MATCH
Communications in Mathematical and in Computer Chemistry

MATCH Commun. Math. Comput. Chem. **75** (2016) 233-242

ISSN 0340 - 6253

Atom–Bond Connectivity Index Versus Graovac–Ghorbani Analog

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(Received September 30, 2015)

Abstract

The atom–bond connectivity index was introduced almost twenty years ago as an improvement of the well-known Randić index. Its mathematical properties and theory are well established and chemical usefulness confirmed in various research projects. On the other hand, recently introduced quantity that was named as "second" ABC index resembles to the original–one, but it is not validated anywhere as a molecular descriptor. Also its mathematical properties are examined to a limited extent. This paper is devoted to the comparison of these two topological invariants.

1 Introduction

Molecular descriptors play an important role in various disciplines intimately connected to chemistry such are chemoinformatics, mathematical chemistry, drug development, QSPR/QSAR research, etc. [1–4] Among them, frequently applied in research projects are so-called topological descriptors [2]. A legion of such invariants exists, but, minority of them have been employed in some kind of chemical investigations. Probably the most prominent topological index is Randić connectivity index [5]. This index has been deeply investigated both by chemists and mathematicians. Several books appeared reporting results connected with Randić index [6–9]. Many topological indices have appeared inspired by this index, aiming to extend its application's scope. The atom–bond connectivity index ($ABC(G)$) is certainly the most succeeded descendant of Randić index.

In order to define the $ABC(G)$ and its analog some graph theoretical elements must be defined. Let's G be a connected graph with vertex set $\mathbf{V}$ and edge set $\mathbf{E}$. The degree of a vertex v (d_v) is equal to the number of edges that are incident to it. The distance between vertices u and v ($d(u,v)$) in a graph is equal to the number of edges in the shortest path that connects these vertices.

The $ABC(G)$ was introduced in 1998 [10], and index is defined as:

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

where summation goes over all edges in a graph G.

Authors, already, in the seminal paper, showed that this index has significant prediction power. It is, hereof, inexplicable why this descriptor remained in shadow for almost ten years. It was revived in 2008 by one of its inventors [11]. This paper attracted attention of researchers and nowadays there exists few dozens of papers dealing with atom–bond connectivity index. As an illustration of vivid researching of ABC index see the most recent publications dealing with it [12–18].

This index has characteristics that made it as one of the best degree–based molecular descriptors [19–22]. Researchers were started to introduce topological invariants that resemble to ABC index hoping that these indices could be successful as the atom–bond connectivity index is. One of such invariants was appeared in literature in 2010 [23].

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

where summation goes over all edges in a graph G. n_u and n_v are defined as cardinalities of the following sets:

$$N_u(e,G) = \{x \in \mathbf{V} \quad | \quad d(u,x \,|\, G) < d(v,x \,|\, G)\}$$

$$N_v(e,G) = \{x \in \mathbf{V} \quad | \quad d(v,x \,|\, G) < d(u,x \,|\, G)\}$$

In the seminal paper [23], this index was erroneously named as new version of atom–bond connectivity index, and labeled as ABC_2. Etymology of the atom–bond connectivity index lies in the fact that in its definition exiting atom connectivity as degree of a vertex, and bond connectivity as degree of a bond. Such descriptors of atom or bond connectivity cannot be recognized in the Graovac–Ghorbani analog. Therefore, here, this index is denoted as ABC_{GG}, and will be called as Graovac–Ghorbani index.

There are just a few mathematical papers dealing with Graovac–Ghorbani index [24–27], but its chemical usability issues and comparison with atom–bond connectivity index are matter of current researches [28, 29].

2 Prediction power of ABC_{GG}

Earlier has been pointed out that atom–bond connectivity index shows a reasonable prediction power. It was mainly tested on alkanes and here the prediction power of Graovac–Ghorbani index is compared on the same test set. Namely, dataset of all octanes have been taken from http://www.moleculardescriptors.eu . This dataset contains 13 physico–chemical properties of octanes, but we are interested in those for which ABC_{GG} shows better correlation coefficient than atom–bond connectivity index. Finally, the properties for which the absolute value of correlation coefficient with ABC_{GG} is greater than 0.8 were selected. After cleaning database from missing values and taking into account above mentioned conditions, the Graovac–Ghorbani index gave better prediction in the case of entropy and acentric factor (see Figure 1).

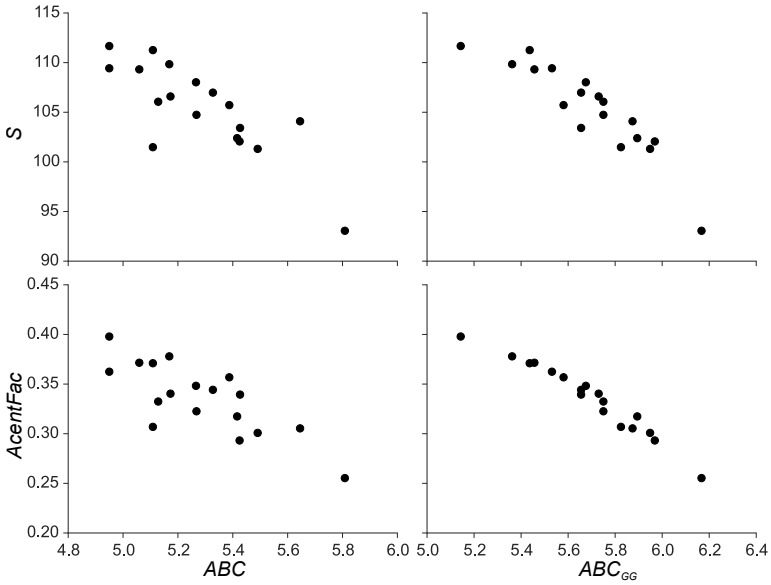

Figure 1. Correlations between ABC and ABC_{GG} with entropy and acentric factor.

From Figure 1 it is evident that correlations between Graovac–Ghorbani index and these two physico–chemical parameters are far more better than with atom–bond connectivity index. Correlation coefficients support this and are given in the following table:

	ABC	ABC_{GG}
S	-0.807	-0.905
Acentric Factor	-0.788	-0.977

However, ABC_{GG} is a distance–based topological descriptor, while ABC is a degree–based one. Therefore, Graovac–Ghorbani index should be compared with best representatives of the same kind of molecular structure descriptors. The prediction potential of ABC_{GG} is compared with Wiener (W), Balaban (J), and Harary (H) indices. Reasons for choosing these distance–based molecular descriptors are evident for people who are working in this area of science. Namely, W is the oldest topological index, and frequently employed in various QSPR/QSAR investigations; J is descriptor whose degeneracy is smallest among distance–based indices, and it also proved to be valuable predictor of physico–chemical properties and biological activities of molecules; H is the least studied index in this group, but its definition is chemically sound and easily explicable. Therefore it is expected to be a useful tool in a such kind of researches.

The physico–chemical properties used for the comparison of these topological indices have been chosen from same dataset as above. This dataset has been cleaned from missing values, and the properties were selected based on criterion that the absolute value of correlation coefficient between each of them and Graovac–Ghorbani index is greater than 0.8. Only three physico–chemical properties of initial 13 were survived these stipulations. Entropy, acentric factor, and heat of vaporization of octanes are well correlated with ABC_{GG}. Correlations between Balaban, Harary, Wiener, and Graovac–Ghorbani indices with these three physico–chemical properties are displayed in Figure 2. Plots depicted in it show that there is no visible difference in predicting entropy, acentric factor, and heat of vaporization among these four indices. Howsoever, the correlation coefficients are given in Table 1. They demonstrate that Graovac–Ghorbani index is predicting the heat of vaporization of octanes somewhat better than other three distance–based descriptors. It is interesting that in the case of entropy and acentric factor the best predicting tool among these descriptors is Harary index.

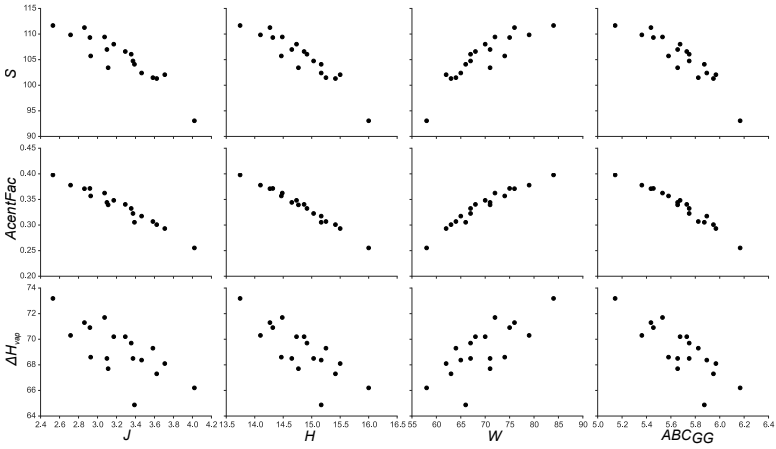

Figure 2. Correlations between Balaban, Harary, Wiener, and Graovac–Ghorbani indices with heat of vaporization, acentric factor, and entropy, respectively.

	J	H	W	ABC_{GG}
S	-0.906	-0.929	0.878	-0.905
AcentFac	-0.979	-0.992	0.966	-0.977
ΔH_{VAP}	-0.707	-0.779	0.738	-0.810

Table 1. Correlation coefficients between Balaban, Harary, Wiener, and Graovac–Ghorbani indices and entropy, acentric factor and, heat of vaporization of octanes.

Findings presented in this section suggest that Graovac–Ghorbani index might be interesting for further investigations. It has been shown that for particular physico–chemical properties ABC_{GG} gives significantly better correlations than atom–bond connectivity index. On the other hand, comparison of Graovac–Ghorbani index with other distance–based descriptors reveals quite similar prediction power. Thence, ABC_{GG} could be used as well as other descriptors of the same kind.

3 Connected graphs with extremal Graovac–Ghorbani index

A first mathematical question in researching of a molecular descriptor is usually addressed to characterization of graphs with fixed number of vertices having its extremal values.

From a chemical point of view, the most interesting part of this problem is related to connected graphs. Therefore, from now on, our attention will be narrowed down to them.

Since the atom–bond connectivity index demonstrated respectable power for modeling of physical, chemical, and biological qualities of molecules, several articles appeared dealing with its mathematical features. Majority of them are devoted to characterization of connected graphs with minimal ABC. These results are compiled in [30] and references cited in it.

The unique connected graph with given order n having maximal atom–bond connectivity index is complete graph K_n. It is known that connected graph with minimal ABC must be a tree and it need not to be unique. Characterization of these trees is a matter of current researches [12, 13, 15].

Contrary to atom–bond connectivity index, characterization of a connected graph with given order n having minimum value of Graovac–Ghorbani index is an easy task. It is the complete graph, K_n [26]. It is quite easy to learn this from the definition of ABC_{GG} (see Eq. (2)). Its minimal value is 0, and it can be achieved if and only if $n_1 = n_2 = 1$ for all edges in a connected graph. Only such graph is K_n.

Characterizing connected graphs that maximize ABC_{GG} is much more serious problem. It is, here, tackled in assistance of computers.

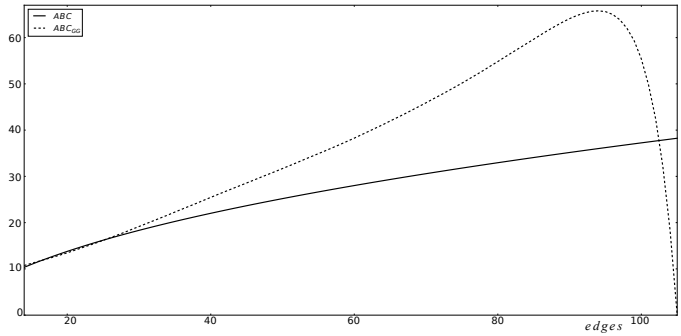

Figure 3

For this project it was used in-house computer with processor IntelCore i5-3470 (3.2 GHz) and 8 GB of memory. The program has been written in Python. It starts from the complete graph with given order n and calculates ABC and ABC_{GG}. Then, randomly delete an edge and recalculate these indices. Random deletion of edges with checking the connectivity of obtained graph and calculation of indices goes to a tree. In order to

smoothening curves, such procedure was repeated 1000 times with calculating the average of indices. An example is shown in Figure 3 for connected graphs with 15 vertices. Values of atom–bond connectivity index are drawn by the solid line. As it was above pointed out the minimal value of ABC is attained for a connected graph with the smallest number of edges, i.e. for a tree. The maximal value of ABC reached for a connected graph with the greatest number of edges, i.e. the complete graph.

Trend of values of Graovac–Ghorbani index has been shown in Figure 3 by dashed line. As it was proven in [26] the complete graph is the unique connected graph with smallest ABC_{GG}. However, it appears that a connected graph(s) with the maximal Graovac–Ghorbani index is also an edge–rich graph.

In order to characterize graphs that maximize Graovac–Ghorbani index, scanning of all connected ones up to 10 vertices has been performed. As an illustration of the complexity of this task we will mention that the number of connected graphs with ten vertices is 11716571. These graphs are generated using `nauty` package [31]. Obtained graphs with maximal ABC_{GG} are depicted in Figure 4.

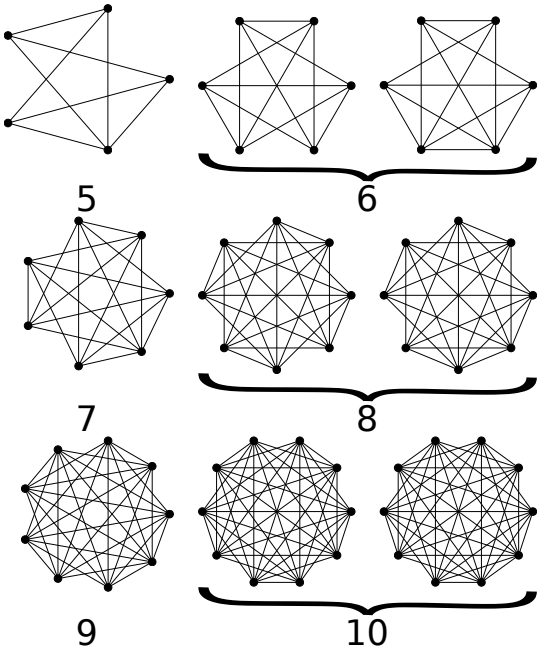

Figure 4

This figure shows 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 with even number. These graphs with odd number of vertices have exactly one vertex of degree equal to $n-1$, and $n-1$ vertices with degree equal to $n-2$. Among two graphs with even number of vertices one is a regular graph with degree equal to $n-2$ (called cocktail party graph), while other graph that maximizes ABC_{GG} has exactly 2 vertices of degree equal to $n-1$, and other vertices are of degree equal to $n-2$. It is easy to envisage that the Graovac–Ghorbani index of these graphs can be calculated by following formulas:

$$ABC(G) = \begin{cases} \dfrac{(n-1)^2}{4}\sqrt{2} & \text{if } n \text{ is odd} \\ \dfrac{n\,(n-2)}{4}\sqrt{2} & \text{if } n \text{ is even} \end{cases}$$

where number of edges in graphs with maximum ABC_{GG} and odd number of vertices is $(n-1)^2/2$, while in those with even number of vertices is $n\,(n-2)/2$ for $(n-2)$-regular graph (other extremal graph has $n\,(n-2)/2+1$ edges). For each of these edges value of $\sqrt{\frac{n_u+n_v-2}{n_u\,n_v}}$ is equal to $\sqrt{2}/2$.

Brutal force scanning of all connected graphs up to 10 vertices, hypothesizing which graphs maximize Graovac–Ghorbani index. Unfortunately, lack of computer resources makes such procedure inapplicable on all connected graphs with number of vertices greater than 10. However, the number of edges of extremal graphs depicted in Figure 4 helped us to deduce theirs number of edges, m. Thence, using `nauty` package we narrowed our search by constructing all connected graphs having number of edges in range $[m-5, m+5]$. Then this set of graphs was scanned for graphs that maximize Graovac–Ghorbani index. This investigations was conducted on connected graphs up to 20 vertices and obtained results corroborated hypothesizes on graphs having maximal ABC_{GG}.

4 Conclusions

This paper is devoted to the investigations of Graovac–Ghorbani index, and it is clearly divided into two distinct parts. First part of the paper was presented results dealing with evaluation of the prediction power of ABC_{GG}. In spite of the fact that this index showed comparable prediction capability with other topological descriptors, the reason for its designing is questionable. Second part of the paper dealing with characterization of connected graphs that maximize Graovac–Ghorbani index. This was done solely by computer help. Connected graphs with maximal ABC_{GG} are described, but the rigorous mathematical proof is needful.

Acknowledgment: This work has been supported by the *Ministry of Education, Science, and Technological Development* of Republic of Serbia through the grant no. 174033.

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