Relation of ABC and ABSC Index of regular graphs and its operations

Abstract

Atom-Bond Connectivity (ABC) index by Cuban mathematician Ernesto Estrada was introduced and developed for predicting chemical properties of molecular structures. It was an elaborate development from Randić's connectivity index, which aimed to capture molecular properties beyond simply branching. The atom-bond sum-connectivity (ABSC) index is a recent topological index, first introduced in 2022 by amalgamating the atom-bond connectivity (ABC) index with the sum-connectivity index (SC). In this study, we establish some results which directly gives the ABC and ABSC values of graphs obtained by some well known operations on regular graphs.

Keywords: Degree of vertex, Atom Bond Connectivity Index, Atom Bond Sum Connectivity index.
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1 Introduction

Chemical graph theory applies the conventional graph theory directly to chemical structures and help analyse a simplified yet detailed study. It provides a framework for establishing connections between molecular structures of compounds with their chemical properties through graph theoretic approaches.

Numerical values namely topological indices which are derived from molecular structure of chemicals help describe as well as predict various behaviours and chemical properties based on arrangement and connectivity of atoms and bonds within a molecule. The first Zagreb index measures degree based connectivity in a molecular graph which is given by,

$$M_1(G) = \sum_{uv \in E(G)} (d(u) + d(v))$$

Based on the above, the second Zagreb index of graph is also defined on product of degree of two adjacent vertices which is,

$$M_2(G) = \sum_{uv \in E(G)} (d(u)d(v))$$

In 1998, Estrada and his collaborators introduced a novel topological descriptor in the field of chemical graph theory, which came to be known as the atom-bond connectivity (ABC) index in [1] as,

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

The ABC index was originally introduced to investigate the stability of alkanes—a class of hydrocarbons composed solely of single bonds—and to estimate the strain energy of cycloalkanes, which are ring-shaped alkanes. These chemical properties are crucial in understanding how molecules behave and react under different conditions.

A molecular graph is a mathematical representation of a molecule, where atoms are represented as vertices (nodes) and bonds as edges (connections). In this context, the degree of a vertex refers to the number of bonds (edges) connected to an atom.

Due to its simplicity and effectiveness, the ABC index has been widely used in quantitative structure–activity relationships (QSAR) and quantitative structure–property relationships (QSPR) to predict the behavior of organic compounds without the need for experimental data.

Building upon the concept of the ABC index, Ali and his fellow researchers introduced another related topological index in [2], referred to as the atom-bond sum-connectivity (ABSC) index which is mentioned as,

$$ABSC(G) = \sum \sqrt{\frac{d_u+d_v-2}{d_u+d_v}}$$

This topological index is employed in mathematical chemistry to analyze the stability of alkanes and the strain energy in cycloalkanes. It provides a graph-theoretical representation of a molecule's structure, allowing researchers to relate it to various chemical and physical properties.

2 Relation between Atom Bond Connectivity Index of regular graphs and graph operations

Definition 2.1. *[3] The splitting graph $S'(G)$ of a graph G is obtained by adding to each vertex v a new vertex v' such that v' is adjacent to every vertex that is adjacent to $v \in V(G)$.*

Definition 2.2. *[3] The m - splitting graph $Spl_m(G)$ of a graph G is obtained by adding to each vertex $v \in V(G)$ new m vertices, say $v_1, v_2, v_3 \dots v_m$ such that $v_i, 1 \leq i \leq m$ is adjacent to each vertex that is adjacent to $v \in G$.*

Theorem 2.3. *Let $G(n,m)$ be a r-regular graph and $Spl_m(G)$ be its m - splitting graph then,*

$$ABC(Spl_m(G)) = ABC(G)\Big[\sqrt{\tfrac{rm+r-1}{(r-1)(m+1)^2}} + 2m\sqrt{\tfrac{rm+2(r-1)}{2(r-1)(m+1)}}\Big].$$

Proof. The ABC index of any graph $G(n,m)$ is defined as

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

Let $G(n,m)$ be a r-regular graph then for a non-negative integer r, the degree of every vertex $u \in V(G)$ is $d_u = r$. So, the number of edges is $m = \frac{nr}{2}$.
Thus,

$$\begin{aligned} ABC(G) &= \frac{nr}{2}\sqrt{\frac{2r-2}{r^2}} \\ &= \frac{n}{2}\sqrt{2(r-1)}. \end{aligned}$$

Now, the $m-$splitting graph of r-regular graph $G(n,m)$ has $\frac{nr}{2}$ edges having degree of both end vertices is $r(m+1)$ and rnm edges having degree of end vertices r and $r(m+1)$ respectively. So, ABC Index of m-splitting graph of G can be calculated as,

$$\begin{aligned} ABC(Spl_m(G)) &= \frac{nr}{2}\sqrt{\frac{2r(m+1)-2}{r^2(m+1)^2}} + rmn\sqrt{\frac{r+r(m+1)-2}{r^2(m+1)}} \\ &= \frac{n}{2(m+1)}\sqrt{2(r(m+1)-1)} + mn\sqrt{\frac{2r+rm-2}{(m+1)}} \\ &= \frac{n}{2(m+1)}\sqrt{2rm+2r-2)} + 2\frac{mn}{2}\sqrt{\frac{2(r-1)+rm)}{(m+1)}} \\ &= \frac{n}{2}\Big[\frac{\sqrt{2rm+2(r-1)}}{m+1} + 2m\sqrt{\frac{rm+2(r-1)}{m+1}}\Big]\sqrt{\frac{2(r-1)}{2(r-1)}} \\ &= ABC(G)\Big[\sqrt{\frac{r(m+1)-1}{(r-1)(m+1)^2}} + 2m\sqrt{\frac{rm+2(r-1)}{2(r-1)(m+1)}}\Big]. \end{aligned}$$

□

Definition 2.4. *[4] Given a graph G with vertex set $V(G)$ and edge set $E(G)$, the middle graph $M(G)$ has a vertex set $V(M(G)) = V(G) \cup E(G)$. Two vertices u and v in $V(M(G))$ are adjacent in $M(G)$ if and only if either u and v are adjacent edges in G or u is a vertex in $V(G)$ and v is an edge in $E(G)$ incident to u.*

Theorem 2.5. *Let $G(n,m)$ be a r-regular graph and $M(G)$ be its Middle graph then,*

$$ABC(M(G)) = ABC(G)\Big[\sqrt{\tfrac{3r-2}{r-1}} + \tfrac{\sqrt{(2r-1)(r-1)}}{2}\Big].$$

Proof. The ABC index of a r-regular graph $G(n,m)$ is

$$ABC(G) = \frac{n}{2}\sqrt{2(r-1)}.$$

Formation of a Middle graph of r regular graph leads to edges of two categories, where nr edges are formed between vertices of degree r and $2r$ and $\frac{nr(r-1)}{2}$ edges between vertices of degree $2r$ only.

$$\begin{aligned}
ABC(M(G)) &= \sum_{uv\in E(M(G))}\sqrt{\frac{d_u+d_v-2}{d_ud_v}}\\
&= nr\sqrt{\frac{r+2r-2}{2r^2}} + \frac{nr(r-1)}{2}\sqrt{\frac{2r+2r-2}{4r^2}}\\
&= n\sqrt{\frac{3r-2}{2}} + \frac{n(r-1)}{4}\sqrt{4r-2}\\
&= n\Big[\sqrt{\frac{3r-2}{2}} + \frac{(r-1)}{2\sqrt{2}}\sqrt{2r-1}\Big]\\
&= \frac{n}{\sqrt{2}}\Big[\sqrt{3r-2} + \frac{(r-1)}{2}\sqrt{2r-1}\Big]\\
&= n\sqrt{\frac{r-1}{2}}\Big[\sqrt{\frac{3r-2}{r-1}} + \frac{\sqrt{(2r-1)(r-1)}}{2}\Big]\\
&= ABC(G)\Big[\sqrt{\frac{3r-2}{r-1}} + \frac{\sqrt{(2r-1)(r-1)}}{2}\Big].
\end{aligned}$$

□

Definition 2.6. *The subdivision graph $S(G)$ of a graph G is the graph obtained from G by replacing each of its edges by a path of length 2, or equivalently by inserting an additional vertex into each edge of G.*

Theorem 2.7. *Let G be a r-regular graph on n vertices viz., $v_1, v_2, \ldots v_n \in V(G)$ with m edges and $S(G)$ be its graph subdivision then,*

$$ABC(S(G)) = ABC(G)\Big[\tfrac{r}{r-1}\Big].$$

Proof. As mentioned prior for a regular graph, $ABC(G) = \frac{n}{\sqrt{2}}\sqrt{r-1}$
In case of graph subdivision of a regular graph, the total number of edges are nr where

degree of end vertices of each edge is r and 2 respectively. Thus,

$$\begin{aligned} ABC(S(G)) &= \sum_{uv \in E(S(G))} \sqrt{\frac{d_u + d_v - 2}{d_u d_v}} \\ &= nr\sqrt{\frac{r+2-2}{2r}} \\ &= nr\sqrt{\frac{1}{2}} \\ &= nr\sqrt{\frac{1}{2}}\sqrt{\frac{r-1}{r-1}} \\ &= ABC(G)\Big[\frac{r}{\sqrt{r-1}}\Big]. \end{aligned}$$

□

Definition 2.8. *[5] The corona product of graphs G and H, denoted $G \circ H$, can be obtained by taking one copy of G, called the center graph, and a number of copies of H equal to the order of G. Then, each copy of H is assigned a vertex in G, and that one vertex is attached to each vertex in its corresponding H copy by an edge.*

Theorem 2.9. *Let G be a r-regular graph on n vertices and H be a s-regular graph on m vertices then,*

$$ABC(G \circ H) = \frac{ABC(G)ABC(H)}{\sqrt{(r-1)(s-1)}}\left[\frac{r}{m(r+1)}\sqrt{2(r+m-1)} + \frac{s\sqrt{2s}}{s+1} + 2\sqrt{\frac{r+m+s-1}{(r+m)(s+1)}}\right].$$

Proof. Let the graphs G and H both be r- regular then the resultant corona product $G \circ H$ also becomes r- regular. In this case, relation of ABC of index of both trivially exists. Suppose G be r-regular on n vertices and H be s-regular on m vertices then,

$$ABC(G) = \tfrac{n}{2}\sqrt{2(r-1)} \text{ and } ABC(H) = \tfrac{m}{2}\sqrt{2(s-1)}$$

The corona product of two graphs has three types of edges. $\frac{nr}{2}$ edges which are formed by vertices of degree $r+m$ within the graph G, $\frac{nms}{2}$ edges formed between vertices of degree

$s+1$ within the graph H alongwith edges formed between vertices of graph G and H.

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

$$= \frac{nr}{2}\sqrt{\frac{(r+m)+(r+m)-2}{(r+m)^2}} + \frac{nms}{2}\sqrt{\frac{(s+1)+(s+1)-2}{(s+1)^2}}$$

$$+ mn\sqrt{\frac{(r+m)+(s+1)-2}{(r+m)(s+1)}}$$

$$= \frac{nr}{2}\sqrt{\frac{2(r+m-1)}{(r+m)^2}} + \frac{nms}{2}\sqrt{\frac{2s}{(s+1)^2}} + mn\sqrt{\frac{r+m+s-1}{(r+m)(s+1)}}$$

$$= \frac{mn}{2}\left[\frac{r}{m}\sqrt{\frac{2(r+m-1)}{(r+m)^2}} + s\sqrt{\frac{2s}{(s+1)^2}} + 2\sqrt{\frac{r+m+s-1}{(r+m)(s+1)}}\right]$$

$$= \frac{ABC(G)ABC(H)}{\sqrt{(r-1)(s-1)}}\left[\frac{r}{m(r+1)}\sqrt{2(r+m-1)} + \frac{s\sqrt{2s}}{s+1} + 2\sqrt{\frac{r+m+s-1}{(r+m)(s+1)}}\right].$$

Thus, the result is justified. □

3 Relation between Atom Bond Sum Connectivity Index of regular graphs and graph operations

Theorem 3.1. *Let G be a r-regular graph on n vertices with m edges and $Spl_m(G)$ be its m - splitting graph then,*

$$ABSC(Spl_m(G)) = ABSC(G)\left[\sqrt{\tfrac{r(m+1)-1}{(r-1)(m+1)}} + 2m\sqrt{\tfrac{rm+2(r-1)}{(r-1)(m+2)}}\right].$$

Proof. Atom Bond Sum Connectivity index is given by,

$$ABSC(G) = \sum_{uv \in E(G)} \sqrt{\tfrac{d_u + d_v - 2}{d_u + d_v}}$$

For a r-regular graph G, $d_u = r$ where $u \in V(G)$.
Thus,

$$ABSC(G) = \frac{nr}{2}\sqrt{\frac{2r-2}{2r}}$$

$$= \frac{nr}{2}\sqrt{\frac{r-1}{r}}.$$

Now, for the case of an m-splitting graph $Spl_m(G)$, there are $\frac{nr}{2}$ edges which are formed by the vertices of degree $r(m+1)$ and rmn edges formed by edges having degree r and $r(m+1)$ respectively.

$$\begin{aligned}
ABSC(Spl_m(G)) &= \sum_{uv\in E(Spl_m(G))} \sqrt{\frac{d_u+d_v-2}{d_u+d_v}} \\
&= \frac{nr}{2}\sqrt{\frac{2r(m+1)-2}{2r(m+1)}} + rmn\sqrt{\frac{r+r(m+1)-2}{r+r(m+1)}} \\
&= \frac{nr}{2}\sqrt{\frac{r(m+1)-1}{r(m+1)}} + rmn\sqrt{\frac{rm+2(r-1)}{r+r(m+1)}} \\
&= \frac{nr}{2}\left[\sqrt{\frac{r(m+1)-1}{r(m+1)}} + 2m\sqrt{\frac{rm+2(r-1)}{r+r(m+1)}}\right] \\
&= \frac{nr}{2}\sqrt{\frac{r-1}{r}}\left[\sqrt{\frac{r(m+1)-1}{(r-1)(m+1)}} + 2m\sqrt{\frac{rm+2(r-1)}{(m+2)(r-1)}}\right] \\
&= ABSC(G)\left[\sqrt{\frac{r(m+1)-1}{(r-1)(m+1)}} + 2m\sqrt{\frac{rm+2(r-1)}{(r-1)(m+2)}}\right].
\end{aligned}$$

□

Theorem 3.2. *Let G be a r-regular graph on n vertices with m edges and $M(G)$ be its Middle graph then,*

$$ABSC(M(G)) = ABSC(G)\left[2\sqrt{\frac{3r-2}{3(r-1)}} + \frac{\sqrt{(2r-1)(r-1)}}{2}\right].$$

Proof. $ABSC(M(G)) = \sum_{uv\in E(M(G))} \sqrt{\frac{d_u+d_v-2}{d_u+d_v}}$

For a r-regular graph, $d_u = r$ where $u \in V(G)$. However, for the graph $M(G)$, there are nr edges having degree of end vertices r and $2r$ alongwith $\frac{nr(r-1)}{2}$ edges with degree of end vertices as $2r$ each. Thus,

$$\begin{aligned}
ABSC(M(G)) &= nr\sqrt{\frac{r+2r-2}{3r}} + \frac{nr(r-1)}{2}\sqrt{\frac{2r+2r-2}{4r}} \\
&= nr\sqrt{\frac{3r-2}{3r}} + \frac{nr(r-1)}{2}\sqrt{\frac{2r-1}{2r}} \\
&= \frac{nr}{2}\sqrt{\frac{r-1}{r}}\left[2\sqrt{\frac{3r-2}{3(r-1)}} + \sqrt{\frac{(2r-1)(r-1)}{2}}\right] \\
&= ABSC(G)\left[2\sqrt{\frac{3r-2}{3(r-1)}} + \frac{\sqrt{(2r-1)(r-1)}}{2}\right].
\end{aligned}$$

□

Theorem 3.3. *For a r-regular graph G on n vertices with m edges and its subdivision graph $S(G)$,*

$$ABSC(S(G)) = ABSC(G)\left[\frac{r}{\sqrt{(r+2)(r-1)}}\right]$$

Proof. For a Subdivision graph $S(G)$, the Atom Bond Sum Connectivity index can be evaluated as,

$$\begin{aligned}
ABSC(S(G)) &= \sum_{uv\in E(S(G))} \sqrt{\frac{d_u + d_v - 2}{d_u + d_v}} \\
&= nr\sqrt{\frac{r}{r+2}} \\
&= \frac{nr}{2}\sqrt{\frac{r}{r+2}}\frac{2\sqrt{r(r-1)}}{\sqrt{r(r-1)}} \\
&= \frac{nr}{2}\sqrt{\frac{r-1}{r}}\sqrt{\frac{r^2}{(r+2)(r-1)}} \\
&= ABSC(G)\left[\frac{r}{\sqrt{(r+2)(r-1)}}\right].
\end{aligned}$$

□

Theorem 3.4. *Lets G be a r-regular graph on n vertices and H be a s-regular graph on m vertices then,*

$$ABSC(G \circ H) = ABSC(G)\cdot ABSC(H)\sqrt{\frac{rs}{(r-1)(s-1)}}\left[\frac{1}{ms}\sqrt{\frac{r+m-1}{r+m}} + \frac{1}{r}\sqrt{\frac{s}{s+1}} + \frac{2}{rs}\sqrt{\frac{r+m+s-1}{r+m+s+1}}\right].$$

Proof. If both G and H are r-regular, then the resultant $G \circ H$ will also be r-regular, for which the result already exists. Thus for both the regular graphs, we take different degrees for corresponding vertices.

$$ABSC(G) = \frac{nr}{2}\sqrt{\frac{r-1}{r}}, ABSC(H) = \frac{ms}{2}\sqrt{\frac{s-1}{s}}$$

$$
\begin{aligned}
ABSC(G \circ H) &= \sum_{uv \in E((G \circ H)} \sqrt{\frac{d_u + d_v - 2}{d_u + d_v}} \\
&= \frac{nr}{2}\sqrt{\frac{2(r+m)-2}{2(r+m)}} + \frac{nms}{2}\sqrt{\frac{2(s+1)-2}{2(s+1)}} + mn\sqrt{\frac{(r+m)(s+1)-2}{r+m+s+1}} \\
&= \frac{nr}{2}\sqrt{\frac{r+m-1}{r+m}} + \frac{nms}{2}\sqrt{\frac{s}{s+1}} + mn\sqrt{\frac{r+m+s-1}{r+m+s+1}} \\
&= \frac{mnrs}{2}\left[\frac{1}{ms}\sqrt{\frac{r+m-1}{r+m}} + \frac{1}{r}\sqrt{\frac{s}{s+1}} + \frac{2}{rs}\sqrt{\frac{r+m+s-1}{r+m+s+1}}\right]
\end{aligned}
$$

Multiplying and dividing the factor $\sqrt{\frac{(r-1)(s-1)}{rs}}$ in the above equation,

$$
\begin{aligned}
ABSC(G \circ H) = ABSC(G) \cdot ABSC(H)\sqrt{\frac{rs}{(r-1)(s-1)}} \\
\cdot \left[\frac{1}{ms}\sqrt{\frac{r+m-1}{r+m}} + \frac{1}{r}\sqrt{\frac{s}{s+1}} + \frac{2}{rs}\sqrt{\frac{r+m+s-1}{r+m+s+1}}\right].
\end{aligned}
$$

□

4 Conclusion

In this paper, we explored the Atom-Bond Connectivity (ABC) index and the recently introduced Atom-Bond Sum-Connectivity (ABSC) index in the context of regular graphs. By applying well-known graph operations, we derived explicit results that allow direct computation of ABC and ABSC indices for the resulting graphs. Future work may focus on extending these results to irregular graphs or investigating correlations with additional molecular descriptors.

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