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Computing Topological Indices by Pulling a Few Strings

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Abstract

A thread in a graph G is any maximal connected subgraph induced by a set of vertices of degree 2 in G. A string in G is a subgraph induced by a thread and the vertices adjacent to it. A graph G consists of s strings if it can be represented as a union of s strings so that any two strings have at most two vertices in common. In this paper we compute several recently introduced graph invariants for all graphs that consist of at most three strings.

1 Introduction

A topological index is a numerical quantity related to a graph and invariant under graph automorphisms. Hundreds of topological indices have been studied and used in structure-property relationship studies over the course of several decades, and the new ones have been constantly introduced.

In order to be useful, topological indices must somehow encode the information about structural properties of the underlying graph. Most of them do it in a quite intricate manner. Besides making them useful, such intricacies usually make them difficult (or at least not easy) to compute. In particular, nice closed formulas are usually available only for very narrow classes of graphs. Typical examples are complete graphs, complete bipartite graphs, cycles, paths, stars and some other special trees. Sometimes it is also possible to use the symmetry-related properties of graphs to obtain closed formulas, but such graphs are only of limited interest.

The main goal of this paper is to consider a class of graphs that admit decomposition in a small number of path- or cycle-like structures that we call strings. We follow the idea of a paper by Lukovits [18], where he computed Wiener indices for such graphs. Our main results are explicit formulas for values of several recently introduced topological indices for the considered graphs.

2 Definitions and preliminaries

All graphs considered here are finite and simple. Also, as most of the considered invariants are connectivity-related, we assume the graphs to be connected unless explicitly stated otherwise.

Let G be a graph on p vertices. The vertex and the edge set of G are denoted by $V(G)$ and $E(G)$, respectively. A **thread** in G is any maximal connected subgraph induced by a set of vertices of degree 2 in G. It is clear from the definition that a thread can have at most two other vertices of G adjacent to it. A (sub)graph induced by a thread and the vertices adjacent to it is called a **string**. Any string in G is either an induced path or an induced cycle in G. The converse is not generally true - an induced cycle in G with at least two vertices of degree greater than two is not a string. The **length** of a string is the number of edges in it.

Every edge from $E(G)$ incident to a vertex of degree 2 in G belongs to one (and only one) string in G, and the length of that string is at least 2. In order to allow the length of a string to achieve its natural minimum value of 1, we consider the edges of G connecting two vertices of degree other than two as strings of length 1. Those strings are special, since they do not contain threads as subgraphs. Hence we call them **trivial**. Besides minimizing the length function, trivial strings allow for a decomposition of any graph into a finite union of strings; in the worst case, there will be exactly $|E(G)|$ strings in the decomposition. Such decompositions are somewhat similar to ear decompositions from the structural theory of matchings [17]; there are, however, enough differences to justify the use of different terminology.

We say that a graph G consists of s strings if it can be decomposed into s strings so that any two strings have at most two vertices in common. Of special interest are the cases when s is small with respect to the number of vertices or edges of G; it implies that most strings are non-trivial. In the extreme case $s = 1$, G is either a path or a cycle, and this, together with the number of vertices, gives us complete information on G. In general, the smaller s, the more information on G is packed into its string decomposition. Our goal here is to investigate how that information can be converted into information about the values of certain topological indices of such graphs.

Up to our best knowledge, the first attempt on a systematic investigation of topological indices of graphs consisting of a few strings was made in a paper by Lukovits [18]. There he considered graphs consisting of at most three strings and presented explicit formulas for the values of Wiener index of such graphs in terms of lengths of the strings. The eight classes of graphs considered in his paper are shown in Fig. 1.

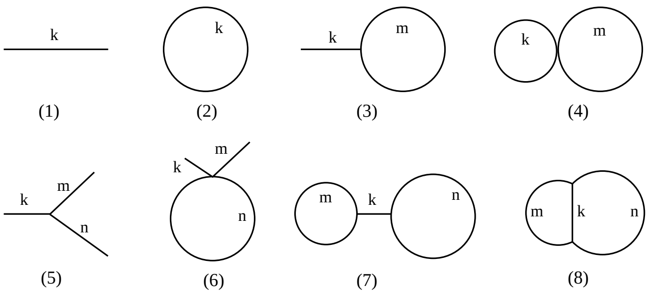

Figure 1: Graphs from Lukovits' paper including at most three strings.

In this paper we take further the line of research of reference [18] by considering two more classes of graphs (shown in Fig. 2). Together with eight classes of Lukovits' paper they exhaust the graphs consisting of at most three strings. We then proceed to compute and present explicit formulas for the values of several topological indices (the eccentric connectivity index, the reverse Wiener index, the geometric-arithmetic index, two connectivity indices and two Zagreb indices) for all graphs consisting of at most three strings in terms of the string lengths.

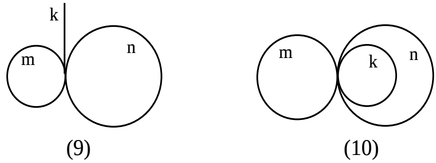

Figure 2: Two more graphs with three strings.

It is clear from the above illustrations that for a given number of vertices there are exactly two graphs that are single strings. Further, for any given pair of meaningful lengths there are exactly two graphs consisting of two strings. (Here we consider length of a cycle meaningful if it is at least three.) Finally, for any three (meaningful) lengths there are six graphs consisting of three strings with given lengths. In order to avoid notational overcrowding we will suppress the length parameters in our notation, and denote the considered graphs by G_i, where i is the number that appears in the parenthesis below the graph in Fig. 1 or Fig. 2. Hence, through the rest of the paper, G_1 denotes a path of length k, G_4 denotes two cycles of length k and m spliced in one vertex, and G_5 denotes three paths of lengths k, m and n spliced together in one of their respective endvertices. Further, whenever referring to the strings of the same type, we assume that the lengths (weakly) increase with the lexicographic order of the corresponding notational parameter. For example, we assume $k \leq m$ in G_4, G_6 and $k \leq m \leq n$ in G_5, G_8 and G_{10}. Similarly, we take $m \leq n$ in G_7 and G_9, but do not make any assumptions about the relationship of either of them with k. Those notational conventions will enable us to formulate results in a more compact way. However, sometimes it will be necessary to refer to the values of the string lengths. In such cases we put the lengths in the superscripts in the alphabetic order. For example, $G_5^{1,1,n}$ denotes a graph of type (5) whose two path-like strings have length 1. Similarly, $G_9^{1,m,n}$ denotes a graph of type (9) whose path-like string is trivial.

In the rest of this section we define the topological indices considered in this paper.

For two vertices u and v of $V(G)$ their **distance** $d(u,v)$ is defined as the length of a shortest path connecting u and v in G. For a given vertex u of $V(G)$ its **eccentricity** $\varepsilon(u)$ is the largest distance between u and any other vertex v of G. Hence, $\varepsilon(u) = \max_{v \in V(G)} d(u,v)$. The maximum eccentricity over all vertices of G is called the **diameter** of G and denoted by $D(G)$; the minimum eccentricity among the vertices of G is called

radius of G and denoted by $R(G)$. The **eccentric connectivity index** $\xi(G)$ of a graph G is defined as

$$\xi(G) = \sum \delta_u \varepsilon(u),$$

where δ_u denotes the degree of vertex u, i. e., the number of its neighbors in G. The eccentric connectivity index was introduced by Madan *et al* and employed in a series of QSAR/QSPR oriented papers over the last couple of years [13–15,19,20]. Its mathematical properties also attracted a lot of attention recently [1, 5–8, 12, 23].

The eccentric connectivity index belongs to a large family of distance-based indices. The most prominent of them, the Wiener index $W(G)$, is defined as the sum of distances between all pairs of distinct vertices,

$$W(G) = \sum_{u,v \in V(G)} d(u, v).$$

Introduced by H. Wiener [22] in 1947, it became one of the most used, the best researched and most generalized topological indices. The literature on Wiener index and its generalizations is vast; we refer the reader to [3, 4] for a survey of recent results concerning some classes of graphs of chemical interest. Among its many generalizations we consider here the reverse Wiener index, introduced in 2000 by Balaban *et al* [2]. The **reverse Wiener index** of a graph G is defined as

$$\Lambda(G) = \binom{p}{2} D(G) - W(G),$$

where $D(G)$ denotes the diameter of G.

The **geometric-arithmetic index** $GA(G)$ of a graph G is defined as

$$GA(G) = \sum_{uv \in E(G)} \frac{2\sqrt{\delta_u \delta_v}}{\delta_u + \delta_v}.$$

Here δ_u stands for the degree of a vertex u. It was introduced in a paper by Vukičević and Furtula [21]. A number of generalizations can be obtained by replacing degrees by any other numerical quantities associated with the endvertices of an edge. For some recent developments we refer the reader to [9, 24].

The **zeroth-order connectivity index** ${}^0\chi(G)$ and the **first-order connectivity index** ${}^1\chi(G)$ or simply the connectivity index (also called the **Randić index** [10, 16]) of the graph G are defined respectively as:

$$\begin{aligned} {}^0\chi(G) &= \sum_{v \in V(G)} (\delta_v)^{-\frac{1}{2}} \\ {}^1\chi(G) &= \sum_{uv \in E(G)} (\delta_u \delta_v)^{-\frac{1}{2}} \end{aligned}$$

The Randić index ${}^1\chi(G)$ is one of the most popular descriptors and has found numerous QSPR and QSAR applications. The quantity ${}^0\chi(G)$ has been also used to investigate structure-based correlations for physical properties.

The list of invariants considered in this paper is concluded by a pair of topological indices introduced some 30 years ago [11] under the name of Zagreb indices. The first $M_1(G)$ and the second $M_2(G)$ Zagreb index of a graph G are defined as follows.

$$\begin{aligned} M_1(G) &= \sum_{v \in V(G)} (\delta_v)^2 \\ M_2(G) &= \sum_{uv \in E(G)} \delta_u \delta_v \end{aligned}$$

3 Main results

3.1 Eccentric connectivity index

In this subsection we compute eccentric connectivity indices of graphs G_i, $1 \le i \le 10$. The first two cases were treated in earlier works [8, 23] and we quote the results without proofs.

Lemma 3.1

$$\xi(G_1) = \xi(P_k) = \begin{cases} \frac{3}{2}k^2 + \frac{1}{2} & \text{k is odd} \\ \frac{3}{2}k^2 & \text{k is even} . \end{cases}$$

Lemma 3.2

$$\xi(G_2) = \xi(C_k) = \begin{cases} k^2 & \text{k is even} \\ k(k-1) & \text{k is odd} . \end{cases}$$

Most of the results that follow are obtained by straightforward calculations. As a rule, we omit the computational details and proofs.

Lemma 3.3

$$\xi(G_3) = \begin{cases} \begin{cases} \frac{5m^2+20mk+12k^2+4}{8} & \text{m is even, } \frac{2k+m}{2} \text{ is odd} \\ \frac{5m^2-2m-3+20mk-4k+12k^2}{8} & \text{m is odd, } \frac{2k+m-1}{2} \text{ is even} \\ \frac{5m^2+20mk+12k^2}{8} & \text{m, } \frac{2k+m}{2} \text{ are even} \\ \frac{5m^2-2m+1+20mk-4k+12k^2}{8} & \text{m, } \frac{2k+m-1}{2} \text{ are odd} \end{cases} & \lfloor \frac{m}{2} \rfloor \le k \\ \begin{cases} 3k^2+mk+m^2 & \text{m is even} \\ 3k^2+mk+k-m+m^2 & \text{m is odd} \end{cases} & \lfloor \frac{m}{2} \rfloor > k \end{cases}$$

Proof

We consider two cases. If $\lfloor \frac{m}{2} \rfloor \leq k$, then

$$\xi(G_3) = \xi(P_{k+\lfloor \frac{m}{2} \rfloor+1}) + \begin{cases} \frac{m^2}{4} + mk & \text{m is even} \\ \frac{(m-1)^2}{4} + mk + m + k - 1 & \text{m is odd} \end{cases}.$$

On the other hand, if $\lfloor \frac{m}{2} \rfloor > k$ we have:

$$\xi(G_3) = \begin{cases} 3(k^2-1) + mk + m^2 + 3 & \text{m is even} \\ 3(k^2-1) + mk + k + m + (m-1)^2 + 2 & \text{m is odd} \end{cases}$$

This completes the proof. ∎

Lemma 3.4

$$\xi(G_4) = \begin{cases} m^2 + mk + k^2 & \text{m, k are even} \\ m^2 - 1 + k^2 + mk - m - k & \text{m, k are odd} \\ m^2 + k^2 - k + mk & \text{k is odd and m is even} \\ m^2 + k^2 - m + mk & \text{m is odd and k is even} \end{cases}$$

Lemma 3.5

$$\xi(G_5) = \begin{cases} \frac{3n^2+6mn+3m^2+4kn+2k^2+1}{2} & \text{m + n + 1 is even} \\ \frac{3}{2}(m+n)^2 + (2n+k)k & \text{m + n + 1 is odd} \end{cases}$$

Proof

It is easy to see that $G_5 - E(P_k) = P_{m+n+1}$. Hence,

$$\begin{aligned} \xi(G_5) &= \sum_{i=1}^{m+n+k+1} \delta v_i \varepsilon(v_i) = \sum_{i=1}^{m+n+1} \delta v_i \varepsilon(v_i) \\ &+ \sum_{i=m+n+2}^{m+n+k+1} \delta v_i \varepsilon(v_i) + n \\ &= \xi(P_{m+n+1}) + 2n + k + 2((n+1) + (n+2) + \ldots + (n+k-1)). \end{aligned}$$

The claim now follows by lemma 3.1. ∎

Lemma 3.6

$$\xi(G_6) = \begin{cases} \xi(G_3^{m,n}) + k(2\lfloor \frac{n}{2} \rfloor + k) & k \leq m < \lfloor \frac{n}{2} \rfloor \\ \xi(G_3^{m,n}) + k(2m + k) & k \leq \lfloor \frac{n}{2} \rfloor \leq m \\ \begin{cases} \xi(P_{m+k}) + \frac{n(n+4m)}{2} & \text{n is even} \\ \xi(P_{m+k}) + \frac{n^2+4mn-1}{2} & \text{n is odd} \end{cases} & \lfloor \frac{n}{2} \rfloor \leq k \leq m \end{cases}$$

Lemma 3.7 *For G_7 we distinguish two cases.*

(A). *If $\lfloor \frac{n}{2} \rfloor \leq k + \lfloor \frac{m}{2} \rfloor$ then*

$$\xi(G_7) = \xi(P_{a+b+k}) + \begin{cases} \frac{1}{4}(m^2+n^2) + mn + mk + kn & \text{m, n are even} \\ \frac{n^2+2n+4nm+4nk-10+2m+8k+m^2+4mk}{4} & \text{m, n are odd} \\ \frac{n^2+4nm+4nk+m^2+4mk-3+4k+2m}{4} & \text{n even , m odd} \\ \frac{n^2+4nm+4nk+m^2+4mk-3+4k+2n}{4} & \text{n odd , m even} \end{cases}$$

(B). *If* $\lfloor \frac{n}{2} \rfloor > k + \lfloor \frac{n}{2} \rfloor$ *then*

$$\xi(G_7) = \begin{cases} n^2+nm+m^2+nk+4mk+3k^2 & \text{m, n are even} \\ n^2-n+nm-1-m+m^2+nk-k+4mk+3k^2 & \text{m, n are odd} \\ n^2+nm+m^2-m+nk+4mk-2k+3k^2 & \text{n even , m odd} \\ n^2+nm-n+m^2+nk+k+4mk+3k^2 & \text{n odd , m even} \end{cases}$$

Lemma 3.8

$$\xi(G_8) = \begin{cases} \begin{cases} R & \text{m, n are odd} \\ R+k-n-m-1 & \text{m, n are even} \\ R-n-2k & \text{n even and m odd} \\ R-k-m & \text{n odd and m even} \end{cases} & \text{k is odd} \\ \begin{cases} R+k-n-m-1 & \text{m, n are odd} \\ R & \text{m, n are even} \\ R-n-2k & \text{n is odd, m is even} \\ R-k-m & \text{m is odd, n is even} \end{cases} & \text{k is even} \end{cases}$$

Here $R = n^2 + 2nk + nm + m^2 + mk.$

Lemma 3.9

$$\xi(G_9) = \begin{cases} \xi(G_3^{k,n}) + \begin{cases} \frac{4mk+m^2}{2} & \text{m is even} \\ \frac{m^2+4mk-1}{2} & \text{m is odd} \end{cases} & \lfloor \frac{n}{2} \rfloor < k \\ \xi(G_3^{k,n}) + \begin{cases} \frac{2mn+m^2}{2} & \text{m, n even} \\ \frac{2mn+m^2-2m-1}{2} & \text{m, n odd} \\ \frac{2mn+m^2-1}{2} & \text{n even, m odd} \\ \frac{2mn+m^2-2m}{2} & \text{n odd, m even} \end{cases} & \lfloor \frac{m}{2} \rfloor \leq k \leq \lfloor \frac{n}{2} \rfloor \\ \xi(G_4^{m,n}) + \begin{cases} k(n+k) & \text{n is even} \\ k(n+k-1) & \text{n is odd} \end{cases} & k < \lfloor \frac{m}{2} \rfloor \end{cases}$$

Lemma 3.10

$$\xi(G_{10}) = \xi(G_4^{m,n}) + \begin{cases} \begin{cases} \frac{k^2+2kn}{2} & \text{n is even} \\ \frac{k^2+2kn-2k}{2} & \text{n is odd} \end{cases} & \text{k is even} \\ \begin{cases} \frac{k^2+2kn-1}{2} & \text{n is even} \\ \frac{k^2+2kn-2k-1}{2} & \text{n is odd} \end{cases} & \text{k is odd} \end{cases}$$

3.2 Reverse Wiener index

As mentioned before, the reverse Wiener index was introduced by Balaban in 2000 [2]. It is defined in terms of Wiener index and the diameter of a graph. Hence we start this subsection by computing the diameters of the graphs considered in this paper. The diameters are presented in Table I. We then proceed by combining them with Lukovits' results in order to obtain explicit formulas. Again, we omit most of the computational details.

G	$remark$	$\lvert V(G)\rvert$	$D(G)$
P_k		$k+1$	k
C_k		k	$\lfloor \frac{k}{2} \rfloor$
G_3		$k+m$	$\lfloor \frac{m}{2} \rfloor + k$
G_4		$k+m-1$	$\lfloor \frac{m}{2} \rfloor + \lfloor \frac{k}{2} \rfloor$
G_5	$k \le m \le n$	$k+m+n+1$	$m+n$
G_6	$k \le m$	$k+m+n$	$m + \lfloor \frac{n}{2} \rfloor$
G_7	$m \le n$	$k+m+n-1$	$\lfloor \frac{n}{2} \rfloor + \lfloor \frac{m}{2} \rfloor + k$
G_8	$k \le m \le n$	$k+m+n-1$	$\begin{cases} \frac{n+m}{2} & \text{m, n are even or odd} \\ \frac{n+m-1}{2} & \text{otherwise} \end{cases}$
G_9	$m \le n$	$k+m+n-1$	$\begin{cases} \lfloor \frac{n}{2} \rfloor + \lfloor \frac{m}{2} \rfloor & \text{k} \le \lfloor \frac{\text{m}}{2} \rfloor \\ k + \lfloor \frac{n}{2} \rfloor & \text{k} \ge \lfloor \frac{\text{m}}{2} \rfloor \end{cases}$
G_{10}	$k \le m \le n$	$k+m+n-2$	$\lfloor \frac{n}{2} \rfloor + \lfloor \frac{m}{2} \rfloor$

Table I

We start by quoting known results for paths and cycles.

Lemma 3.11 *Let C_k and P_k be a cycle and a path of length k.*

$$\Lambda(C_k) = \Lambda(G_2) = \begin{cases} \frac{k^2(k-2)}{8} & \text{k is even} \\ \frac{k(k-1)(k-3)}{8} & \text{k is odd} \end{cases}, \qquad \Lambda(P_k) = \Lambda(G_1) = \frac{k(k^2-1)}{3}.$$

The results for two-parameter graphs depend on the parity of the cycle length(s).

Lemma 3.12

$$\Lambda(G_3) = \begin{cases} \frac{8k^3+18k^2m-12k^2-30km+4k+3m^3+18m^2k-6m^2}{24} & \text{m is even} \\ \frac{8k^3+18k^2m-18k^2-42km+16k+3m^3+18m^2k-12m^2+9m}{24} & \text{m is odd} \end{cases}$$

$$\Lambda(G_4) = \begin{cases} \frac{k^3+4k^2m-4k^2+4m^2k-12km+m^3-4m^2+4k+4m}{8} & \text{k, m are even} \\ \frac{(k+m-4)(k^2-4k+3km-4m+m^2+3)}{8} & \text{k, m are odd} \\ \frac{k^3+4k^2m-6k^2+4m^2k-16km+m^3-6m^2+12k+11m-6}{8} & \text{otherwise} \end{cases}$$

Lemma 3.13 *Let us consider G_5 and G_6.*

If $k \le m \le n$, then

$$\begin{aligned} \Lambda(G_5) \ &= - \ \frac{1}{6}k^3 + \frac{1}{2}(km^2 - km + kn^2 - k^2 - kn) + \frac{1}{3}(m^3 + n^3 - k - n - m) \\ &+ \ 2kmn + m^2n + mn^2 \end{aligned}$$

If n is even and $k \le m$, then

$$\begin{aligned} \Lambda(G_6) \ &= \ \frac{1}{3}m^3 + \frac{1}{8}n^3 - \frac{1}{6}k^3 - \frac{1}{2}m^2 - \frac{1}{4}n^2 + \frac{3}{4}m^2n + \frac{3}{4}n^2m - \frac{1}{4}k^2n \\ &- \ \frac{3}{2}km - \frac{3}{4}kn - \frac{5}{4}mn + \frac{1}{2}km^2 + \frac{1}{4}kn^2 + \frac{3}{2}kmn + \frac{1}{6}k + \frac{1}{6}m \end{aligned}$$

If n is odd and $k \leq m$, then

$$\begin{aligned}\Lambda(G_6) &= \frac{1}{3}m^3 + \frac{1}{8}n^3 - \frac{1}{6}k^3 - \frac{3}{4}m^2 - \frac{1}{2}n^2 + \frac{3}{4}m^2n + \frac{3}{4}n^2m - \frac{1}{4}k^2n - \frac{1}{4}k^2 \\ &- 2km - \frac{5}{4}kn - \frac{7}{4}mn + \frac{1}{2}km^2 + \frac{1}{4}kn^2 + \frac{3}{2}kmn + \frac{2}{3}k + \frac{2}{3}m + \frac{3}{8}n\end{aligned}$$

Lemma 3.14 *For G_7 we distinguish three cases:*

(A) *m and n are even*

$$\begin{aligned}\Lambda(G_7) &= \frac{1}{8}(m^3 + n^3) + \frac{1}{3}k^3 - k^2 + \frac{1}{2}(m^2n + n^2m - n^2 - m^2 + m + n) \\ &- \frac{7}{4}km - \frac{7}{4}kn - \frac{3}{2}mn + \frac{3}{4}(km^2 + k^2m + kn^2 + k^2n) + kmn + \frac{2}{3}k\end{aligned}$$

(B) *m and n are odd*

$$\begin{aligned}\Lambda(G_7) &= -\frac{3}{2}(1 + k^2) + \frac{1}{8}(m^3 + n^3) + \frac{3}{4}(kn^2 + k^2n + km^2 + k^2m) - n^2 - m^2 \\ &- \frac{11}{4}(km + kn) - \frac{5}{2}mn + kmn + \frac{8}{3}k + \frac{1}{3}k^3 + \frac{19}{8}(m + n) + \frac{1}{2}(m^2n + n^2m)\end{aligned}$$

(C) *otherwise*

$$\begin{aligned}\Lambda(G_7) &= -\frac{3}{4}(1 + n^2 + m^2) + \frac{1}{8}(m^3 + n^3) + \frac{1}{3}k^3 - \frac{5}{4}k^2 + \frac{1}{2}(m^2n + n^2m) + kmn \\ &- \frac{9}{4}(km + kn) - 2mn + \frac{3}{4}(km^2 + k^2m + kn^2 + k^2n) + \frac{5}{3}k + \frac{3}{2}m + \frac{11}{8}n\end{aligned}$$

Lemma 3.15 *For G_8 we have four cases:*

(A) *k, m and n are all even or all odd.*

$$\begin{aligned}\Lambda(G_8) &= \frac{1}{8}(n^3 + m^3 + mk^2 + nk^2 + kn^2 + km^2) - \frac{1}{4}(k^3 + km + nk) \\ &+ \frac{1}{2}(mn^2 + nm^2 - n^2 - m^2 + m + n + kmn) - \frac{3}{2}mn\end{aligned}$$

(B) *m, k are odd and n is even or m, k are even and n is odd.*

$$\begin{aligned}\Lambda(G_8) &= \frac{1}{8}(n^3 + m^3 + mk^2 + nk^2 + km^2 + kn^2) - \frac{1}{4}(k^3 + k^2) + \frac{1}{2}(mn^2 + m^2n) \\ &- \frac{3}{4}(mk + nk + n^2 + m^2 + 1) - 2mn + \frac{1}{2}knm + \frac{11}{8}n + \frac{3}{2}m + \frac{7}{8}k\end{aligned}$$

(C) *k, n are odd and m is even or k, n are even and m is odd.*

$$\begin{aligned}\Lambda(G_8) &= \frac{1}{8}(n^3 + m^3 + mk^2 + nk^2 + km^2 + kn^2) + \frac{1}{2}(mn^2 + m^2n + kmn) \\ &+ \frac{3}{2}n + \frac{7}{8}k + \frac{11}{8}m - 2nm - \frac{1}{4}(k^3 + k^2) - \frac{3}{4}(n^2 + m^2 + km + kn + 1)\end{aligned}$$

(D) *m, n are even and k is odd or m, n are odd and k is even.*

$$\begin{aligned}\Lambda(G_8) &= \frac{1}{8}(m^3+n^3+mk^2+nk^2+m^2k+n^2k)-\frac{1}{4}(k^3+k+mk+nk)\\ &+ \frac{7}{8}(m+n)-\frac{1}{2}(n^2+m^2-mn^2-m^2n-kmn+1)-\frac{3}{2}mn\end{aligned}$$

Graph G_9 is the most complicated, since we have to take care of many possible combinations of parities of cycle lengths and their relationships with the length of the path part.

Lemma 3.16 *For G_9 we have two cases, each of them with four subcases:*

(A) $k \le \lfloor \frac{m}{2} \rfloor$

If m and n are even then

$$\begin{aligned}\Lambda(G_9) &= -\frac{1}{6}k^3+\frac{1}{2}nm^2+\frac{1}{4}km^2+\frac{1}{2}m+\frac{1}{2}k^2-\frac{1}{2}n^2+\frac{1}{8}n^3+\frac{1}{8}m^3+\frac{1}{2}n+mnk\\ &+ \frac{2}{3}k+\frac{1}{2}mn^2-\frac{1}{2}m^2-\frac{3}{2}mn-\frac{5}{4}mk-\frac{5}{4}nk-\frac{1}{4}(nk^2+mk^2-kn^2)\end{aligned}$$

If m and n are odd then

$$\begin{aligned}\Lambda(G_9) &= -\frac{1}{6}k^3+\frac{1}{2}nm^2+\frac{19}{8}(m+n)-(n^2+m^2)+\frac{1}{8}(n^3+m^3)+\frac{8}{3}k+mnk\\ &+ \frac{1}{2}mn^2-\frac{5}{2}mn-\frac{9}{4}(mk+nk)-\frac{1}{4}(nk^2+mk^2-kn^2-km^2)-\frac{3}{2}\end{aligned}$$

If m is even and n is odd then

$$\begin{aligned}\Lambda(G_9) &= -\frac{1}{6}k^3+\frac{1}{2}nm^2+\frac{3}{2}m+\frac{11}{8}n-\frac{3}{4}(n^2+m^2)+\frac{1}{8}(n^3+m^3)+\frac{5}{3}k+mnk\\ &+ \frac{1}{2}mn^2-2mn-\frac{7}{4}(mk+nk)-\frac{1}{4}(nk^2+mk^2-kn^2-km^2-k^2)-\frac{3}{4}\end{aligned}$$

If n is even and m is odd then

$$\begin{aligned}\Lambda(G_9) &= -\frac{1}{6}k^3+\frac{1}{2}nm^2+\frac{3}{2}n+\frac{11}{8}m-\frac{3}{4}(n^2+m^2)+\frac{1}{8}(n^3+m^3)+\frac{5}{3}k+mnk\\ &+ \frac{1}{2}mn^2-2mn-\frac{7}{4}(mk+nk)-\frac{1}{4}(nk^2+mk^2-kn^2-km^2-k^2)-\frac{3}{4}\end{aligned}$$

(B) $k \ge \lfloor \frac{m}{2} \rfloor$

If m and n are even then

$$\begin{aligned}\Lambda(G_9) &= \frac{1}{3}k^3+\frac{1}{4}km^2-k^2-\frac{1}{2}n^2+\frac{1}{8}n^3-\frac{1}{8}m^3+\frac{1}{2}n+\frac{3}{2}mnk+\frac{1}{2}mk^2\\ &+ \frac{5}{3}k+\frac{1}{4}mn^2+\frac{1}{4}m^2-\frac{3}{4}mn-2mk-\frac{11}{4}nk+\frac{3}{4}(nk^2+kn^2)\end{aligned}$$

If m and n are odd then

$$\begin{aligned}\Lambda(G_9) &= \frac{1}{3}k^3+\frac{1}{4}km^2-\frac{5}{4}k^2-\frac{3}{4}n^2+\frac{1}{8}n^3-\frac{1}{8}m^3+\frac{13}{8}n+\frac{3}{2}mnk+\frac{1}{2}mk^2\\ &+ \frac{35}{12}k+\frac{9}{8}m+\frac{1}{4}mn^2-\frac{5}{4}mn-\frac{5}{2}mk-\frac{13}{4}nk+\frac{3}{4}(nk^2+kn^2)-1\end{aligned}$$

If m is even and n is odd then

$$\begin{aligned}\Lambda(G_9) &= \frac{1}{3}k^3+\frac{1}{4}km^2-k^2-\frac{1}{2}n^2+\frac{1}{8}n^3-\frac{1}{8}m^3+\frac{5}{8}n+\frac{3}{2}mnk+\frac{1}{2}mk^2+\frac{1}{4}m^2\\ &+ \frac{23}{12}k+\frac{1}{4}m+\frac{1}{4}mn^2-\frac{3}{4}mn-2mk-\frac{11}{4}nk+\frac{3}{4}(nk^2+kn^2)-\frac{1}{4}\end{aligned}$$

If n is even and m is odd then

$$\begin{aligned}\Lambda(G_9) &= \frac{1}{3}k^3+\frac{1}{4}km^2-\frac{5}{4}k^2-\frac{3}{4}n^2+\frac{1}{8}n^3-\frac{1}{8}m^3+\frac{3}{2}(n+mnk)+\frac{1}{2}mk^2\\ &+ \frac{8}{3}k+\frac{7}{8}m+\frac{1}{4}mn^2-\frac{5}{4}mn-\frac{5}{2}mk-\frac{13}{4}nk+\frac{3}{4}(nk^2+kn^2)-\frac{3}{4}\end{aligned}$$

Lemma 3.17

$$\Lambda(G_{10}) = \begin{cases} \begin{cases} R & \text{m, n are even} \\ S & \text{m, n are odd} \\ T & \text{m is even, n is odd} \\ T+\frac{n-m}{8} & \text{m is odd, n is even} \end{cases} & \text{k is even} \\ \begin{cases} R+\frac{2n+2m+k-4}{8} & \text{m, n are even} \\ S+\frac{2n+2m+k-4}{8} & \text{m, n are odd} \\ T+\frac{2n+2m+k-4}{8} & \text{m is even, n is odd} \\ T+\frac{3n+m+k-4}{8} & \text{m is odd, n is even} \end{cases} & \text{k is odd} \end{cases}$$

Here

$R = \frac{(m^3+n^3-k^3)+2(km^2-3n^2+kn^2-3m^2-5mk-5nk)+4(nm^2+3m+k^2+3n+mn^2-5mn)+8mnk}{8}$

$S = \frac{(m^3+n^3-k^3+35m+35n)+2(km^2-5n^2+kn^2-5m^2-9mk-9nk)+4(nm^2+mn^2-7mn)+8(3k+mnk-4)}{8}$

$T = \frac{(m^3+n^3-k^3+23n)+2(km^2+k^2+kn^2-7mk-7nk)+4(nm^2+3k+mn^2)+8(-m^2+3m-3mn+mnk-2)}{8}$.

3.3 Geometric - arithmetic index

Since the majority of edges in our graphs are in threads, and hence have both ends of degree two, their contributions to the geometric-arithmetic index will be, in most cases, equal to one. Hence the values of the geometric-arithmetic indices will be, on average, close to the number of edges, and the deviations will be determined by the number and type of the out-of-thread edges. Further deviations arise when some of the threads are trivial. In order to emphasize the deviations, we express $GA(G_i)$ in terms of the number of edges q, which is equal to the sum of lengths of all strings in G_i.

All results of this subsection follow by a straightforward calculation. Hence we present them omitting the details and proofs.

Proposition 3.18 *Let q denote the number of edges in G_i. Then*

(1) $GA(G_1) = q - 2 + \frac{4\sqrt{2}}{3}$; $GA(G_1^1) = 1$.

(2) $GA(G_2) = q$.

(3) $GA(G_3) = q - 4 + \frac{6\sqrt{6}}{5} + \frac{2\sqrt{2}}{3}$; $GA(G_3^{1,m}) = q - 3 + \frac{4\sqrt{6}}{5} + \frac{\sqrt{3}}{2}$.

(4) $GA(G_4) = q - 4 + \frac{8\sqrt{2}}{3}$.

(5) $GA(G_5) = q - 6 + \frac{6\sqrt{6}}{5} + 2\sqrt{2}$; $GA(G_5^{1,m,n}) = q - 5 + \frac{4\sqrt{6}}{5} + \frac{4\sqrt{2}}{3}\frac{\sqrt{3}}{2}$; $GA(G_5^{1,1,n}) = q - 4 + \frac{2\sqrt{6}}{5} + \frac{2\sqrt{2}}{3} + \sqrt{3}$; $GA(G_5^{1,1,1}) = \frac{3\sqrt{3}}{2}$.

(6) $GA(G_6) = q - 6 + 4\sqrt{2}$; $GA(G_6^{1,m,n}) = q - \frac{21}{5} + \frac{8\sqrt{2}}{3}$; $GA(G_6^{1,1,n}) = q - \frac{12}{5} + \frac{4\sqrt{2}}{3}$.

(7) $GA(G_7) = q - 6 + \frac{12\sqrt{6}}{5}$; $GA(G_7^{1,m,n}) = q - 4 + \frac{8\sqrt{6}}{5}$.

(8) $GA(G_8) = q - 6 + \frac{12\sqrt{6}}{5}$; $GA(G_8^{1,m,n}) = q - 4 + \frac{8\sqrt{6}}{5}$.

(9) $GA(G_9) = q - 6 + \frac{10\sqrt{10}}{7} + \frac{2\sqrt{2}}{3}$; $GA(G_9^{1,m,n}) = q - 5 + \frac{8\sqrt{10}}{7} + \frac{\sqrt{5}}{3}$.

(10) $GA(G_{10}) = q - 6 + 3\sqrt{3}$.

A few things are immediately obvious from the above formulas. First, we note that among the graphs with at most three strings the geometric-arithmetic index assumes rational values only on cycles and on the trivial string K_2. Further, the index is quite discriminative on the considered class of graphs; given the number of edges, the graph type can be in most cases reconstructed from the index value. The only exceptions are G_7 and G_8. The same two graphs also show anomalous behavior with respect to the deviations of $GA(G)$ from q. Namely, the quantity $q - GA(G_i)$ introduces an ordering into the set of ten graph classes considered here. Its numerical values range from 0 for G_2 and 0.11438 for G_1 to 0.53965 for G_9 and 0.80385 for G_{10}, and, for the most part, agree with an intuitive sense of complexity of the graphs. (We have restricted our attention only on the graphs without trivial strings.) If we agree that $G_i \leq G_j$ means $q - GA(G_i) \leq q - GA(G_j)$, we can write

$$G_2 \leq G_1 \leq G_3 \leq G_7 = G_8 \leq G_4 \leq G_5 \leq G_6 \leq G_9 \leq G_{10}.$$

This supports the conclusion that the geometric-arithmetic index measures both diversity of edge types and a disparity of their end-vertices.

3.4 Connectivity indices

The results for the connectivity indices have a similar flavor as those for the geometric-arithmetic index. For example, all of them (with two trivial exceptions) contain irrationalities and they do not distinguish between G_7 and G_8. That is the reason we present them next.

Proposition 3.19 *Let G_i be graphs in figures 1 and 2. Then*

(1) ${}^0\chi(G_1) = 2 + \frac{\sqrt{2}}{2}(k-1);$
${}^1\chi(G_1) = \sqrt{2} - 1 + \frac{1}{2}k;\ {}^1\chi(G_1^1) = 1.$

(2) ${}^0\chi(G_2) = \frac{\sqrt{2}}{2}k;$
${}^1\chi(G_2) = \frac{1}{2}k.$

(3) ${}^0\chi(G_3) = 1 + \frac{\sqrt{3}}{3} + \frac{\sqrt{2}}{2}(k+m-2);$
${}^1\chi(G_3) = -2 + \frac{\sqrt{2}+\sqrt{6}}{2} + \frac{1}{2}(k+m);\ {}^1\chi(G_3^{1,m}) = \frac{\sqrt{3}+\sqrt{6}}{3} + \frac{m-2}{2}.$

(4) ${}^0\chi(G_4) = \frac{1}{2} + \frac{\sqrt{2}}{2}(k+m-2);$
${}^1\chi(G_4) = -2 + \sqrt{2} + \frac{1}{2}(k+m).$

(5) ${}^0\chi(G_5) = 3 + \frac{\sqrt{3}}{3} + \frac{\sqrt{2}}{2}(k+m+n-3);$
${}^1\chi(G_5) = -3 + \frac{3\sqrt{2}+\sqrt{6}}{2} + \frac{1}{2}(k+m+n);\ {}^1\chi(G_5^{1,m,n}) = \frac{3\sqrt{2}+\sqrt{3}+\sqrt{6}}{3} + \frac{m+n-4}{2};$
${}^1\chi(G_5^{1,1,n}) = \frac{4\sqrt{3}+\sqrt{6}+3\sqrt{2}}{6} + \frac{n-2}{2};\ {}^1\chi(G_5^{1,1,1}) = \sqrt{3}.$

(6) ${}^0\chi(G_6) = \frac{5}{2} + \frac{\sqrt{2}}{2}(k+m+n-3);$
${}^1\chi(G_6) = 2\sqrt{2} - 3 + \frac{1}{2}(k+m+n);\ {}^1\chi(G_6^{1,m,n}) = \frac{5\sqrt{2}-2}{4} + \frac{m+n}{2};$
${}^1\chi(G_6^{1,1,n}) = \frac{\sqrt{2}+n}{2}.$

(7) ${}^0\chi(G_7) = \frac{2\sqrt{3}}{3} + \frac{\sqrt{2}}{2}(k+m+n-3);$
${}^1\chi(G_7) = \sqrt{6} - 3 + \frac{1}{2}(k+m+n);\ {}^1\chi(G_7^{1,m,n}) = \frac{2\sqrt{6}-5}{3} + \frac{m+n}{2};$

(8) ${}^0\chi(G_8) =^0 \chi(G_7);$
${}^1\chi(G_8) =^1 \chi(G_7);\ {}^1\chi(G_8^{1,m,n}) =^1 \chi(G_7^{1,m,n});\ {}^1\chi(G_8^{1,1,n}) = \frac{\sqrt{6}-1}{3} + \frac{n}{2};$
${}^1\chi(G_8^{1,1,1}) = 1$

(9) ${}^0\chi(G_9) = \frac{5+\sqrt{5}}{5} + \frac{\sqrt{2}}{2}(k+m+n-3)$;
${}^1\chi(G_9) = \frac{\sqrt{2}+\sqrt{10}-6}{2} + \frac{1}{2}(k+m+n)$; ${}^1\chi(G_9^{1,m,n}) = \frac{\sqrt{5}+2\sqrt{10}-10}{5} + \frac{m+n}{2}$;

(10) ${}^0\chi(G_{10}) = \frac{\sqrt{6}}{6} + \frac{\sqrt{2}}{2}(k+m+n-3)$;
${}^1\chi(G_{10}) = \sqrt{3} - 3 + \frac{1}{2}(k+m+n)$

3.5 Zagreb Indices

The Zagreb indices exhibit somewhat larger degeneracy than the connectivity indices and the geometric-arithmetic index. For example, neither of them discriminates between G_6, G_7 and G_8.

Proposition 3.20 *Let G_i be graphs from figures 1 and 2.*

(1) $M_1(G_1) = 4k - 2$;
$M_2(G_1) = 4(k-1)$; $M_2(G_1^1) = 1$.

(2) $M_1(G_2) = M_2(G_2) = 4k$.

(3) $M_1(G_3) = 4(k+m) + 2$;
$M_2(G_3) = 4(k+m) + 4$;
$M_2(G_3^{1,m}) = 4m + 7$.

(4) $M_1(G_4) = 4(m+k+2)$;
$M_2(G_4) = 4(m+k+4)$.

(5) $M_1(G_5) = M_2(G_5) = 4(k+m+n)$;
$M_2(G_5^{1,m,n}) = 4(m+n) + 3$; $M_2(G_5^{1,1,n}) = 4n + 6$; $M_2(G_5^{1,1,1}) = 9$.

(6) $M_1(G_6) = 4(k+m+n) + 6$;
$M_2(G_6) = 4(k+m+n) + 12$;
$M_2(G_6^{1,m,n}) = 4(m+n) + 14$; $M_2(G_6^{1,1,n}) = 4n + 16$.

(7) $M_1(G_7) = M_1(G_6)$;
$M_2(G_7) = M_2(G_6)$; $M_2(G_7^{1,m,n}) = 4(m+n) + 17$;

(8) $M_1(G_8) = M_1(G_6)$;
$M_2(G_8) = M_2(G_6)$; $M_2(G_8^{1,m,n}) = M_2(G_7^{1,m,n})$; $M_2(G_8^{1,1,n}) = 4n + 22$;
$M_2(G_8^{1,1,1}) = 27$

(9) $M_1(G_9) = 4(k+m+n)+14$;
$M_2(G_9) = 4(k+m+n)+28$; $M_2(G_9^{1,m,n}) = 4(m+n)+29$;

(10) $M_1(G_{10}) = 4(k+m+n)+24$;
$M_2(G_{10}) = 4(k+m+n)+48$.

We see than the expressions for $M_1(G)$ have basically the same form as those for ${}^0\chi(G)$ for all considered graphs. This fact is readily explained by noticing that the only differences come from the vertices of degree 3 and more. Another consequence of this observation is that $M_1(G)$ and ${}^0\chi(G)$ will order our graphs (on the same number of edges) in roughly the opposite ways. Similar, but less pronounced, is the parallelism between ${}^1\chi(G)$ and $M_2(G)$ for the considered graphs.

4 Concluding remarks

In this paper we have presented explicit formulas for values of several important graph-theoretical invariants of graphs that consist of at most three strings. In spite of the simple description, this class contains many chemically interesting graphs. Hence, it could be worthwhile to continue this line of research by finding formulas for values of other chemically interesting invariants.

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