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Remarks on the Graovac–Ghorbani index of bipartite graphs

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ABSTRACT

The atom–bond connectivity (ABC) index is a well-known degree-based molecular structure descriptor with a variety of chemical applications. In 2010 Graovac and Ghorbani introduced a distance-based analog of this index, the Graovac–Ghorbani (GG) index, which yielded promising results when compared to analogous descriptors. In this paper, we investigate the structure of graphs that maximize and minimize the GG index. Specifically, we show that amongst all bipartite graphs, the minimum GG index is attained by a complete bipartite graph, while the maximum GG index is attained by a path or a cycle-like graph; the structure of the resulting graph depends on the number of vertices. Through the course of the research, we also derive an asymptotic estimate of the GG index of paths. In order to obtain our results, we introduce a normalized version of the GG index and call it the normalized Graovac–Ghorbani (NGG) index. Finally, we discuss some related open questions as a potential extension of our work.

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1. Introduction

Let G be a simple undirected graph of order $n = |V(G)|$ and size $m = |E(G)|$. The degree of a vertex $v \in V(G)$, denoted by $d(v)$, is the number of edges incident to v. Then the *atom–bond connectivity (ABC) index* of G is defined as

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

This degree-based molecular structure descriptor was introduced in 1998 by Estrada et al. [16], who showed that it can be a valuable predictive tool in the study of the heat of formation in alkanes. Later the physico-chemical applicability of the ABC index was confirmed and extended in several studies [9,15,24,26]. In addition, some comparative studies reported results that favor the ABC index over other mathematically similar molecular structure descriptors [19,27]. As a consequence, the mathematical properties of the ABC index were studied with increasing interest over the last several years. More results about the mathematical and computational aspect of the ABC index can be found in [1–5,7,11–14,20,21,23,25,28–31] and the references cited therein.

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Several natural extensions and variants of the ABC index were introduced with a hope to obtain other successful molecular structure descriptors. Thus, in 2010, Graovac and Ghorbani [24] proposed the following distance-based analog of the ABC index:

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

where n_u is defined as the number of vertices of G lying closer to u than to v and similarly n_v as the number of vertices of G lying closer to v than to u, namely

$$n_u = |\{w \in V(G) : d(w,u) < d(w,v)\}| \quad \text{and} \quad n_v = |\{w \in V(G) : d(w,v) < d(w,u)\}|. \tag{1}$$

Here $d(i, j)$ denotes the distance between vertices i and j, i.e., the number of edges on the shortest path connecting i and j.

This index was named after its authors as the *Graovac–Ghorbani index*. Since it resembles the ABC index, it is also known as the *second atom–bond connectivity index* and is often denoted by ABC_2. However, as it was indicated in [17], this name and notation are inappropriate since the expression $\sqrt{(n_u + n_v - 2)/(n_u n_v)}$ is not related to atom connectivity (as the degree of a vertex) and bond connectivity (as the degree of a bond/edge). Therefore, we refer to this index as the Graovac–Ghorbani index and denote it by GG. Some initial studies indicate that the Graovac–Ghorbani index could be an effective predictive tool in chemistry. For instance, it can be used to model both the boiling and the melting points of molecules [22].

Due to its recentness, the Graovac–Ghorbani index was studied only to a limited extent. In [10] maximal unicyclic graphs with respect to the GG index were determined. Some upper bounds on the GG index were presented in [33]. This work was extended in [32], where lower and additional upper bounds for the GG index of graphs were given. The authors also determined the trees with minimal and maximal GG indices. Throughout the paper, we will need the result about trees with minimal GG indices. For later reference, we state it explicitly.

Theorem 1.1 (Rostami and Sohrabi-Haghighat [32])**.** *The path P_n is the n-vertex tree with the minimum Graovac–Ghorbani index.*

Further upper and lower bounds on the GG index were presented in [6]. The GG indices of several special chemical molecular structures including the unilateral polyomino chain, the unilateral hexagonal chain, the V-phenylenic nanotubes and the nanotori were presented in [22]. Recently, in [17], the structure of graphs with maximal GG was conjectured based on computational results. The relation between the GG index and the original ABC index was also investigated very recently in [8,17,18]. In addition, in [17], some physico-chemical properties of the GG index were compared with the physico-chemical properties of a few other well-known distance-based molecular descriptors, and the obtained results suggest that it might be worth investigating the GG index further.

To simplify the derivation of the results presented in the paper, we find it useful to introduce the notion of a *normalized Graovac–Ghorbani index*. We denote it by NGG, and define it as

$$\mathrm{NGG}(G) = \sum_{uv \in E(G)} \frac{1}{\sqrt{n_u n_v}}.$$

This measure is of purely technical importance to us. The Graovac–Ghorbani index GG can be expressed very conveniently using NGG when dealing with bipartite graphs.

Proposition 1.2. *Let G be a bipartite graph on n vertices. Then*

$$\mathrm{GG}(G) = \mathrm{NGG}(G)\sqrt{n-2}.$$

Proof. Following the definition of n_u and n_v in (1), one can conclude that in the case of a bipartite graph, $n_u + n_v = n$ holds for any edge uv of G. Indeed, assume that this does not hold, i.e., assume that $n_u + n_v < n$ for some edge $uv \in E(G)$. Then there exists a vertex w such that $d(u,w) = d(v,w)$ and therefore G contains an odd cycle, which in turn is a contradiction to the fact that G is a bipartite graph.

Hence, the desired equality holds:

$$\mathrm{GG}(G) = \sum_{uv \in E(G)} \sqrt{\frac{n-2}{n_u n_v}} = \sqrt{n-2} \cdot \mathrm{NGG}(G).$$

□

Notice that Proposition 1.2 implies that in any subclass of bipartite graphs of fixed order n, the extremal graphs for the NGG index and the extremal graphs for the GG index are the same.

In the rest of the paper, we first consider the GG index of very long paths in Section 2. In Section 3, we present all bipartite graphs with minimal and maximal GG indices. We conclude and state some open problems in Section 4.

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