MATCH
Communications in Mathematical and in Computer Chemistry

MATCH Commun. Math. Comput. Chem. **89** (2023) 517–525
ISSN: 0340–6253
doi: 10.46793/match.89-2.517F

Connected Graphs with Maximal Graovac–Ghorbani Index

Slobodan Filipovski[a,*]

[a] *FAMNIT, University of Primorska, Glagoljaška ulica 8, 6000 Koper, Slovenia*
slobodan.filipovski@famnit.upr.si

(Received June 17, 2022)

Abstract

Based on computer search, Furtula characterized the connected graphs with maximal ABC_{GG} index. In this paper we give a mathematical proof of the established hypothesizes.

1 Introduction

Let $G = (V, E)$ be a simple, undirected and connected graph on n vertices. The degree of a vertex $v \in V(G)$, denoted by d_v, is equal to the number of edges that are adjacent to v. For any two vertices u and v, the distance $d(u, v)$ is defined as the length of the shortest path between u and v. The atom-bond connectivity index $ABC(G)$ was introduced in 1998 in [6], as follows:

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

This index has significant prediction ability and represents one of the most studied successors of Randić index. In the last two decades various topological invariants of ABC index were defined and studied. In this paper

*Corresponding author.

we focus on the Graovac-Ghorbani index introduced in [10] as follows

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

where n_u is the number of vertices closer to vertex u than vertex v of the edge $(u, v) \in E(G)$, and n_v is defined on the same way. The Graovac-Ghorbani index is distance-based topological descriptor which gives better prediction in the case of entropy and acentric factor than ABC index, see in [3, 4, 7–9, 11, 12].

In the last decade the graphs with maximal Graovac-Ghorbani index were studied in several publications. Rostami et al. in [11] give lower and upper bounds for the trees with a given number of pendent vertices. Das et al. in [3] obtain upper bounds for the unicyclic graphs. Dimitrov et al. in [5] proved that among all bipartite graphs on n vertices, the maximal Graovac-Ghorbani index is uniquely attained by the complete bipartite graph $K_{\lfloor \frac{n}{2} \rfloor, \lceil \frac{n}{2} \rceil}$.

It is easy to notice that among all connected graphs on n vertices, the minimum value of ABC_{GG} is achieved for the complete graphs. From the definition of the Graovac-Ghorbani index we observe that $ABC_{GG} = 0$ if and only if $n_u = n_v = 1$ for each edge (u, v) from K_n.

Based on computer search, Furtula in [7] characterized the connected graphs with maximal ABC_{GG} index. It was shown that for connected graphs with odd number of vertices there is a unique graph that maximizes ABC_{GG}, while there are two of them for graphs on even number of vertices. These graphs with odd number of vertices have exactly one vertex of degree $n - 1$, and $n - 1$ vertices have degree equal to $n - 2$. In this case the expected upper bound for the ABC_{GG} is $\frac{(n-1)^2}{4}\sqrt{2} = B_1$. Among two graphs with even number of vertices one is regular graph with degree equal to $n - 2$, known as a cocktail party graph, while the other graph that maximizes ABC_{GG} has exactly two vertices of degree equal to $n - 1$, and all other vertices are of degree equal to $n - 2$. In both cases ABC_{GG} is equal to $\frac{n(n-2)}{4}\sqrt{2} = B_2$.

Despite the fact that the connected graphs with maximal ABC_{GG} index are described, in [7] was pointed out that the rigorous mathematical confirmation of this characterization is needful. In this paper we support Furtula's hypothesizes giving a mathematical proof of the existence of the extremal graphs with maximal Graovac-Ghorbani index.

2 Proof

Let G be a connected graph on n vertices and m edges. First, we observe that the Graovac-Ghorbani index for triangle-free graphs on n vertices is less than the bounds B_1 and B_2. If G is a triangle-free graph on m edges and n vertices, from Mantel's theorem [13] we have $m \leq \frac{n^2}{4}$. On the other hand, since $\sqrt{\frac{n_u+n_v-2}{n_u n_v}} < 1$ for which edge (u,v), we have $ABC_{GG}(G) < m$. Now, for $n \geq 7$ we easily prove that

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

The cases when $n < 7$ are considered in [7].
From now on we assume that the graph G contains at least one triangle. For an edge (u,v) of G we define $n_{uv} = |\{z \mid d(z,v) = d(z,u)\}|$. Note that $0 \leq n_{uv} \leq n-2$. Moreover, for any edge (u,v) of G it holds the relation $n_u + n_v = n - n_{uv}$.
By $t(G)$ we denote the number of triangles of a graph G. We use the following result:

Lemma 1. *[1] For the number of triangles of G it holds*

$$\frac{m(4m-n^2)}{n} \leq 3t(G) \leq \sum_{(u,v)} n_{uv}. \tag{3}$$

The left inequality is derived by Bollobás [1]. Since n_{uv} counts cycles of odd length containing an edge (u,v), the right inequality is obvious. In our proof we also use the following lemma obtained by Cambie in [2].

Lemma 2. *[2] For any edge $e = (u,v) \in E(G)$, we have*

$$n_u + n_v + d_u + d_v \leq 2n. \tag{4}$$

As a consequence of Lemma 1 (the same result also follows from Lemma 2) we derive the following lemma.

Lemma 3. *If G is a connected graph on m edges and n vertices, then*

$$\sum_{(u,v)\in E(G)} (n_u + n_v) \leq 2mn - \frac{4m^2}{n}. \tag{5}$$

Using Lemma 1 is not hard to prove that, if n is an even number and if $n_u > 1, n_v > 1$ for each edge $(u,v) \in E(G)$, then the maximum value of ABC_{GG} is achieved for the cocktail party graphs.

Proposition 1. *Let G be a connected graph on n vertices and m edges. If n is an even number and if $n_u \geq 2, n_v \geq 2$ for each edge $(u,v) \in E(G)$, then*

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

The maximum value is achieved for the cocktail party graphs.

Proof. First we show that $n_u n_v \geq 2(n - n_{uv} - 2)$ for each edge $(u,v) \in E(G)$. Let $s = n - n_{uv} = n_u + n_v$. The inequality $n_u n_v \geq 2(n - n_{uv} - 2)$ is equivalent to $n_u(s - n_u) \geq 2(s-2)$, which is true because $s \geq n_u + 2$ and $n_u \geq 2$. Thus we have

$$\begin{aligned} ABC_{GG}(G) &= \sum_{(u,v)\in E(G)} \sqrt{\frac{n_u + n_v - 2}{n_u n_v}} \\ &\leq \sum_{(u,v)\in E(G)} \sqrt{\frac{n - n_{uv} - 2}{2(n - n_{uv} - 2)}} = \frac{m\sqrt{2}}{2}. \end{aligned}$$

From $n_u \geq 2$ and $n_v \geq 2$ we get $n_{uv} = n - n_u - n_v \leq n - 4$. Now from Lemma 1 we get

$$\frac{m(4m - n^2)}{n} \leq \sum_{(u,v)\in E(G)} n_{uv} \leq m(n-4)\ .$$

Hence $m \leq \frac{n(n-2)}{2}$ and $ABC_{GG}(G) \leq \frac{n(n-2)}{4}\sqrt{2}$. The equality holds if $n_u = n_v = 2$ for each edge $(u,v) \in E(G)$ and $m = \frac{n(n-2)}{2}$. The graph

G does not contain a vertex u of degree $n-1$; in such case $n_v = 1$ for each vertex v which is connected to u. From $2m = n(n-2) = \sum_{i=1}^{n} d_i \geq n(n-2)$, we obtain that all vertices of G are of degree $n-2$. ■

It is clear that the above approach does not work if G contains edges (u, v) for which $n_u = 1$ or $n_v = 1$. In order to characterize the graphs on n vertices with maximal ABC_{GG} we apply the Lagrange multipliers method.

Theorem 2. *Let G be a connected graph on n vertices. If n is even, then*

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

The 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

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

The equality holds for the graphs with one vertex of degree $n-1$ and $n-1$ vertices of degree $n-2$.

Proof. Let G be a connected graph on n vertices and m edges.
Let $F : (x_1, x_2, \ldots, x_{2m}) \to \mathbb{R}$ be a real-valued function defined by

$$F(x_1, x_2, \ldots, x_{2m}) = \sum_{i=1}^{m} \sqrt{\frac{x_{2i-1} + x_{2i} - 2}{x_{2i-1}x_{2i}}}.$$

It is clear that $ABC_{GG}(G) = F(x_1', x_2', \ldots, x_{2m}')$ where $x_{2i-1}' = n_u$ and $x_{2i}' = n_v$ for each edge $e_i = (u, v) \in E(G)$, $1 \leq i \leq m$. In order to maximize the index $ABC_{GG}(G)$ we maximize the function F by applying the Lagrange multipliers method under the side condition $2m \leq g(x_1, x_2, \ldots, x_{2m}) = x_1 + x_2 + \ldots + x_{2m} \leq 2m(n - \frac{2m}{n})$. The bounds for the function $g(x_1, x_2, \ldots, x_{2m})$ come from $2 \leq n_u + n_v$ and Lemma 3.
We calculate $\frac{\partial F}{\partial x_{2i-1}} = \frac{1}{2(x_{2i-1}x_{2i})^{\frac{3}{2}}} \cdot \frac{x_{2i}(2-x_{2i})}{\sqrt{x_{2i-1}+x_{2i}-2}}$ and $\frac{\partial F}{\partial x_{2i}} = \frac{1}{2(x_{2i-1}x_{2i})^{\frac{3}{2}}} \cdot \frac{x_{2i-1}(2-x_{2i-1})}{\sqrt{x_{2i-1}+x_{2i}-2}}$. Hence $\frac{\partial F}{\partial x_i} = 0$ if and only if $x_i = 2$. Thus, the point

$(2, 2, \ldots, 2)$ is the unique critical point for the function F. If $n_u = n_v = 2$ for each edge of the graph G, then

$$F(2, 2, \ldots, 2) = ABC_{GG}(G) = \frac{m\sqrt{2}}{2} \tag{6}$$

From $\nabla g = \langle 1, 1, \ldots, 1\rangle$ and $\nabla F = \lambda \cdot \nabla g$, for each $i = 1, \ldots, m$ we get

$$\frac{1}{2(x_{2i-1}x_{2i})^{\frac{3}{2}}} \cdot \frac{x_{2i}(2 - x_{2i})}{\sqrt{x_{2i-1} + x_{2i} - 2}} = \lambda \tag{7}$$

$$\frac{1}{2(x_{2i-1}x_{2i})^{\frac{3}{2}}} \cdot \frac{x_{2i-1}(2 - x_{2i-1})}{\sqrt{x_{2i-1} + x_{2i} - 2}} = \lambda \tag{8}$$

Dividing (7) by (8) we get $x_{2i-1} = x_{2i} = c$ or $x_{2i-1} + x_{2i} = 2$, that is, $x_{2i-1} = x_{2i} = 1$. The case $x_{2i-1} = x_{2i} = 1$ contributes with 0 in the index formula, thus we omit it. From the boundary constraint $g = 2m(n - \frac{2m}{n})$ we have $2mc = 2m(n - \frac{2m}{n})$, that is, $x_i = n - \frac{2m}{n}$. Now if we assume that $n_u = n_v = n - \frac{2m}{n}$ for each edge $(u, v) \in E(G)$, we get

$$F(n-\frac{2m}{n}, n-\frac{2m}{n}, \ldots, n-\frac{2m}{n}) = ABC_{GG}(G) = \frac{m}{n^2 - 2m}\sqrt{n(2n^2 - 2n - 4m)}. \tag{9}$$

Comparing (6) and (9) we easily prove that the inequality

$$\frac{m}{n^2 - 2m}\sqrt{n(2n^2 - 2n - 4m)} \leq \frac{m\sqrt{2}}{2}$$

is equivalent to

$$n^4 + 4n^2 + 4m^2 - 4n^3 - 4mn^2 + 8mn \geq 0 \Leftrightarrow (n^2 - 2n - 2m)^2 \geq 0.$$

The equality between the bounds in (6) and (9) holds if $m = \frac{n(n-2)}{2}$. Therefore, for each connected graph on m edges and n vertices holds

$$F(x_1, x_2, \ldots, x_{2m}) \leq \frac{m\sqrt{2}}{2} \Leftrightarrow ABC_{GG}(G) \leq \frac{m\sqrt{2}}{2}. \tag{10}$$

In the second part of the proof we consider when the equality in (10) does hold.

Let n be an odd number. Since the maximum of F is achieved for $n_u = n_v = 2$, we get $n_{uv} = n - 4$. Now from Lemma 1 we get $m \leq \frac{n(n-2)}{2}$, but clearly the equality is not attained. Since each edge of the extremal graph contributes with $\frac{\sqrt{2}}{2}$ in the index-formula, we can assume that there are edges (u, v) for which $\sqrt{\frac{n_u+n_v-2}{n_u n_v}} = \frac{\sqrt{2}}{2}$ and $n_u \neq n_v$. Easy calculations show that for each such edge it holds $n_u = 2$ or $n_v = 2$. In order to maximize the value for m, from Lemma 1, we maximize the value of $\sum_{(u,v)\in E(G)} n_{uv}$. Thus we assume that $n_u = 1$, i.e., we assume that the graph G contains edges for which $(n_u, n_v) = (1, 2)$. Let G contains k vertices of degree $n - 1$. Then we have $2m \leq k(n - 1) + (n - k)(n - 2)$, from where $m \leq \frac{n^2-2n+k}{2}$. There are $\binom{k}{2}$ edges between these k vertices. If for (u, v) holds $d_u = d_v = n - 1$, then $n_u = n_v = 1$. In this case we have $\sqrt{\frac{n_u+n_v-2}{n_u n_v}} = 0$. Thus

$$ABC_{GG}(G) \leq \left(m - \frac{k(k-1)}{2}\right)\frac{\sqrt{2}}{2} \leq \left(\frac{n^2 - 2n + 2k - k^2}{2}\right)\frac{\sqrt{2}}{2}$$
$$\leq \left(\frac{n^2 - 2n + 1}{2}\right)\frac{\sqrt{2}}{2} \qquad (11)$$

The equality in (11) holds for $k = 1$, i.e., if G contains exactly one vertex of degree $n - 1$ and $n - 1$ vertices of degree $n - 2$. The Graovac-Ghorbani index of these graphs is equal to

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

If n is even and if $n_u = n_v = 2$ for each edge, then G does not contain a vertex of degree $n - 1$ and $m \leq \frac{n(n-2)}{2}$. Thus, $m = \frac{n(n-2)}{2}$ if and only if all vertices of G are of degree $n - 2$; in this case we obtain the cocktail party graph. If there are edges for which $(n_u, n_v) = (1, 2)$, then we can suppose that G contains k vertices of degree $n - 1$. Using the bounds in (11), we find that the largest value of m is achieved for $k = 0$, (we already consider this case), and for $k = 2$. In this case we have exactly two vertices of degree $n - 1$ and all other vertices of degree $n - 2$. In both cases ($k = 0$

or $k = 2$) we obtain

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

■

***Acknowledgment*:** The author is supported by the Slovenian Research Agency through the grants P1-0285, J1-1695, J1-9108 and J1-9110.

References

[1] B. Bollobás, *Extremal Graph Theory*, *Acad. Press*, London, 1978, pp. 297–297.

[2] S. Cambie, Five results on maximizing topological indices of graphs, *Discr. Math. Theor. Comput. Sci.* **23** (2021) #6896.

[3] K. C. Das, K. Xu, A. Graovac, Maximal unicyclic graphs with respect to new atom–bond connectivity index, *Acta Chim. Slov.* **60** (2013) 34–42.

[4] K. C. Das, M. A. Mohammed, I. Gutman, K. A. Atan, Comparison between atom-bond connectivity indices of graphs, *MATCH Commun. Math. Comput. Chem.* **76** (2016) 159–170.

[5] D. Dimitrov, B. Ikica, R. Škrekovski, Remarks on the Graovac-Ghorbani index of bipartite graphs, *Appl. Math. Comp.* **293** (2017) 370–376.

[6] E. Estrada, L. Torres, L. Rodríguez, I. Gutman, An atom–bond connectivity index: Modelling the enthalpy of formation of alkanes, *Indian J. Chem.* **37A** (1998) 849–855.

[7] B. Furtula, Atom-bond connectivity index versus Graovac-Ghorbani analog, *MATCH Commun. Math. Comput. Chem.* **75** (2016) 233-242.

[8] B. Furtula, I. Gutman, K. C. Das, On atom–bond molecule structure descriptors, *J. Serb. Chem. Soc.* **81** (2016) 271–276.

[9] W. Gao, W. Wang, Second atom–bond connectivity index of special molecular structures, *J. Chem.* **2014** (2014) #906254.

[10] A. Graovac, M. Ghorbani, A new version of atom-bond connectivity index, *Acta Chim. Slov* **57** (2010) 609–612.

[11] M. Rostami, M. Sohrabi–Haghighat, M. Ghorbani, On second atom–bond connectivity index, *Iranian J. Math. Chem.* **4** (2013) 265–270.

[12] M. Rostami, M. Sohrabi–Haghighat, Further results on new version of atom–bond connectivity index, *MATCH Commun. Math. Comput. Chem.* **71** (2014) 21–32.

[13] W. Mantel, Solution to Problem 28, by H. Gouwentak, W. Mantel, J. Teixeira de Mattes, F. Schuh, and W. A. Wythoff, *Wiskundige Opgaven* **10** (1907) 60–61.