

On the geometric–arithmetic index by decompositions-CMMSE

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Abstract The concept of geometric–arithmetic index was introduced in the chemical graph theory recently, but it has shown to be useful. There are many papers studying different kinds of indices (as Wiener, hyper–Wiener, detour, hyper–detour, Szeged, edge–Szeged, PI, vertex–PI and eccentric connectivity indices) under particular cases of decompositions. The main aim of this paper is to show that the computation of the geometric–arithmetic index of a graph G is essentially reduced to the computation of the geometric–arithmetic indices of the so-called primary subgraphs obtained by a general decomposition of G . Furthermore, using these results, we obtain formulas for the geometric–arithmetic indices of bridge graphs and other classes of graphs, like bouquet of graphs and circle graphs. These results are applied to the computation

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of the geometric-arithmetic index of Spiro chain of hexagons, polyphenylenes and polyethene.

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1 Introduction

A topological index is defined as a single number that represents a chemical structure in graph-theoretical terms via the molecular graph, and that correlates with a molecular property; it is used to understand physicochemical properties of chemical compounds. Topological indices are interesting since they capture some of the properties of a molecule in a single number. Hundreds of topological indices have been introduced and studied, starting with the seminal work by Wiener [25] in which he used the sum of all shortest-path distances of a (molecular) graph for modeling physical properties of alkanes.

Topological indices based on end-vertex degrees of edges have been used over 40 years. Among them, several indices are recognized to be useful tools in chemical researches. Probably, the best known such descriptor is the Randić connectivity index (R) [15]. There are more than thousand papers and a couple of books dealing with this index (see e.g., [7, 8, 16] and the references therein). During many years, scientists were trying to improve the predictive power of the Randić index. This led to the introduction of a large number of new topological descriptors resembling the original Randić index. The first geometric-arithmetic index GA_1 , defined in [24] as

$$GA_1(G) = \sum_{uv \in E(G)} \frac{\sqrt{d_u d_v}}{\frac{1}{2}(d_u + d_v)}$$

where uv denotes the edge of the graph G connecting the vertices u and v , and d_u is the degree of the vertex u , is one of the successors of the Randić index. Although GA_1 was introduced just six years ago, there are many papers dealing with this index (see e.g., [5, 13, 17, 18, 21, 24] and the survey [4]). There are other geometric-arithmetic indices, like $Z_{p,q}$ ($Z_{0,1} = GA_1$), but the results in [4, p. 598] show empirically that the GA_1 index gathers the same information on observed molecules as other $Z_{p,q}$ indices.

The reason for introducing a new index is to gain prediction of some property of molecules somewhat better than obtained by already presented indices. Therefore, a test study of predictive power of a new index must be done. As a standard for testing new topological descriptors, the properties of octanes are commonly used. We can find 16 physico-chemical properties of octanes at www.moleculardescriptors.eu.

Although only about 1000 benzenoid hydrocarbons are known, the number of possible benzenoid hydrocarbons is huge. For instance, the number of possible benzenoid hydrocarbons with 35 benzene rings is 5851000265625801806530 [23]. Therefore, the modeling of their physico-chemical properties is very important in order to predict properties of currently unknown species.

The graphic in [4, Fig. 7] (from [4, Table 2], [22]) shows that there exists a good linear correlation between GA_1 and the heat of formation of benzenoid hydrocarbons (the correlation coefficient is equal to 0.972). Furthermore, the improvement in prediction with GA_1 index comparing to Randić index in the case of standard enthalpy of vaporization is more than 9%. Hence, one can think that GA_1 index should be considered in the QSPR/QSAR researches.

We say that a family of subgraphs $\{G_1, \dots, G_r\}$ of G is a *decomposition* of G if $G_1 \cup \dots \cup G_r = G$ and $G_i \cap G_j$ is either empty or a vertex for every $i, j \in \{1, \dots, r\}, i \neq j$. The subgraphs G_1, \dots, G_r are usually called *primary subgraphs* of the decomposition.

Particular cases of decompositions are the T-decompositions (equivalent to the concept of graphs obtained by point-attaching, see [6, 19]); they are a very useful tool in different areas of graph theory, as Gromov hyperbolic graphs (see e.g., [2, 3, 12]), polynomials on graphs (see [6]) and metric dimension of graphs (see [19]). We say that a vertex v of a graph G is a *cut-vertex* if $G \setminus \{v\}$ is not connected. A graph is *biconnected* if it does not contain cut-vertices. Given a graph G , we say that a family of subgraphs $\{G_1, \dots, G_r\}$ of G is a *T-decomposition* of G if $G_1 \cup \dots \cup G_r = G$ and $G_i \cap G_j$ is either empty or a cut-vertex for every $i, j \in \{1, \dots, r\}, i \neq j$. Every graph has a T-decomposition, as the following example shows. Given any edge in G , let us consider the maximal two-connected subgraph containing it: this is the well-known *biconnected decomposition* of G .

In [9] and [10] the authors introduce the concept of bridge and chain graphs, which are particular cases of T-decompositions (a chain graph is a graph with a T-decomposition in which every cut-vertex belongs at most to two primary subgraphs; bridge graphs are a subset of chain graphs). For bridge and chain graphs the PI index was determined in [9] and for bridge graphs the Szeged index (and the vertex PI index) was considered in [11]. Recently, the Wiener index was considered in [1] for a class of graphs containing as special cases the bridge and chain graphs. Also, in [10] appear formulas for the Wiener, hyper-Wiener, detour and hyper-detour indices of bridge and chain graphs. Besides, [20] contains formulas for the Szeged, edge-Szeged, PI, vertex-PI and eccentric connectivity indices of splice graphs (another class of graphs with T-decompositions). More classes of graphs can be obtained as particular cases of T-decompositions: bouquets of graphs, rooted product graphs, corona product graphs and block graphs (see [19]).

Since the papers [1, 9–11, 20] (studying different kinds of indices under particular cases of decompositions) are useful, it is natural to show that the computation of the geometric-arithmetic index of a graph G is essentially reduced to the computation of the geometric-arithmetic indices of the primary subgraphs obtained by a general decomposition of G . This is the main aim of the present paper. Using these results, we obtain formulas for the geometric-arithmetic indices of bridge graphs and other classes of graphs, like bouquet of graphs and circle graphs. These results are applied in Sect. 3 to the computation of the geometric-arithmetic index of Spiro chain of hexagons, Polyphenylenes and Polyethylene (see Examples 3.2, 3.4 and 3.8, respectively).

Throughout this paper, $G = (V(G), E(G))$ denotes a (non-oriented) finite simple (without multiple edges and loops) connected graph with $E(G) \neq \emptyset$. Note that the connectivity of G is not an important restriction, since if G has connected components

G_1, \dots, G_r , then $GA_1(G) = GA_1(G_1) + \dots + GA_1(G_r)$; furthermore, every molecular graph is connected.

2 Geometric–arithmetic index and decompositions

If $v \in V(G)$, then we denote by $N_G(v)$ or $N(v)$ the set of neighbors of v , i.e.,

$$N_G(v) = N(v) = \{u \in V(G) \mid uv \in E(G)\}.$$

Given a decomposition $\{G_1, \dots, G_r\}$ of G , denote by \mathcal{W} the set of vertices v in G belonging at least at two G_i 's. Given a vertex $v \in \mathcal{W}$, denote by G_{i_1}, \dots, G_{i_k} the set of primary subgraphs containing v and by d_{i_j} the number of neighbors of v in G_{i_j} (then $d_v = d_{i_1} + \dots + d_{i_k}$). If $v \in \mathcal{W}$, then we define $W(v)$ as

$$W(v) = \sum_{u \in N_G(v) \setminus \mathcal{W}} \frac{\sqrt{d_u d_v}}{\frac{1}{2}(d_u + d_v)} - \sum_{j=1}^k \sum_{u \in N_{G_{i_j}}(v) \setminus \mathcal{W}} \frac{\sqrt{d_u d_{i_j}}}{\frac{1}{2}(d_u + d_{i_j})}.$$

Denote by \mathcal{Z} the set of edges in G with both endpoints in \mathcal{W} . If $e = uv \in \mathcal{Z}$, then $e \in G_i$ for some i , and we denote by d_u^*, d_v^* the degrees of u, v in G_i . If $e = uv \in \mathcal{Z}$, then we define $Z(e)$ as

$$Z(e) = \frac{\sqrt{d_u d_v}}{\frac{1}{2}(d_u + d_v)} - \frac{\sqrt{d_u^* d_v^*}}{\frac{1}{2}(d_u^* + d_v^*)}.$$

The following result allows to compute the precise value of $GA_1(G)$ in terms of the geometric–arithmetic indices of the primary subgraphs in any decomposition.

Theorem 2.1 *Let $\{G_1, \dots, G_r\}$ be a decomposition of the graph G . Then*

$$GA_1(G) = \sum_{i=1}^r GA_1(G_i) + \sum_{v \in \mathcal{W}} W(v) + \sum_{e \in \mathcal{Z}} Z(e).$$

Proof First of all, note that if $u, v \notin \mathcal{W}$ and $uv \in E(G)$, then the term in $GA_1(G)$ corresponding to uv in G is equal to its corresponding term in $\sum_{i=1}^r GA_1(G_i)$.

For each $v \in \mathcal{W}$ and $u \notin \mathcal{W}$ with $uv \in E(G)$, $W(v)$ replaces in the sum $\sum_{i=1}^r GA_1(G_i)$ the corresponding term to uv by its correct value as edge in G . This fact holds since the degree of u is d_u both in G and in its (unique) corresponding primary subgraph.

Finally, for each $u, v \in \mathcal{W}$ with $uv \in E(G)$, $Z(uv)$ replaces in the sum $\sum_{i=1}^r GA_1(G_i)$ the corresponding term to uv by its correct value as edge in G . \square

In order to estimate the difference between $GA_1(G)$ and $\sum_{i=1}^r GA_1(G_i)$, Proposition 2.4 will provide bounds for $W(v)$ and $Z(uv)$. We need first the following technical result.

Lemma 2.2 Given any positive integer a , let h_a be the function $h_a(x) = \frac{2\sqrt{x}}{a+x}$ on the interval $[1, \infty)$. Then h_a strictly increases in $[1, a]$, strictly decreases in $[a, \infty)$, and $|h'_a(x)| \leq \frac{1}{8}$ for every $x \in [1, \infty)$.

Proof Since

$$h'_a(x) = \frac{\frac{1}{\sqrt{x}}(a+x) - 2\sqrt{x}}{(a+x)^2} = \frac{a-x}{\sqrt{x}(a+x)^2},$$

$h'_a > 0$ on $[1, a)$ and $h'_a < 0$ on (a, ∞) . A computation gives

$$\begin{aligned} h''_a(x) &= \frac{-\sqrt{x}(a+x)^2 + (x-a)\left(\frac{1}{2\sqrt{x}}(a+x)^2 + 2\sqrt{x}(a+x)\right)}{x(a+x)^4} \\ &= \frac{3x^2 - 6ax - a^2}{2x^{3/2}(a+x)^3}. \end{aligned}$$

We have $3x^2 - 6ax - a^2 = 0$ if and only if

$$x = \frac{3a \pm \sqrt{9a^2 + 3a^2}}{3} = \frac{3 \pm 2\sqrt{3}}{3} a.$$

Thus, $h''_a \leq 0$ on $\left[1, \frac{3+2\sqrt{3}}{3} a\right]$ and $h''_a \geq 0$ on $\left[\frac{3+2\sqrt{3}}{3} a, \infty\right)$. Since $\lim_{x \rightarrow \infty} h'_a(x) = 0$ and $a \geq 1$,

$$|h'_a(x)| \leq \max \left\{ h'_a(1), -h'_a \left(\frac{3+2\sqrt{3}}{3} a \right) \right\} = \max \left\{ \frac{a-1}{(a+1)^2}, \frac{c_0}{a^{3/2}} \right\}$$

for every $x \in [1, \infty)$, where

$$c_0 = \frac{\frac{2\sqrt{3}}{3}}{\sqrt{\frac{3+2\sqrt{3}}{3} \left(\frac{6+2\sqrt{3}}{3}\right)^2}} \sim 0.079.$$

Consider the function

$$H(t) = \frac{t^{3/2}(t-1)}{(t+1)^2} = \frac{t^{5/2} - t^{3/2}}{(t+1)^2}$$

for $t \in [2, \infty)$. Since

$$H'(t) = \frac{\left(\frac{5}{2}t^{3/2} - \frac{3}{2}t^{1/2}\right)(t+1)^2 - (t^{5/2} - t^{3/2})2(t+1)}{(t+1)^4} = \frac{t^{1/2}t^2 + 6t - 3}{2(t+1)^3} > 0$$

for $t \in [2, \infty)$, we have

$$\frac{t^{3/2}(t - 1)}{(t + 1)^2} = H(t) \geq H(2) = \frac{2^{3/2}}{9} > c_0, \quad \frac{t - 1}{(t + 1)^2} > \frac{c_0}{t^{3/2}},$$

for every $t \in [2, \infty)$. Therefore,

$$|h'_a(x)| \leq \max \left\{ \frac{a - 1}{(a + 1)^2}, \frac{c_0}{a^{3/2}} \right\} = \begin{cases} c_0, & \text{if } a = 1, \\ \frac{a-1}{(a+1)^2}, & \text{if } a \geq 2. \end{cases}$$

for every $x \in [1, \infty)$. Since $u(t) = \frac{t-1}{(t+1)^2}$ satisfies

$$u'(t) = \frac{(t + 1)^2 - (t - 1)2(t + 1)}{(t + 1)^4} = \frac{3 - t}{(t + 1)^3},$$

we obtain $u'(t) \geq 0$ for every $t \in [2, 3]$ and $u'(t) \leq 0$ for every $t \in [3, \infty)$. Hence, $u(a) \leq u(3) = \frac{1}{8} > c_0$ for every $a \geq 2$ and $|h'_a(x)| \leq \frac{1}{8}$ for every $x \in [1, \infty)$. \square

We also need the following result (see e.g., [17, Corollary 2.3]).

Lemma 2.3 *Let g be the function $g(x, y) = \frac{2\sqrt{xy}}{x+y}$ with $0 < a \leq x, y \leq b$. Then*

$$\frac{2\sqrt{ab}}{a + b} \leq g(x, y) \leq 1.$$

The equality in the lower bound is attained if and only if either $x = a$ and $y = b$, or $x = b$ and $y = a$, and the equality in the upper bound is attained if and only if $x = y$. Besides, $g(x, y) = g(x', y')$ if and only if x/y is equal to either x'/y' or y'/x' .

Given a decomposition $\{G_1, \dots, G_r\}$ of G and $e = uv \in \mathcal{Z}$, we say that e is maximal or minimal if $d_u = d_v$ or $d_u^* = d_v^*$, respectively.

Given a graph G , denote by Δ, δ the maximum and minimum degrees of G , respectively.

Proposition 2.4 *Let $\{G_1, \dots, G_r\}$ be a decomposition of the graph G . Given $e \in \mathcal{Z}$, denote by Δ_e, δ_e the maximum and minimum degrees of the primary subgraph G_i with $e \in G_i$, respectively. Then*

$$-1 \leq \frac{2\sqrt{\Delta\delta}}{\Delta + \delta} - 1 \leq Z(e) \leq 1 - \frac{2\sqrt{\Delta_e\delta_e}}{\Delta_e + \delta_e} \leq 1,$$

for every $e \in \mathcal{Z}$. If e is maximal or minimal, then $Z(e) \geq 0$ or $Z(e) \leq 0$, respectively. Furthermore,

$$|W(v)| \leq \frac{1}{8} \sqrt{\Delta} d_v(d_v - 1),$$

for every $v \in \mathcal{W}$.

Proof If $e = uv \in \mathcal{Z}$, then Lemma 2.3 gives

$$-1 \leq \frac{2\sqrt{\Delta\delta}}{\Delta + \delta} - 1 \leq Z(e) = \frac{\sqrt{d_u d_v}}{\frac{1}{2}(d_u + d_v)} - \frac{\sqrt{d_u^* d_v^*}}{\frac{1}{2}(d_u^* + d_v^*)} \leq 1 - \frac{2\sqrt{\Delta_e \delta_e}}{\Delta_e + \delta_e} \leq 1.$$

If e is maximal or minimal, then

$$Z(e) = \frac{\sqrt{d_u d_v}}{\frac{1}{2}(d_u + d_v)} - \frac{\sqrt{d_u^* d_v^*}}{\frac{1}{2}(d_u^* + d_v^*)} = 1 - \frac{\sqrt{d_u^* d_v^*}}{\frac{1}{2}(d_u^* + d_v^*)} \geq 0$$

or

$$Z(e) = \frac{\sqrt{d_u d_v}}{\frac{1}{2}(d_u + d_v)} - 1 \leq 0,$$

respectively.

Finally, fix $v \in \mathcal{W}$. As in the definition of $W(v)$, denote by G_{i_1}, \dots, G_{i_k} the set of primary subgraphs containing v and by d_{i_j} the number of neighbors of v in G_{i_j} for $j = 1, \dots, k$. Fix j and $u \in N_{G_{i_j}}(v) \setminus \mathcal{W}$. Mean value theorem and Lemma 2.2 give

$$\left| \frac{2\sqrt{d_u d_v}}{d_u + d_v} - \frac{2\sqrt{d_u d_{i_j}}}{d_u + d_{i_j}} \right| = \sqrt{d_u} |h_{d_u}(d_v) - h_{d_u}(d_{i_j})| = \sqrt{d_u} |h'_{d_u}(t)| (d_v - d_{i_j})$$

for some $t \in (d_{i_j}, d_v) \subset [1, d_v]$, where h_a is the function appearing in Lemma 2.2.

Since $|h'_{d_u}(t)| \leq \frac{1}{8}$ for every $t \in [1, \infty)$ by Lemma 2.2, we deduce

$$\left| \frac{2\sqrt{d_u d_{i_j}}}{d_u + d_{i_j}} - \frac{2\sqrt{d_u d_v}}{d_u + d_v} \right| \leq \sqrt{\Delta} \frac{1}{8} (d_v - 1).$$

Hence,

$$|W(v)| \leq \frac{1}{8} \sqrt{\Delta} d_v (d_v - 1),$$

for every $v \in \mathcal{W}$. □

We have the following direct consequence of Theorem 2.1, since $|Z(e)| \leq 1$ for every $e \in \mathcal{Z}$ by Proposition 2.4.

Corollary 2.5 *Let $\{G_1, \dots, G_r\}$ be a decomposition of the graph G . Then*

$$\left| GA_1(G) - \sum_{i=1}^r GA_1(G_i) \right| \leq \frac{1}{8} \Delta^{3/2} (\Delta - 1) \text{card } \mathcal{W} + \text{card } \mathcal{Z}.$$

Proposition 2.6 *Let $\{G_1, \dots, G_r\}$ be a decomposition of the graph G . If $d_v \leq d_u$ for every $v \in \mathcal{W}$ and $u \in N_G(v) \setminus \mathcal{W}$, then*

$$GA_1(G) \geq \sum_{i=1}^r GA_1(G_i) - \text{card } \mathcal{Z}.$$

Furthermore, if every edge in \mathcal{Z} is maximal, then

$$GA_1(G) \geq \sum_{i=1}^r GA_1(G_i).$$

Proof Fix $v \in \mathcal{W}$. We are going to prove $W(v) \geq 0$. Denote by G_{i_1}, \dots, G_{i_k} the set of primary subgraphs containing v and by d_{i_j} the number of neighbors of v in G_{i_j} , as in the definition of $W(v)$. Fix j and $u \in N_{G_{i_j}}(v) \setminus \mathcal{W}$. Since

$$h_{d_u}(x) = \frac{2\sqrt{x}}{d_u + x}$$

is an increasing function on $[1, d_u]$ by Lemma 2.2, and $d_{i_j} \leq d_v \leq d_u$,

$$\frac{\sqrt{d_u d_{i_j}}}{\frac{1}{2}(d_u + d_{i_j})} \leq \frac{\sqrt{d_u d_v}}{\frac{1}{2}(d_u + d_v)}.$$

Hence, $W(v) \geq 0$ for every $v \in \mathcal{W}$. Since $|Z(e)| \leq 1$ for every $e \in \mathcal{Z}$ by Proposition 2.4, Theorem 2.1 gives the result.

Furthermore, if every edge in \mathcal{Z} is maximal, then Proposition 2.4 gives $Z(e) \geq 0$ for every $e \in \mathcal{Z}$, and the second inequality follows by Theorem 2.1. \square

Corollary 2.7 *Let $\{G_1, \dots, G_r\}$ be a decomposition of the graph G with minimum degree δ . If $d_v = \delta$ for every $v \in \mathcal{W}$, then*

$$GA_1(G) \geq \sum_{i=1}^r GA_1(G_i) - \text{card } \mathcal{Z}.$$

Furthermore, if every edge in \mathcal{Z} is maximal, then

$$GA_1(G) \geq \sum_{i=1}^r GA_1(G_i).$$

The obtention of bounds for the geometric arithmetic index is a very active topic of research (see e.g., [5, 13, 17, 21, 24], the survey [4] and the references therein). The following result provides an upper bound for it involving the numbers of vertices and the diameters of the primary subgraphs in the biconnected decomposition.

Let us define $M(n, r)$ as follows: $M(n, r) := r + \frac{1}{2}(n - r - 1)(n - r + 4)$.

We denote by $\text{diam}(G)$ the diameter of G , i.e., $\text{diam}(G) := \max\{d(u, v) \mid u, v \in V(G)\}$.

Theorem 2.8 *If $\{G_1, \dots, G_k\}$ is the biconnected decomposition of a graph G and G_j has n_j vertices for $1 \leq j \leq k$, then*

$$GA_1(G) \leq \sum_{j=1}^k M(n_j, \text{diam}(G_j)).$$

Proof If G_j has n_j vertices and m_j edges for $1 \leq j \leq k$, then G has $m = \sum_{j=1}^k m_j$ edges. Since each G_j is two-connected, the classical Ore's result in [14, Theorem 3.1] gives $m_j \leq \sum_{j=1}^k M(n_j, \text{diam}(G_j))$ for every $1 \leq j \leq k$. Since $GA_1(G)$ is bounded by the number of edges in G , we have

$$GA_1(G) \leq m = \sum_{j=1}^k m_j \leq \sum_{j=1}^k M(n_j, \text{diam}(G_j)).$$

□

3 Applications to mathematical chemistry

Next, we apply our results on decompositions in order to compute the geometric-arithmetic indices of several chemical graphs.

Let $\{G_i\}_{i=1}^d$ be a set of finite pairwise disjoint graphs and $v_i, w_i \in V(G_i)$. The *chain graph*

$$C(G_1, G_2, \dots, G_d) = C(G_1, G_2, \dots, G_d; v_1, w_1, v_2, w_2, \dots, v_d, w_d)$$

of $\{G_i\}_{i=1}^d$ with respect to the vertices $\{v_i, w_i\}_{i=1}^d$ is the graph obtained from the graphs G_1, \dots, G_d by identifying the vertex w_i and the vertex v_{i+1} for every $i \in \{1, 2, \dots, d-1\}$.

We denote by u_i the vertex in $C(G_1, G_2, \dots, G_d; v_1, w_1, \dots, v_d, w_d)$ obtained by identifying the vertices w_i and v_{i+1} . It is clear that $\{G_1, \dots, G_d\}$ is a T-decomposition of the chain graph:

$$C(G_1, \dots, G_d; v_1, w_1, \dots, v_d, w_d).$$

Following the notation in [9], given any graph H , $v, w \in V(H)$ and an integer $d > 1$, let us define

$$T_d(H, v, w) = C(H, \dots, H; v, w, \dots, v, w),$$

where H appears d times. Theorem 2.1 has the following direct consequence.

Corollary 3.1 Consider any graph H , $v, w \in V(H)$ and an integer $d > 1$.

(1) If $vw \notin E(H)$, then

$$GA_1(T_d(H, v, w)) = d GA_1(H) + (d - 1)W(u_1).$$

(2) If $vw \in E(H)$, then

$$GA_1(T_d(H, v, w)) = d GA_1(H) + (d - 1)W(u_1) + (d - 2)Z(vw).$$

Example 3.2 Spiro chain of hexagons. Consider the chain graph $T_d(C_6)$, where C_6 is the cycle graph with vertices v_1, v_2, \dots, v_6 (labeled clockwise), $v = v_1$ and $w = v_4$. Since $vw \notin E(C_6)$, Corollary 3.1 gives

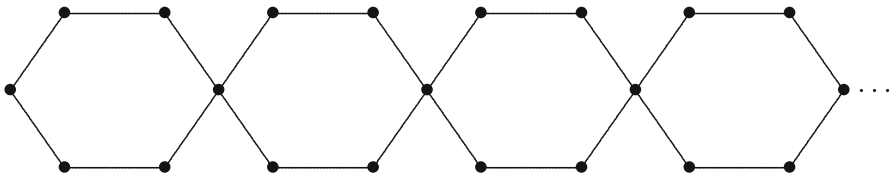
$$\begin{aligned} GA_1(T_d(C_6)) &= d GA_1(C_6) + (d - 1)W(u_1) \\ &= 6d + (d - 1) \left(4 \frac{2\sqrt{8}}{6} - 4 \right) = \left(2 + \frac{8\sqrt{2}}{3} \right) d + 4 - \frac{8\sqrt{2}}{3}. \end{aligned}$$

Note that if we take $v = v_3$ or $w = v_5$ in Example 3.2, then we obtain graphs with the same geometric-arithmetic index than the previous one.

Given any graph H , $v, w \in V(H)$, P_2 a graph of one edge connecting the two vertices v', w' , and an integer $d > 1$, let us define

$$U_d(H) = C(H, P_2, \dots, H, P_2, H; v, w, v', w', \dots, v, w, v', w', v, w),$$

where H appears d times. Theorem 2.1 also has the following consequence.



Spiro chain of hexagons

Corollary 3.3 Consider any graph H , $v, w \in V(H)$ and an integer $d > 1$. Denote by d_v, d_w the degrees of v, w in H , respectively.

(1) If $vw \notin E(H)$, then

$$GA_1(U_d(H)) = d GA_1(H) + (d - 1) \left(W(u_1) + W(u_2) + \frac{2\sqrt{(d_v + 1)(d_w + 1)}}{d_v + d_w + 2} \right).$$

(2) If $vw \in E(H)$, then

$$GA_1(U_d(H)) = d GA_1(H) + (d - 1) \left(W(u_1) + W(u_2) + \frac{2\sqrt{(d_v + 1)(d_w + 1)}}{d_v + d_w + 2} \right) + (d - 2)Z(vw).$$

Proof Consider the T-decomposition $\{H, P_2, \dots, H, P_2, H\}$ of $U_d(H)$. Note that $GA_1(P_2) = 1$ and $Z(P_2) = \frac{2\sqrt{(d_v+1)(d_w+1)}}{d_v+d_w+2} - 1$. If $vw \notin E(H)$, then \mathcal{Z} is just the set of copies of P_2 . Hence, Theorem 2.1 gives

$$\begin{aligned} GA_1(U_d(H)) &= d GA_1(H) + d - 1 + (d - 1)W(u_1) + (d - 1)W(u_2) \\ &\quad + (d - 1) \left(\frac{2\sqrt{(d_v + 1)(d_w + 1)}}{d_v + d_w + 2} - 1 \right) \\ &= d GA_1(H) + (d - 1) \left(W(u_1) + W(u_2) + \frac{2\sqrt{(d_v + 1)(d_w + 1)}}{d_v + d_w + 2} \right). \end{aligned}$$

If $vw \in E(H)$, then \mathcal{Z} is the set of copies of P_2 and the copies of vw which are not in the first and last copies of H . Therefore, we just need to add the term $(d - 2)Z(vw)$ to the formula in (1). \square

Example 3.4 Polyphenylenes. Consider the chain graph $U_d(C_6)$, where C_6 is the cycle graph with vertices v_1, v_2, \dots, v_6 (labeled clockwise), $v = v_1$ and $w = v_4$. Since $vw \notin E(C_6)$, Corollary 3.3 gives

$$\begin{aligned} GA_1(U_d(C_6)) &= d GA_1(C_6) + (d - 1) \left(W(u_1) + W(u_2) + \frac{2\sqrt{(d_v + 1)(d_w + 1)}}{d_v + d_w + 2} \right) \\ &= 6d + (d - 1) \left(2 \left(2 \frac{2\sqrt{6}}{5} - 2 \right) + 1 \right) = \left(3 + \frac{8\sqrt{6}}{5} \right) d + 3 - \frac{8\sqrt{6}}{5}. \end{aligned}$$

If we take $v = v_3$ or $w = v_5$ in Example 3.4, then we obtain graphs with the same geometric-arithmetic index than the previous one.

Let $\{G_i\}_{i=1}^d$ be a set of finite pairwise disjoint graphs and $v_i \in V(G_i)$. The *bridge graph*

$$B(G_1, G_2, \dots, G_d) = B(G_1, G_2, \dots, G_d; v_1, v_2, \dots, v_d)$$

of $\{G_i\}_{i=1}^d$ with respect to the vertices $\{v_i\}_{i=1}^d$ is the graph obtained from the graphs G_1, \dots, G_d by connecting the vertices v_i and v_{i+1} by an edge for every $i \in \{1, 2, \dots, d - 1\}$. Theorem 2.1 has the following consequence.

Theorem 3.5 Let $\{G_i\}_{i=1}^d$ be a set of finite pairwise disjoint graphs and $v_i \in V(G_i)$. Then

$$GA_1(B(G_1, \dots, G_d; v_1, \dots, v_d)) = \sum_{i=1}^d GA_1(G_i) + d - 1 + \sum_{i=1}^d W(v_i) + \sum_{i=1}^{d-1} Z(v_i v_{i+1}).$$

Proof Consider the T-decomposition $\{G_1, \dots, G_d, v_1 v_2, \dots, v_{d-1} v_d\}$ of

$$B(G_1, \dots, G_d; v_1, \dots, v_d).$$

We have in this case $\mathcal{W} = \{v_1, \dots, v_d\}$, $\mathcal{Z} = \{v_1 v_2, \dots, v_{d-1} v_d\}$ and $GA_1(v_i v_{i+1}) = 1$ for $i \in \{1, \dots, d - 1\}$. Hence, Theorem 2.1 gives the result. \square

Given any graph H , $v \in V(H)$ and an integer $d > 1$, let us define

$$G_d(H, v) = B(H, \dots, H; v, \dots, v),$$

where H appears d times. Theorem 3.5 has the following corollary.

Corollary 3.6 Consider a graph H , $v \in V(H)$ and an integer $d > 1$. Denote by v_i the copy of v in the i -th copy of H in $G_d(H, v)$ and by d_v the degree of v in H .

(1) If $d = 2$, then

$$GA_1(G_d(H, v)) = d GA_1(H) + 1 + 2W(v_1).$$

(2) If $d \geq 3$, then

$$GA_1(G_d(H, v)) = d GA_1(H) + d - 3 + 2W(v_1) + (d - 2)W(v_2) + \frac{4\sqrt{(d_v + 1)(d_v + 2)}}{2d_v + 3}.$$

Proof We prove first the case (2). Note that $Z(v_1 v_2) = Z(v_{d-1} v_d) = \frac{2\sqrt{(d_v+1)(d_v+2)}}{2d_v+3} - 1$ and $Z(v_i v_{i+1}) = 1 - 1 = 0$ for every $i \in \{2, 3, \dots, d - 2\}$. Theorem 3.5 gives

$$\begin{aligned} GA_1(G_d(H, v)) &= d GA_1(H) + d - 1 + \sum_{i=1}^d W(v_i) + \sum_{i=1}^{d-1} Z(v_i v_{i+1}) \\ &= d GA_1(H) + d - 1 + 2W(v_1) + (d - 2)W(v_2) \\ &\quad + Z(v_1 v_2) + Z(v_{d-1} v_d) \\ &= d GA_1(H) + d - 1 + 2W(v_1) + (d - 2)W(v_2) \\ &\quad + \frac{4\sqrt{(d_v + 1)(d_v + 2)}}{2d_v + 3} - 2. \end{aligned}$$

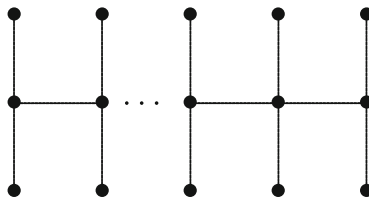
In case (1) we have $\mathcal{Z} = \{v_1 v_2\}$ and $Z(v_1 v_1) = 1 - 1 = 0$, and so the previous argument gives the formula. \square

Example 3.7 As an application of the previous result, we consider $k \geq 3$, $d \geq 3$ and the bridge graph $G_d(P_k, w_1)$, where P_k is the path graph with vertices w_1, w_2, \dots, w_k . Corollary 3.6 gives

$$\begin{aligned} GA_1(G_d(P_k, w_1)) &= d GA_1(P_k) + d - 3 + 2W(v_1) + (d - 2)W(v_2) \\ &\quad + \frac{4\sqrt{(d_v + 1)(d_v + 2)}}{2d_v + 3} \\ &= \left(k - 3 + \frac{4\sqrt{2}}{3}\right)d + d - 3 + 2\left(1 - \frac{2\sqrt{2}}{3}\right) \\ &\quad + (d - 2)\left(\frac{2\sqrt{3}}{4} - \frac{2\sqrt{2}}{3}\right) + \frac{4\sqrt{6}}{5} \\ &= \left(k - 2 + \frac{2\sqrt{2}}{3} + \frac{\sqrt{3}}{2}\right)d - 1 - \sqrt{3} + \frac{4\sqrt{6}}{5}. \end{aligned}$$

Example 3.8 Polyethene. For $d \geq 3$, consider the bridge graph $G_d(P_3, w_2)$. Note that $G_4(P_3, w_2)$ is the graph corresponding to Polyethene. Corollary 3.6 gives

$$\begin{aligned} GA_1(G_d(P_3, w_2)) &= d GA_1(P_3) + d - 3 + 2W(v_1) + (d - 2)W(v_2) \\ &\quad + \frac{4\sqrt{(d_v + 1)(d_v + 2)}}{2d_v + 3} \\ &= \frac{4\sqrt{2}}{3}d + d - 3 + 2\left(2\left(\frac{2\sqrt{3}}{4} - \frac{2\sqrt{2}}{3}\right)\right) \\ &\quad + (d - 2)\left(2\left(\frac{2\sqrt{4}}{5} - \frac{2\sqrt{2}}{3}\right)\right) + \frac{4\sqrt{12}}{7} \\ &= \frac{13}{5}d - \frac{31}{5} + \frac{22\sqrt{3}}{7}. \end{aligned}$$



$G_d(P_3, w_2)$ (Polyethene when $d = 4$).

Note that in the previous results we have used always T-decompositions. We deal now with a class of graphs obtained by decompositions which are not T-decompositions.

Let $\{G_i\}_{i=1}^d$ ($d \geq 3$) be a set of finite pairwise disjoint graphs and $v_i \in V(G_i)$. The circle graph $F(G_1, G_2, \dots, G_d) = F(G_1, G_2, \dots, G_d; v_1, v_2, \dots, v_d)$ of $\{G_i\}_{i=1}^d$ with respect to the vertices $\{v_i\}_{i=1}^d$ is the graph obtained from the graphs G_1, \dots, G_d by connecting the vertices v_i and v_{i+1} by an edge for every $i \in \{1, 2, \dots, d\}$, where v_{d+1} is defined as $v_{d+1} = v_1$. Theorem 2.1 has the following consequence.

Theorem 3.9 *Let $\{G_i\}_{i=1}^d$ be a set of finite pairwise disjoint graphs with $d \geq 3$ and $v_i \in V(G_i)$. Then*

$$GA_1(F(G_1, \dots, G_d; v_1, \dots, v_d)) = \sum_{i=1}^d GA_1(G_i) + d + \sum_{i=1}^d W(v_i) + \sum_{i=1}^d Z(v_i v_{i+1}).$$

Proof Consider the decomposition $\{G_1, \dots, G_d, v_1 v_2, \dots, v_d v_{d+1}\}$ of

$$F(G_1, \dots, G_d; v_1, \dots, v_d).$$

Since we have $\mathcal{W} = \{v_1, \dots, v_d\}$, $\mathcal{Z} = \{v_1 v_2, \dots, v_d v_{d+1}\}$ and $GA_1(v_i v_{i+1}) = 1$ for $i \in \{1, \dots, d\}$, Theorem 2.1 gives the result. □

Given any graph H , $v \in V(H)$ and an integer $d > 1$, let us define $F_d(H, v) = F(H, \dots, H; v, \dots, v)$, where H appears d times. Theorem 3.9 has the following corollary.

Corollary 3.10 *Consider a graph H , $v \in V(H)$ and an integer $d \geq 3$. Denote by v_1 the copy of v in the first copy of H in $F_d(H, v)$. Then*

$$GA_1(F_d(H, v)) = d GA_1(H) + d + d W(v_1).$$

Proof Note that $Z(v_i v_{i+1}) = 1 - 1 = 0$ for every $i \in \{1, \dots, d\}$. Theorem 3.9 gives

$$GA_1(F_d(H, v)) = d GA_1(H) + d + \sum_{i=1}^d W(v_i) + \sum_{i=1}^d Z(v_i v_{i+1}) = d GA_1(H) + d + d W(v_1).$$

□

Let $\{G_i\}_{i=1}^d$ be a set of finite pairwise disjoint graphs and $v_i \in V(G_i)$. The bouquet $S(G_1, G_2, \dots, G_d) = S(G_1, G_2, \dots, G_d; v_1, v_2, \dots, v_d)$ of $\{G_i\}_{i=1}^d$ with respect to the vertices $\{v_i\}_{i=1}^d$ is the graph obtained from the graphs G_1, \dots, G_d by identifying the vertices $\{v_i\}_{i=1}^d$ with a new vertex v . Theorem 2.1 has the following consequence.

Theorem 3.11 Let $\{G_i\}_{i=1}^d$ be a set of finite pairwise disjoint graphs and $v_i \in V(G_i)$. Then $GA_1(S(G_1, \dots, G_d; v_1, \dots, v_d)) = \sum_{i=1}^d GA_1(G_i) + W(v)$.

Proof Consider the T-decomposition $\{G_1, \dots, G_d\}$ of $S(G_1, \dots, G_d; v_1, \dots, v_d)$. Note that we have in this case $\mathcal{W} = \{v\}$ and so $\mathcal{Z} = \emptyset$. Hence, Theorem 2.1 gives the result. \square

Given any graph H , $v \in V(H)$ and an integer $d > 1$, let us define

$$S_d(H, v) = S(H, \dots, H; v, \dots, v),$$

where H appears d times. Theorem 3.11 has the following corollary.

Corollary 3.12 Consider a graph H , $v \in V(H)$ and an integer $d > 1$. Denote by d_v the degree of v in H . Then

$$GA_1(S_d(H, v)) = d \left(GA_1(H) + \sum_{u \in N_H(v)} \frac{2\sqrt{d} d_u d_v}{d_u + d} - \sum_{u \in N_H(v)} \frac{2\sqrt{d_u d_v}}{d_u + d_v} \right).$$

Proof Since $\mathcal{W} = \{v\}$, we have $N_H(v) \setminus \mathcal{W} = N_H(v)$. Each copy of H contributes to $W(v)$ with

$$\sum_{u \in N_H(v)} \frac{2\sqrt{d} d_u d_v}{d_u + d} - \sum_{u \in N_H(v)} \frac{2\sqrt{d_u d_v}}{d_u + d_v},$$

and so Theorem 3.11 gives the result. \square

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