Math. Comput. Chem.* **82** (2019) 29–41.

[16] Y. Yao, M. Liu, K. C. Das, Y. Ye, Some extremal results for vertex-degree-based invariants, *MATCH Commun. Math. Comput. Chem.* **81** (2019) 325–344.

[17] Z. Zhu, H. Lu, On the general sum-connectivity index of tricyclic graphs, *J. Appl. Math. Comput.* **51** (2016) 177–188.