Kuwait J. Sci. **46 (4)** pp. 14-22, 2019

On the inverse degree index and decompositions in graphs

Jesús Romero-Valencia*, Juan C. Hernández-Gómez, Gerardo Reyna-Hernández
Facultad de Matemáticas, Universidad Autónoma de Guerrero, Chilpancingo, Gro. 39087, México.
Corresponding author: jromv@yahoo.com

Abstract

The inverse degree index of a graph $G = (V,E)$ without isolated vertices is defined as $\mathrm{ID}(G) = \sum_{v \in V} \frac{1}{dv}$, where dv is the degree of the vertex v in G. In this paper, we show a relation between the inverse degree of a graph and the inverse degree indices of the primary subgraphs obtained by a general decomposition of G, we establish some relations between the inverse degree index and other known indices and an application to a specific chemical structure is given.

Keywords: Decomposition; inverse degree index; polyethylene graph; topological indices.

1. Introduction

The study of topological indices becomes increasingly important due to the information they provide about the chemical structure of molecules in terms of graph theory. Topological indices condense information of some properties of a molecule into a real number that is computed from the representative graph of the molecule, through parameters of vertices, edges or matrices associated to the graph (the adjacency matrix $\mathbf{A}(G)$, the distance matrix $\mathbf{D}(G)$ or the incidence matrix $\mathbf{T}(G)$). A graph invariant is a graph-theoretic property which is preserved under isomorphisms (Harary 1969; Read & Corneil 1977), and topological indices are precise examples of graph invariants. Some molecules, such as alkanes, can be seen as graphs in which the atoms are represented by vertices and the covalent chemicals bonds by the edges of a simple graph. The later are called molecular graphs in mathematical chemistry. In this way, graphs are models of the spacial structure of a molecule and the molecular topology (the pattern of connectedness of atoms).

Topological indices have been studied in order to improve the understanding of the chemical structures of molecules. Gutman (2013) investigated some familiar topological indices. Xu *et al.* (2014) researched the first and second Zagreb indices and coindices of connected graphs. In addition, the authors gave closed formulae for the Zagreb coindices as functions of Zagreb indices and their orders and sizes. Other authors have established bounds for topological indices. Elumalai *et al.* (2018), for example, obtained several lower and upper bounds for inverse degree and compared it to other topological indices.

Researchers are interested in the study of two-dimensional structures formed by atoms because they make up carbon nanotubes, structures formed by sheets of graphite with the thickness of an atom. Nanotube technology is in its infancy but is a promising field because of increasing applications. These include but are not limited to, electronics and batteries, medical applications, purification and oil cleanup. This research presents grid and cylinder results that may represent nanotube structures

One of the best known indices is the Randić connectivity index R (Randić 1975). Several papers on this index include those by Gutman & Furtula (2008); Li & Gutman (2006); Rodríguez & Sigarreta (2005); Gutman (2013). Since its introduction, there have been many efforts to improve this index, and other chemical and mathematical indices have been proposed. The Randić index is defined as

$$\mathrm{R}(G) = \sum_{uv\in E} \frac{1}{\sqrt{du\,dv}},$$

where du and dv denote the degrees of vertices u and v, respectively.

The inverse degree index of G, denoted by $\mathrm{ID}(G)$ is defined by the following formula

$$\mathrm{ID}(G) = \sum_{u\in V} \frac{1}{du}, \tag{1}$$

but it can be equivalently defined in terms of edges as follows

$$\mathrm{ID}(G) = \sum_{uv\in E} \frac{du^2+dv^2}{du^2\,dv^2}. \tag{2}$$

Formula (1), is called the *vertex-definition* for the inverse degree and (2) the *edge-definition*.

The *general forgotten index* $\mathrm{F}_\alpha(G)$ is defined by

$$\mathrm{F}_\alpha(G) = \sum_{u\in V} du^\alpha.$$

Note that $\mathrm{ID}(G)$ is a particular case (with $\alpha = -1$) of the *general forgotten index*.

Throughout this paper, our graphs $G=(V,E)$ are non-oriented, finite, simple (without multiple edges or loops) and connected, we consider that a graph $G'=(V',E')$ is a subgraph of $G=(V,E)$ if $V'\subset V$ and $E'\subset E$. For $v\in V$, dv denotes its degree, $N(v)$ is its set of neighbors, that is,

$$N(v) = \{u \in V \,:\, uv \in E\}$$

and $N_{G'}(v)$ is its set of neighbors in G'

$$N_{G'}(v) = \{u \in V' \,:\, uv \in E'\}.$$

For a graph G, n is its order ($|V|$), m its size ($|E|$), and δ and Δ are its minimum and maximum degrees, respectively.

2. Examples of computing the inverse degree index of some families of graphs

Now we use the edge-definition for computing the inverse degree index for some known graph families. To make easier our computations, we use the following identity for any real numbers a,b:

$$\frac{a^2+b^2}{a^2b^2} = \frac{1}{a^2} + \frac{1}{b^2}.$$

Proposition 2.1. *The inverse degree indices of the following graphs are*

i. *If P_n is the path graph of order n ($m=n-1$), then* $\mathrm{ID}(P_n) = \frac{n+2}{2} = \frac{m+3}{2}$,

ii. *if G is a $k-$regular graph ($2m = kn$), then* $\mathrm{ID}(G) = \frac{n}{k} = \frac{2m}{k^2}$,

iii. *if S_n is the star graph of order $n+1$ ($m=n$),* $\mathrm{ID}(S_n) = \frac{n^2+1}{n} = \frac{m^2+1}{m}$,

iv. *for the wheel graph W_n of order $n+1$ ($m = 2n$),* $\mathrm{ID}(W_n) = \frac{n^2+3}{3n} = \frac{m^2+6}{3m}$,

v. *for the grid graph $G_{r,s} = P_r \times P_s$ ($m = 2rs - r - s$),* $\mathrm{ID}(G_{r,s}) = \frac{3rs+2(r+s)+4}{12}$,

vi. *for the cylinder graph $C_{r,s} = C_r \times P_s$ ($m = r(2s-1)$),* $\mathrm{ID}(C_{r,s}) = \frac{r(3s+2)}{12}$.

Proof. Every proof is elementary, we show only three cases, the others are analogous.

For P_n, note that there are two edges whose endpoint vertices have degree 1 and 2 and $m-2$ edges with endpoints of degree 2. Thus

$$\mathrm{ID}(P_n) = \sum_{uv\in E}\left(\frac{1}{du^2} + \frac{1}{dv^2}\right)$$

$$= (2)\frac{5}{4} + (m-2)\frac{1}{2} = \frac{m+3}{2}.$$

If G is $k-$regular, every vertex of G has degree k. Hence

$$\mathrm{ID}(G) = \sum_{uv\in E}\left(\frac{1}{du^2} + \frac{1}{dv^2}\right)$$
$$= \sum_{uv\in E}(2)\frac{2}{k^2} = \frac{2m}{k^2}.$$

The grid graph $G_{r,s}$ has four kinds of edges uv: eight of degrees 2 and 3 (on the corners), $2(r-3)+2(s-3)$ of degrees 3 and 3 (on the borders), $2(r-2)+2(s-2)$ of degrees 3 and 4 (exactly one endpoint on the border), and $(r-3)(s-2)+(r-2)(s-3)$ edges of degrees 4 and 4. Thus

$$\begin{aligned}\mathrm{ID}(G) &= \sum_{uv\in E}\left(\frac{1}{du^2}+\frac{1}{dv^2}\right)\\ &= 8\left(\frac{1}{4}+\frac{1}{9}\right)+2(r+s-3)\left(\frac{1}{9}+\frac{1}{9}\right)\\ &\quad +2(r+s-4)\left(\frac{1}{9}+\frac{1}{16}\right)\\ &\quad +\big(2(rs+6)-5(r+s)\big)\left(\frac{1}{16}+\frac{1}{16}\right)\\ &= \frac{3rs+2(r+s)+4}{12}.\end{aligned}$$

□

3. The inverse degree index and its relation with other indices

In this section we give some relations between the inverse degree index and other indices.

3.1 The inverse degree and Randić indices

The Randić index (Randić, 1975) has proved to be the most prominent of all topological indices as it is vital in applications for modeling the chemical properties of organic molecules. Recall that for a graph G without isolated vertices, the Randić index is defined as

$$\mathrm{R}(G) = \sum_{uv\in E}\frac{1}{\sqrt{du\,dv}}.$$

There is a generalization to the last expression

$$\mathrm{R}_\lambda(G) = \sum_{uv\in E}(du\,dv)^\lambda,$$

which is known as the generalized Randić index (Gutman 2013). Note that $\mathrm{R}(G) = \mathrm{R}_{-1/2}(G)$.

To compare the inverse degree and Randić indices, the following elementary lemma will be useful.

Lemma 3.1. *Let a,b,l and L be positive real numbers such that $1\le l\le a,b\le L$. Then*

$$2\sqrt{\frac{l}{L^3ab}}\le\frac{a^2+b^2}{a^2b^2}\le 2\sqrt{\frac{L}{l^3ab}},$$

and the equality in each bound is attained if and only if $l=a=b=L$.

Proposition 3.2. *Let G be a graph without isolated vertices. Then*

$$2\sqrt{\frac{\delta}{\Delta^3}}\,\mathrm{R}(G)\le\mathrm{ID}(G)\le 2\sqrt{\frac{\Delta}{\delta^3}}\,\mathrm{R}(G).$$

The equalities in each bound are attained if and only if G is regular.

Proof. Since $\delta\le du,dv\le\Delta$, the above relations imply

$$2\sqrt{\frac{\delta}{\Delta^3du\,dv}}\le\frac{du^2+dv^2}{du^2\,dv^2}\le 2\sqrt{\frac{\Delta}{\delta^3du\,dv}}.$$

Summing over all edges of G, we obtain

$$\begin{aligned}2\sqrt{\frac{\delta}{\Delta^3}}\sum_{uv\in E}\frac{1}{\sqrt{du\,dv}} &\le \sum_{uv\in E}\frac{du^2+dv^2}{du^2\,dv^2}\\ &\le 2\sqrt{\frac{\Delta}{\delta^3}}\sum_{uv\in E}\frac{1}{\sqrt{du\,dv}},\end{aligned}$$

so we get

$$2\sqrt{\frac{\delta}{\Delta^3}}\,\mathrm{R}(G)\le\mathrm{ID}(G)\le 2\sqrt{\frac{\Delta^2}{\delta^3}}\,\mathrm{R}(G).$$

The equalities are attained in each bound if and only if G is regular. □

3.2 The inverse degree and harmonic indices

Insofar as we know, the harmonic index appeared for the first time in S. Fajtlowicz (1987) as a variant of the Randić index. Since its introduction several papers have presented min and max values for it. The *Harmonic index of G* is defined as

$$\mathrm{H}(G) = \sum_{uv\in E}\frac{1}{du+dv}.$$

Proposition 3.3. *Let G be a graph. Then*

$$\mathrm{H}(G)+\frac{m(4\delta-\Delta^2)}{2\delta\Delta^2}\le\mathrm{ID}(G)\le\mathrm{H}(G)+\frac{m(4\Delta-\delta^2)}{2\delta^2\Delta}.$$

The equalities are attained in each inequality if and only if G is regular.

Proof. Since $\delta \le du, dv \le \Delta$, we have

$$\frac{du^2+dv^2}{du^2\,dv^2} \le \frac{2}{\delta^2} \quad \text{and} \quad -\frac{1}{du+dv} \le -\frac{1}{2\Delta}.$$

Thus,

$$\mathrm{ID}(G) \le \frac{2m}{\delta^2} \quad \text{and} \quad -\mathrm{H}(G) \le -\frac{m}{2\Delta}$$

obtaining

$$\mathrm{ID}(G) \le \mathrm{H}(G) + \frac{m(4\Delta-\delta^2)}{2\delta^2\Delta}.$$

Analogously, we obtain the other inequality. The equalities are attained in each bound if and only if G is regular. □

3.3 The inverse degree and second Zagreb indices

Formerly known as "Zagreb group indices" the first and second Zagreb indices, M_1 and M_2, have mostly been studied in regards to lower and upper bounds or for determining graphs for which these values are extremal. Furtula *et al.* (2010) proposed a modified version of these indices named "the augmented Zagreb index". Other authors have established properties thereto. See Ali, Raza & Bhatti (2016). Gutman & Trinajstić (1972) proposed the structure-dependency of total $\pi-$electron energy. The authors proved that the value depends on the sums $\sum_{v\in V} dv^2$ and $\sum_{v\in V} dv^3$ of the molecular graph (the first Zagreb index and the forgotten index, respectively). This sum showed notable applications. Finally, work by Abdo, Dimitrov & Gutman (2017) examined the trees extremal with respect to the index.

The *second Zagreb index of G* is defined as the sum of the products of the degrees of pairs of adjacent vertices of G, that is

$$\mathrm{M}_2(G) = \sum_{uv\in E} du\,dv.$$

Proposition 3.4. *Let G be a graph. Then*

$$\mathrm{M}_2(G) + \frac{m(2-\Delta^4)}{\Delta^2} \le \mathrm{ID}(G) \le \mathrm{M}_2(G) + \frac{m(2-\delta^4)}{\delta^2}.$$

The equalities are attained in each inequality if and only if G is regular.

Proof. Since $\delta \le du, dv \le \Delta$, we have

$$\frac{2}{\Delta^2} \le \frac{1}{du^2} + \frac{1}{dv^2} \le \frac{2}{\delta^2} \quad \text{and} \quad \delta^2 \le du\,dv \le \Delta^2.$$

Considering the identity $\frac{du^2+dv^2}{du^2\,dv^2} = \frac{1}{du^2} + \frac{1}{dv^2}$ and adding up over all edges, we obtain

$$\frac{2m}{\Delta^2} \le \mathrm{ID}(G) \le \frac{2m}{\delta^2} \quad \text{and} \quad m\delta^2 \le \mathrm{M}_2(G) \le m\Delta^2.$$

Thus,

$$\mathrm{ID}(G) \le \mathrm{M}_2(G) + m\left(\frac{2}{\delta^2} - \delta^2\right).$$

Analogously, we obtain the other inequality. The equalities are attained in each bound if and only if G is regular. □

Example 3.1. We show explicit computations of the indices considered in the last sections for the *Polyethylene graph*.

Figure 1 shows the associated graph of polyethylene. Polyethylene is the most common plastic which has many forms. Most have the chemical formula $(C_2H_4)_n$.

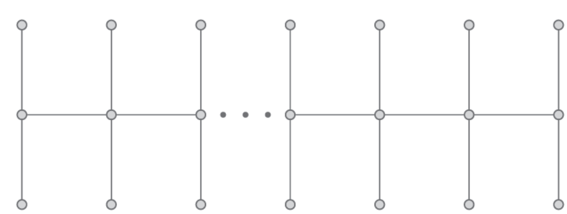

Fig. 1. A polyethylene graph

First note that the polyethylene graph has four types of edges: two whose endpoints vertices have degrees 4 and 3, $n-3$ with vertices of degrees 4 and 4, four of degrees 3 and 1 and $2(n-2)$ of degrees 4 and 1. Thus, we get

$$\begin{aligned}\mathrm{ID}(G) &= \sum_{uv\in E}\left(\frac{1}{du^2}+\frac{1}{dv^2}\right)\\ &= 2\left(\frac{1}{9}+\frac{1}{16}\right) + (n-3)\left(\frac{1}{16}+\frac{1}{16}\right)\\ &\quad + 4\left(\frac{1}{1}+\frac{1}{9}\right) + 2(n-2)\left(\frac{1}{1}+\frac{1}{16}\right)\\ &= \frac{9}{4}n + \frac{1}{6},\end{aligned}$$

$$\begin{aligned}
\mathrm{R}(G) &= \sum_{uv\in E} \frac{1}{\sqrt{du\,dv}} \\
&= 2\left(\frac{1}{\sqrt{3\cdot 4}}\right) + (n-3)\left(\frac{1}{\sqrt{4\cdot 4}}\right) \\
&\quad + 4\left(\frac{1}{\sqrt{3\cdot 1}}\right) + 2(n-2)\left(\frac{1}{\sqrt{4\cdot 1}}\right) \\
&= \frac{5}{4}n + \frac{5}{\sqrt{3}} - \frac{11}{4}, \\
\mathrm{H}(G) &= \sum_{uv\in E} \frac{1}{\sqrt{du+dv}} \\
&= 2\left(\frac{1}{3+4}\right) + (n-3)\left(\frac{1}{4+4}\right) \\
&\quad + 4\left(\frac{1}{3+1}\right) + 2(n-2)\left(\frac{1}{4+1}\right) \\
&= \frac{21}{4}n + \frac{31}{280} \\
\mathrm{M}_2(G) &= \sum_{uv\in E} du\,dv \\
&= 2(4\cdot 3) + (n-3)(4\cdot 4) \\
&\quad + 4(3\cdot 1) + 2(n-2)(4\cdot 1) \\
&= 24n - 28.
\end{aligned}$$

For the polyethylene graph, we have $3n$ vertices, $3n-1$ edges, $\delta = 1$ and $\Delta = 4$. Notice that the inequalities obtained in the last sections are strict. ♢

4. The inverse degree index and decompositions

Given a graph G, we say that a family of subgraphs $\{G_1, \dots, G_r\}$ is a *(primary) decomposition* of G if the following conditions hold:

- ⋄ $G = G_1 \cup \cdots \cup G_r$ and
- ⋄ the intersection of any two of these subgraphs is at most a vertex, that is

$$G_i \cap G_j = \begin{cases} \emptyset, & \text{or;} \\ \{v\}, & \text{for some } v \in V. \end{cases}$$

These subgraphs are called *primary subgraphs of the decomposition of G*.

Note that for any graph G, we can always construct a decomposition, at least the trivial one

$$G = G_1 \cup \cdots \cup G_m,$$

where G_i is an edge with its two endpoints being vertices of G.

Hernández-Gómez *et al.* (2017) used the $T-$decomposition concept for finding some relations between geometric-arithmetic index of a graph and of its components. A $T-$decomposition is a particular case of a primary decomposition, since the intersection of any two of the induced subgraphs is at most a cut-vertex. $v \in V$ is a cut-vertex if removing it disconnects the graph.

In this section, we use a (primary) decomposition of a graph to show a relation between the inverse degree of the graph and the inverse degree indices of the primary subgraphs induced by this decomposition.

Given a decomposition $\{G_1, \dots, G_r\}$ of G, we use the following notation: $\mathscr{W}$ is the set of vertices $v \in G$ belonging to at least to two G_i's, for $v \in \mathscr{W}$, we can assume without loss of generality that $G_1, \dots, G_k$ are the primary subgraphs containing v. We denote by d_j the number of neighbors of v in G_j (thus $dv = d_1 + \cdots + d_k$, since an edge belongs to a unique primary subgraph). For $v \in \mathscr{W}$, we define the function W as

$$\begin{aligned}
W(v) = &\sum_{u\in N(v)-\mathscr{W}} \frac{du^2+dv^2}{du^2\,dv^2} \\
&- \sum_{j=1}^{k} \sum_{u\in N_j(v)-\mathscr{W}} \frac{d_ju^2+d_jv^2}{d_ju^2\,d_jv^2},
\end{aligned}$$

where $N_j(v) = N_{G_j}(v)$.

Let $\mathscr{Z}$ be the set of edges in G with both endpoints in $\mathscr{W}$. If $e = uv \in \mathscr{Z}$, then $e \in G_i$ for a unique i. For $e = uv \in \mathscr{Z}$, we define a function Z by the rule

$$Z(e) = \frac{du^2+dv^2}{du^2\,dv^2} - \frac{d_iu^2+d_iv^2}{d_iu^2\,d_iv^2}.$$

The following result allows to compute the precise value of the inverse degree index of G in terms of the inverse degrees indices of the primary subgraphs in any decomposition.

Theorem 4.1. *Let G be a graph and $\{G_1,\dots,G_r\}$ a decomposition of G. Then,*

$$\mathrm{ID}(G)=\sum_{i=1}^{r}\mathrm{ID}(G_i)+\sum_{v\in\mathscr{W}}W(v)+\sum_{e\in\mathscr{Z}}Z(e).$$

Proof. Let $uv\in E$ be an edge of G. We have three cases.

a. $u,v\notin\mathscr{W}$. For this case uv belongs to a unique primary subgraph G_j, so the term in $\mathrm{ID}(G)$ corresponding to uv in G is equal to its corresponding term in $\mathrm{ID}(G_j)$.

b. $u\notin\mathscr{W}$ and $v\in\mathscr{W}$. Here there are two subcases.

b. 1 $u\in G_i$, for some $1\le i\le k$. Thus, $u,v\in G_i$, the edge uv gives the term $\frac{d_iu^2+d_iv^2}{d_iu^2\,d_iv^2}$ in $\mathrm{ID}(G_i)$, and for $W(v)$ the term

$$\frac{du^2+dv^2}{du^2\,dv^2}-\frac{d_iu^2+d_iv^2}{d_iu^2\,d_iv^2},$$

when adding these terms, we obtain the term given in $\mathrm{ID}(G)$.

b. 2 $u\notin G_i$, for $i=1,\dots,k$. Thus the edge uv gives the term

$$\frac{du^2+dv^2}{du^2\,dv^2},$$

in $W(v)$, which is the term in $\mathrm{ID}(G)$.

c. $u,v\in\mathscr{W}$. The edge uv belongs to a unique primary subgraph G_i. The corresponding term given by uv in $\mathrm{ID}(G_i)$ is $\frac{d_iu^2+d_iv^2}{d_iu^2\,d_iv^2}$. This edge does not give any term for $W(v)$ and

$$Z(uv)=\frac{du^2+dv^2}{du^2\,dv^2}-\frac{d_iu^2+d_iv^2}{d_iu^2\,d_iv^2}.$$

Again, adding these terms, we get the corresponding term in $\mathrm{ID}(G)$.

□

For a more precise estimation of the difference between $\mathrm{ID}(G)$ and $\sum_{i=1}^{r}\mathrm{ID}(G_i)$, the next result provides bounds for $W(v)$ and $Z(uv)$. First observe that if $0<l\le x\le a\le L$ and $0<l\le y\le b\le L$, then

$$0\ge\left(\frac{1}{a^2}+\frac{1}{b^2}\right)-\left(\frac{1}{x^2}+\frac{1}{y^2}\right)\ge 2\left(\frac{1}{L^2}-\frac{1}{l^2}\right). \quad (3)$$

Proposition 4.2. *Let $\{G_1,\dots,G_r\}$ be a decomposition of G. Then*

(i) $-2\le 2\left(\frac{1}{\Delta^2}-\frac{1}{\delta^2}\right)\le Z(e)\le 0$, *for every edge $e\in\mathscr{Z}$,*

(ii) $2dv\left(\frac{1}{\Delta^2}-\frac{1}{\delta^2}\right)\le W(v)\le 0$, *for every vertex $v\in\mathscr{W}$.*

Proof. Since $\delta\le d_iu\le du\le\Delta$ and $\delta\le d_iv\le dv\le\Delta$, relation (3) gives

$$0\ge\left(\frac{1}{du^2}+\frac{1}{dv^2}\right)-\left(\frac{1}{d_iu^2}+\frac{1}{d_iv^2}\right)\ge 2\left(\frac{1}{\Delta^2}-\frac{1}{\delta^2}\right),$$

Hence, *(i)* is true.
Now note that $W(v)$ can be written as a sum of differences

$$\frac{du^2+dv^2}{du^2\,dv^2}-\frac{d_iu^2+d_iv^2}{d_iu^2\,d_iv^2},$$

one for each edge uv. Thus, we obtain *(ii)*. □

As a consequence of this proposition we get the following corollary.

Corollary 4.3. *If $\{G_1,\dots,G_r\}$ is a decomposition of G, then*

$$\mathrm{ID}(G)\le\sum_{i=1}^{r}\mathrm{ID}(G_i).$$

Proof. We know, by Theorem 4.1 that

$$\mathrm{ID}(G)=\sum_{i=1}^{r}\mathrm{ID}(G_i)+\sum_{v\in\mathscr{W}}W(v)+\sum_{e\in\mathscr{Z}}Z(e),$$

but $W(v),Z(e)\le 0$ for $v\in\mathscr{W}$ and $e\in\mathscr{Z}$. Hence,

$$\mathrm{ID}(G)\le\sum_{i=1}^{r}\mathrm{ID}(G_i).$$

□

Example 4.1. Figure 2 shows a decomposition for the polyethylene graph, defined in example

3.1. Note that the decomposition considered is

$$\{G_1, \ldots, G_n\},$$

where $G_1, \ldots, G_{n-1}$ are star graphs S_3, and G_n is a P_3 graph. Considering the notation in figure 2, we have

$$\mathscr{W} = \{v_2, v_3, \ldots, v_n\} \quad \text{and}$$
$$\mathscr{Z} = \{e_2 = v_2v_3, e_3 = v_3v_4, \ldots, e_{n-1} = v_{n-1}v_n\}.$$

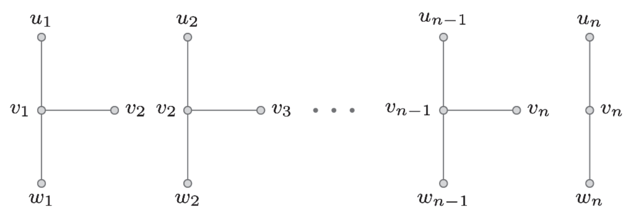

Fig. 2. A decomposition for the polyethylene graph

For $v \in \mathscr{W}$, we defined

$$W(v) = \sum_{u \in N(v) - \mathscr{W}} \frac{du^2 + dv^2}{du^2\, dv^2} - \\ - \sum_{j=1}^{k} \sum_{u \in N_j(v) - \mathscr{W}} \frac{d_ju^2 + d_jv^2}{d_ju^2\, d_jv^2},$$

and observe that $v_i \in G_{i-1} \cap G_i$. Thus,

$$W(v_2) = \left[\left(\frac{1}{3^2} + \frac{1}{4^2}\right) + \left(\frac{1}{1^2} + \frac{1}{4^2}\right) + \left(\frac{1}{1^2} + \frac{1}{4^2}\right)\right] - \\ - \left[\left(\frac{1}{3^2} + \frac{1}{1^2}\right) + \left(\left(\frac{1}{1^2} + \frac{1}{3^2}\right) + \left(\frac{1}{1^2} + \frac{1}{3^2}\right)\right)\right] \\ = -\frac{149}{144}.$$

Analogously, we obtain

$$W(v_i) = -\frac{7}{72} \quad \text{for } i = 3, \ldots, n-1 \quad \text{and}$$
$$W(v_n) = -\frac{5}{18}.$$

This implies

$$\sum_{v \in \mathscr{W}} W(v) = -\frac{149}{144} - (n-3)\frac{7}{72} - \frac{5}{18} = -\frac{7}{72}n - \frac{49}{48}.$$

Now recall that if $e = uv$ then

$$Z(e) = \frac{du^2 + dv^2}{du^2\, dv^2} - \frac{d_iu^2 + d_iv^2}{d_iu^2\, d_iv^2},$$

where G_i is the unique component such that $e \in G_i$. Thus, we have

$$Z(e_i) = \left(\frac{1}{4^2} + \frac{1}{4^2}\right) - \left(\frac{1}{3^2} + \frac{1}{1^2}\right) = -\frac{71}{72}$$

for $i = 2, \ldots, n-2$ and

$$Z(e_{n-1}) = \left(\frac{1}{4^2} + \frac{1}{3^2}\right) - \left(\frac{1}{3^2} + \frac{1}{1^2}\right) = -\frac{15}{16}.$$

Hence,

$$\sum_{e \in \mathscr{Z}} Z(e) = -\frac{71}{72}(n-3) - \frac{15}{16} = -\frac{71}{72}n + \frac{97}{48}.$$

And computing the values $\mathrm{ID}(G_i)$, for $i = 1, \ldots, n$ we obtain

$$\mathrm{ID}(G_i) = \frac{3^2 + 1}{3} = \frac{10}{3}, \quad \text{for } i = 1, \ldots, n-1$$
$$\mathrm{ID}(G_n) = \frac{3+2}{2} = \frac{5}{2}.$$

Then,

$$\sum_{i=1}^{n} \mathrm{ID}(G_i) = (n-1)\frac{10}{3} + \frac{5}{2} = \frac{10}{3}n - \frac{5}{6}.$$

Finally, we may observe that the formula obtained in theorem 4.1 holds for this construction

$$\sum_{i=1}^{n} \mathrm{ID}(G_i) + \sum_{v \in \mathscr{W}} W(v) + \sum_{e \in \mathscr{Z}} Z(e) = \\ = \frac{10}{3}n - \frac{5}{6} - \frac{7}{72}n - \frac{49}{48} - \frac{71}{72}n - \frac{419}{144} \\ = \frac{9}{4}n + \frac{1}{6} = \mathrm{ID}(G).$$

◇

References

Abdo H., Dimitrov D. & Gutman I. (2017). On extremal trees with respect to the F—index. Kuwait Journal of Science, **44(3)**: 1-8.

Ali A., Raza Z. & Bhatti A.A. (2016). On the augmented Zagreb index. Kuwait Journal of Science, **43(2)**: 48-63.

Dankelmann P., Swart H.C. & Van den Berg P. (2008). Diameter and inverse degree. Discrete Mathematics, **308(5-6)**: 670-673.

Dankelmann P., Hellvig A. & Volkmann L. (2009). Inverse degree and edge-connectivity. Discrete Mathematics, **309(9)**: 2943-2947.

Das K.Ch. (2010). On comparing Zagreb indices of graphs. MATCH Commununications in Mathematical and in Computer Chemistry, **63**: 433-440.

Elumalai S., Hosamani S.M., Mansour T. & Rostami M.A. (2018). More on inverse degree and topological inidices of graphs. Filomat, **32(1)**: 165-178.

Fajtlowicz S. (1987). On conjectures of Graffiti - II. Congressus Numerantium, **60**: 187-197.

Gutman I. (2013). Degree-based topological indices. Croatica Chemica Acta, **86(4)**: 351-361

Gutman I. & Furtula B. (eds) (2008). Recent Results in the Theory of Randić Index. University Kragujevac, Kragujevac.

Harary F. (1969). Graph Theory. Addison-Wesley, Reading, MA, 3.

Hernández-Gómez J.C., Rodríguez J.M. & Sigarreta J.M. (2017). On the geometric-arithmetic index by decomposition. Journal of Mathematical Chemistry, **55**: 1376-1391.

Li X. & Gutman I. (2006). Mathematical aspects of Randić-Type molecular structure descriptors. Croatica Chemica Acta, **79(3)**: A31-A32.

Mansour T. & Schork M. (2009). The PI index of bridge and chain graphs. MATCH Commununications in Mathematical and in Computer Chemistry, **61**: 723-734.

Randić M. (1975). On characterization of molecular branching. Journal of the American Chemical Society, **97(23)**: 6609-6615.

Read R.C. & Corneil D.G. (1977). The graph isomorphism disease. Journal of Graph Theory, **1**: 339-363.

Rodríguez J.A. & Sigarreta J.M. (2005). On the Randić index and conditional parameters of a graph. MATCH Commununications in Mathematical and in Computer Chemistry, **54**: 403-416.

Xu K., Das K.Ch. & Balachandran S. (2014). Maximizing the Zagreb indices of (n, m)—graphs. MATCH Communications in Mathematical and in Computer Chemistry, **72**: 641-654.

Xu K. & Das K.Ch. (2016). Some extremal graphs with respect to inverse degree. Discrete Applied Mathematics, **203**: 171-183.

Submitted : 07/06/2018

Revised : 13/11/2018

Accepted : 20/11/2018

حول مؤشر درجة الانعكاس والتحليل في الرسوم البيانية

*جيسوس روميرو – فالنسيا، خوان سي هرنانديز – جوميز، جيراردو رينا هيرنانديز
كلية الرياضيات، جامعة غيريرو المستقلة، تشيلبانجو، غرو، المكسيك

الملخص

يتم تعريف مؤشر درجة الانعكاس للرسم البياني $G = (V;E)$ بدون رؤوس معزولة على أنه $\mathrm{ID}(G) = \sum_{v\in V} \frac{1}{dv}$، حيث أن dv هي درجة قمة الرأس v في G. في هذا البحث، نوضح العلاقة بين درجة الانعكاس للرسم البياني ومؤشراتها للرسومات الفرعية الأولية التي تم الحصول عليها من خلال تحليل عام لـ G، ونُنشيء بعض العلاقات بين مؤشر درجة الإنعكاس والمؤشرات المعروفة الأخرى وتم تقديم تطبيق على تركيب كيميائي محدد.