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On Some Vertex–Degree–Based Graph Invariants

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Abstract

Let $G = (V, E)$ be a graph, d_u the degree of its vertex u, and uv the edge connecting the vertices u and v. The atom–bond connectivity index and the sum–connectivity index of G are defined as $ABC = \sum_{uv \in E} \sqrt{(d_u + d_v - 2)/(d_u\, d_v)}$ and $\chi = \sum_{uv \in E} 1/\sqrt{d_u + d_v}$, respectively. Continuing the recent researches on ABC [B. Furtula, A. Graovac, D. Vukičević, Atom-bond connectivity index of trees, *Discr. Appl. Math.* **157** (2009) 2828–2835] and χ [B. Zhou, N. Trinajstić, On a novel connectivity index, *J. Math. Chem.* **46** (2009) 1252–1270] we obtain novel upper bounds on these vertex–degree–based graph invariants.

1 Introduction

In mathematical chemistry a variety graph invariants, usually referred to as topological indices, are used for predicting molecular properties [10]. Among these are some that are defined by means of the vertex degree sequence of the underlying (molecular) graph.

Let $G = (V(G), E(G))$ be a simple graph with $n = |V(G)|$ vertices and $m = |E(G)|$ edges. The degree (= number of first neighbors) of a vertex $u \in V(G)$ will be denoted by d_u. The edge connecting the vertices u and v will be denoted by uv.

The oldest and most studied vertex–degree–based topological indices are the Randić index $R(G) = \sum_{uv \in E(G)} 1/\sqrt{d_u\, d_v}$ and the so-called first and second Zagreb indices:

$$M_1(G) = \sum_{u \in V(G)} d_u^2 \qquad \text{and} \qquad M_2(G) = \sum_{uv \in E(G)} d_u\, d_v$$

respectively [10].

A few years ago Estrada et al. [5] introduced a further vertex–degree–based graph invariant, nowadays known as the *atom–bond connectivity index*. It is defined as:

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

Furtula et al. [6] have recently characterized trees with the maximum and minimum values of the ABC index. In particular, they proved that among n-vertex trees, ABC is maximal for the star $K_{1,n-1}$.

Also quite recently, Zhou and Trinajstić [16] introduced and studied the so-called *sum–connectivity index*, defined as:

$$\chi(G) = \sum_{uv \in E(G)} \frac{1}{\sqrt{d_u + d_v}} \, .$$

They established lower and upper bounds for χ in terms of number of vertices, number of edges, maximum vertex degree Δ, and minimum vertex degree δ. They also determined the unique n-vertex tree with a given number of pendent vertices, having minimum χ.

The Zagreb indices have been much studied in the past (see [4, 7, 12, 14] and references cited therein). De Caen [3] gave an upper bound on the first Zagreb index in terms of the number of vertices and edges. Bollobás and Erdős [1, 2] determined the graph with the given number of edges, having the maximum value of the second Zagreb index.

In this paper we present a relationship between ABC and M_2 for a graph with n vertices and m edges. Using this and some previous results, we obtain upper bounds for ABC for some classes of graphs. Also upper bounds for the sum–connectivity index are given.

2 Preliminaries

In this section we list some previously known results that will be needed in the subsequent sections. Bollobás and Erdős [1] proved that if $m = \binom{k}{2}$ then the maximum second Zagreb index of a graph with m edges is $m(k-1)^2$, with equality holding if and only if G is the union of K_k and isolated vertices. This result can be reformulated as follows.

Lemma 2.1. [1] *Let G be a graph with m edges. Then*

$$M_2(G) \leq m\left(\sqrt{2m+\frac{1}{4}}-\frac{1}{2}\right)^2$$

with equality if and only if m is of the form $m = \binom{k}{2}$ for some natural number k, and G is the union of the complete graph K_k and isolated vertices.

In [4] the following upper bound for the second Zagreb index was obtained:

Lemma 2.2. [4] *Let G be a graph with n vertices, m edges and minimum vertex degree δ. Then*

$$M_2(G) \leq 2m^2 - m\delta(n-1) + \frac{1}{2}m(\delta-1)\left(\frac{2m}{n-1}+n-2\right)$$

with equality if and only if $G \cong K_{1,n-1}$ or $G \cong K_n$.

The eccentricity of a vertex v is the greatest distance between v and any other vertex. The radius of a graph is the minimum eccentricity of any vertex. Yamaguchi [12] studied maximum values of the Zagreb indices for triangle– and quadrangle–free connected graphs, and obtained:

Lemma 2.3. [12] *Let G be a triangle– and quadrangle–free connected graph with n vertices, m edges, and radius r. Then $M_1(G) \leq n(n+1-r)$ and $M_2(G) \leq m(n+1-r)$, with equality in either place if and only if G is isomorphic to a Moore graph of diameter two or is the cycle of length six.*

3 Atom-bond connectivity index

A bipartite graph is called semiregular if each vertex in the same part of a bipartition has the same degree.

Theorem 3.1. *Let G be a graph with n vertices and m edges. Then*

$$ABC(G) \leq \sqrt{m\left(n - \frac{2m^2}{M_2(G)}\right)} \tag{1}$$

with equality if and only if G is a regular or a semiregular bipartite graph.

Proof. By the arithmetic–harmonic mean inequality,

$$\sum_{uv \in E(G)} \frac{1}{d_u\, d_v} \geq \frac{m^2}{\sum_{uv \in E(G)} d_u\, d_v} = \frac{m^2}{M_2(G)} \,. \tag{2}$$

Let n_0 be the number of isolated vertices of G. Then

$$\sum_{uv \in E(G)} \left(\frac{1}{d_u} + \frac{1}{d_v}\right) = \sum_{u \in V(G),\, d_u \neq 0} \left(d_u \cdot \frac{1}{d_u}\right) = n - n_0 \,. \tag{3}$$

Bearing this in mind, by the Cauchy–Schwarz inequality we get

$$\begin{aligned} ABC(G) &= \sum_{uv \in E(G)} \sqrt{\frac{1}{d_u} + \frac{1}{d_v} - \frac{2}{d_u\, d_v}} \leq \sqrt{m} \sqrt{\sum_{uv \in E(G)} \left(\frac{1}{d_u} + \frac{1}{d_v} - \frac{2}{d_u\, d_v}\right)} \\ &= \sqrt{m} \sqrt{n - n_0 - 2 \sum_{uv \in E(G)} \frac{1}{d_u\, d_v}} \end{aligned}$$

and thus

$$ABC(G) \leq \sqrt{m\,n - 2m \sum_{uv \in E(G)} \frac{1}{d_u\, d_v}} \,. \tag{4}$$

Combining (2) and (4), we get the inequality in (1).

Suppose now that equality holds in (1). Then all inequalities in the above argument must be equalities. Thus from (2), $d_u\, d_v$ is a constant for each $uv \in E(G)$. Then we prove that each component of G is a regular graph or a semiregular bipartite graph. Let $C(G)$ be a component of G and u be a vertex in $C(G)$. Since $d_u\, d_v$ is a constant, neighbors of vertex u must have the same degree. Hence $C(G)$ has only two types of degrees d_u and d_v because $C(G)$ is connected. If $C(G)$ contains an odd cycle, then clearly all vertices on this cycle have equal degrees. Hence it is easy to see that $d_u = d_v$. Thus $C(G)$ is regular. If $C(G)$ does not contain an odd cycle, then it is bipartite. Hence $C(G)$ is semiregular bipartite. Then from (4) follows that $n_0 = 0$ and $(d_u + d_v - 2)/(d_u\, d_v)$ is a constant for each $uv \in E(G)$. Since $d_u\, d_v$ is a constant, $d_u + d_v$ is also constant for each $uv \in E(G)$. Hence G is a regular graph or a semiregular bipartite graph.

Conversely, if G is a regular graph then one can easily see that the equality holds in (1). Now, suppose that G is a semiregular bipartite graph with two types of degrees d_u and d_v. Then we have

$$m\left(\frac{1}{d_u}+\frac{1}{d_v}\right)=n$$

that is

$$\frac{m(d_u+d_v-2)}{d_u\,d_v}=n-\frac{2m^2}{m\,d_u\,d_v}\,.$$

Multiplying both sides of the above equality by m and taking the square root, we get equality in (1). This completes the proof. □

At this point is should be noted that nowadays a large number of upper bounds for the second Zagreb index M_2 is known, either in terms of other graph invariants or valid for special classes of graphs (see e. g. [8,9,11,13–15]). By means of Theorem 3.1, from each of these we could deduce upper bounds for ABC.

The following theorems are immediate consequences of Theorem 3.1, and are obtained by using the lemmas from the previous section.

Theorem 3.2. *Let G be a graph with n vertices and m edges. Then*

$$ABC(G)\le\sqrt{m\left(n-\frac{8m}{(\sqrt{8m+1}-1)^2}\right)}$$

with equality holding if and only if $G\cong K_n$.

Moore graphs are regular graphs of degree k and diameter d that have the maximum possible number of vertices, namely $1+k+k(k-1)+\cdots+k(k-1)^{d-1}$. Hoffman and Singleton proved that Moore graphs of diameter two are the pentagon, the Petersen graph, a 7-regular graph with 50 vertices (the Hoffman–Singleton graph) and possibly a 57-regular graph with 57^2+1 vertices (which still is an open problem).

Theorem 3.3. *Let G be a triangle– and quadrangle–free connected graph with n vertices, m edges, and radius r. Then*

$$ABC(G)\le\sqrt{m\left(n-\frac{2m}{n+1-r}\right)}$$

with equality if and only if G is isomorphic to a Moore graph of diameter two or is the cycle of length six.

Let us denote

$$\varphi(n,m,\delta) := 2m - \delta(n-1) + \frac{1}{2}(\delta-1)\left(\frac{2m}{n-1} + n - 2\right).$$

Theorem 3.4. *Let G be a graph with n vertices, m edges, and minimum degree δ. Then*

$$ABC(G) \le \sqrt{m\left(n - \frac{2m}{\varphi(n,m,\delta)}\right)} \tag{5}$$

with equality if and only if $G \cong K_{1,n-1}$ or $G \cong K_n$.

Corollary 3.1. [6] *Let T be a tree with n vertices. Then*

$$ABC(T) \le \sqrt{(n-1)(n-2)} \tag{6}$$

with equality holding if and only if $T \cong K_{1,n-1}$.

Proof. Since T is a tree, $m = n-1$ and $\delta = 1$. Hence $\varphi(n,m,\delta) = n-1$ and inequality (6) follows from (5). □

4 Sum–connectivity index

Zhou and Trinajstić [16] established several bounds for the sum–connectivity index in terms of basic graph invariants. Most of these are lower bounds. In particular, they showed that $\chi(G) < \sqrt{n\,m/2}$. We now improve this bound and, in addition, give an upper bound for triangle– and quadrangle–free connected graphs in terms of the number of vertices n and radius r.

Theorem 4.1. *Let G be a graph with n vertices and m edges. Then*

$$\chi(G) \le \frac{1}{2}\sqrt{n\,m} \tag{7}$$

with equality holding if and only if G is regular.

Proof. For each edge uv of G, we have

$$\frac{1}{d_u + d_v} \le \frac{1}{4}\left(\frac{1}{d_u} + \frac{1}{d_v}\right). \tag{8}$$

As before, let n_0 be the number of isolated vertices of G. Taking the sum of both sides of (8) over all $uv \in E(G)$ and using (3), we get

$$\sum_{uv\in E(G)} \frac{1}{d_u + d_v} \le \frac{1}{4}\sum_{uv\in E(G)}\left(\frac{1}{d_u} + \frac{1}{d_v}\right) = \frac{n-n_0}{4} \le \frac{n}{4} \tag{9}$$

which by the Cauchy–Schwarz inequality yields

$$\chi(G) \leq \sqrt{m} \left(\sum_{uv \in E(G)} \frac{1}{d_u + d_v} \right)^{1/2} . \tag{10}$$

Combining (9) and (10) we arrive at the inequality in (7).

Suppose now that equality holds in (7). Then all inequalities in the above argument must be equalities. Then $n_0 = 0$ and $d_u = d_v$ for all $uv \in E(G)$. Hence G is without isolated vertices and every component of G is regular. From (10), $d_u + d_v$ is a constant for each $uv \in E(G)$. Hence G is regular. $\square$

Lemma 4.1. *Let G be a triangle– and quadrangle–free connected graph with n vertices, m edges, and radius r. Then*

$$2m \leq n\sqrt{n+1-r} \tag{11}$$

with equality if and only if G is isomorphic to a Moore graph of diameter two or is the cycle of length six.

Proof. It is easy to see that by the Cauchy–Schwarz inequality, $n\,M_1(G) \geq 4m^2$, with equality if and only if G is a regular graph. Hence by Lemma 2.3, we get (11). The Moore graphs and C_6 are regular, and thus the proof is completed. $\square$

Using Theorem 4.1 and Lemma 4.1 we deduce the following upper bound for the sum–connectivity index:

Theorem 4.2. *Let G be a triangle– and quadrangle–free connected graph with n vertices and radius r. Then*

$$\chi(G) \leq \frac{n}{2}\sqrt{\frac{1}{2}\sqrt{n+1-r}}$$

with equality if and only if G is isomorphic to a Moore graph of diameter two or is the cycle of length six.

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