WIENER AND ZAGREB INDICES FOR LINE GRAPHS

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Abstract: The line graph $L(G)$ of a connected graph G, has vertex set identical with the set of edges of G, and two vertices of $L(G)$ are adjacent if and only if the corresponding edges are adjacent in G. Ivan Gutman et al examined the dependency of certain physio-chemical properties of alkanes in boiling point, molar volume, and molar refraction, heat of vapourization, critical temperature, critical pressure and surface tension on the Bertz indices of $L^i(G)$ Dobrynin and Melnikov conjectured that there exists no nontrivial tree T and $i \geq 3$, such that $W(L^i(T)) = W(T)$. In this paper we study Wiener and Zagreb indices for line graphs of Complete graph, Complete bipartite graph and wheel graph.

Keywords: Distance, Degree, Graphs, Topological indices.

AMS Classification: 05C12, 05C25.

1. Introduction

In this paper all graphs are finite, simple and undirected. For a graph G, we denote by $V(G)$ and $E(G)$ its vertex and edge sets, respectively. All paths and cycles are simple, i.e., they contain no repeated vertices[3]. A path $P_n = x_1, x_2, ..., x_n$ is given by the sequence of its consecutive vertices. A path whose end vertices are u and v is called an uv-path. The length of a path P, denoted $|P|$, is the number of its edges. A cycle of length k is denoted by C_k.

Given a graph G, its line graph $L(G)$ [1] is a graph such that the vertices of $L(G)$ are the edges of G; and two vertices of $L(G)$ are adjacent if and only if their corresponding edges in G share a common end vertex[7]. These graphs are defined as follows:

$$L^i(G) = \begin{cases} G & if\ i=0 \\ L(L^{i-1}(G)) & if\ i>0 \end{cases}$$

where L is the line graph operator. The use of line graphs in chemistry can be traced back to 1952, when Lennard-Jones and Hall [2] published a work on the ionization of paraffin molecules, in which they used on the ionization of paraffin molecules, C-C and H-C bonds as equivalent orbitals. Line graph based models of saturated molecules were elaborated by sana and Leory[3] . Line graphs have application in an algebraic formulation of Clar's aromatic sextet theory[5]. The first connections between topological indices of line graphs and physico-chemical properties of alkanes were communicated in 1995, independently by Diudea and Estrada [4]. In the work of Estrada a correlation between molar volumes and connectivity index of $L(G)$ was reported. An example of hydrogen depleted molecular graph of 2,3,4 trimethylpentane and its line graph is shown in figure 1

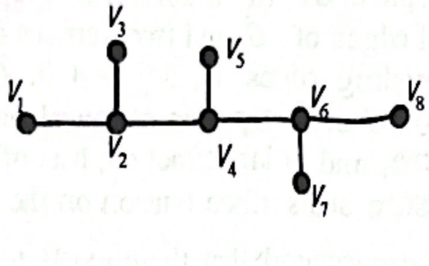

Figure 1: The graph G

The graph G representing the chemical compound 2,3,4 trimethylpentane

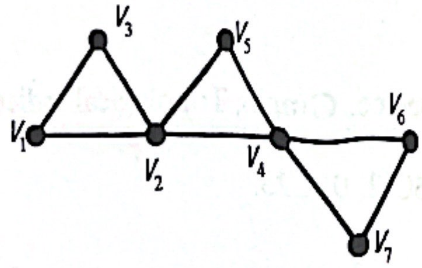

Figure 2 : The line graph of G

For a vertex $v \in V(G)$, we denote by $d_G(v)$ or $d(v)$ the degree of v in G. For $(u,v) \in V(G)$ we denote by $d_G(u,v)$ (or simply $d(u,v)$ the length of a shortest path in G between u and v. For $e_1, e_2 \in E(G)$, we define $d_G(e_1,e_2) = d_{LG}(e_1,e_2)$.

Definition 2.1: The Wiener index [5] $W(G)$ of a graph G is defined as the sum of half of the distances between every pair of vertices of G. $W(G) = \frac{1}{2}\sum_{i=1}^{N}\sum_{j=1}^{N} d(v_i, v_j)$, where $d(v_i, v_j)$ is the number of edges in a shortest path connecting the vertices v_i, v_j. We have an equivalent definition of Wiener index $W(G) = \frac{1}{2}\sum_{k,l} d(v_i, v_j)$.

Definition 2.2: The Zagreb group indexes [5] of a graph G denoted by $M_1(G)$ (first Zagreb index) and $M_2(G)$ (second Zagreb index) are defined as

$M_1(G)=\sum_{i=1}^{N} D_i^2$, $M_2(G)=\sum_{(i,j)} D_i D_j$ where D_i stands for the degree of a vertex i. The sum in $M_1(G)$ is over all vertices of G, while the sum in $M_2(G)$ is over all edges of G. where D_i stands for the degree of the vertex V_i. In this paper we have investigated the Wiener and Zagreb indices of the line graph of Wheel graph, Complete bipartite graph and complete graph.

2. Main Results

Theorem 2.1: The Wiener index of a line graph of complete graph with n vertices is $W(L(K_n))=\frac{n(n-1)^2(n-2)}{4}$.

Proof: Let K_n be a complete graph with n vertices. Degree sequence of K_n be $(d_1,d_2,...,d_n)$ each vertex in complete graph K_n has $n-1$ degrees. The line graph of complete graph K_n has $\frac{n(n-1)}{2}$ vertices and each vertex has degree $2(n-2)$. In the graph $L(K_n)$, $2(n-1)$ vertices has distance one and $\left(\frac{n(n-1)}{2}-2(n-2)-2\right)$ vertices has distance two. By definition

$$W(L(K_n))=\frac{1}{2}\left(\frac{n(n-1)}{2}\right)\left(2(n-1)\right.$$
$$\left.+2\left(\frac{n(n-1)}{2}-2(n-2)-2\right)\right)$$

$$W(L(K_n))=\frac{n(n-1)}{4}\left(2(n-1)+\left(n^2-5n+4\right)\right)$$

$$W(L(K_n))=\frac{n(n-1)}{4}\left(n^2-3n+2\right)$$

$$W(L(K_n))=\frac{n(n-1)^2(n-2)}{4}.$$

Theorem 2.2: The Wiener index of line graph of complete bipartite graph is $W(L(K_{m,n}))=(m+n-2)(3m+3n-8)$.

Proof: Let $K_{m,n}$ be complete bipartite graph have $(m+n)$ vertices. The line graph of complete bipartite graph $K_{m,n}$ has mn vertices and the degree sequence be $(m+n-2)$

By definition

$$W\left(L\left(K_{m,n}\right)\right)=\frac{1}{2}\Big(2(m+n-2)$$

$$\Big(\underbrace{1+1+\ldots+1}_{m+n-2}+\underbrace{2+2+\ldots+2}_{m+n-3}\Big)\Big)$$

$$W\left(L\left(K_{m,n}\right)\right)=\frac{1}{2}\big(2(m+n-2)\big((m+n-2)$$

$$+2(m+n-3)\big)\big)$$

$$W\left(L\left(K_{m,n}\right)\right)=(m+n-2)$$

$$(m+n-2+2m+2n-6)$$

$$W\left(L\left(K_{m,n}\right)\right)=(m+n-2)(3m+3n-8).$$

Theorem 2.3: The line graph of first Zagreb index and second Zagreb index of complete graph is $M_1\left(L\left(K_n\right)\right)=2n(n-1)(n-2)^2$ and $M_2\left(L\left(K_n\right)\right)=2n(n-1)(n-2)^3$.

Proof: Let K_n be a complete graph with n vertices. Degree sequence of K_n be $(d_1,d_2,d_3,\ldots d_n)$. Each vertex in complete graph K_n has degree n-1 and the the line graph of complete graph K_n has $\frac{n(n-1)}{2}$ vertices and each vertex has degree $2(n-2)$.

Then by the definition the first Zagreb indices of complete graph is $M_1\left(L\left(K_n\right)\right)=2n(n-1)(n-2)^2$.

By definition $M_2(G)=\sum_{(i,j)} D_iD_j$

$$M_2(L(K_n))=\frac{n(n-1)(n-2)(2n-4)(2n-4)}{2}$$

$$M_2\left(L\left(K_n\right)\right)=2n(n-1)(n-2)^3.$$

Theorem 2.4: The line graph of first Zagreb index and second Zagreb index of Wheel graph is $M_1\left(L(W_n)\right)=(n-1)\left(n^2+16\right)$ and $M_2\left(L(W_n)\right)=\frac{1}{2}(n-1)\left(n^3-2n^2+16n+32\right)$.

Proof: Let W_n be a Wheel graph with n vertices. Degree sequence of W_n be $(3,3,3,\ldots,(n-1))$. Number of edges in the wheel graph is $2(n-1)$.

The line graph of wheel graph W_n has $2(n-1)$ vertices and the degree sequence be $2(4,4,4,\ldots,4,n,n,n,\ldots,n)$. In the graph $L(W_n),(n-1)$ vertices has degree four and $(n-1)$ vertices has degree n. Then by the definition of first Zagreb index $M_1\left(L(W_n)\right)=(n-1)\left(n^2+16\right)$.

By the definition of second Zagreb index $M_2(G)=\sum_{(i,j)} D_i D_j$

$$M_2\left(L(W_n)\right)=16(n-1)+8n(n-1)+\frac{n^2(n-1)(n-2)}{2}.$$

$$M_2\left(L(W_n)\right)=\frac{1}{2}(n-1)\left(n^3-2n^2+16n+32\right).$$

Theorem 2.5: The line graph of first Zagreb index and second Zagreb index of a complete bipartite is given by $M_1\left(L\left(K_{m,n}\right)\right)=mn(m+n-2)^2$ and $M_2\left(L\left(K_{m,n}\right)\right)=\frac{mn(m+n-2)^3}{2}$.

Proof: Let $K_{m,n}$ be complete bipartite graph have $(m+n)$ vertices. The line graph of complete bipartite graph $K_{m,n}$ has mn vertices and the degree sequence be $(m+n-2,m+n-2,\ldots,m+n-2)$.

By definition the first Zagreb index of $M_1\left(L\left(K_{m,n}\right)\right)$ is $mn(m+n-2)^2$.

The graph $L\left(K_{m,n}\right)$ has $\frac{mn(m+n-2)}{2}$ edges. Then by the definition of second Zagreb index $M_2\left(L\left(K_{m,n}\right)\right)=\frac{mn(m+n-2)^3}{2}$.

3. Conclusion

The construction and investigation of topological indices that could be used to describe molecular structures is one of the important directions of mathematical chemistry. Accordingly they have been used in designing several measures of branching and related topological indices. We would like to extend our study in finding the iterated line graph of generalized graphs.

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