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# Maximizing Graovac–Ghorbani Index of Trees with Fixed Maximum Degree

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**Abstract**

The Graovac-Ghorbani ($ABC_{GG}$) index of a graph is a distance-based topological descriptor which is an analog of the atom-bond connectivity (ABC) index. In [9], Furtula showed that, tested on alkans, $ABC_{GG}$ gives better prediction in the case of entropy and acentric factor than $ABC$ index.

In [5] Dimitrov et al. conjectured that among all trees on $n$ vertices with the maximum degree $\Delta$ almost dendrimers are trees which maximize $ABC_{GG}$ index. In this paper we present a mathematical proof of the established conjecture by showing that almost dendrimers are extremal trees among all trees with $n$ vertices and maximum degree at most $\Delta$.

# 1 Introduction

Topological descriptors are molecular descriptors which are frequently applied in various research projects. Among them, Randić connectivity index is the most conspicuous one and has countless applications in chemistry and pharmacology [19]. The mathematical properties of this index are also well elaborated. Thorough investigation of this index has motivated

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scientists to introduce other molecular descriptors that could match for Randić index. One of them is the atom-bond connectivity ($ABC$) index introduced in 1998 by Estrada et al. [7]. For a finite, simple and undirected graph $G$ with the vertex set $V(G)$ and the edge set $E(G)$, $ABC$ index is defined as follows

$$ABC(G) = \sum_{uv \in E(G)} \sqrt{\frac{d(u) + d(v) - 2}{d(u)d(v)}}, \tag{1}$$

with $d(w)$ being the degree of a vertex $w \in V(G)$. According to [9], $ABC$ index is one of the best degree–based molecular descriptors [9, 11, 14].

In the hope of being successful as $ABC$ index, in 2010 another topological invariant appeared, afterwards known as Graovac-Ghorbani ($ABC_{GG}$) index [12]. It is defined as

$$ABC_{GG}(G) = \sum_{uv \in E(G)} \sqrt{\frac{n_u + n_v - 2}{n_u n_v}}, \tag{2}$$

where $n_u$ is the number of vertices which are closer to vertex $u$ than to vertex $v$ and $n_v$ is the number of vertices which are closer to $v$ than to $u$. In [9] Furtula studied prediction power of $ABC_{GG}$ index and showed that this distance-based topological descriptor gives better prediction in the case of entropy and acentric factor than ABC index.

Despite the fact that $ABC_{GG}$ index was introduced thirteen years ago, there are only several publications concerned with its mathematical properties. In [20] Rostami et al. proved that among all connected graphs on $n$ vertices, the minimum value of $ABC_{GG}$ is achieved for the complete graphs $K_n$. Additionally, they determined lower and upper bounds of $ABC_{GG}$ index for trees with given number of pendant vertices. Das et al. in [3] obtained bounds of $ABC_{GG}$ index for unicyclic graphs, while Pacheco et al. [18] studied $ABC_{GG}$ index for some types of bicyclic graphs. Dimitrov et al. in [5] showed that amongst all bipartite graphs with $n$ vertices, the minimum $ABC_{GG}$ index is attained by a complete bipartite graph $K_{\lfloor \frac{n}{2} \rfloor, \lceil \frac{n}{2} \rceil}$, while the maximum $ABC_{GG}$ index is attained by a path or a cycle-like graph. Brand new results concerning $ABC_{GG}$ index were obtained in [8], where Filipovski solved a conjecture posed in [9] by characterizing graphs with given number of vertices that maximize $ABC_{GG}$ index.

In this paper we solve one of the conjectures posed in [5] concerning extremal values of $ABC_{GG}$ index of trees. Namely, we prove that almost dendrimers are trees which maximize $ABC_{GG}$ index among all trees on $n$ vertices with maximum degree at most $\Delta$.

# 2 Proof

All graphs in this paper will be finite, simple and undirected, and we follow the standard graph-theoretic terminology, see for example [4]. For a simple graph $G$, by $d_G(u, v)$ we denote the distance between vertices $u$ and $v$ in $G$, i.e. the length of a shortest path between $u$ and $v$. The *distance of a vertex* $u$, $\sigma_G(u) = \sigma(u)$, in a connected graph $G$ is defined by $\sigma(u) := \sum_{v \in V(G)} d(u, v)$. A vertex $v$ in $G$ of minimum distance is called the *centroid* of $G$. Centroid of a tree is either a single vertex or a set of two adjacent vertices, see Jordan [16]. We will need the following two lemmas:

**Lemma 1.** [1] *A vertex $v$ is the centroid of an $n-$vertex tree $T$ if and only if the largest component of $T - v$ has at most $n/2$ vertices.*

Notice that if $v$ is the centroid of $T$ and the largest component of $T - v$ has exactly $n/2$ vertices, then the neighbor of $v$ which is in the largest component of $T - v$ is also the centroid of $T$. If the largest component of $T - v$ has less than $n/2$ vertices, then $T$ has a single centroid.

**Lemma 2.** [6] *Suppose $a$ and $b$ are vertices of a connected graph $G$. Let $A$ be the set of vertices closer to $a$ than $b$ and let $B$ be the set of vertices closer to $b$ then $a$. Then $\sigma(a) - \sigma(b) = |B| - |A| = |B'| - |A'|$, where $A' = A - a$ and $B' = B - b$.*

It follows that if $v = v_1, v_2, \ldots, v_k = w$ is an arbitrary path from a centroid $v$ to an end vertex $w$, then

$$\sigma_T(v_1) \leq \sigma_T(v_2) < \cdots < \sigma_T(v_k). \tag{3}$$

If both $v_1$ and $v_2$ are centroids of $T$, then equality holds in (3), that is $\sigma_T(v_1) = \sigma_T(v_2)$.

Let us consider a tree $T$ with the vertex set $V$ and the edge set $E$ *rooted at the vertex* $r$. The *level* or *depth* $l(v)$ of a vertex $v$ in $T$ is the length of the path from the root $r$ to $v$. The depth $l = l(T)$ of $T$ is the maximum depth among all vertices in $T$. For $1 \leq k \leq l$, vertex at the level $k$ which is adjacent to a vertex $v$ at the level $k-1$ is called a *child* of $v$.

For $n \geq 3$ and $\Delta \geq 2$, by $\mathcal{T}_{n,\Delta}$ we denote the set of trees with $n$ vertices and with maximum degree at most $\Delta$. If we consider such trees to be rooted at some vertex, then the root has at most $\Delta$ children, and all other vertices have at most $\Delta - 1$ children.

Let us consider trees $T, T' \in \mathcal{T}_{n,\Delta}$ with roots $r$ and $r'$, respectively. If there exists an edge-preserving bijection $f : V \to V'$, then $T$ and $T'$ are isomorphic trees and we write $T \cong T'$. If $f$ is such that $f(r) = r'$, we write $T \cong^r T'$.

Let us introduce special types of trees with the maximum degree at most $\Delta$ which are cruical in our study. For $\Delta \geq 2$, let $T^1_{\Delta+1,\Delta} \in \mathcal{T}_{n,\Delta}$ be a star with $\Delta + 1$ vertices rooted at the vertex $v^0$ of a degree $\Delta$. For $l \geq 2$, let $T^l_{n,\Delta}$ be a rooted tree obtained by attaching $\Delta - 1$ new pendant vertices to each pendant vertex in $m-$vertex tree $T^{l-1}_{m,\Delta}$. The tree $T^l_{n,\Delta}$ is called a *dendrimer*. Notice that $T^l_{n,\Delta}$ has $\Delta(\Delta-1)^{i-1}$ vertices at level $i = 1, \ldots, l$ and

$$|V(T^l_{n,\Delta})| = 1 + \sum_{i=0}^{l-1} \Delta(\Delta-1)^i = \begin{cases} 1 + \frac{\Delta}{\Delta-2}[(\Delta-1)^l - 1], \ \Delta \geq 3 \\ 1 + 2l, \ \Delta = 2. \end{cases} \tag{4}$$

For convenience, neighbors, i.e. children of $v^0$ in $T^l_{n,\Delta}$ are denoted by $v^1_i$, $i = 1, \ldots, \Delta$. For $2 \leq k \leq l$ and $j = 1, \ldots, \Delta(\Delta-1)^{k-2}$ children of $v^{k-1}_j$ are denoted by $v^k_{1+(j-1)(\Delta-1)}, \ldots, v^k_{j(\Delta-1)}$.

*An almost dendrimer* $T_{n,\Delta}$ is a tree with $n$ vertices obtained from $T^l_{n,\Delta}$ by removing $s$ pendant vertices $v^l_{\Delta(\Delta-1)^{l-1}-i}$, $i = 0, \ldots, s$, $0 \leq s \leq \Delta(\Delta-1)^{l-1} - 1$. Therefore, every non-pendant vertex in $T_{n,\Delta}$ except perhaps one (which is at level $l-1$), has degree $\Delta$. It is clear that $T_{n,\Delta}$ belongs to $\mathcal{T}_{n,\Delta}$ and if $n$ is given by equation (4), then $T_{n,\Delta} \cong^r T^l_{n,\Delta}$.

Example of an almost dendrimer is presented in Figure 1.

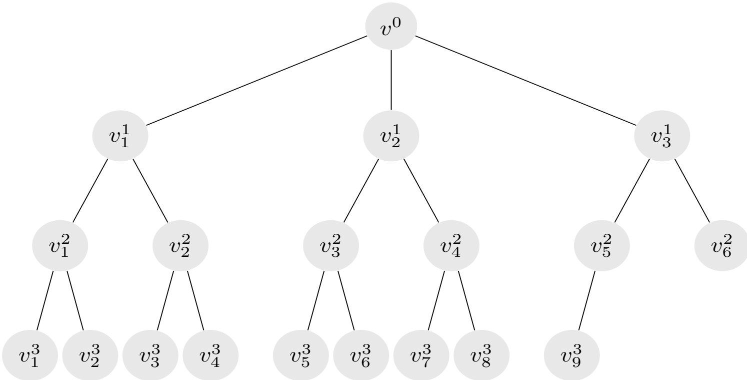


**Figure 1.** An almost dendrimer $T_{19,3}$.

Now we introduce another family of trees which is slightly different from almost dendrimers. Let $p \geq 2$ and let $T(p+1,p)^1$ be a star with $p+1$ vertices rooted at the vertex $u^0$ of a degree $p$. For $l \geq 2$, let $T(n,p)^l$ be a rooted tree obtained by attaching $p$ new pendant vertices to each pendant vertex in $m-$vertex tree $T(m,p)^{l-1}$. A tree $T(n,p)^l$ has $p^i$ vertices at level $i = 1, \ldots, l$ and

$$|V(T_{n,p}^l)| = 1 + \sum_{i=1}^{l} p^i = \frac{p^{l+1} - 1}{p - 1} \ . \tag{5}$$

For $i = 1, \ldots, p$ children of $u^0$ in $T(n,p)^l$ are denoted by $u_i^1$. For $2 \leq k \leq l$ and $j = 1, \ldots, p^{k-1}$ children of $u_j^{k-1}$ are denoted by $u_{1+(j-1)p}^k, \ldots, u_{jp}^k$. By $T(n,p)$ we denote a tree with $n$ vertices obtained from $T(n,p)^l$ by removing $s$ pendant vertices $v_{p^l-i}^l$, $i = 0, \ldots, s$, $0 \leq s \leq p^l - 1$. Therefore, every non-pendant vertex in $T(n,p)$ except perhaps one (which is at level $l-1$), has $p$ children. It is clear that for $p = \Delta - 1$, $p \geq 3$ tree $T(n, \Delta - 1)$ belongs to $\mathcal{T}_{n,\Delta}$ and if $n$ is given by equation (5), then $T(n,p) \cong^r T(n,p)^l$. Example of $T(n,p)$ is presented in Figure 2.

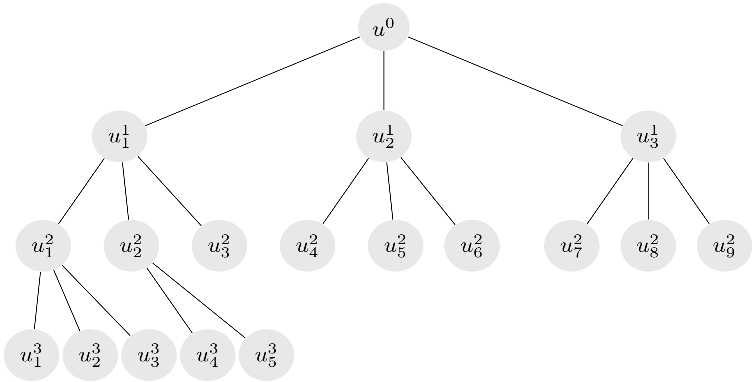


**Figure 2.** Tree $T(18,3)$.

Notice that $T_{n,2} \cong P_n$ and its depth is $l = \lfloor \frac{n}{2} \rfloor$. A tree $T_{n,2} - v^0$ consists of two paths with $\lfloor \frac{n}{2} \rfloor$ vertices and according to Lemma 1, vertex $v^0$ is its centroid. If $n$ is odd, centroid of $T_{n,2}$ is not unique, it is the set $\{v^0, v^1_1\}$.

Let $\Delta \geq 3$ and let $T_i$ be a component of $T_{n,\Delta} - v^0$, $i = 1, \ldots, \Delta$. Notice that $|T_1| \geq |T_2| \geq \cdots \geq |T_\Delta|$ and $|T_i| \leq \frac{(\Delta-1)^l-1}{\Delta-2}$, with equality holding for each $i$ if and only if $T_{n,\Delta} \cong^r T^l_{n,\Delta}$.

**Lemma 3.** *For $n \geq 4$ and $\Delta \geq 3$ we have $|V(T_{n,\Delta})| = \frac{2[(\Delta-1)^l-1]}{\Delta-2}$ if and only if $T_1$ has the maximum number of vertices, i.e. $|T_1| = \frac{(\Delta-1)^l-1}{\Delta-2}$ and $T_i$ has the smallest number of vertices, i.e. $|T_i| = \frac{(\Delta-1)^{l-1}-1}{\Delta-2}$, $i = 2, \ldots, \Delta$.*

*Proof.* Proof of necessity is straightforward. Conditions on $T_1$ and $T_i$, $i = 2, \ldots, n$ imply $n = 1 + \sum_{i=1}^{\Delta} |T_i| = \frac{2[(\Delta-1)^l-1]}{\Delta-2}$. Let us prove sufficiency. If $n = \frac{2[(\Delta-1)^l-1]}{\Delta-2}$, then $T_1$ has the maximum number of vertices, otherwise $|T_1| < \frac{(\Delta-1)^l-1}{\Delta-2}$ would imply $|T_i| = \frac{(\Delta-1)^{l-1}-1}{\Delta-2}$, $i = 2, \ldots, \Delta$, which is impossible since it leads to $n < \frac{2[(\Delta-1)^l-1]}{\Delta-2}$. However, if $T_1$ has the maximum number of vertices, then $T_i$, $i = 2, \ldots, \Delta$ has the smallest number of vertices, i.e. $|T_i| = \frac{(\Delta-1)^{l-1}-1}{\Delta-2}$, otherwise $n$ would be larger than $\frac{2[(\Delta-1)^l-1]}{\Delta-2}$. ■

The following proposition is useful for further observations.

**Proposition 1.** *Let $n \geq 4$ and $\Delta \geq 3$.*
*(i) Set $\{v^0, v_1^1\}$ is the centroid of $T_{n,\Delta}$ if and only if $n = \frac{2[(\Delta-1)^l-1]}{\Delta-2}$.*
*(ii) Vertex $v^0$ is a single centroid of $T_{n,\Delta}$ if and only if $n \neq \frac{2[(\Delta-1)^l-1]}{\Delta-2}$.*

*Proof.* $(i)$ It holds $n = \frac{2[(\Delta-1)^l-1]}{\Delta-2}$ if and only if $|T_1| = \frac{n}{2}$ and $|R| := 1 + \sum_{i=2}^{\Delta} |T_i| = \frac{n}{2}$. Since $T_1$ and $R$ are the largest components of $T_{n,\Delta} - v^0$, according to Lemma 1, $\{v^0, v_1^1\}$ is the centroid of $T_{n,\Delta}$.
$(ii)$ Let $n \neq \frac{2[(\Delta-1)^l-1]}{\Delta-2}$. According to Lemma 3, $|T_1| < \frac{(\Delta-1)^l-1}{\Delta-2}$ or there exists $k \in \mathbb{N}$, $1 < k \leq \Delta$ such that $|T_k| > \frac{(\Delta-1)^{l-1}-1}{\Delta-2}$. If $|T_1| < \frac{(\Delta-1)^l-1}{\Delta-2}$, then $|T_i| = \frac{(\Delta-1)^{l-1}-1}{\Delta-2}$, $i = 2, \ldots, \Delta$ (otherwise, tree is not an almost dendrimer) and $n < \frac{2[(\Delta-1)^l-1]}{\Delta-2}$. If we assume that $|T_1| \geq n/2$, then $1 + \sum_{i=2}^{\Delta} |T_i| = \frac{(\Delta-1)^l-1}{\Delta-2} \leq \frac{n}{2}$, which is impossible. Therefore, $|T_1| < n/2$ and we conclude that $v^0$ is a single centroid of $T_{n,\Delta}$.
We are left with the case $|T_k| > \frac{(\Delta-1)^{l-1}-1}{\Delta-2}$ for some $k$, $1 < k \leq \Delta$. Then $|T_1| = \frac{(\Delta-1)^l-1}{\Delta-2}$ and we conclude $n > \frac{2[(\Delta-1)^l-1]}{\Delta-2}$. But this implies $|T_i| < n/2$ for all $i = 1, \ldots, \Delta$. Therefore, $v^0$ is the centroid of $T_{n,\Delta}$. ■

Proposition 1 claims that centroid of an arbitrary tree $T_{n,\Delta}$ is its root. That is not the case for $T(n,p)$. For example, the single centroid of $T(22,3)$ is the vertex $u_1^1$.

For proving the main result in our paper, we will need some tools from the the theory of majorization, see Marshall, Olkin and Arnold [17].
Let $\mathbb{R}^s := \{(x_1, \ldots, x_s) : x_i \in \mathbb{R}, i = 1, \ldots, s\}$. For any $x = (x_1, \ldots, x_s) \in \mathbb{R}^s$, let

$$x_{(1)} \leq x_{(2)} \leq \cdots \leq x_{(s)}$$

denote the components of $x$ in increasing order, and let

$$x_{\uparrow} = (x_{(1)}, x_{(2)}, \ldots, x_{(s)})$$

denote the *increasing rearrangement* of $x$.

**Definition 1.** Let $x, y \in \mathbb{R}^s$. We say that $x$ is *majorized* by $y$ ($y$ *majorizes*

$x$) and write $x \prec y$ if

$$\begin{cases} \sum_{i=1}^{k} x_{(i)} \geq \sum_{i=1}^{k} y_{(i)}, \quad k = 1, \dots, s-1, \\ \sum_{i=1}^{s} x_{(i)} = \sum_{i=1}^{s} y_{(i)}. \end{cases} \tag{6}$$

By replacing equality in (6) by an inequality leads to the concept of weak majorization.

**Definition 2.** Let $x, y \in \mathbb{R}^s$. We say that $x$ is *weakly supermajorized* by $y$ ($y$ *weakly supermajorizes* $x$) and write $x \prec^w y$ if

$$\sum_{i=1}^{k} x_{(i)} \geq \sum_{i=1}^{k} y_{(i)}, \quad k = 1, \dots, s. \tag{7}$$

There are numerous ways to verify that $x$ is majorized by $y$. One of them is crucial for our main result and characterizes majorization by using order-preserving functions.

**Theorem 2.** [17] *Let $x, y \in \mathbb{R}^s$. Inequality*

$$\sum_{i=1}^{s} f(x_i) \leq \sum_{i=1}^{s} f(y_i) \tag{8}$$

*holds for all continuous decreasing convex functions $f : \mathbb{R} \to \mathbb{R}$ if and only if $x \prec^w y$.*

Let $T$ be a rooted tree of depth $l$. For $e = w^{k-1}w^k \in E$, $k = 1, \dots, l$ by $n_T(e)^k$ we denote the number of vertices in $T$ which are closer to $w^k$ than $w^{k-1}$, that is

$$n_T(e)^k = |\{z : d_T(w^k, z) < d_T(w^{k-1}, z)\}|. \tag{9}$$

Similarly, by $n_T(e)^{k-1}$ we denote the number of vertices in $T$ which are closer to $w^{k-1}$ than $w^k$. Notice that $n_T(e)^k$ is the number of vertices in component of $T - e$ that contains $w^k$. Moreover, all vertices in $T$ which are closer to $w^k$ have depth greater than or equal to $k$.

If we consider a tree in which a root and a centroid coincide, then Lemma 2 and inequality (3) imply

$$n_T(e)^k \leq n_T(e)^{k-1}. \tag{10}$$

Let us consider the sequence $N(T) = (n_T(e)^k)_{e \in E}$. In 2003 Jelen and Triesch [15] considered $(n,p)-$ary treese. i.e., $n-$vertex trees in which any vertex has at most $p$ children. They proved the following theorem.

**Theorem 3.** *Let $n, p \in \mathbb{N}$ with $n \geq 2$ and $p \geq 2$ and let $T$ be an $(n,p)-$ary tree. Then $N(T) \prec^w N(T(n,p))$ with equality if and only if $T \cong^r T(n,p)$.*

Note that for any $n-$vertex tree $T$, equation (2) can be written as

$$ABC_{GG}(T) = (n-2) \sum_{uv \in E} \sqrt{\frac{1}{n_u(n-n_u)}} \tag{11}$$

since $n_u + n_v = n$. Without the loss of generality we can assume $n_u \leq n_v$ $\forall uv \in E$. Let $n \geq 2$ and let us consider a function $f_n : \left[1, \frac{n}{2}\right] \to \mathbb{R}$ given by

$$f_n(t) = \sqrt{\frac{1}{t(n-t)}}. \tag{12}$$

By examining properties of $f_n$, we conclude that it is a continuous, strictly decreasing and strictly convex function. Now $ABC_{GG}(T)$ can be written as

$$ABC_{GG}(T) = (n-2) \sum_{uv \in E} f_n(n_u), \tag{13}$$

and if we assume that $T$ is rooted at its centroid, then according to (10) we can write

$$ABC_{GG}(T) = (n-2) \sum_{e \in E} f_n(n_T(e)^k). \tag{14}$$

Bearing in mind properties of $f_n$, according to Theorem 2 the problem of maximizing $ABC_{GG}(T)$ given by (14) is equivalent to the problem of maximizing $N(T) = (n_T(e)^k)_{e \in E}$ in the sense of weak supermajorization.

Now we are ready to state and prove the main result.

**Theorem 4.** *Let $n, \Delta \in \mathbb{N}$ with $n \geq 3$ and $\Delta \geq 2$. If $T \in \mathcal{T}_{n,\Delta}$ has the maximum Graovac-Ghorbani index, then $T \cong T_{n,\Delta}$.*

*Proof.* Path $P_n$ is a unique $n-$vertex tree with maximum degree at most 2, so $T(n,2) \cong P_n$. Let $\Delta \geq 3$. For $n = \Delta + 1$ we have a unique tree: a star $S_n$, therefore $T(\Delta+1, \Delta) \cong S_{n+1}$.

Suppose now that $n > \Delta + 1$. Let $T^* \in \mathcal{T}_{n,\Delta}$ be a tree rooted at a centroid $z$ and $T^*$ has the maximum Graovac-Ghorbani index. Then, as we concluded earlier, $N(T^*) = (n_{T^*}(e)^k)_{e \in E}$ is maximum in the sense of weak supermajorization. By $z_i$, $1 \leq i \leq d_{T^*}(z)$ we denote neighbors of $z$ and by $T^*(z_i)$ the components of $T^* - z$ rooted at $z_i$. Furthermore, by $T_i^*$ we denote the subtree induced by $V \setminus V(T^*(z_i))$ and that is rooted at $r$. Notice that $d_{T^*}(z) \geq 2$, otherwise $z$ is not a centroid (it is a pendant vertex and $n \geq 4$). Each vertrex in $T_i^*$ has at most $\Delta - 1$ children so it is $(|V(T_i^*)|, \Delta - 1)-$ary tree. From Theorem 3 it follows that

$$T_i^* \cong^z T(|V(T_i^*)|, \Delta - 1)$$

for all $i = 1, \ldots, d_{T^*}(z)$. This implies $d_{T^*}(z) = \Delta$ and $T^* \cong^z T(n, \Delta)$. ∎

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