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A Survey on Graovac–Ghorbani Index

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Abstract

Let $G = (V, E)$ be a simple undirected and connected graph on n vertices. The *Graovac–Ghorbani* (ABC_{GG}) index of a graph G is defined as

$$ABC_{GG}(G) = \sum_{uv \in E} \sqrt{\frac{n(u) + n(v) - 2}{n(u)n(v)}},$$

where $n(u)$ is the number of vertices closer to vertex u than vertex v and $n(v)$ is defined analogously. This paper is a survey of topological *Graovac–Ghorbani* index of a graph G. It contains results on ABC_{GG} which are known until this moment and some conjectures.

1 Introduction

Molecular descriptors are mathematical quantities that describe the structure or shape of molecules, helping to predict the activity and properties of molecules in complex experiments [10]. Among them, topological

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indices have a prominent place [13]. The concept of topological indices came from the work done by Wiener [11] while he was working on boiling point of paraffin. According to Furtula et al. [14], topological indices are quantities that are calculated from the molecular graphs and they are used for modeling physico-chemical, pharmacological, toxicological and other properties of the underlying chemical compounds. Inspired by Randić, Estrada [12] proposed a topological index based on the degrees of vertices of graphs, which is called the atom-bond connectivity (ABC) index. It provides a good model for the stability of linear and branched alkanes as well as the strain energy of cycloalkanes [12, 18]. A new justification of the quantum theory [18] for this topological index has been attracting much interest in recent years, both in the mathematical and chemical research communities. Many results and structural properties of the ABC index have been determined in [1–6, 14, 19–24] and in the works cited therein.

Let $G = (V, E)$ be a simple undirected graph with vertex and edge set $V = V(G)$ and $E = E(G)$, respectively, such that $n = |V|$ and $m = |E|$. The degree of a vertex $v \in V$, denoted by $d(v)$, is the number of edges incidents to v. In [12], the ABC index of G is defined as

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

Graovac and Ghorbani [7] proposed a new version of the ABC index [12], called *Graovac–Ghorbani* index (or ABC_{GG} index), defined as

$$ABC_{GG}(G) = \sum_{uv \in E} \sqrt{\frac{n(u) + n(v) - 2}{n(u)n(v)}} \ ,$$

where $n(u)$ is the number of vertices closer to vertex u than vertex v and $n(v)$ is defined analogously. Vertices equidistant from u and v are not taken into account.

The main goal of this paper is to present a survey about the *Graovac–Ghorbani* index, providing a complete bibliography for future research.

This survey is organized in the following way: in Section 2 we present basic concepts that are needed in this paper. In Section 3, the results so far existing in the literature are presented, as well as the open problems for the *Graovac-Ghorbani* index. Finally, in Section 4 we make the final considerations.

2 Preliminaries

Let K_n, T_n, C_n and P_n be the complete graph, cycle, tree and path on n vertices, respectively. A bipartite graph G is a graph whose vertices set $V(G)$ can be partitioned into two disjoint and independent sets V_1 and V_2 with cardinality a and b vertices respectively, such that every edge connects a vertex V_1 to one in V_2. If G contains every possible edge joining V_1 and V_2, then G is the complete bipartite graph, denoted as $K_{a,b}$. A connected graph G with n vertices and m edges is called unicyclic if $m = n$ and called bicyclic if G has $n+1$ edges.

Let $\mathrm{S}(t_1, t_2, \ldots, t_k)$ be a unicyclic graph of order n with girth k and $n-k$ pendent vertices, where t_i is the number of pendent vertices adjacent to the i-th vertex of the cycle [3] (see Figure 1). It easy to see that $\sum_{i=1}^{k} t_i = n-k$ and $S(0, 0, \ldots, 0) \simeq C_n$.

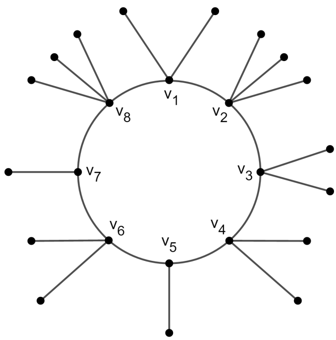

Figure 1. Unicyclic graph S(2,3,2,2,1,2,1,3) [3].

Let $p, q, l \in \mathbb{N}$, such that p, $q \geq 3$ and $l \geq 1$. Let $B_1(p, q)$ a bicyclic graph obtained from two vertex-disjoint cycles C_p and C_q by identifying a vertex u of C_p and a vertex v of C_q such that $n = p+q-1$. So, let $B_1(n) = \bigcup_{p,q\geq 3} B_1(p, q)$(see Figure 2). Let $B_2(p, l, q)$ a bicyclic graph obtained from a cycle $C_{p+q-2l} : v_1v_2v_3, \ldots, v_{p-l}v_{p-l+1}v_{p-l+2}v_{p-l+3}v_{p-l+4}, \ldots, v_{p+q-2l-1}$

$v_{p+q-2l}v_1$ by joining vertices v_1 and v_{p-l-2} by a new path $v_1u_1u_2,\ldots,u_{l-2}$ $u_{l-1}u_lv_{p-l-2}$ with length l, where $p+q-l-1=n$. So, let $B_2(n) = \bigcup_{p,q\geq 3,l\geq 1} B_2(p,l,q)$ (see Figure 2).

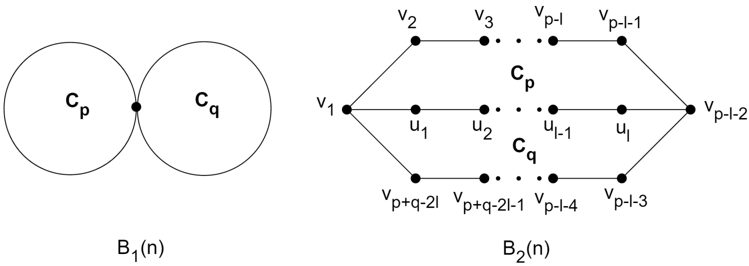

Figure 2. $B_1(n)$ and $B_2(n)$ families of bicyclic graphs with no pendent vertices, respectively [16].

A graph is said k-regular if all vertices have degree k. As described in [5], we say that a graph is (almost) k-regular if all vertices have degree k except for one which has degree $k-1$.

3 General results for the ABC_{GG} index

In 2013, the first results about ABC_{GG} index appeared. The results involve unicyclic graphs [3], complete bipartite graphs and trees [9] and bipartite graphs [5].

Rostami and Sohrabi-Haghighat [9], determined the graph with minimum value with respect to ABC_{GG} index among all graphs (Theorem 1). Besides, determined the lower and upper bounds for complete bipartite graphs (Theorem 2) and for trees (Theorem 3) with respect to ABC_{GG} index, which are presented below.

Theorem 1. *[9] Among all $n-$vertex graphs, the complete graph K_n has the smallest ABC_{GG} index..*

Theorem 2. *[9] Let G be a complete bipartite graph with $n \geq 4$ vertices. Then*

$$ABC_{GG}(K_{1,n-1}) \leq ABC_{GG}(G) \leq ABC_{GG}(K_{\lfloor \frac{n}{2} \rfloor \lceil \frac{n}{2} \rceil}), \tag{1}$$

with equality if and only if $G \simeq K_{1,n-1}$ *(left) and* $G \simeq K_{\lfloor \frac{n}{2} \rfloor \lceil \frac{n}{2} \rceil}$ *(right).*

Theorem 3. *[9] The star* $K_{1,n-1}$ *is the tree with the maximum Graovac-Ghorbani index and the path* P_n *is the tree with the minimum Graovac-Ghorbani index.*

In 2013, Das [3] determined within the family of unicyclic graphs the ones which maximize the ABC_{GG} index. The upper bound for the ABC_{GG} index for unicyclic graphs is described below.

Theorem 4. *[3] Let* G *be a connected unicyclic graph of order* n. *Then, for* $10 \leq n \leq 15$, *we have*

$$ABC_{GG}(G) \leq (n-3)\sqrt{\frac{n-2}{n-1}} + \sqrt{\frac{2}{3}} + \sqrt{\frac{n-5}{n-4}} + \sqrt{\frac{n-3}{3(n-4)}}, \tag{2}$$

with equality holds if and only if $G \simeq S(n-5,2,0)$. *For* $n \geq 16$, *we have*

$$ABC_{GG}(G) \leq (n-3)\sqrt{\frac{n-2}{n-1}} + \sqrt{\frac{n-4}{n-3}} + \sqrt{2}, \tag{3}$$

with equality if and only if $G \simeq S(n-4,1,0)$ *(Figure 3).*

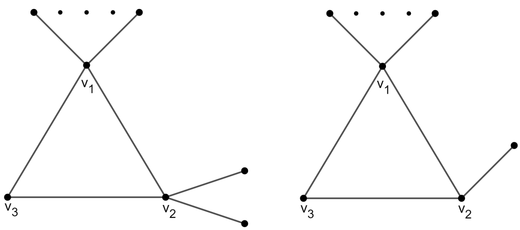

Figure 3. Extremal unicyclic graphs for $10 \leq n \leq 15$ and $n \geq 16$, respectively.

Table 1 describes the unicyclic graphs that maximize the ABC_{GG} index for $4 \leq n \leq 9$. Das [3] describes that the minimum value of ABC_{GG} index for unicyclic graphs is an open problem, which in fact remains up to this moment.

In 2017, Dimitrov et al. [5] determined the graphs with the maximum and minimum value of ABC_{GG} index among all bipartite graphs.

n	ABC_{GG}	Maximal unicyclic graphs
4	$2\sqrt{2}$	C_4
5	$\sqrt{3}+\frac{3}{\sqrt{2}}$	S(1,1,0)
6	$3\sqrt{\frac{4}{5}}+\sqrt{2}+\sqrt{\frac{2}{3}}$	S(2,1,0)
7	$4\sqrt{\frac{5}{6}}+2\sqrt{\frac{2}{3}}+\frac{2}{3}$	S(2,2,0)
8	$5\sqrt{\frac{6}{7}}+\sqrt{\frac{2}{3}}+\sqrt{\frac{3}{4}}+\sqrt{\frac{5}{12}}$	S(3,2,0)
9	$6\sqrt{\frac{7}{8}}+\sqrt{3}+\sqrt{\frac{3}{8}}$	S(3,3,0)

Table 1. Maximal unicyclic graphs with respect to the ABC_{GG} index for $4 \leq n \leq 9$.

As described in [5], we denote by C_n' (see Figure 4) as a cycle with a pendent edge, that is, a unicyclic graph on n (odd) vertices composed of a cycle C_{n-1} and a pendent vertex. Consider a cycle with a *hook*, that is, a graph with an odd number of n vertices composed of two even cycles C_{n-1} and C_4 which share three vertices and two edges in common, denoted by C_n'' (see Figure 4). Next results involve bipartite graphs.

Theorem 5. *[5] Amongst all bipartite graphs on n vertices, the maximum Graovac–Ghorbani index is uniquely attained by the complete bipartite graph $K_{\lfloor \frac{n}{2} \rfloor, \lceil \frac{n}{2} \rceil}$.*

Theorem 6. *[5] Amongst all bipartite graphs on $n \geq 8$ vertices, the minimum Graovac–Ghorbani index is attained by the cycle C_n for even n, by C_n' for odd $n \leq 15$ and by C_n'' for odd $n \geq 17$. For $n < 8$, the graph that minimizes the Graovac–Ghorbani index is the path P_n on n vertices. Furthermore, these are the unique graphs with the respective properties.*

Figure 4 shows examples of the bipartite graphs that minimize *Graovac–Ghorbani* index among all bipartite graphs.

In 2021 Pacheco et al. [16] gave a lower bound on the ABC_{GG} index for all graphs in $B_1(n)$ and proved it is sharp.

Theorem 7. *[16] Let $G \in B_1(n)$ be a graph of order $n \geq 9$. If n is odd, then*

$$ABC_{GG}(G) \geq \frac{2(n-3)}{\sqrt{n-1}} + 2\sqrt{\frac{n-3}{n-2}} + \frac{2\sqrt{n-5}}{n-3}.$$

If n is even, then

$$ABC_{GG}(G) \geq 2\sqrt{\frac{n-3}{n-2}} + \frac{2\,(n-2)}{\sqrt{n+2}}.$$

Equality holds in both cases if and only if $G \simeq B_1(3, n-2)$.

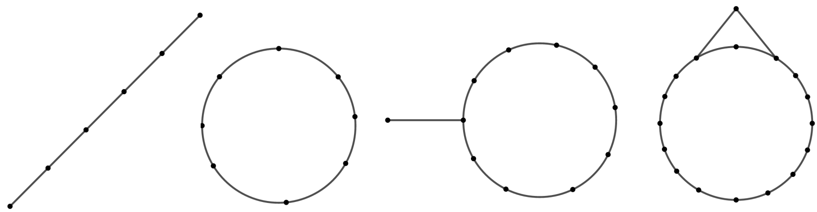

Figure 4. Example of bipartite graphs with minimum ABC_{GG} index: P_6, C_8, C'_{13} and C''_{17}, respectively.

Furtula in [6] characterized all the connected graphs with $5 \leq n \leq 10$ vertices which maximize the ABC_{GG} index. These graphs are presented in Figure 5 and we can observe that with an odd number of vertices, there is only one which maximizes the ABC_{GG} index, while there are two of them for graphs with an even number of vertices. Moreover, these graphs with an odd number of vertices have exactly one vertex of degree equal to $n-1$ and $n-1$ vertices of degree equal to $n-2$, [6].

In 2023, Filipovski [17] proved the result above, which is presented in the next theorem.

Theorem 8. *[17] Let G be a connected graph on n vertices. If n is even, then*

$$ABC_{GG} \leq \frac{n(n-2)}{4}\sqrt{2}.$$

Equality holds for the $(n-2)$-regular cocktail party graph and for a graph which contains two vertices of degree $n-1$ and all other vertices are of degree $n-2$. If n is an odd number, then

$$ABC_{GG} \leq \frac{(n-1)^2}{4}\sqrt{2}.$$

Equality holds for the graphs with one vertex of degree $n-1$ and $n-1$

vertices of degree $n-2$.

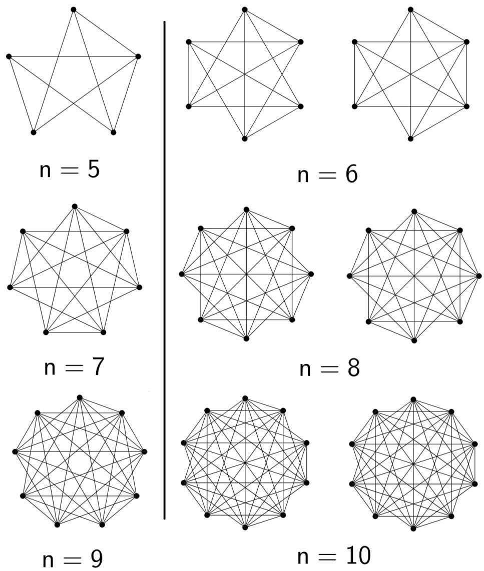

Figure 5. Graphs obtained for $5 \leq n \leq 10$ that maximize the ABC_{GG} index [6].

There are more results in the literature which can be verified in [1–3, 8, 15]. Rostami et al. [8] determined some upper and lower bounds for the ABC_{GG} index, as well as characterized its extremal graphs. Das [1] presented the upper and lower bounds for the ABC_{GG} index and characterized the extremal graphs. Das et al. [2] determined the relations between the ABC and ABC_{GG} indices and certain classes of graphs for which the ABC index is greater than (respectively equal to or less than) the ABC_{GG} index. Ghorbani et al. [15] computed the ABC_{GG} index for a family of fullerenes. Das [3] reported that extremal graphs related to certain chemical structures, such as fullerenes, benzenoid hydrocarbons are open problems.

3.1 Conjectures for the ABC_{GG} index

In this section, we present some conjectures related to ABC_{GG} index. In 2014, Dimitrov et al. [5] presented some conjectures about the maximal and minimal ABC_{GG} index which are described below.

Conjecture 1. *[5] Let G be a graph with maximal ABC_{GG} index amongst all graphs on $n \gg \Delta$ vertices. Then G is an (almost) Δ-regular graph.*

Conjecture 2. *[5] Let G be a graph with minimal ABC_{GG} index amongst all graphs on $n \gg \Delta$ vertices. Then G is the cycle C_n.*

According to Dimitrov et al. [5] an almost dendrimer $T_{n,d}$ is a rooted tree with n vertices in which every non-pendent vertex, except perhaps one, has degree d and the inequality $d(u) \geq d(v)$ holds for every vertex u that occurs before vertex v in the breadth-first traversal (Figure 6). The following conjecture involves these families of graphs.

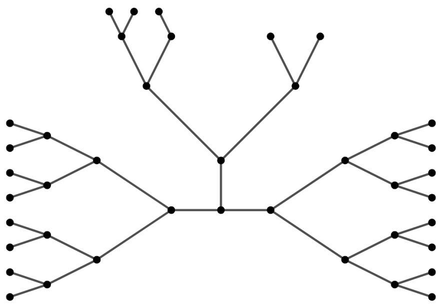

Figure 6. An almost dendrimer $T_{41,3}$ [5].

Conjecture 3. *[5] Let G be a tree with maximal $ABC_{GG}(G)$ index amongst all trees on n vertices with maximum degree $\Delta \leq n-1$. Then G is an almost dendrimer $T_{n,\Delta}$.*

Let $\mathcal{B'}_n$ be the family of all bicyclic graphs on n vertices and $B_2(p,l,q)$ the graphs defined in the Section 2. In [16], the conjecture on lower bounds of the ABC_{GG} index among all graphs in $\mathcal{B'}_n$ is presented.

Conjecture 4. *[16] Let $G \in \mathcal{B}'_n$ with order $n \geq 9$ vertices. If n is odd, then*

$$ABC_{GG}(G) \geq 2(n+1)\sqrt{\frac{n-2}{n^2-1}}\ .$$

If n is even, then

$$ABC_{GG}(G) \geq \frac{6}{n}\sqrt{n-2} + 2(n-2)\sqrt{\frac{1}{n+2}}\ .$$

For n odd, equality holds if and only if $G \simeq B_2(4,2,n-1)$ and for n even, equality holds if and only if $G \simeq B_2(6,3,n-2)$.

Figure 7 displays the extremal graphs of Conjecture 4 according to the parity of n.

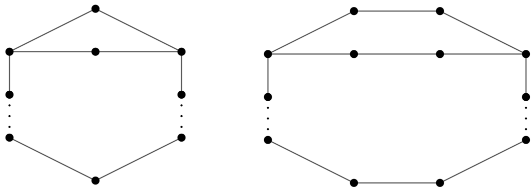

Figure 7. Bicyclic graphs with minimal value of ABC_{GG} index for $n \geq 9$ odd (left) and even (right), respectively [16].

Before presenting the last conjecture, consider the graph K_4 minus one edge ($K_4 - e$). Let H be a graph obtained from $K_4 - e$ by adding $n-4$ pendent vertices to one vertex of degree 3, as shown in Figure 8. Pacheco et al. [16] presented a conjecture about the upper bound to the ABC_{GG} index for all bicyclic graphs.

Conjecture 5. *[16] Let $G \in \mathcal{B}'_n$ with order $n \geq 8$ vertices. Then,*

$$ABC_{GG}(G) \leq (n-4)\sqrt{\frac{n-2}{n-1}} + \sqrt{\frac{n-4}{n-3}} + 2\sqrt{\frac{n-3}{n-2}} + \sqrt{2}.$$

Equality holds if and only if G is isomorphic to H.

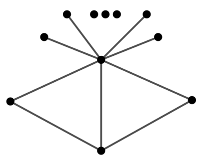

Figure 8. Graph H, for $n \geq 8$ [16].

4 Conclusion

This survey gathers all the existing results in the literature until this moment and presents open problems in order to inspire researchers to obtain new results about the *Graovac–Ghorbani* index.

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