

Lanzhou Indices of First Transformation Graph

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Abstract:—In molecular science, one of the major challenges is the precise modeling and prediction of a molecule's chemical properties. To overcome this difficulty, researchers have proposed several theoretical methodologies, among which topological indices have gained considerable importance. These indices are numerical parameters derived from the structural graph of a molecule and are widely applied to estimate its chemical and physical properties. In particular, degree-based topological indices constitute an important category within chemical graph theory and significantly contribute to such predictive analyses. In the present study, we introduce a new degree-based topological index and compute its values for some kind of transformation graphs.

Keywords: Chemical graph theory, degree-based topological index, Transformation graph.

1. Introduction

Graph theory serves as a powerful mathematical tool that is widely applied in many scientific disciplines, particularly in chemistry. Within the framework of chemical graph theory, a molecule is modeled as a graph in which atoms correspond to vertices and chemical bonds correspond to edges. This graphical representation facilitates a systematic and quantitative examination of molecular structure, characteristics, and behavior.

One of the most significant contributions of graph theory to chemistry is the formulation of topological indices. These are numerical descriptors derived from the structural features of a molecular graph and are extensively employed in Quantitative Structure–Property/Activity Relationship (QSPR/QSAR) studies. Such indices play a pivotal role in estimating the physical, chemical, and biological properties of compounds, thereby supporting advancements in areas such as drug design, materials development, and environmental chemistry.

Topological indices reflect fundamental structural features of molecular graphs, including connectivity patterns, symmetry, and branching characteristics, thereby offering valuable insight into molecular reactivity and stability without relying on laboratory experimentation. Classical descriptors such as the Wiener index, Randić index, and Zagreb indices have been widely investigated and successfully applied in the modeling of molecular systems with notable precision.

Quantitative Structure–Property/Activity Relationship (QSPR/QSAR) models function as effective predictive frameworks, enabling the estimation of physical, chemical, and biological properties of compounds using only structural data, thus reducing dependence on expensive and time-consuming experimental methods. Since topological indices are computed from graph-based representations of molecules, they provide a systematic numerical means of encoding molecular connectivity and geometry. Consequently, these indices substantially strengthen the accuracy, reliability, and overall performance of QSPR/QSAR predictive models.

Topological indices are powerful tools to connect graph theory with other areas. The first degree based topological indices were introduced by Gutman *et al.* [1, 2] in 1972. They are defined for a connected graph G as $M_1(G) = \sum_{ab \in E(G)} (\theta_G(a) + \theta_G(b))$ and $M_2(G) = \sum_{ab \in E(G)} (\theta_G(a)\theta_G(b))$. Furtula and Gutman [3] introduced forgotten topological index (also called F-index) which is defined as $F(G) = \sum_{ab \in E(G)} (\theta_G(a)^2 + \theta_G(b)^2)$.

In [L4], Vukicevic et al. considered a linear combination of $M_1(G)$ and $F(G)$ of the form $M_1(G) + F(G)$, where was a free parameter ranging from -20 to 20. From the above linear combination, Vukicevic et al. introduced in the same paper a new topological index named as Lanzhou index. It is denoted by $LZD(G)$ and defined by $LZD(G) = (|V(G)| - 1)\sum_{ab \in E(G)} (\theta_G(a) + \theta_G(b)) - \sum_{ab \in E(G)} (\theta_G(a)^2 + \theta_G(b)^2)$. For its mathematical properties see the paper [4]. In chemical graph theory, many vertex degree based topological indices and their properties have been investigated in [5-12]. In this sequence, we present the mathematical properties for Lanzhou indices of first transformation graph.

2. First Transformation of graphs $T_1^{xy}(G)$

The graph $T_1^{xy}(G)$ is a graph with $V(T_1^{xy}(G)) = (V(G) \cup E(G))$ such that two vertices x and y in $V(T_1^{xy}(G))$ are adjacent if and only if the following holds

- (i) $x, y \in V(G), xy \in E(G)$ if $x = +$ and x and y are not adjacent if $x = -$.
- (ii) $x \in V(G)$ and $y \in E(G), xy \in E(G)$ if $y = +$ and $xy \notin E(G)$ if $y = -$.

One can observe that this transformation graph $T_1^{xy}(G)$ has four graphs like $T_1^{++}(G), T_1^{+-}(G), T_1^{-+}(G)$ and $T_1^{--}(G)$. Now we establish the results for Lanzhou indices for these transformation graphs. The graph $K_{1,3}$ and its transformation graph is given in Figure 1.

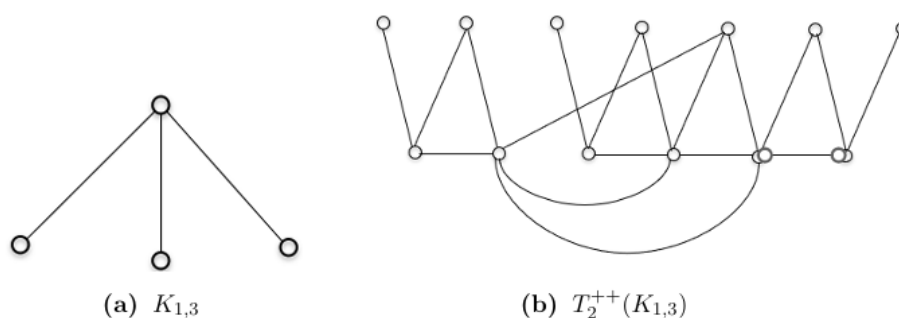


Figure 1: The graph $K_{1,3}$ and its transformation graph.

Theorem 2.1. For a (p, q) graph G , the exact value of LZD index of $T_1^{++}(S(G))$ is $T_1^{++}(S(G)) = 4(p + 3q - 1)(M_1(G) + 4q) - F(G) + 8q(p + 2q - 3)$.

Proof. From the structure of $T_1^{++}(S(G))$, the number of vertices and edges are respectively, $p + 3q$ and $6q$. By the definition of LZD index of $T_1^{++}(S(G))$,

$$LZD(T_1^{++}(S(G))) = (p + 3q - 1) \sum_{x \in V(T_1^{++}(S(G)))} \theta^2(x) - \sum_{x \in V(T_1^{++}(S(G)))} \theta^3(x)$$

In addition, the degree of $x \in V(T_1^{++}(S(G))) \cap V(S(G))$ is $2\theta(x)$ and degree of $xy \in V(T_1^{++}(S(G))) \cap E(S(G))$ is 2.

Hence,

$$\begin{aligned} LZD(T_1^{++}(S(G))) &= (p + 3q - 1) \sum_{x \in V(T_1^{++}(S(G))) \cap V(S(G))} \theta^2(x) \\ &+ (p + 3q - 1) \sum_{xy \in V(T_1^{++}(S(G))) \cap E(S(G))} \theta^2(x) \\ &- \sum_{x \in V(T_1^{++}(S(G))) \cap V(S(G))} \theta^3(x) - \sum_{xy \in (T_1^{++}(S(G))) \cap E(S(G))} \theta^3(x) \end{aligned}$$

Hence,

Thus,

$$LZD(T_1^{++}(S(G))) = 4(p + 3q - 1)(M_1(G) + 4q) - F(G) + 8q(p + 2q - 3).$$

Theorem 2.2. For a (p, q) -graph G , the exact value of LZD index of $T_1^{--}(S(G))$ is

$$\begin{aligned} LZD(T_1^{--}(S(G))) &= (p + 3q - 1)[p(p + 3q - 1)^2 - 8(p + 3q - 1) - 4M_1(G) + q(p + 3q - 5)^2 + 2q(p + q - 2)^2] - p(p + 3q - 1)^3 + 8F(G) - 12(p + 3q - 1)M_1(G) + 12q(p + 3q - 1)^2 - q(p + 3q - 5)^3 - 2q(p + q - 2)^3 \end{aligned}$$

Proof. By the definition of LZD index of $T_1^{--}(S(G))$, we get

$$LZD(T_1^{--}(S(G))) = (|V(T_1^{--}(S(G)))| - 1) \sum_{x \in V(T_1^{--}(S(G)))} \theta^2(x) - \sum_{x \in V(T_1^{--}(S(G)))} \theta^3(x)$$

From the structure of $T_1^{--}(S(G))$, it has $p + 3q$ vertices and $2(p + q)^2 - 9q - p$ edges.

The degree of a vertex $x \in V(T_1^{--}(S(G))) \cap V(S(G))$ is $p + 3q - 2\theta(x) - 1$ and an edge

$xy \in V(T_1^{--}(S(G))) \cap E(S(G))$ is $p + q - 2$.

Thus,

$$\begin{aligned} LZD(T_1^{--}(S(G))) &= (p + 3q - 1) \left[\sum_{x \in V(S(G))} (p + 3q - 2\theta(x) - 1)^2 + \sum_{xy \in E(S(G))} (p + q - 2)^2 \right] - \\ &\sum_{x \in V(S(G))} (p + 3q - 2\theta(x) - 1)^3 - \sum_{xy \in E(S(G))} (p + q - 2)^3 \end{aligned} \tag{2.1}$$

We shall calculate the above sums separately.

$$\begin{aligned} \sum_{x \in V(S(G))} (p + 3q - 2\theta(x) - 1)^2 &= p(p + 3q - 1)^2 - 8(p + 3q - 1) + 4M_1(G) + q(p + 3q - 5)^2 \end{aligned} \tag{2.2}$$

Similarly,

$$\begin{aligned} \sum_{x \in V(S(G))} (p + 3q - 2\theta(x) - 1)^3 &= p(p + 3q - 1)^3 - 8F(G) + 12(p + 3q - 1)M_1(G) - 12(p + 3q - 1)^2q \\ &+ q(p + 3q - 5)^3 \end{aligned} \tag{2.3}$$

Using the equations (2.2) and (2.3) in (2.1), we have

$$\begin{aligned} Lz(T_1^{+-}(S(G))) &= (p + 3q - 1) \left[\sum_{x \in V(T_1^{+-}(S(G))) \cap V(S(G))} \theta^2(x) + \sum_{xy \in V(T_1^{+-}(S(G))) \cap E(S(G))} \theta^2(x) \right] \\ &\quad - \left[\sum_{x \in V(T_1^{+-}(S(G))) \cap V(S(G))} \theta^3(x) + \sum_{xy \in V(T_1^{+-}(S(G))) \cap E(S(G))} \theta^3(x) \right] \\ &= (p + 3q - 1) \left[\sum_{x \in V(S(G))} (2q)^2 + \sum_{xy \in E(S(G))} (p + q - 2)^2 \right] \\ &\quad - \left[\sum_{x \in V(S(G))} (2q)^3 + \sum_{xy \in E(S(G))} (p + q - 2)^3 \right] \\ &= 4q^2(p + q)(p + 3q - 1) + 2q(p + 3q - 1)(p + q - 2)^2 - 8q^3(p + q) \\ &\quad - 2q(p + q - 2)^3. \end{aligned}$$

Theorem 2.3. For a (p, q) graph G ,

$$\begin{aligned} Lz(T_1^{-+}(S(G))) &= (p + 3q - 1)(p + q - 1)^2(p + q) + 8q(p + 3q - 1) \\ &\quad - (p + q - 1)^3(p + q) - 16q. \end{aligned}$$

Proof. From the structure of $T_1^{-+}(S(G))$, the number of vertices and edges are $p + 3q$ and $(p + q)(p + q - 1)$ respectively. In addition, the degree of a vertex $x \in V(T_1^{-+}(S(G)))$ is $p + q - 1$ and an edge $xy \in V(G) \cap E(S(G))$ is 2. Thus,

$$\begin{aligned} Lz(T^{-+}(S(G))) &= (p + 3q - 1) \left[\sum_{x \in V(T^{-+}(S(G))) \cap V(S(G))} \theta^2(x) + \sum_{xy \in V(T^{-+}(S(G))) \cap E(S(G))} \theta^2(x) \right] \\ &\quad - \left[\sum_{x \in V(T^{-+}(S(G))) \cap V(S(G))} \theta^3(x) + \sum_{xy \in V(T^{-+}(S(G))) \cap E(S(G))} \theta^3(x) \right] (p + 3q \\ &\quad - 1) \left[\sum_{x \in V(S(G))} (p + q - 1)^2 + \sum_{xy \in E(S(G))} 2^2 \right] - \left[\sum_{x \in V(S(G))} (p + q - 1)^3 + \sum_{xy \in E(S(G))} 2^3 \right] \end{aligned}$$

$$Lz(T^{-+}(S(G))) = (p + 3q - 1)(p + q - 1)^2(p + q) + 8q(p + 3q - 1) - (p + q - 1)^3(p + q) - 16q.$$

3. Discussion

In this paper, we investigated the Lanzhou degree index for several first transformation graphs associated with subdivision graphs. Explicit formulae for the Lanzhou degree index of the transformation graphs were derived by utilizing graph-theoretical techniques and degree-based computations. The obtained results establish direct relationships between the Lanzhou degree index and well-known graph invariants such as the first Zagreb index and forgotten index.

The study demonstrates that graph transformations significantly influence the structural behavior of degree-based topological descriptors. The derived expressions provide a systematic approach for computing the Lanzhou degree index of transformed graphs and reveal how subdivision operations and transformation parameters affect the corresponding index values. The obtained results further highlight the applicability of Lanzhou indices in analyzing structural characteristics of graphs arising in chemical graph theory.

Since topological indices play an important role in QSPR/QSAR investigations, the results obtained in this work may be useful in predicting physicochemical properties of molecular structures represented by transformation graphs. Furthermore, the mathematical techniques developed in this paper can be extended to other graph operations, transformation graphs, and newly defined degree-based descriptors. Thus, the present work contributes to the advancement of chemical graph theory and opens new directions for further investigations involving transformation graphs and molecular modeling.

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