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Vertex-Degree-Based Topological Indices of Trees and Unicyclic Graphs with Perfect Matchings

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Abstract

Let graph G be an ordered pair $(V(G), E(G))$ consisting of a set $V(G)$ of vertices and a set $E(G)$ of edges. The formal definition of a vertex-degree-based topological index (VDB topological index) of G is $TI_f(G) = \sum_{v_i v_j \in E(G)} f(d(v_i), d(v_j))$, where $f(x, y) > 0$ is a symmetric real function with $x \geq 1$ and $y \geq 1$, and $d(v_i)$ denotes the degree of vertex v_i in G. When $f(x, y) = (\frac{x+y-2}{xy})^{\alpha}$, where α is an arbitrary non-zero real number, this VDB topological index is called the generalized atom-bond connectivity index (or ABC_α index for short) of G, which was introduced as a topological index by Furtula et al.

In this paper, we present several conditions on the function $f(x, y)$ and prove that if a VDB topological index satisfies these conditions, then its extremal graphs are almost regular. Based on this conclusion, we derive the maximum VDB indices of trees and unicyclic graphs with perfect matchings, and characterize the corresponding extremal graphs. As an application, we verify that the ABC_α index for $0 < \alpha \leq 1$ satisfies the conditions given in this paper, present the maximum ABC_α index of trees and unicyclic graphs

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with perfect matchings, and characterize the corresponding extremal graphs. Our work thereby extends several previously known results.

1 Introduction

Let G be a graph with vertex set $V(G) = \{v_1, v_2, \ldots, v_n\}$ and edge set $E(G)$. Denote by $d_G(v_i)$ (or $d(v_i)$ for short) the degree of the vertex v_i in G. A vertex $v_i \in V(G)$ is called a pendent vertex of G if $d_G(v_i) = 1$, and an edge $v_iv_j \in E(G)$ is called a pendent edge of G if v_i or v_j is a pendent vertex. Use $N_G(v_i)$ to denote the set of all neighbors of v_i. The graph that arises from G by deleting the vertex $u \in V(G)$ (and its incident edges) or the edge $uv \in E(G)$ will be denoted by $G-u$ or $G-uv$, respectively. Similarly, the graph $G+uv$ arises from G by adding an edge $uv \notin E(G)$ between the endpoints $u, v \in V(G)$. A graph G is called a tree if $|E(G)| = |V(G)| - 1$, and a unicycle graph if $|E(G)| = |V(G)|$.

In mathematical chemistry, there are a large number of topological indices. We are mostly interested in vertex-degree-based topological indices (VDB topological index), 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 VDB topological index of G is as follows

$$TI_f(G) = \sum_{v_iv_j \in E(G)} f(d(v_i), d(v_j)),$$

where $f(x, y) > 0$ is a pertinently chosen symmetric real function with $x \geq 1$ and $y \geq 1$. The most popular topological indices of this kind can be found in [1–3].

The atom-bond connectivity index (or ABC index for short) of G, introduced by Estrada et al. As a topological index, is defined to be the sum of weights $\sqrt{\frac{d(v_i)+d(v_j)-2}{d(v_i)d(v_j)}}$ over all edges v_iv_j of G, that is

$$ABC(G) = \sum_{v_iv_j \in E(G)} \sqrt{\frac{d(v_i) + d(v_j) - 2}{d(v_i)d(v_j)}} \ .$$

The ABC index was shown to be well correlated with the heat of formation of alkanes [4]. Estrada later [5] provided a quantum-chemical explanation for this descriptive capacity of the ABC index based on the ratio of 1,3-interactions with respect to the total number of 1,2-, 1,3-and 1,4-interactions in alkanes. Gutman et al. [6] further confirmed that the ABC index can reproduce the heat of formation with an accuracy comparable to that of high-level abinitio and DFT (MP2, B3LYP) quantum chemical calculations. These (chemical) applications have led to a great deal of mathematical investigations on the ABC index; see [7–15] for details.

On the other hand, in order to explore the better correlation abilities of the ABC index for the heat of formation of alkanes, Furtula et al. [16] made a generalization of this index by replacing $\frac{1}{2}$ with an arbitrary non-zero real number α, i.e.,

$$ABC_\alpha(G) = \sum_{v_iv_j \in E(G)} \left(\frac{d(v_i) + d(v_j) - 2}{d(v_i)d(v_j)} \right)^\alpha ,$$

and showed that $ABC_{-3}(G)$ has a better prediction power than the ABC index when studying the heat of formation of octanes and heptanes, which was named the augmented Zagreb index .

A matching M of the graph G is a subset of $E(G)$ such that no two edges in M share a common vertex. If M is a matching of a graph G and vertex $v \in V(G)$ is incident with an edge of M, then v is said to be M-saturated, and if every vertex of G is M-saturated, then M is a perfect matching.

The main purpose of this paper is to investigate the maximum VDB index of trees and unicyclic graphs with perfect matchings. In Section 2, we give some conditions related to the function $f(x, y)$. In Section 3 and 4, we show that if a VDB topological index satisfies these conditions, then the extremal graphs are almost regular. Based on this conclusion, we derived the maximum VDB index for trees and unicyclic graphs with perfect matching, and characterized the corresponding extreme trees and unicyclic graphs.

As an application, in Section 5, we show that the ABC$_\alpha$ index for $0 < \alpha \leq 1$ satisfies the conditions given in this paper. We then present the maximum ABC$_\alpha$ index of trees and unicyclic graphs with perfect matchings and characterize the corresponding extremal graphs, thereby extending the results in [12, 13] for the ABC index.

2 Preliminaries

In this section, we define the following two functions.

Definition 1. Let $f(x, y)$ be a symmetric real function with $x \geq 1$ and $y \geq 1$. Then

(1) The function $f(1, y)$ is monotonically increasing on $y \geq 1$.
(2) For $x > 2$ is fixed, $f(x, y)$ is monotonically decreasing on $y \geq 2$.
(3) $f(2, y) = A$, where A is fixed number.
(4) $2A < f(3, 3) + 2f(3, 1) - f(4, 1) < f(3, 3) + f(3, 1)$.
(5) $3A < 2f(3, 3) + f(3, 1)$.
(6) $4A + f(3, 2) + f(4, 1) < 3(f(3, 3) + f(3, 1))$.

Definition 2. Let $g(x, y) = f(x, y) - f(x, y - 1)$ with $x \geq 1$ and $y \geq 2$. Then

(1) For $x \geq 2$ and $y \geq 2$, $g(x, y) \leq g(2, y) = 0 < g(1, y)$.
(2) The function $g(1, y)$ is monotonically decreasing on $y \geq 3$.

3 The maximum VDB topological index of trees with perfect matchings

For a positive integer $m \geq 3$, let $T(m)$ be the set of trees on $2m$ vertices with perfect matchings. In this section, we consider the VDB topological indices $TI_f(T)$ satisfying the Definitions 1 and 2.

Theorem 3.1. *Let $f(x, y) > 0$ be a symmetric real function satisfied the Definitions 1, 2, and $T \in T(m)$ with $m \geq 3$. Then*

$$TI_f(T) \leq (m - 3)f(3, 3) + (m - 2)f(3, 1) + 4A,$$

with equality holds if and only if $T \cong T_m^*$ (where T_m^* is depicted in Figure 1).

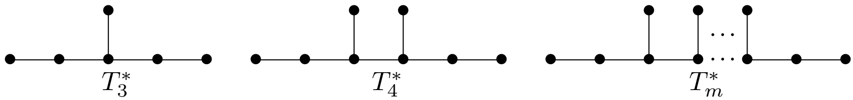


Figure 1. Trees T_3^*, T_4^*, and T_m^* $(m \geq 5)$.

Proof. Let

$$\varphi(m) = (m-3)f(3,3) + (m-2)f(3,1) + 4A. \tag{1}$$

We prove the result by induction on m.

It is easy to see that $T(3)$ contains exactly T_3^* and the path P_6. Note that $TI_f(P_6) = 4A + f(2,1), TI_f(T_3^*) = 4A + f(3,1)$. By Definition 1, the function $f(1,y)$ is monotonically increasing on $y \geq 1$. So, $TI_f(P_6) < TI_f(T_3^*)$. The result holds for $m = 3$.

If $m = 4$ and $T \in T(m)$, then $T \cong T_4^*, P_8$, or F_i $(i = 1,2,3$, see Figure 2). By direct calculation, we can get that $TI_f(T_4^*) = f(3,3) + 2f(3,1) + 4A$, $TI_f(P_8) = 7A$, $TI_f(F_1) = f(3,1) + 6A$, $TI_f(F_2) = 7A$, and $TI_f(F_3) = f(3,1) + 6A$. By Definition 1, the function $f(1,y)$ is monotonically increasing on $y \geq 1$, and for $x > 2$ is fixed, $f(x,y)$ is monotonically decreasing on $y \geq 2$, and $2f(2,1) < f(3,3) + f(3,1)$. Since $TI_f(P_8) = TI_f(F_2) = 7A = 4A + f(3,2) + 2f(2,1) < 4A + f(3,3) + 2f(3,1) = TI_f(T_4^*) = \varphi(4)$, $TI_f(F_1) = TI_f(F_3) = f(3,1)+6A = f(3,1)+2f(2,1)+4A < f(3,3)+2f(3,1)+4A = TI_f(T_4^*) = \varphi(4)$, the result follows for $m = 4$.

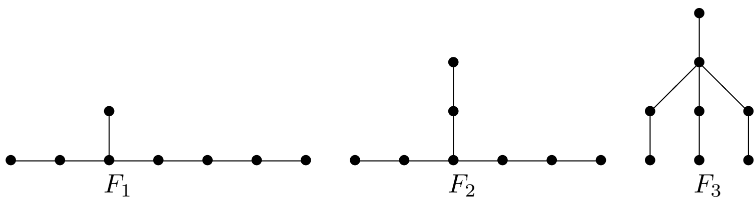


Figure 2. Trees F_i $(i = 1,2,3)$.

Suppose that $m \geq 5$ and the result holds for the trees in $T(n)$ with $n < m$. Let $T \in T(m)$ with a perfect matching M. Then there is a pendent vertex u in T adjacent to a vertex v of degree 2, and so $uv \in M$

and $T_1 = T - u - v \in T(m-1)$. Let w be the neighbor of v different from u in T. Then $d_T(w) \geq 2$. Thus

$$\begin{aligned} TI_f(T) &= TI_f(T_1) + f(d_T(u), d_T(v)) + f(d_T(v), d_T(w)) \\ &\quad + \sum_{x \in N_T(w) \setminus \{v\}} g(d_T(x), d_T(w)) \\ &= TI_f(T_1) + 2A + \sum_{x \in N_T(w) \setminus \{v\}} g(d_T(x), d_T(w)), \end{aligned}$$

where the functions $f(x, y)$ and $g(x, y)$ are defined as Definitions 1 and 2, respectively.

By the induction hypothesis, we have $TI(T_1) \leq \varphi(m-1)$, and so

$$TI_f(T) \leq \varphi(m-1) + 2A + \sum_{x \in N_T(w) \setminus \{v\}} g(d_T(x), d_T(w)), \qquad (2)$$

with equality if and only if $T_1 \cong T^*_{m-1}$.

Denote $N_T(w) \setminus \{v\} = \{w_1, \ldots, w_t\}$, where $t = d_T(w) - 1 \geq 1$. Note that T is a tree with a perfect matching. If $t = 1$, then $d_T(w_1) \geq 2$. If $t \geq 2$, then $N_T(w) \setminus \{v\}$ has at most one pendent vertex of T. So we consider the following two cases.

Case 1. $d_T(w_i) \geq 2$ for $i = 1, \ldots, t$.

By Definition 2, we have

$$\sum_{x \in N_T(w) \setminus \{v\}} g(d_T(x), d_T(w)) = \sum_{i=1}^{t} g(d_T(w_i), d_T(w)) \leq 0.$$

From (1) and (2),

$$TI_f(T) \leq \varphi(m-1) + 2A < \varphi(m).$$

Case 2. $N_T(w) \setminus \{v\}$ has exactly one pendent vertex of T.

Without loss of generality, we assume that $d_T(w_1) = 1$, $d_T(w_i) \geq 2$ for $i = 2, \ldots, t$. Note that in this case, $t \geq 2$, and $d_T(w) = t + 1 \geq 3$.

Subcase 2.1. $t \geq 3$.

Then $d_T(w) = t + 1 \geq 4$. By Definition 2, we have

$$\begin{aligned}\sum_{x \in N_T(w) \setminus \{v\}} g(d_T(x), d_T(w)) &= g(d_T(w_1), d_T(w)) + \sum_{i=2}^{t} g(d_T(w_i), d_T(w)) \\ &\leq g(d_T(w_1), d_T(w)) \\ &= f(t+1, 1) - f(t, 1) \\ &\leq f(4, 1) - f(3, 1).\end{aligned}$$

From (1) and (2),

$$TI_f(T) \leq \varphi(m-1) + 2A + f(4,1) - f(3,1) < \varphi(m).$$

Subcase 2.2. $t = 2$.

Then $d_T(w) = t + 1 = 3$, $N_T(w) \setminus \{v\} = \{w_1, w_2\}$, $d_T(w_1) = 1$, and $d_T(w_2) \geq 2$.

If $d_T(w_2) \geq 3$, then by Definition 1, we have

$$\begin{aligned}&\sum_{x \in N_T(w) \setminus \{v\}} g(d_T(x), d_T(w)) \\ &= g(d_T(w_1), d_T(w)) + g(d_T(w_2), d_T(w)) \\ &= (f(3,1) - f(2,1)) + (f(d_T(w_2), 3) - f(2,1)) \\ &= f(3,1) - 2A + f(d_T(w_2), 3) \\ &\leq f(3,1) - 2A + f(2,3).\end{aligned}$$

From (1) and (2),

$$TI_f(T) \leq \varphi(m-1) + 2A + (f(3,1) - 2A + f(2,3)) = \varphi(m).$$

If $d_T(w_2) = 2$, then it is easy to see the edges $uv, ww_1 \in M$, and $T_2 = T - u - v - w - w_2 \in T(m-2)$. Denote $N_T(w) \setminus \{v, w_1\} = \{z\}$. Note that $d_T(z) \geq 2$. By Definition 2 and the induction hypothesis, we have

$$\begin{aligned} TI_f(T) &= TI_f(T_2) + f(d_T(u), d_T(v)) + f(d_T(v), d_T(w)) \\ &\quad + f(d_T(w), d_T(w_1)) + f(d_T(w), d_T(w_2)) + g(d_T(z), d_T(w_2)) \\ &= TI_f(T_2) + 3A + f(3,1) + g(d_T(z), d_T(w_2)) \\ &\leq \varphi(m-2) + 3A + f(3,1) < \varphi(m). \end{aligned}$$

Combining the above three cases, we now get $TI_f(T) \leq \varphi(m)$, and with equality if and only if $T_1 \cong T^*_{m-1}$, $d_T(w) = 3$, $d_T(w_1) = 1$, and $d_T(w_2) = 3$, that is, $T \cong T^*_m$.

This completes the proof. ■

4 The maximum VDB topological index of unicyclic graphs with perfect matchings

For positive integer $m \geq 2$, let $U(m)$ be the set of unicyclic graphs on $2m$ vertices with perfect matchings. In this section, we consider the VDB topological indices $TI_f(G)$ satisfing the Definitions 1 and 2.

Theorem 4.1. *Let $f(x, y) > 0$ be a symmetric real function satisfied the Definitions 1, 2, and $G \in U(m)$ with $m \geq 2$. Then*

$$TI_f(G) \leq \begin{cases} 3A + f(3,1), & \text{if } m = 2, \\ m(f(3,3) + f(3,1)), & \text{if } m \geq 3, \end{cases}$$

with equality holds if and only if $G \cong U^*_m$ (where U^*_m is depicted in Figure 3).

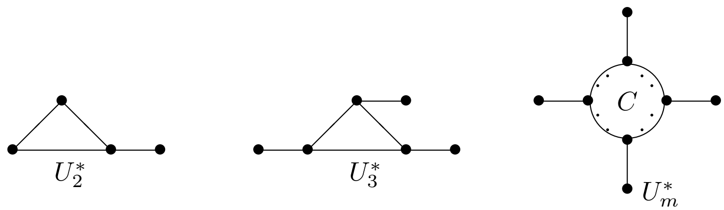


Figure 3. Trees U^*_2, U^*_3, and U^*_m ($m \geq 4$).

Proof. Let

$$\chi(m) = \begin{cases} 3A + f(3,1), & \text{if } m = 2, \\ m(f(3,3) + f(3,1)), & \text{if } m \geq 3. \end{cases} \tag{3}$$

We prove the result by induction on m.

It is easily seen that $U(2)$ contains exactly U_2^* and the cycle C_4. Note that $TI_f(C_4) = 4A = 3A + f(2,1) < 3A + f(3,1) = TI_f(U_2^*) = \chi(2)$, and thus the result holds for $m = 2$.

If $m = 3$ and $G \in U(m)$, then $G \cong U_3^*$, C_6 or H_i ($i = 1, 2, 3, 4, 5, 6$ see Figure 4). By direct calculation, we can get that $TI_f(U_3^*) = 3(f(3,3) + f(3,1)) = \chi(3)$, $TI_f(C_6) = 6A$, $TI_f(H_1) = 5A + f(4,1)$, $TI_f(H_2) = 4A + f(3,3) + f(3,1)$, $TI_f(H_3) = 6A$, $TI_f(H_4) = 6A$, $TI_f(H_5) = 3A + f(3,3) + 2f(3,1)$, $TI_f(H_6) = 5A + f(3,1)$. Since

$TI_f(C_6) = TI_f(H_3) = TI_f(H_4) = 3 \times 2A < 3(f(3,3) + f(3,1)) = TI_f(U_3^*) = \chi(3)$,

$TI_f(H_2) = 4A + f(3,3) + f(3,1) < 4A + f(3,2) + f(4,1) = TI_f(H_1) < 3(f(3,3) + f(3,1)) = TI_f(U_3^*) = \chi(3)$,

$TI_f(H_6) = 3A + 2A + f(3,1) < 3A + f(3,3) + 2f(3,1) = TI_f(H_5) < 3(f(3,3) + f(3,1)) = TI_f(U_3^*) = \chi(3)$, The result follows for $m = 3$.

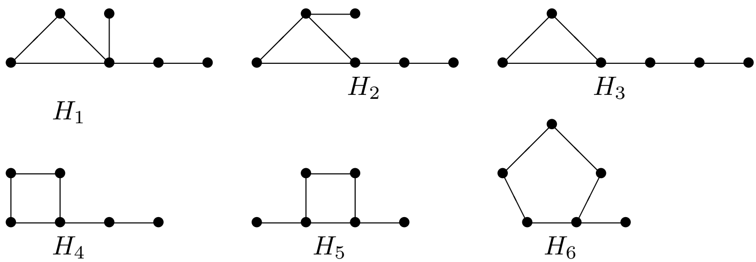


Figure 4. Graphs H_i $(i = 1, 2, \ldots, 6)$

Suppose that $m \geq 4$ and the result holds for the unicyclic graphs in $U(n)$ with $n < m$. Let $G \in U(m)$ with a perfect matching M, and C be the cycle of G.

If $G \cong C_{2m}$, then

$$TI_f(G) = TI_f(C_m) = 2mA < \chi(m).$$

In the following we assume that $G \ncong C_{2m}$. Then G has at least one pendent vertex. Consider the following two cases.

Case 1. There is a pendent vertex u_0 such that $N_G(u_0) \cap V(C) = \phi$.

In this case, there is a pendent vertex u adjacent to a vertex v of degree 2. It is clear that $uv \in M$, and $G_1 = G - u - v \in U(m-1)$. Let w be the neighbor of v different from u in G. Then $d_G(w) \geq 2$. By the induction hypothesis, $TI_f(G_1) \leq \chi(m-1)$, and

$$\begin{aligned} TI_f(G) &= TI_f(G_1) + f(d_G(u), d_G(v)) + f(d_G(v), d_G(w)) \\ &\quad + \sum_{x \in N_G(w) \setminus \{v\}} g(d_G(x), d_G(w)) \\ &\leq \chi(m-1) + 2A + \sum_{x \in N_G(w) \setminus \{v\}} g(d_G(x), d_G(w)), \end{aligned} \tag{4}$$

where the functions $f(x, y)$ and $g(x, y)$ are defined as Definitions 1 and 2, and the equality in (4) holds if and only if $G_1 \cong U^*_{m-1}$. Denote $N_G(w) \setminus \{v\} = \{w_1, \ldots, w_t\}$, where $t = d_G(w) - 1 \geq 1$.

Subcase 1.1. $d_G(w_i) \geq 2$ for $i = 1, \ldots, t$.

By Definition 2,

$$\sum_{x \in N_G(w) \setminus \{v\}} g(d_G(x), d_G(w)) = \sum_{i=1}^{t} g(d_G(w_i), d_G(w)) \leq 0.$$

From (3) and (4), we have

$$TI_f(G) \leq \chi(m-1) + 2A < \chi(m).$$

Subcase 1.2. There is $1 \leq i \leq t$ such that $d_G(w_i) = 1$.

Without loss of generality, we assume that $d_T(w_1) = 1$. Since G has a perfect matching, we have $d_T(w_i) \geq 2$ for $i = 2, \ldots, t$, and $d_G(w) = t+1 \geq 3$.

If $d_G(w)=t+1\geq 4$ (that is, $t\geq 3$), then by Definition 2, we have

$$\begin{aligned}\sum_{x\in N_G(w)\setminus\{v\}} g(d_G(x),d_G(w)) &= g(d_G(w_1),d_G(w))+\sum_{i=1}^{t} g(d_G(w_i),d_G(w))\\ &\leq g(d_G(w_1),d_G(w))=f(t+1,1)-f(t,1)\\ &\leq f(4,1)-f(3,1).\end{aligned}$$

From (3) and (4), we have

$$TI_f(G)\leq \chi(m-1)+2A+f(4,1)-f(3,1)<\chi(m).$$

If $d_G(w)=t+1=3$ (that is, $t\geq 3$, and $N_G(w)\setminus\{v\}=\{w_1,w_2\}$) and $d_G(w_2)\geq 3$, then by Definition 1, we have

$$\begin{aligned}&\sum_{x\in N_G(w)\setminus\{v\}} g(d_G(x),d_G(w))\\ &= g(d_G(w_1),d_G(w))+g(d_G(w_2),d_G(w))\\ &=(f(3,1)-f(2,2))+(f(3,d_G(w_2))-f(2,2))\\ &=f(3,1)-2f(2,2)+f(3,d_G(w_2)\\ &\leq f(3,1)-2A+f(3,3).\end{aligned}$$

Note that $G_1\ncong U^*_{m-1}$ for this case. Then $TI_f(G_1)<\chi(m-1)$. From (3) and (4), we have

$$TI_f(G)<\chi(m-1)+2A+(f(3,1)-2A+f(3,3))=\chi(m).$$

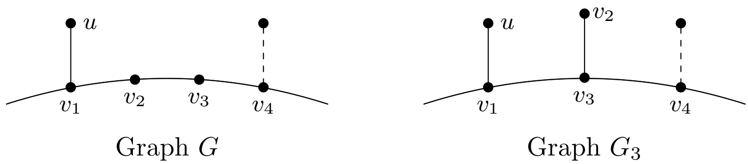
If $d_G(w)=t+1=3$ and $d_G(w_2)=2$, then it is easy to see the edges $uv,ww_1\in M$, and $G_2=G-u-v-w-w_2\in U(m-2)$. Denote $N_G(w)\setminus\{v,w_1\}=\{z\}$. Note that $d_G(z)\geq 2$. By Definition 2 and the induction hypothesis, we have

$$\begin{aligned}TI_f(G)&=TI_f(G_2)+3A+f(3,1)+g(d_G(z),d_G(w_2))\\ &\leq \chi(m-2)+3A+f(3,1)<\chi(m).\end{aligned}$$

So far, we get $TI_f(G) < \chi(m)$ for Case 1.

Case 2. For each pendent vertex u_0 of G, $N_G(u_0) \cap V(C) \neq \phi$.

Since G has a perfect matching M, we have that for each vertex $v_i \in V(C)$, $N_G(v_i)$ has at most one pendent vertex. It implies that $2 \leq d_G(v_i) \leq 3$ for each $v_i \in V(C)$. If $|V(C)| = m/2$, then $G \cong U^*_m$, and by direct calculation, $TI_f(G) = \chi(m)$. If $|V(C)| > m/2$, then there is some vertex of C with degree 2. Since $G \ncong C_{2m}$, there is also some vertex of C with degree 3. Without loss of generality, we assume that $v_1, v_2 \in V(C)$ such that v_1 and v_2 are adjacent, $d_T(v_1) = 3$, and $d_T(v_2) = 2$. Denote $N_G(v_2) \setminus \{v_1\} = \{v_3\}$. Since G has a perfect matching M, each pendent edge of G must be in M. Then $d_T(v_3) = 2$. Consider the graph $G_3 = G - v_1v_2 + v_1v_3$.



Denote $N_G(v_3) \setminus \{v_2\} = \{v_4\}$. Then $2 \leq d_G(w_4) \leq 3$, and so

$$\begin{aligned}
& TI_f(G) - TI_f(G_3) \\
= & f(d_G(v_1), d_G(v_2)) + f(d_G(v_2), d_G(v_3)) + f(d_G(v_3), d_G(v_4)) \\
& - f(d_{G_3}(v_1), d_{G_3}(v_3)) - f(d_{G_3}(v_2), d_{G_3}(v_3)) - f(d_{G_3}(v_3), d_{G_3}(v_4)) \\
= & 3A - f(3,3) - f(3,1) - f(3, d_{G_3}(v_4)) \\
\leq & 3A - f(3,3) - f(3,1) - f(3,3) < 0,
\end{aligned}$$

that is, $TI_f(G) < TI_f(G_3)$.

Thus $TI_f(G) \leq \chi(m)$ for Case 2, with equality holds if and only if $G \cong U^*_m$.

This completes the proof. ∎

5 The maximum ABC_α index of trees and unicyclic graphs with perfect matchings

In this section, as an application, we consider the ABC_α index of trees and unicyclic graphs with perfect matchings, where the parameter α satisfies $0 < \alpha \leq 1$.

Lemma 5.1. *Let* $f(x, y) = (\frac{x+y-2}{xy})^\alpha$ *with* $x \geq 1$, $y \geq 1$ *and* $0 < \alpha \leq 1$. *Then*

(1) *The function* $f(1, y)$ *is monotonically increasing on* $y \geq 1$.

(2) *For* $x > 2$ *is fixed,* $f(x, y)$ *is monotonically decreasing on* $y \geq 2$.

(3) $f(2, y) = A = \left(\frac{1}{2}\right)^\alpha$.

(4) $2A < f(3, 3) + 2f(3, 1) - f(4, 1) < f(3, 3) + f(3, 1)$.

(5) $3A < 2f(3, 3) + f(3, 1)$.

(6) $4A + f(3, 2) + f(4, 1) < 3(f(3, 3) + f(3, 1))$.

Proof. We just have to prove the claims (1) and (2).

(1) Note that $f(1, y) = \left(1 - \frac{1}{y}\right)^\alpha$. Then $f(1, y)$ is monotonically increasing on $y \geq 1$.

(2) For $x > 2$ and $y \geq 2$,

$$\begin{aligned} f(x, y+1) - f(x, y) &= \left(\frac{x+y-1}{x(y+1)}\right)^\alpha - \left(\frac{x+y-2}{xy}\right)^\alpha \\ &= \left(\frac{xy+y^2-y}{xy(y+1)}\right)^\alpha - \left(\frac{xy+y^2-y+x-2}{xy(y+1)}\right)^\alpha < 0. \end{aligned}$$

So $f(x, y)$ is a monotonically decreasing function on $y \geq 2$. ■

Lemma 5.2. *Let* $g(x, y) = \left(\frac{x+y-2}{xy}\right)^\alpha - \left(\frac{x+y-3}{x(y-1)}\right)^\alpha$ $x \geq 1$, $y \geq 1$ *and* $0 < \alpha \leq 1$. *Then*

(1) *For* $x \geq 2$ *and* $y \geq 2$, $g(x, y) \leq g(2, y) = 0 < g(1, y)$.

(2) *The function* $g(1, y)$ *is monotonically decreasing on* $y \geq 3$.

Proof. The claim (1) is clear by Lemma 5.1(1)(3). In the following, we prove the claim (2). For $y \geq 3$,

$$\begin{aligned}\frac{\mathrm{d}g(1,y)}{\mathrm{d}y} &= \frac{\mathrm{d}}{\mathrm{d}y}\left(\left(\frac{y-1}{y}\right)^{\alpha} - \left(\frac{y-2}{y-1}\right)^{\alpha}\right) \\ &= \frac{\alpha}{y^2}\left(\frac{y-1}{y}\right)^{\alpha-1} - \frac{\alpha}{(y-1)^2}\left(\frac{y-2}{y-1}\right)^{\alpha-1} < 0.\end{aligned}$$

So g(1,y) is monotonically decreasing on $y \geq 3$. ■

By Definitions 1, 2, Theorems 3.1, 4.1, Lemmas 5.1, 5.2, we have the following results.

Theorem 5.1. *Let $T \in T(m)$ with $m \geq 3$. Then*

$$ABC_{\alpha}(T) \leq 4\left(\frac{1}{2}\right)^{\alpha} + (m-3)\left(\frac{4}{9}\right)^{\alpha} + (m-2)\left(\frac{2}{3}\right)^{\alpha},$$

with equality holds if and only if $T \cong T_m^*$ (where T_m^* is depicted in Figure 1).

Theorem 5.2. *Let $G \in U(m)$ with $m \geq 2$. Then*

$$ABC_{\alpha}(G) \leq \begin{cases} 3\left(\frac{1}{2}\right)^{\alpha} + \left(\frac{2}{3}\right)^{\alpha}, & \text{if } m = 2, \\ \left(\left(\frac{2}{3}\right)^{\alpha} + \left(\frac{4}{9}\right)^{\alpha}\right)m, & \text{if } m \geq 3, \end{cases}$$

with equality holds if and only if $G \cong U_m^*$ (where U_m^* is depicted in Figure 3).

When $\alpha = \frac{1}{2}$, this corresponds to the results in [12, 13] for the ABC index.

Corollary 5.3. *[12] Let $T \in T(m)$ with $m \geq 3$. Then*

$$ABC(T) \leq \frac{2+\sqrt{6}}{3}m + 2\sqrt{2} - 2 - \frac{2\sqrt{6}}{3},$$

with equality holds if and only if $T \cong T_m^*$ (where T_m^* is depicted in Figure 1).

Corollary 5.4. *[13] Let $G \in U(m)$ with $m \geq 2$. Then*

$$ABC(G) \leq \begin{cases} \frac{3\sqrt{2}}{2} + \frac{\sqrt{6}}{3}, & \textit{if } m = 2, \\ \frac{2+\sqrt{6}}{3} m, & \textit{if } m \geq 3, \end{cases}$$

with equality holds if and only if $G \cong U_m^*$ (where U_m^* is depicted in Figure 3).

6 Conclusions

In this paper, we investigate the maximum VDB index of trees and unicyclic graphs with perfect matchings. 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 are almost regular. Leveraging this result, we derive the maximum VDB index values for the graph classes mentioned and characterize the corresponding extremal graphs. As an application, we show that ABC_α index for $0 < \alpha \leq 1$ satisfies the conditions given in this paper. We then present the maximum ABC_α index of trees and unicyclic graphs with perfect matchings and characterize the corresponding extremal graphs, thereby extending the results in [12, 13] for the ABC index.

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