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Extremal Graphs with respect to the Modified First Zagreb Connection Index

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Abstract

Topological indices (TIs) have an important role in studying properties of molecules. A main problem in mathematical chemistry is finding extreme graphs with respect to a given TI. In this paper extremal graphs with respect to the modified first Zagreb connection index for trees, unicyclic graphs with or without a fixed girth and connected graphs are determined. These graphs are relevant since they are chemical graphs.

Keywords : *topological index, Zagreb indices, trees, unicyclic graphs*

1 Introduction

Molecular descriptors are numerical values that characterize different properties of molecules. They are used mainly in the construction of Quantitative Structure-Activity Relationship (QSAR) or Quantitative Structure-Property Relationship (QSPR) models to generate predictions about the biological activity or physico-chemical properties of new untested or even yet to be synthesized substances. Such models have an accuracy up to 90% in predicting the effects of different medicines on some species of parasites which cause a large number of deaths or viruses known for their aggressivity, like Hepatitis B and C, Cytomegalovirus and HIV-1 ([4, 5]). Moreover, these models provides new drugs much more active than those already existing on the market ([2]).

A special family of molecular descriptors is represented by the topological indices (TIs), invariants that characterize the topology of a graph, indicating its ramification. TIs are mainly studied in connection with chemical graphs, which are undirected, connected graphs that model organic compounds by considering only the carbon-carbon and carbon-hydrogen type atomic bonds. Analysed in this context, the TIs appeared from the desire of studying structural properties of chemical compounds. Since the structures of substances, even modelled as graphs, cannot be readily investigated as such, numerical quantities associated with these structures have to be considered for successful studies in this area ([2, 4, 5]). Thus TIs participate, along with other molecular descriptors, in the construction of QSAR or QSPR models that generate predictions about the biological activity or physico-chemical properties of new substances. Consequently, more and more topological indices are being introduced in the literature with the purpose of being used mainly in applications within different areas of chemistry.

One of the most important and intensely studied TIs are the Zagreb indices, introduced in [6] from the desire to examine the dependence of the total π -electron energy on the molecular structure. They are defined by

$$M_1(G) = \sum_{v \in V(G)} d_G(v)^2 \quad \text{and} \quad M_2(G) = \sum_{(u,v) \in E(G)} d_G(u)d_G(v),$$

where $G = (V(G), E(G))$ is a connected graph and $d_G(v)$ denotes the degree of the vertex v .

Starting from these, a whole family of Zagreb indices appeared, including the multiplicative Zagreb indices ([8]), the reformulated Zagreb indices ([9]) and the modified Zagreb connection index ([6]).

This class of indices has been used to study molecular complexity, chirality, *ZE*-isomerism, heterosystems and has been used with good results in QSAR and QSPR models. Thus, mathematical chemistry experts note that the best descriptor models considered in the literature contains the Zagreb M_2 -index. ([7])

An important direction in the field of mathematical chemistry is given by the determination of the extreme graphs with respect to a given TI. This field started with the leading article of Bollobás and Erdős ([3]), in which they determine the extremal graphs with respect to the Randić index, a well-known and intensely used in QSAR and QSPR models TI.

In this paper we study a modified Zagreb index introduced by Gutman and Trinajstić in [6], but studied for the first time in [1], and named the modified first Zagreb connection index:

$$ZC_1^*(G) = \sum_{v \in V(G)} d_G(v)\tau_G(v),$$

where $\tau_G(v)$ denotes the number of vertices at distance 2 from v , also called the connection number of v . The latter article determines the extremal graphs with respect to the $ZC_1^*(G)$ -index in the class of chemical trees (in which every vertex has degree at most four). In this paper we extend the above study by considering general trees and unicyclic graphs with given or arbitrary girth, all of them representing classes of graphs of interest for the field of mathematical chemistry, due to their topology that closely resembles molecular structures.

The main method used in determining the extremal graphs is defining graph transformations that, under certain conditions, strictly increase/decrease the value of the topological index. This leads us to the extremal graph(s) by the following principle: whenever a graph is not yet of the desired shape, there is a way to apply one of the transformations mentioned above to yield a new graph; since the class of graphs under investigation is finite, this process is finite; since the process gives the same end result regardless of the graph it starts with, it exhibits the extremal graph(s) of the class in question.

We propose a new method with higher degree of generality with respect to the transformation techniques usually used in such context. It allows to find transformations that strictly increases the index by seeing the graph as a result of join operations of subgraphs and study the changes in the index when replacing a subgraph with another. This is useful, since various types of decomposition of graphs exists in literature, such as block decompositions.

2 Results on graph operations and transformations

Let G, H be two connected graphs and consider one vertex from each graph: $a \in V(G)$, $b \in V(H)$. Denote by $(G, a) \odot (H, b)$ the graph obtained from the union of graphs G and H by identifying vertices a and b . Note that if a graph has cut vertices, it can be seen as a vertex-joins of its biconnected components.

For a graph G denote by $d(G)$ the set of the degrees of its vertices and, for a vertex $v \in V(G)$, by $s_G(v)$ the sum of the degrees of its neighbors. In order to determine the ZC_1^* -index for graphs obtained from vertex-join operations, we define the following constants:

$$\epsilon_n = \begin{cases} 4, & \text{if } n \geq 5, \\ 2, & \text{if } n = 4, \\ 0, & \text{if } n = 3. \end{cases} \quad \alpha_n = \begin{cases} 6, & \text{if } n \geq 5, \\ 5, & \text{if } n = 4, \\ 4, & \text{if } n = 3. \end{cases}$$

Lemma 1 *Let G, H be two connected graphs and two vertices $a \in V(G)$, $b \in V(H)$. Let $\Omega = (G, a) \odot (H, b)$. Then*

$$ZC_1^*(\Omega) = ZC_1^*(G) + ZC_1^*(H) + (s_G(a) + \tau_G(a))d_H(b) + d_G(a)(s_H(b) + \tau_H(b)).$$

Since for the classes of graphs considered in this paper are results of applying vertex-join operations on trees and cycles or of moving pendant edges from one vertex to another, we derive formulas for the case when one of the graphs is a path with one edge or a cycle.

Corollary 1 Let G, H be two connected graphs and two vertices $a \in V(G), b \in V(H)$. Let $\Omega = (G, a) \odot (H, b)$.

1. If $H \simeq P_2$, then $ZC_1^*(\Omega) = ZC_1^*(G) + d_G(a) + \tau_G(a) + s_G(a)$.

2. If $H \simeq C_n, n \geq 3$, then $ZC_1^*(\Omega) = ZC_1^*(G) + \epsilon_n n + \alpha_n d_G(a) + 2\tau_G(a) + 2s_G(a)$.

We define the following transformation on a connected graph G . If G contains a pendant edge yx with y of degree at least 2 (non-pendant) and u is a vertex of $G, u \neq y$ and $u \neq x$, define transformation t_1 through which we obtain the graph

$$t_1(G, yx, u) := G - yx + ux$$

by removing the pendant edge yx from y and attaching it to vertex u .

A similar transformation can be defined by removing a cycle C from a vertex y and attaching it to a vertex u . We calculate the effect of these transformations on $ZC_1^*(G)$ by seeing G and the obtained graph as results of vertex-join operations.

Lemma 2 Let G be a connected graph and t_1 the transformation defined above. Then

$ZC_1^*(t_1(G, yx, u)) - ZC_1^*(G) = (s_G(u) - s_G(y)) + (\tau_G(u) - \tau_G(y)) + (d_G(u) - d_G(y)) + 2\gamma_{G,y,u}$ where

$$\gamma_{G,y,u} = \begin{cases} 0, & \text{if } u \text{ and } y \text{ are adjacent,} \\ 1, & \text{otherwise.} \end{cases}$$

3 Trees

In [1] it is proven that, for $n \geq 5$, the path graph P_n has minimum ZC_1^* value among all trees with n vertices and this minimum value is $4n - 10$. In this section the trees with n vertices having maximum ZC_1^* value are determined. Let \mathcal{S}_n be the family of trees with n vertices and diameter at most 3. Note that the only trees in \mathcal{S}_n are the star and double stars.

Theorem 1 The trees with $n \geq 4$ vertices having the maximum value of modified first Zagreb connection index are the trees in \mathcal{S}_n and this value is $(n - 2)(n - 1)$.

Proof : For a tree $T \notin \mathcal{S}_n$ there are two vertices u, y at distance at least 2 in which are incident pendant edges denoted such that $s_T(u) \geq s_T(y)$. Consider the tree $T' = t_1(T, yx, u)$. By Lemma 2 we obtain $ZC_1^*(T') - ZC_1^*(T) = 2(s_T(u) - s_T(y)) + 2 > 0$ \square

4 Unicyclic graphs

A unicyclic graph is a connected graph containing exactly one cycle. Let $n \geq 5$ and $g < n$. In this section we consider first unicyclic graphs with n vertices and fixed girth g , that is having the length of the cycle equal to g .

Denote by $\mathcal{U}_{n,g}$ the family of unicyclic graphs with n vertices and girth g such that any two non-pendant vertices incident to pendant edges are adjacent vertices on the cycle.

Theorem 2 Let $n \geq 5$ and $g < n$. The unicyclic graphs with n vertices and girth g having the maximum value of modified first Zagreb connection index are the graphs in $\mathcal{U}_{n,g}$ and this value is $(n - g)^2 + (\alpha_g + 1)(n - g) + \epsilon_g g$.

Proof : Let $G \notin \mathcal{U}_{n,g}$. We construct a graph with higher index using previous results. More exactly, if there are in G two non-pendant vertices u, y both incident to at least one pendant edge, such that $d(u, y) \geq 2$ and $s_G(u) + d_G(u) + \tau_G(u) \geq s_G(y) + d_G(y) + \tau_G(y)$, we consider the graph $G' = t_1(G, yx, u)$. Otherwise the vertices of the cycle of G have degree 2, with one exception, a vertex denoted y . Then $G = (T_G, y) \odot (C_g, y)$ where T_G is a tree. In this case, we consider $G' = (S_{n-g}, a) \odot (C_g, y)$ where a is the center of star S_{n-g} (G' is obtained from G by replacing tree T_G rooted in y with star S_{n-g} rooted in the center). \square

Let G be a unicyclic graph and C its unique cycle. Note that the connected components of $G - E(C)$ are trees rooted in vertices belonging to C . In order to obtain unicyclic graphs with smaller ZC_1^* index we study the changes of this index when replacing such a component with paths (with the same number of vertices) rooted in one extremity. Moreover, if one such component is a path, consider the graph obtained by attaching this component to a pendant vertex of G instead of a vertex from cycle C . The following result holds.

Theorem 3 Let $n \geq 5$ and $g < n$. The unicyclic graph with n vertices and girth g having the minimum value of modified first Zagreb connection index is $T_{g,n-g} = (C_g, a) \odot (P_{n-g+1}, v)$, where v is a pendant vertex in P_{n-g+1} (the $(g, n-g)$ -tadpole graph). Moreover,

$$ZC_1^*(T_{g,n-g}) = \begin{cases} 4(n-g) + \epsilon_g g + \alpha_g, & \text{if } g \leq n-2, \\ \epsilon_g g + \alpha_g + 2, & \text{if } g = n-1. \end{cases}$$

We use the results on extremal unicyclic graph with fixed girth to study how the maximum and minimum value of ZC_1^* evolves when girth is variable, in particular to find the extremal unicyclic graphs with n vertices.

Theorem 4 Let $n \geq 5$.

1. The unicyclic graphs with n vertices having the maximum value of the ZC_1^* -index are the graphs in $\mathcal{U}_{n,5}$ if $n < 8$, in $\mathcal{U}_{n,5} \cup \mathcal{U}_{n,3}$ if $n = 8$ and in $\mathcal{U}_{n,3}$ if $n > 8$.
2. The unicyclic graph with n vertices having the minimum value of the ZC_1^* -index is $T_{3,n-3}$.

5 Connected graphs with n vertices

One important problem is to find the structure of an extremal connected graph with respect to ZC_1^* , having n vertices and no other constraints, that is to know the possible structure of molecules with n atoms that have minimum or maximum value of ZC_1^* .

Theorem 5 Let $n \geq 5$.

1. The complete graph K_n is the unique graph that minimizes the index ZC_1^* among all n -vertex connected graphs.
2. A connected graph G with n vertices maximizes the index ZC_1^* among all n -vertex connected graphs if and only if it has diameter 2 and:
 - $d(G) \subseteq \{\frac{n}{2} - 1, \frac{n}{2}\}$, if $n \in \{4k, 4k + 2 | k \in \mathbb{N}\}$
 - $d(G) = \{\frac{n-1}{2}\}$, if $n \in \{4k + 1 | k \in \mathbb{N}\}$
 - there exists a vertex $x \in V(G)$ such that $d(G) \setminus \{d(x)\} = \{\frac{n-1}{2}\}$ and $d(x) \in \{\frac{n-1}{2} - 1, \frac{n-1}{2} + 1\}$, if $n \in \{4k + 3 | k \in \mathbb{N}\}$

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