

On The Atom-Bond Connectivity Index and Coindex

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Abstract
In this paper we find a bound for the first eigenvalue of the atom-bond connectivity matrix. Also, we obtain an inequality consepting atom-bond connectivity index and we give some relations including atom-bond connectivity coindex.

Keywords: Atom-bond connectivity index, coindex.

1. Introduction

Let G be a simple, connected graph on the vertex set V(G) and the edge set E(G). For $v_i \in V(G)$, the degree of the vertex v_i denoted by d_i, the maximum degree is denoted by Δ and the minimum degree is denoted by δ.

The $[ABC](G)$ atom-bond connectivity matrix of graphs is defined as

$$[ABC]_{ij} = \begin{cases} \sqrt{\dfrac{d_i + d_j - 2}{d_i d_j}} & if\ i\ is\ adjacent\ to\ j \\ 0 & otherwise. \end{cases}$$

The eigenvalues of $[ABC](G)$ is denoted by μ_i^{ABC}, $i = 1,2, \ldots, n$. We set new bounds for μ_1^{ABC} in terms of the vertices and the degrees.

The Atom-bond connectivity (ABC) index of G is a topolojical index that is defined as [2]

$$\sum_{v_i v_j \in E(G)} \sqrt{\frac{d_i + d_j - 2}{d_i d_j}}.$$

The Randic index of G is described as [7],

$$\sum_{v_i v_j \in E(G)} \frac{1}{\sqrt{d_i d_j}}.$$

The Reformulated Zagreb index of G is specified that [9],

$$RZ(G) = \sum_{v_i v_j \in E(G),} (d_G(i) + d_G(j) - 2)^2.$$

In this study, we have an inequalty using the Randic index, the Reformulated Zagreb index and the degrees for ABC index.

The ABC Estrada index of the graph G in [4] as

$$E^{ABC}(G) = \sum_{i=1}^{n} e^{\mu_i^{ABC}}$$

where μ_i^{ABC} is the eigenvalue of $ABC(G)$.

The Zagreb co index of G is described in [6] as

$$\overline{Z_1}(G) = \sum_{v_i v_j \notin E(G),} (d_G(i) + d_G(j)),$$

$$\overline{Z_2}(G) = \sum_{v_i v_j \notin E(G),} (d_G(i) d_G(j)).$$

Using topological indices, we will obtain some relations and conclusions deal with ABC index and coindex.

(See [1], [10] for more details.)

2. Preliminaries

In this section, we will give some known lemmas that will be used in the next section.

Lemma 2.1. [5] Let $M = (m_{ij})$ be an nxn irreducible nonnegative matrix and $\lambda_1(M)$ be the greatest eigenvalue with $R_i(M) = \sum_{j=1}^{m} m_{ij}$. Then,

$$(minR_i(M): 1 \leq i \leq n) \leq \lambda_1(M) \leq (maxR_i(M): 1 \leq i \leq n).$$

Lemma 2.2. [3] If G is a simple connected graph and $\lambda_1(G)$ is the spectral radius, then

$$\lambda_1(G) \leq max\left(\sqrt{m_i m_j}: 1 \leq i, j \leq n, v_{i,} v_j \in E\right).$$

Lemma 2.3. [8] If $0 \leq n_1 \leq a_j \leq N_1$ and $0 \leq n_2 \leq b_j \leq N_2$ then

(1.1) $$\left(\sum_{j=1}^{k} (a_j)^2\right)^{\frac{1}{2}} \left(\sum_{j=1}^{k} (b_j)^2\right)^{\frac{1}{2}} \leq \frac{1}{2}\left(\sqrt{\frac{N_1 N_2}{n_1 n_2}} + \sqrt{\frac{n_1 n_2}{N_1 N_2}}\right)\left(\sum_{j=1}^{k} a_j b_j\right)$$

for $1 \leq j \leq k$.

Lemma 2.4. [6] If G is a regular graph, then

$$\overline{Z_1}(G) \leq \frac{-4m^2}{n} + 2m(n-1),$$

$$\overline{Z_2}(G) \leq 2m^2\left(1 - \frac{2m}{n^2} - \frac{1}{n}\right).$$

3. Main Results

Firstly, we define ABC coindex in this section. Secondly, we obtain an inequality for the first eigenvalue of ABC matrix of G and we conclude ABC Estrada index. In addition, we establish different relations for ABC coindex in terms of degrees and some indices.

Definition 3.1. Let G be a simple, connected graph. ABC coindex is defined as follows:

$$\overline{ABC}(G) = \sum_{v_i v_j \notin E(G)} \sqrt{\frac{d_G(i) + d_G(j) - 2}{d_G(i) \cdot d_G(j)}}.$$

Theorem3.2. If G is a simple, connected graph then,

$$\mu_1^{ABC}(G) \leq \frac{n(\Delta + \delta - 2)}{d_n\sqrt{\Delta\delta}}.$$

where d is the degree of G.

Proof. Let us multiply the atom-bond connectivity matrix with the diagonal matrix and the inverse of diagonalmatrix. Let us show this multiplication by $D(G)^{-1}ABC(G)D(G)$. Let us consider an eigenvector of $D(G)^{-1}ABC(G)D(G)$ and this eigenvector be $X = (x_1, x_2, \ldots, x_n)^T$. Let one eigencomponent $x_i = 1$ and the other eigencomponent $0 \leq x_k \leq 1$ for every k.

Let $x_j = max_k(x_k : v_i v_j \in E, i \sim k)$. We know $(D(G)^{-1}ABC(G)D(G))X = \mu_1^{ABC}(G)X$. The i_th equation as follows:

$$\mu_1^{ABC}(G)x_i = \sum_k \sqrt{\frac{d_i + d_k - 2}{d_i d_k}} x_k$$

$$\leq \sqrt{\sum_k \frac{d_i + d_k - 2}{d_i d_k}} x_k$$

$$\leq \sqrt{\sum_k \frac{1}{d_k} + \sum_k \frac{1}{d_i} - \frac{2}{d_i}\sum_k \frac{1}{d_k}} x_k$$

$$\leq \sqrt{\left(\frac{n}{d_n}\right) + \left(\frac{n}{d_i}\right) - \left(\frac{2n}{d_i d_n}\right)} x_k$$

$$\leq \sqrt{n\left(\frac{d_i + d_n - 2}{d_i d_n}\right)} x_k.$$

Lemma 2.1 says that

$$\mu_1^{ABC}(G)x_i \leq \sqrt{n\left(\frac{d_i+d_n-2}{d_i d_n}\right)}.$$

The j-th inequality of $\mu_1^{ABC}(G)$ is

$\mu_1^{ABC}(G)x_j \leq \sqrt{n\left(\frac{d_j+d_n-2}{d_j d_n}\right)}.$

By Lemma 2.2, we get

$$\mu_1^{ABC}(G) \leq \left(n^2\left(\frac{d_i+d_n-2}{d_id_n}\right)\left(\frac{d_j+d_n-2}{d_jd_n}\right)\right)^{\frac{1}{4}}.$$

We know that $\Delta = d_1 \geq d_2 \geq \cdots \geq d_n = \delta$. Hence,

$$\mu_1^{ABC}(G) \leq \sqrt{n\left(\frac{\Delta+\delta-2}{\Delta\delta}\right)}.$$

Corollary 3.3. Let G be a graph with n vertices m edges and E_{ABC} be ABC Estrada index of G. Then,

$$E_{ABC} \geq e^K + \frac{n-1}{e^{\frac{1}{n-1}}}$$

where

$$K = \sqrt{n\left(\frac{\Delta+\delta-2}{\Delta\delta}\right)}.$$

Proof. Using the Arithmetic-Geometric Mean Inequality,

$$E_{ABC} = \sum_{j=1}^{n} e^{\mu_j^{ABC}}$$

$$\geq e^{\mu_1^{ABC}} + (n-1)\left(\prod_{j=2}^{n} e^{\mu_j^{ABC}}\right)^{\frac{1}{n-1}}$$

$$= e^{\mu_1^{ABC}} + \frac{n-1}{e^{\frac{1}{n-1}}}.$$

By Theorem 3.2, we get

$$E_{ABC} \geq e^K + \frac{n-1}{e^{\frac{1}{n-1}}}.$$

Lemma 3.4. Let G be a graph on n vertices and m edges. Then,

$$ABC(G) \geq \sqrt{\left(\frac{\sqrt{2}\delta\Delta}{2\Delta^2+\delta^2}\right)RZ(G)R^2(G)}.$$

Proof. Let us choose

$$a_j = d_i + d_j - 2 \text{ , } b_j = \frac{1}{d_id_j} \text{ , } N_1 = 2\Delta \text{ , } N_2 = \frac{1}{2\delta} \text{ , } n_1 = \delta \text{ , } n_2 = \frac{1}{2\Delta}.$$

By Lemma 2.3,

$$\left(\sum_{j=1}^{k}(d_i+d_j-2)^2\right)^{\frac{1}{2}}\left(\sum_{j=1}^{k}\left(\frac{1}{d_id_j}\right)^2\right)^{\frac{1}{2}} \leq \frac{1}{2}\left(\sqrt{\frac{2\Delta\frac{1}{2\delta}}{\frac{\delta}{2\Delta}}}+\sqrt{\frac{\frac{\delta}{2\Delta}}{2\Delta\frac{1}{2\delta}}}\right)\left(\sum_{j=1}^{k}(d_i+d_j-2)\left(\frac{1}{d_id_j}\right)\right).$$

So, we have that

$$\left(\left(\sum_{j=1}^{k} d_i + d_j - 2\right)^2\right)^{\frac{1}{2}} \sum_{j=1}^{k}\left(\frac{1}{\sqrt{d_i d_j}}\right)^2 \le \frac{1}{2}\left(\sqrt{\frac{2\Delta^2}{\delta^2}} + \sqrt{\frac{\delta^2}{2\Delta^2}}\right)\left(\sum_{j=1}^{k}\frac{d_i + d_j - 2}{d_i d_j}\right).$$

By the definition of the following indices,

$$((RZ(G))^2)^{\frac{1}{2}}\big(R(G)\big)^2 \le \frac{1}{2}\left(\frac{2\Delta^2 + \delta^2}{\sqrt{2}\delta\Delta}\right)\big(ABC(G)\big)^2.$$

Hence, we conclude that

$$ABC(G) \ge \sqrt{\left(\frac{\sqrt{2}\delta\Delta}{2\Delta^2 + \delta^2}\right) RZ(G)\big(R(G)\big)^2}.$$

Theorem 3.6. Let G be a regular graph with n vertices and m edges and $(\bar{G})$ be the complement of G. Then,

$$ABC(\bar{G}) \ge \sqrt{\frac{(n-2)[n(n-1)-2m] + \frac{4m^2}{n} - 2m(n-1)}{(n-1)^2\left[\frac{n(n-1)-6m}{2}\right] + 2m^2\left(1 - \frac{2m}{n^2} + \frac{2n-3}{n}\right)}}.$$

Proof. We know that

$$ABC\,(\bar{G}) = \sum_{v_i v_j \notin E(G)} \sqrt{\frac{d_{\bar{G}}(i) + d_{\bar{G}}(j) - 2}{d_{\bar{G}}(i)\cdot d_{\bar{G}}(j)}}.$$

Since $d_{\bar{G}}(i) = (n - 1 - d_i)$ then,

$$ABC\,(\bar{G}) = \sum_{v_i,v_j \notin E(G)} \sqrt{\frac{(n-1-d_i) + (n-1-d_j) - 2}{(n-1-d_i)\cdot(n-1-d_j)}}$$

$$= \sum_{v_i,v_j \notin E(G)} \sqrt{\frac{(2n-4) - (d_i + d_j)}{(n-1)^2 - (n-1)(d_i + d_j) + d_i d_j}}$$

$$\ge \sqrt{\sum_{v_i,v_j \notin E(G)} \frac{(2n-4) - (d_i + d_j)}{(n-1)^2 - (n-1)(d_i + d_j) + d_i d_j}}$$

$$\ge \sqrt{\frac{\sum_{v_i,v_j \notin E(G)}(2n-4) - (d_i + d_j)}{\sum_{v_i,v_j \notin E(G)}(n-1)^2 - (n-1)(d_i + d_j) + d_i d_j}}.$$

Since G has $\frac{n(n-1)-2m}{2}$ edges, then

$$ABC\,(\bar{G}) \ge \sqrt{\frac{(2n-4)\left[\frac{n(n-1)-2m}{2}\right] - Z_1(\bar{G})}{(n-1)^2\left[\frac{n(n-1)-2m}{2}\right] - (n-1)\cdot Z_1(\bar{G}) + Z_2(\bar{G})}}.$$

Since $Z_1(\bar{G}) = \bar{Z}_1(G)$ and $Z_2(\bar{G}) = \bar{Z}_2(G)$, then

$$ABC(\bar{G}) \geq \sqrt{\frac{(n-2)[n(n-1)-2m] - \bar{Z}_1(G)}{(n-1)^2\left[\frac{n(n-1)-2m}{2}\right] - (n-1)\cdot \bar{Z}_1(G) + \bar{Z}_2(G)}}.$$

By Lemma 2.4,

$$ABC(\bar{G}) \geq \sqrt{\frac{(n-2)[n(n-1)-2m] + \frac{4m^2}{n} - 2m(n-1)}{(n-1)^2\left[\frac{n(n-1)-2m}{2}\right] + (n-1)\cdot\left(\frac{4m^2}{n} - 2m(n-1)\right) + 2m^2\left(1 - \frac{2m}{n^2} + \frac{2n-3}{n}\right)}}.$$

Hence,

$$ABC(\bar{G}) \geq \sqrt{\frac{(n-2)[n(n-1)-2m] + \frac{4m^2}{n} - 2m(n-1)}{(n-1)^2\left[\frac{n(n-1)-6m}{2}\right] + 2m^2\left(1 - \frac{2m}{n^2} + \frac{2n-3}{n}\right)}}.$$

Theorem 3.7. Let G be a graph with n vertices and $\overline{ABC}(G)$ be ABC coindex of G. Then,

$$\overline{ABC}(G) \geq \frac{\sqrt{2}}{2}\sqrt{\frac{n^2}{\delta} - R^2(G)} - \sqrt{\frac{n}{\delta} + \frac{n}{d_i}\left(1 - \frac{2n}{\delta}\right)} - \sqrt{\left(\frac{\sqrt{2}\delta\Delta}{2\Delta^2 + \delta^2}\right) RZ(G)\big(R(G)\big)^2}\ .$$

Proof. By the sum of ABC index and ABC coindex, we have that

$$ABC(G) + \overline{ABC}(G) = \Big(\sum_{v_i v_j \in E(G)} + \sum_{v_i v_j \notin E(G)}\Big)\sqrt{\frac{d_i + d_j - 2}{d_i d_j}}$$

$$= \frac{1}{2}\left(\sum_{v_i \in V(G)}\sum_{v_j \in V(G)}\sqrt{\frac{d_i + d_j - 2}{d_i d_j}} - \sum_{v_j \in V(G)}\sqrt{\frac{d_i + d_j - 2}{d_i d_j}}\right)$$

$$\geq \frac{1}{2}\left(\sqrt{\sum_{v_i \in V(G)}\sum_{v_j \in V(G)}\frac{d_i + d_j - 2}{d_i d_j}} - \sqrt{\sum_{v_j \in V(G)}\frac{d_i + d_j - 2}{d_i d_j}}\right)$$

$$\geq \frac{1}{2}\sqrt{n\cdot\sum_{v_j \in V(G)}\frac{1}{d_j} + n\cdot\sum_{v_i \in V(G)}\frac{1}{d_i} - 2\sum_{v_i \in V(G)}\sum_{V_j \in V(G)}\frac{1}{d_i d_j}} - \sqrt{\sum_{v_j \in V(G)}\frac{1}{d_j} + \frac{n}{d_i} - \frac{2}{d_i}\sum_{v_j \in V(G)}\frac{1}{d_j}}.$$

Since δ is the minimum degree then,

$$ABC(G) + \overline{ABC}(G) \geq \frac{1}{2}\sqrt{\frac{n^2}{\delta} + \frac{n^2}{\delta} - 2R^2(G)} - \sqrt{\frac{n}{\delta} + \frac{n}{d_i} - \frac{2n}{\delta d_i}}$$

$$= \frac{1}{2}\sqrt{\frac{2n^2}{\delta} - 2R^2(G)} - \sqrt{\frac{n}{\delta} + \frac{n}{d_i}\left(1 - \frac{2n}{\delta}\right)}.$$

Hence, Lemma 3.4 says that

$$ABC(G) + \overline{ABC}(G) \geq \frac{\sqrt{2}}{2}\sqrt{\frac{n^2}{\delta} - R^2(G)} - \sqrt{\frac{n}{\delta} + \frac{n}{d_i}\left(1 - \frac{2n}{\delta}\right)}$$

$$\overline{ABC}(G) \geq \frac{\sqrt{2}}{2}\sqrt{\frac{n^2}{\delta} - R^2(G)} - \sqrt{\frac{n}{\delta} + \frac{n}{d_i}\left(1 - \frac{2n}{\delta}\right)} - \sqrt{\left(\frac{\sqrt{2}\delta\Delta}{2\Delta^2 + \delta^2}\right) RZ(G)\big(R(G)\big)^2} \; .$$

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