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Some Operations on Graph Theory in Zagreb and related Indices

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A B S T R A C T

A topological index is a numerical description computed from a molecular network that represents a molecule. Topological indices linked to the atom-atom connection of the molecular structure represented by the graph G are classical Zagreb indices and the recently developed Zagreb coincides. We investigate their fundamental mathematical features and offer precise equations for these novel graph invariants under a variety of graph operations..

Keywords: Topological Index, Zagreb Indices and Zagreb Coindices, Graph Operations.

1.Introduction

A topological representation of an item is one that simply contains information on the number of elements that make up the object and their connectivity. A molecular graph is a topological representation of a molecule. A molecular graph is made up of dots that represent the atoms in the molecule and lines that indicate the covalent connections. In graph theory, these spots are called vertices, and the lines are called edges. Topological indices have the benefit of being able to be employed directly as simple numerical descriptors in comparisons with physical, chemical, or biological properties of molecules in Quantitative Structure Property Relationships (QSPR) and Quantitative Structure Activity Relationships (QSAR) (QSAR).

2.Preliminaries

Definition 2.1

A diagram H = (W,D) comprises of a bunch of items W = $\{w_1, w_2,..,w_n\}$ called vertices and another set D = $\{d_1, d_2, d_3, \dots d_m\}$ whose components are called edges, to such an extent that each edge d_k is related to an unordered pair (w_i, w_j) of vertices(H).

Definition 2.2

On the off chance that two edges of a chart have a similar end vertex, these edges are called equal edges or numerous edges. δ(H) and the greatest level of vertices of a chart H is indicated by δ. The vertices w_jw_j related with edge d_k are known as the end vertices of d_k. The request of a diagram H is its number of vertices and the size of a chart is its number of edges. On the off chance that the request for a diagram is 'r' and the size is 's' at that point the chart is called as (r,s) diagram.

Definition 2.3

The level of a vertex w is the quantity of edges occurrence with the vertex w, considering each circle two edges and we signify this by d(w).

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The base level of vertices of a diagram H is signified by Pendant Vertex is a vertex whose degree is one. A circle is an edge that interfaces a vertex to itself.

Definition 2.4

Basic diagram contain no-numerous edges or circles. A chart which has different edges is known as a multi diagram. Chart which has the two circles and various edges is known as a pseudo diagram.

Definition 2.5

A chart His a sub-diagram of a diagram Gif every one of its vertices has a place with W(H) and every one of its edges has a place with D(H). Along these lines the chart in Figure 1.2 (a) will be a sub-diagram of the diagram in Figure 1.2 (b).

Definition 2.6

Two vertices of a diagram are contiguous when they are associated by an edge and these two vertices are supposed to be episode to each other. We additionally say that two edges are supposed to be neighbouring on the off chance that they share a vertex for all intents and purpose. Which is double the quantity of edges? So in the event that we think about a diagram 'H' with 'f' edges 'm' vertices $w_1,w_2,\ldots,w_n$. the amount of the levels of all vertices in H, is double the quantity of edges in H, since each edge contribute two degrees.

Definition 2.7

Two graphs H_1 and H_2 are supposed to be isomorphic if there are a one–one correspondence between the vertices of H_1 and those of H_2 such that the quantity of edges joining any two vertices of H_1 approaches the quantity of edges joining the relating vertices of H_2.

Definition 2.8

Two vertices w_1 and w_2 are supposed to be associated if there is a way among w_1 and w_2 in H. A chart H is supposed to be associated if any two vertices in H are associated; in any case H is detached. The detached chart comprise segments, the parts of a diagram H are its maximal associated sub-diagrams.

Definition 2.9

The diagram in which all vertices are of equivalent degree is known as a Regular chart. A normal chart where all the vertices have degree m is called m-Regular diagram. In a diagram, in the event that we provide guidance to each edge, the subsequent chart is called coordinated chart (or) digraph.

Definition 2.10

A Complete Graph is a straightforward diagram in which each pair of particular vertices is nearby. Complete chart is signified by M_q for q vertices. Complete diagram M_n is (n-1) customary.

Definition 2.11

A total bipartite chart is a bipartite diagram where each vertex in U is joined to every vertex in V by precisely one edge. On the off chance that the quantity of vertices in U and V are meant by p and q, individually, at that point a total bipartite diagram is signified by $M_{r,s}$.

Definition 2.12

A diagram is called planar in the event that it very well may be drawn on a plane without Meeting edges aside from the end focuses. A diagram is called non-planar in the event that it's anything but a planar.

Definition 2.13

A stroll in a diagram H is a limited non-invalid succession $F = f_0d_1f_1d_2f_2 \ldots f_kd_k$ whose terms then again vertices and edges to such an extent that for $1 \leq I \leq k$, and F_{i1} and F_i are the two finishes of d_i. On the off chance that the walk closes at a similar vertex where it starts, it is called shut walk. On the off chance that the walk doesn't end at the vertex where it starts called Open walk.

An Open stroll in which a vertex doesn't show up more than whenever is known as a way. The quantity of edges in a way is known as the length of a way. A shut stroll in which no vertex shows up more than whenever is known as a Cycle. A chart without cycle is called non-cyclic diagram.

Definition 2.14

Let H be a graph with m vertices $w_1,\ldots.w_n$. Then m×m adjacency matrix $A=(b_{ij})$ is defined by

$$a_{ij} = \begin{cases} 1, if\ vertex\ v_i\ adjacent\ with\ vertex\ v_j \\ 0, otherwise \end{cases}$$

Definition 2.15

Let H be a graph with n vertices $w_1,\ldots.w_n$ and m edges$d_1,\ldots.d_m$.

Then an incidence matrix m×n matrix is $J = (b_{ij})$ is defined by

$$b_{ij} = \begin{cases} 1, if\ vertex\ v_i\ is\ incident\ with\ the\ edge\ e_j \\ 0, otherwise \end{cases}$$

3.Origin Of Chemical Graph Theory

To get the design movement linkages on which speculative and computational procedures are based, adequate representations of the subatomic structure of synthetic mixes must be discovered. Subatomic descriptors are used to recognise these depictions. Subatomic descriptors are integers that comprise basic data derived from the underlying representation used for particles under inquiry. Topological records are one type of atomic descriptor (Dennis H Rouvray 1991).

A sub-atomic chart can provide a topological representation of a particle. Descriptors are mathematical features associated with synthetic constitution for connecting substance structure with various real attributes, compound reactivity, or natural action. They are derived from a topological representation of particles and may be regarded as design unequivocal descriptors, in contrast to those construct mysterious descriptors, such as quantum compound ones and design verifiable as hydrophobicity and electronic constants.

3.1 *The Growth of Chemical Graph Theory*

Now, in our narrative, we interrupt to gain the upper hand in the general enhancement of compound chart theory. Following the severe choppiness of the 1850s and 1860s caused by the approach of construction and valence assumptions, the need for adequate numerical formalisms for continued scientific growth became obvious. The diagram hypothesis addressed a common formalism for science and had been successfully applied in a variety of verifiable hypotheses. Throughout the years, we have accepted an inexorable explicit structure through the use of schematic hypothesis in science.

The application grew so quickly that the substance chart theory branched in complicated ways, resulting in a collection of diverse specialisms. All things considered, inclusion would result in a section of unmanageable inventions, thus some restriction of our primary point of attention is essential from here on out. To keep up as broad an overview as possible, we shall highlight four main areas of the growth of synthetic diagram hypothesis. When everything is said and done, it should be noted that the progression of the diagram theory has not been particularly smooth. It is true that moments of tremendous interest in the topic have been followed by nearly total disinterest.

3.2 *Topological Representation of Molecules*

A topological depiction of an object is one that just shows the number of components that make up the piece and their availability. A sub-atomic chart is a topological representation of a particle. A sub-atomic diagram is a collection of foci that address the particles in the particle and a set of lines that address the covalent bonds. In diagram hypothesis language, these focuses are called vertices, while the lines are called edges. The following are some important definitions from the atomic charts.

(i)A atomic chart in which hydrogen's are not considered is called hydrogen-exhausted diagram.

(ii) The quantity of bonds episode on v is called valiancy of a molecule or vertex degree w and is meant by deg (w).

(iii) The quantity of bonds contiguous f_k is called edge or bond level of d_k and is meant by deg(d_k). The two bonds are adjoining in the event that they are episode to a similar molecule. The accompanying connection is kept up, deg(d_k) = deg(w_i)+deg(w_j)- 2, vi and w_j are occurrence to d_k.

(iv) Topological distance d(w_i,w_j)is the length of the most brief way between vertices w_i and w_j.

(v) Bond Matrix F is a square and symmetric network of request m whose components d_{ij} are ones or zeros if the relating bonds i and j are adjoining or not.

(vii) Distance Matrix D is a square and symmetric lattice of request n whose components d_{ij} compare to the topological distances between iota's i and j.

(viii) Spectral snapshots of a framework are the follows, i.e., the amount of the principle askew, of the various forces of the relating network.

(ix) Since the vertices addressing hydrogen are pendant vertices, they go with carbon molecules only one way and thus make no commitment to isomorphism. Accordingly we need not show any hydrogen vertices.

(x) Thus the tree addressing D_k I_{2k+2} lessens to one with k vertices, each addressing carbon particle. In this tree no qualification can be made between the vertices, and along these lines it is unlabeled.

There are just two types of trees in butane, D4 I10. Every natural Physicist is aware that there are two distinct types of butanes:

Subatomic charts, also known as compound diagrams, are particle models in which molecules are addressed by vertices and synthetic bonds are addressed by chart edges. Figure 2.1(a) discusses n - butane, whereas Figure 2.1(b) addresses n - butane's subatomic chart. Figure 2.2(a) handles is o -

butane independently, whereas figure 2.2(b) addresses the sub-atomic diagram of is o - butane.

A diagram hypothetical invariant is any numerical articulation based on the components of a chart that does not rely on diagram component numbering. The mathematical aftereffect of any diagram invariant is a topological file. They are numbers derived from a diagram addressing an atom that does not rely on the chart's vertices or edges being numbered.

These atomic descriptors (TI) are believed to include important particle data that may be used to depict physico-synthetic and organic features. Alternatively, topological files might be used as fundamental mathematical descriptors in a connection with physical, chemical, or organic particle boundaries in quantitative construction property relationship (QSPR) and quantitative design action relationship (QDAR) (QSAR).

The bulk of the suggested topological files are linked to either a vertex contiguousness connection (iota particle network) or topological distances in the diagram (atomic design) G. Topological lists may therefore be traced back to either the contiguousness framework of a chart or the distance grid of a diagram.

Case (i): Lists Based on Connectivity

(i) The Zagreb Index
(ii) The network Index
(iii) The Maximum Eigen esteem Index
(iv) The likeness Index
(v) The Z Index

Case (ii): Records Based on Topological Distances

(i) The Wiener Index
(ii) The Platt Number
(iii) The Gordon-Scantlebury Index
(iv) The Altenburg Polynomial
(v) The Balaban Index
(vi) The Smolenskii Function
(vii) The Distance Polynomial
(viii) The data Indices
(ix) The Centric Index

Topological records are also classified according to their temperament in the first, second, and third eras. Topological distances, for example, are based on number chart features of original topological records. Wiener Index W, Platt Index F, Hosoya Index, and the centric record of Balaban B and C are the most delegate lists of this class. The Wiener Index is the only one of these Topological records that has been used in drug disclosure research.

Second-generation Topological lists are actual numbers that are based on whole number chart features. This class contains the majority of the Topological files used in drug disclosure today. Randic presents the optimal organization of such atomic descriptors as sub-atomic availability lists.

Third Generation Topological records are those genuine numbers that are based on the atomic diagram's genuine number neighborhood features. These files are in continuous presentation, have exceptionally little decrease, and provide a large range of options. Other third-generation Topological records are based on data hypotheses applied to distance wholes or recently presented non-balanced frameworks, and these Topological lists have no applicability in drug discovery research.

4.Zagreb Indices and Zagred Coindices

4.1 *Zagreb Indices*

The **First Zagreb Index** of H=G is denoted by $M_1(G)$ and is defined as

$$M_1(G) = \sum_{u \in V(G)} \left(d_G(u)\right)^2$$

The sum over edges in H=G.

$$M_1(G) = \sum_{uv \in E(G)} \left(d_G(u) + d_G(v)\right)$$

The **Second Zagreb Index** of G is denoted by $M_2(G)$ and is defined as

$$M_2(G) = \sum_{uv \in E(G)} d_G(u) d_G(v)$$

4.2 ***Zagreb Coindices***

The **First Zagreb Coindex** of G is denoted by $\overline{M}_1(G)$ and is defined as

$$\overline{M}_1(G) = \sum_{uv \notin E(G)} \left(d_G(u) + d_G(v) \right)$$

The **Second Zagreb Coindex** of G is denoted by $\overline{M}_2(G)$ and is defined as

$$\overline{M}_2(G) = \sum_{uv \notin E(G)} d_G(u) d_G(v)$$

5. Zagreb Indices and Coindices of Some Graph & their Operations

The below conditions are satisfied in the their assumptions.

(i) $$|E(G_1 \times G_2)| = |V(G_2)||E(G_1)| + |V(G_1)||E(G_2)|$$

(ii) $$M_1(G_1 \times G_2) = n_2 M_1(G_1) + n_1 M_1(G_2) + 8 m_1 m_2$$

(iii) $$|E(G_1 \vee G_2)| = |V(G_2)|^2 |E(G_1)| + |V(G_1)|^2 |E(G_2)| - 2|E(G_1)||E(G_2)|$$

(iv) $$|E(G_1 \circ G_2)| = 2|E(G_1)||E(G_2)| + |V(G_2)||E(G_1)| + |V(G_1)||E(G_2)|$$

(v) $$M_1(G_1 \circ G_2) = (4m_1 + n_1) M_1(G_2) + (4m_2 + n_2) M_1(G_1) + 8 m_1 m_2 + M_1(G_1) M_1(G_2)$$

(vi) $$\overline{M}_1(G_1 \circ G_2) = 2 n_1 n_2 m_1 (n_2 - 1) + 2 n_1 n_2 m_2 (n_1 - 1) - 4 m_1 m_2 (n_1 + n_2) + (4m_2 + n_2) M_1(G_1)$$
$$- \overline{M}_1(G_1) \overline{M}_1(G_2) + \overline{M}_1(G_1)(n_2 + 2 m_2 n_2 + 2 m_2) + \overline{M}_1(G_2)(n_1 + 2 m_1 n_1 + 2 m_1)$$

Conclusion

The main notions of diagram hypothesis and Introduction to substance chart hypothesis have been discussed in this work. Furthermore, we clarified Zagreb files and Zagreb coindices, and we examined their fundamental numerical properties and obtained unambiguous formulae for registering their qualities under a few chart tasks, specifically Cartesian item, Disjunction, Composition, Tensor item, and Normal result of diagrams.

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