

An Improved Proof for the Wiener index when $diam(G) \leq 2$

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Abstract: The Wiener index of a connected graph G is denoted by $W(G)$ and is defined as $W(G) = \frac{1}{2} \sum_{u,v \in V(G)} d_G(u,v)$ where $d_G(u,v)$

is the distance between the vertices u and v . In this paper we have established an improved version of the proof of the earlier result of Walikar et. al. [3] on wiener index.

Keywords: Distance; Wiener index.

1 Introduction

Let $G = (V, E)$ be a graph. The number of vertices of G we denote by n and the number of edges we denote by m , thus $|V(G)| = n$ and $|E(G)| = m$. The complement of G , denoted by \bar{G} , is a graph which has the same vertices as G , and in which two vertices are adjacent if and only if they are not adjacent in G . The degree of a vertex v , denoted by $deg(v)$. The distance between two vertices of a graph is the number of edges in a shortest path connecting them it is denoted by $d_G(u,v)$. The eccentricity $e(v)$ of a vertex v in G is defined as $e(v) = \max\{d_G(u,v) \mid u \in V\}$.

The Wiener index is named after Harry Wiener, who introduced it in 1947; at the time, Wiener called it the "path number".[2] It is the oldest topological index related to molecular branching.[3] Based on its success, many other topological indices of chemical graphs [1,2,6], based on information in the distance matrix of the graph, have been developed subsequently to Wiener's work.

Definition 1. let G be any connected graph of order n and size m . Then Wiener index of G is denoted by $W(G)$ and is defined as follows.

$$W(G) = \frac{1}{2} \sum_{u,v \in V(G)} d_G(u,v)$$

2 Results

Theorem 1[3] Let G be a graph of order n and size m . Then $W(G) = n^2 - n - m$ if and only $diam(G) \leq 2$.

In this paper an improved version of the proof of the above theorem is given, which is as follows.

Proof. let $G = (n, m)$ be a graph with $diam(G) \leq 2$. Then $\sum_{u \in V(G)} deg(u)$ contributes 1 to the sum of distance between every pair of adjacent vertices in G and $\sum_{u \in V(\bar{G})} (n - deg(u) - 1)$ contributes 2 to the sum of distance between every pair of adjacent vertices in \bar{G} . i.e

$$\begin{aligned} W(G) &= \frac{1}{2} \left[\left[\sum_{u \in V(G)} deg(u) \right] 1 + \left[\sum_{u \in V(\bar{G})} (n - deg(u) - 1) \right] 2 \right] \\ &= \frac{1}{2} [2m + 2n(n-1) - 4m] \\ &= n(n-1) - m. \end{aligned}$$

Conversely, suppose $W(G) = n(n-1) - m$ and $diam(G) = k \geq 3$. Then define the sets X and Y as $X = \{u \in V \mid e(u) = 2\}$ and $Y = \{u \in V \mid e(u) = k \geq 3\}$ such that $|X| + |Y| = n$. Hence

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$$\begin{aligned}
 W(G) &\geq \frac{1}{2} \left[\left[\sum_{u \in V(\bar{G})} (n - \deg(u) - 1) \right] \cdot 2 \right. \\
 &\quad \left. + \left[\sum_{u \in V(\bar{G})} (n - \deg(u) - 1) \right] \cdot k \right] \\
 &= \frac{1}{2} [2n^2 - 2n - 4m + kn^2 - kn - 2mk] \\
 &\geq \frac{(k+2)}{2} [n(n-1) - m].
 \end{aligned}$$

a contradiction to the fact that $W(G) = n(n-1) - m$.
Hence $\text{diam}(G) \leq 2$.

3 Conclusion

In the field of chemical graph theory Wiener index is the most studied topological index, due to its applications in predicting the boiling points of the alkanes. In this paper, we have improved the proof of the upper bound for Wiener index when diameter of a graph G is less than or equal to two.

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