Iranian J. Math. Chem. 8 (1) (2017) 61−70

Iranian Journal of Mathematical Chemistry

Journal homepage: www.ijmc.kashanu.ac.ir

Splice Graphs and Their Vertex–Degree–Based Invariants

MAHDIEH AZARI[1,•] AND FARZANEH FALAHATI-NEZHAD[2]

[1]Department of Mathematics, Kazerun Branch, Islamic Azad University, P. O. Box: 73135−168, Kazerun, Iran
[2]Department of Mathematics, Safadasht Branch, Islamic Azad University, Tehran, Iran

ARTICLE INFO

Article History:

Received 20 July 2015
Accepted 21 September 2015
Published online : 1 February 2017
Academic Editor: Tomislav Došlić

Keywords:

Vertex degree
Graph invariant
Splice

ABSTRACT

Let G_1 and G_2 be simple connected graphs with disjoint vertex sets $V(G_1)$ and $V(G_2)$, respectively. For given vertices $a_1 \in V(G_1)$ and $a_2 \in V(G_2)$, a splice of G_1 and G_2 by vertices a_1 and a_2 is defined by identifying the vertices a_1 and a_2 in the union of G_1 and G_2. In this paper, we present exact formulas for computing some vertex-degree-based graph invariants of splice of graphs.

1. INTRODUCTION

Let G be a simple connected graph with vertex set $V(G)$ and edge set $E(G)$. For a vertex $u \in V(G)$, we denote by $N_G(u)$ the set of all first neighbors of u in G. The cardinality of $N_G(u)$ is called the *degree* of u in G and denoted by $d_G(u)$. A *graph invariant* (also known as *topological index* or *structural descriptor*) is any function on a graph that does not depend on a labeling of its vertices. Several hundreds of different invariants have been employed to date with various degrees of success in QSAR/QSPR studies. We refer the reader to [1−3] for review.

In 1975, Milan Randić [4] proposed a structural descriptor, based on the end-vertex degrees of edges in a graph, called the *branching index* that later became the well-known *Randić connectivity index*. The Randić index of a graph G is denoted by $R(G)$ and defined as

•Corresponding Author: (Email address: azari@kau.ac.ir)
DOI: 10.22052/ijmc.2017.42671.

$$R(G)=\sum_{uv\in E(G)}\frac{1}{\sqrt{d_G(u)d_G(v)}}.$$

The Randić index is one of the most successful molecular descriptors in QSPR and QSAR studies, suitable for measuring the extent of branching of the carbon-atom skeleton of saturated hydrocarbons.

A closely related variant of the Randić connectivity index called the *sum-connectivity index* was proposed by Zhou and Trinajstić [5] in 2009. The sum-connectivity index $\chi(G)$ of a graph G is defined as

$$\chi(G)=\sum_{uv\in E(G)}\frac{1}{\sqrt{d_G(u)+d_G(v)}}.$$

The sum-connectivity index has been found to correlate well with π-electronic energy of benzenoid hydrocarbons.

Another variant of the Randić connectivity index named the *harmonic index* was introduced by Fajtlowicz [6] in 1987. The harmonic index of a graph G is denoted by $H(G)$ and defined as

$$H(G)=\sum_{uv\in E(G)}\frac{2}{d_G(u)+d_G(v)}.$$

In 1998, Estrada et al. [7] introduced another vertex-degree-based descriptor called the *atom-bond connectivity index*. The atom-bond connectivity index of a graph G is denoted by $ABC(G)$ and defined as

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

This index has been proved to be a valuable predictive index in the study of the formation heat in alkanes and it provides a good model for the stability of linear and branched alkanes as well as the strain energy of cycloalkanes [7, 8].

Motivated by the success of the atom-bond connectivity index, Furtula et al. [9] put forward its modified version, that they somewhat inadequately named it *augmented Zagreb index*. The augmented Zagreb index of a graph G is denoted by $AZI(G)$ and defined as

$$AZI(G)=\sum_{uv\in E(G)}\left(\frac{d_G(u)d_G(v)}{d_G(u)+d_G(v)-2}\right)^3.$$

Preliminary studies [9] indicate that *AZI* index has an even better correlation potential than *ABC* index.

Motivated by definition of the Randić connectivity index, Vukičević and Furtula [10] proposed another vertex-degree-based topological index, named the *geometric-arithmetic index*. The geometric-arithmetic index of a graph G is denoted by $GA(G)$ and defined as

$$GA(G) = \Sigma_{uv\in E(G)} \frac{\sqrt{d_G(u)d_G(v)}}{(d_G(u)+d_G(v))/2} = \Sigma_{uv\in E(G)} \frac{2\sqrt{d_G(u)d_G(v)}}{d_G(u)+d_G(v)}.$$

It has been proved that [10], for physico-chemical properties such as boiling point, entropy, enthalpy of vaporization, standard enthalpy of vaporization, enthalpy of formation and acentric factor, the predictive power of *GA* index is somewhat better than the predictive power of the Randić connectivity index.

Recently, Deng et al. [11] proposed a general mathematical formulation for vertex-degree-based invariants which is defined for a graph G as

$$TI(G) = \Sigma_{uv\in E(G)} F(d_G(u), d_G(v)),$$

where $F(x, y)$ is an appropriately chosen function.

For an arbitrary vertex u of G, we define

$$TI_G(u) = \Sigma_{v\in N_G(u)} F(d_G(u), d_G(v)).$$

In particular,

$F(x, y) = \frac{1}{\sqrt{xy}}$ for the Randić index,

$F(x, y) = \frac{1}{\sqrt{x+y}}$ for the sum-connectivity index,

$F(x, y) = \frac{2}{x+y}$ for the harmonic index,

$F(x, y) = \sqrt{\frac{x+y-2}{xy}}$ for the atom-bond connectivity index,

$F(x, y) = \left(\frac{xy}{x+y-2}\right)^3$ for the augmented Zagreb index, and

$F(x,y)=\frac{2\sqrt{xy}}{x+y}$ for the geometric-arithmetic index.

In this paper, we present an exact formula for computing the general vertex-degree-based invariant of splice of graphs. Using this result, the Randić connectivity index, sum–connectivity index, harmonic index, atom-bond connectivity index, augmented Zagreb index, and geometric–arithmetic index of splice of graphs are computed. Readers interested in more information on computing topological indices of splice of graphs can be referred to [12−22].

2. RESULTS AND DISCUSSION

Let G_1 and G_2 be simple connected graphs with disjoint vertex sets $V(G_1)$ and $V(G_2)$, and edge sets $E(G_1)$ and $E(G_2)$, respectively, and let $a_1 \in V(G_1)$ and $a_2 \in V(G_2)$. Following Došlić [21], a *splice* or *coalescence* of G_1 and G_2 by vertices a_1 and a_2 is denoted by $(G_1 \bullet G_2)(a_1,a_2)$ and defined by identifying the vertices a_1 and a_2 in the union of G_1 and G_2 as shown in Fig. 1. For notational convenience, we denote by n_i, e_i, and δ_i the order of G_i, the size of G_i, and the degree of the vertex a_i in G_i, respectively, where $i \in \{1,2\}$. It is easy to see that, $|V((G_1 \bullet G_2)(a_1,a_2))| = n_1+n_2-1$ and $|E((G_1 \bullet G_2)(a_1,a_2))| = e_1+e_2$.

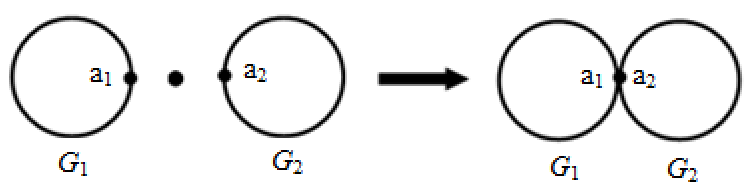

Figure 1. *A splice of* G*1 and* G*2 by vertices a1 and a2.*

In the following lemma, the degree of an arbitrary vertex of the splice of two graphs is computed. The result follows easily from the definition of the splice of graphs, so the proof is omitted.

Lemma 2.1 Let $G=(G_1 \bullet G_2)(a_1,a_2)$. For every vertex $u \in V(G)$,

$$d_G(u)=\begin{cases} d_{G_1}(u) & u\in V(G_1)-\{a_1\},\\ d_{G_2}(u) & u\in V(G_2)-\{a_2\},\\ \delta_1+\delta_2 & u=a_1 \ \ or\ \ u=a_2.\end{cases}$$

In the following theorem, the general vertex-degree-based invariant of the splice of two graphs is computed.

Theorem 2.2 The general vertex-degree-based invariant of $G=(G_1\bullet G_2)(a_1,a_2)$ is given by

$$\begin{aligned} TI(G) \ &= TI(G_1)+TI(G_2)-TI_{G_1}(a_1)-TI_{G_2}(a_2)\\ &+\textstyle\sum_{v\in N_{G_1}(a_1)}F(\delta_1+\delta_2,d_{G_1}(v))\\ &+\textstyle\sum_{v\in N_{G_2}(a_2)}F(\delta_1+\delta_2,d_{G_2}(v)). \end{aligned} \tag{1}$$

Proof. By definition of the general vertex-degree-based invariant and Lemma 2.1,

$$\begin{aligned} TI(G) \ &= \textstyle\sum_{uv\in E(G)}F(d_G(u),d_G(v))\\ &= \textstyle\sum_{uv\in E(G_1);u,v\neq a_1}F(d_{G_1}(u),d_{G_1}(v))\\ &+\textstyle\sum_{uv\in E(G_2);u,v\neq a_2}F(d_{G_2}(u),d_{G_2}(v))\\ &+\textstyle\sum_{v\in N_{G_1}(a_1)}F(\delta_1+\delta_2,d_{G_1}(v))\\ &+\textstyle\sum_{v\in N_{G_2}(a_2)}F(\delta_1+\delta_2,d_{G_2}(v)). \end{aligned}$$

Now, using the fact that

$$\sum_{uv\in E(G_i);u,v\neq a_i}F(d_{G_i}(u),d_{G_i}(v))=TI(G_i)-TI_{G_i}(a_i), \qquad i\in\{1,2\},$$

we can get Eq. (1). ■

Using Eq. (1), one can easily compute the Randić connectivity index, sum–connectivity index, harmonic index, atom–bond connectivity index, augmented Zagreb index, geometric–arithmetic index, and some other vertex-degree-based invariants of splice of two graphs.

By setting $F(x,y)=\dfrac{1}{\sqrt{xy}}$ in Eq. (1), we easily arrive at:

Corollary 2.3 The Randić connectivity index of $G=(G_1\bullet G_2)(a_1,a_2)$ is given by

$$\begin{aligned} R(G) &= R(G_1)+R(G_2)-R_{G_1}(a_1)-R_{G_2}(a_2) \\ &+\frac{1}{\sqrt{\delta_1+\delta_2}}\left(\sum_{v\in N_{G_1}(a_1)}\frac{1}{\sqrt{d_{G_1}(v)}}+\sum_{v\in N_{G_2}(a_2)}\frac{1}{\sqrt{d_{G_2}(v)}}\right). \end{aligned}$$

As a direct consequence of Corollary 2.3, we obtain the following Corollary.

Corollary 2.4 Let G_1 be r_1–regular and G_2 be r_2–regular. The Randić connectivity index of $G=(G_1\bullet G_2)(a_1,a_2)$ is given by

$$R(G)=\frac{e_1}{r_1}+\frac{e_2}{r_2}+\frac{\sqrt{r_1}+\sqrt{r_2}}{\sqrt{r_1+r_2}}-2.$$

By setting $F(x,y)=\frac{1}{\sqrt{x+y}}$ in Eq. (1), we easily arrive at:

Corollary 2.5 The sum–connectivity index of $G=(G_1\bullet G_2)(a_1,a_2)$ is given by

$$\begin{aligned} \chi(G) &= \chi(G_1)+\chi(G_2)-\chi_{G_1}(a_1)-\chi_{G_2}(a_2) \\ &+\sum\nolimits_{v\in N_{G_1}(a_1)}\frac{1}{\sqrt{\delta_1+\delta_2+d_{G_1}(v)}} \\ &+\sum\nolimits_{v\in N_{G_2}(a_2)}\frac{1}{\sqrt{\delta_1+\delta_2+d_{G_2}(v)}}. \end{aligned}$$

As a direct consequence of Corollary 2.5, we obtain the following Corollary.

Corollary 2.6 Let G_1 be r_1–regular and G_2 be r_2–regular. The sum–connectivity index of $G=(G_1\bullet G_2)(a_1,a_2)$ is given by

$$\chi(G)=\frac{e_1-r_1}{\sqrt{2r_1}}+\frac{e_2-r_2}{\sqrt{2r_2}}+\frac{r_1}{\sqrt{2r_1+r_2}}+\frac{r_2}{\sqrt{2r_2+r_1}}.$$

By setting $F(x,y)=\frac{2}{x+y}$ in Eq. (1), we easily arrive at:

Corollary 2.7 The harmonic index of $G=(G_1\bullet G_2)(a_1,a_2)$ is given by

$$\begin{aligned} H(G) &= H(G_1) + H(G_2) - H_{G_1}(a_1) - H_{G_2}(a_2) \\ &+ \Sigma_{v \in N_{G_1}(a_1)} \frac{2}{\delta_1 + \delta_2 + d_{G_1}(v)} \\ &+ \Sigma_{v \in N_{G_2}(a_2)} \frac{2}{\delta_1 + \delta_2 + d_{G_2}(v)}. \end{aligned}$$

As a direct consequence of Corollary 2.7, we obtain the following Corollary.

Corollary 2.8 Let G_1 be r_1–regular and G_2 be r_2–regular. The harmonic index of $G = (G_1 \bullet G_2)(a_1, a_2)$ is given by

$$H(G) = \frac{e_1}{r_1} + \frac{e_2}{r_2} - \frac{r_1}{2r_2 + r_1} - \frac{r_2}{2r_1 + r_2}.$$

By setting $F(x, y) = \sqrt{\frac{x + y - 2}{xy}}$ in Eq. (1), we easily arrive at:

Corollary 2.9 The atom bond connectivity index of $G = (G_1 \bullet G_2)(a_1, a_2)$ is given by

$$\begin{aligned} ABC(G) &= ABC(G_1) + ABC(G_2) - ABC_{G_1}(a_1) - ABC_{G_2}(a_2) \\ &+ \frac{1}{\sqrt{\delta_1 + \delta_2}} \left(\Sigma_{v \in N_{G_1}(a_1)} \sqrt{\frac{\delta_1 + \delta_2 + d_{G_1}(v) - 2}{d_{G_1}(v)}} + \Sigma_{v \in N_{G_2}(a_2)} \sqrt{\frac{\delta_1 + \delta_2 + d_{G_2}(v) - 2}{d_{G_2}(v)}} \right). \end{aligned}$$

As a direct consequence of Corollary 2.9, we obtain the following Corollary.

Corollary 2.10 Let G_1 be r_1–regular and G_2 be r_2–regular. The atom bond connectivity index of $G = (G_1 \bullet G_2)(a_1, a_2)$ is given by

$$ABC(G) = \sqrt{2(r_1 - 1)}(\frac{e_1}{r_1} - 1) + \sqrt{2(r_2 - 1)}(\frac{e_2}{r_2} - 1) + \frac{\sqrt{r_1(2r_1 + r_2 - 2)} + \sqrt{r_2(2r_2 + r_1 - 2)}}{\sqrt{r_1 + r_2}}.$$

By setting $F(x, y) = \left(\frac{xy}{x + y - 2} \right)^3$ in Eq. (1), we easily arrive at:

Corollary 2.11 The augmented Zagreb index of $G = (G_1 \bullet G_2)(a_1, a_2)$ is given by

$$\begin{aligned} AZI(G) &= AZI(G_1) + AZI(G_2) - AZI_{G_1}(a_1) - AZI_{G_2}(a_2) \\ &+ (\delta_1+\delta_2)^3 \left(\Sigma_{v\in N_{G_1}(a_1)} \left(\frac{d_{G_1}(v)}{\delta_1+\delta_2+d_{G_1}(v)-2} \right)^3 + \Sigma_{v\in N_{G_2}(a_2)} \left(\frac{d_{G_2}(v)}{\delta_1+\delta_2+d_{G_2}(v)-2} \right)^3 \right). \end{aligned}$$

As a direct consequence of Corollary 2.11, we obtain the following Corollary.

Corollary 2.12 Let G_1 be r_1–regular and G_2 be r_2–regular. The augmented Zagreb index of $G = (G_1 \bullet G_2)(a_1, a_2)$ is given by

$$AZI(G) = \frac{r_1^6(e_1 - r_1)}{8(r_1-1)^3} + \frac{r_2^6(e_2 - r_2)}{8(r_2-1)^3} + (r_1+r_2)^3 \left(\frac{r_1^4}{(2r_1+r_2-2)^3} + \frac{r_2^4}{(2r_2+r_1-2)^3} \right).$$

By setting $F(x,y) = \frac{2\sqrt{xy}}{x+y}$ in Eq. (1), we easily arrive at:

Corollary 2.13 The geometric–arithmetic index of $G = (G_1 \bullet G_2)(a_1, a_2)$ is given by

$$\begin{aligned} GA(G) &= GA(G_1) + GA(G_2) - GA_{G_1}(a_1) - GA_{G_2}(a_2) \\ &+ 2\sqrt{\delta_1+\delta_2} \left(\Sigma_{v\in N_{G_1}(a_1)} \frac{\sqrt{d_{G_1}(v)}}{\delta_1+\delta_2+d_{G_1}(v)} + \Sigma_{v\in N_{G_2}(a_2)} \frac{\sqrt{d_{G_2}(v)}}{\delta_1+\delta_2+d_{G_2}(v)} \right). \end{aligned}$$

As a direct consequence of Corollary 2.13, we obtain the following corollary.

Corollary 2.14 Let G_1 be r_1–regular and G_2 be r_2–regular. The geometric-arithmetic index of $G = (G_1 \bullet G_2)(a_1, a_2)$ is given by

$$GA(G) = e_1 + e_2 - r_1 - r_2 + 2\sqrt{r_1+r_2} \left(\frac{r_1\sqrt{r_1}}{2r_1+r_2} + \frac{r_2\sqrt{r_2}}{2r_2+r_1} \right).$$

ACKNOWLEDGMENT. The authors would like to thank the referee for his/her insightful comments and valuable suggestions.

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