A Sharp Lower Bound for the Wiener Index of a Graph

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Abstract

Given a simple connected undirected graph G, the Wiener index $W(G)$ of G is defined as half the sum of the distances over all pairs of vertices of G. In practice, G corresponds to what is known as the *molecular graph* of an organic compound. We obtain a sharp lower bound for $W(G)$ of an arbitrary graph in terms of the order, size and diameter of G.

1 Introduction

Let $G = (V(G), E(G))$ be a simple connected undirected graph with $|V(G)| = n$ and $|E(G)| = m$. Given any two vertices u, v of G, let $d(u, v)$ denote the distance (= the number of edges in a shortest path) between u

and v. The Wiener index $W(G)$ of the graph G is defined by

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

where the summation is over all possible pairs u, $v \in V(G)$. Our notation and terminology are as in [1].

The Wiener index is one of the oldest molecular-graph-based structure-descriptors, first proposed by the chemist Harold Wiener [8] as an aid to determine the boiling point of paraffins. In the calculation of graph-theoretic descriptors, an organic chemical molecule is modeled as a graph, where atoms are represented by vertices and covalent bonds by edges (double and triple bonds, if any, are treated as single edges unless specifically mentioned otherwise). It is now recognized that there are good correlations between $W(G)$ and a variety of physico-chemical properties (such as boiling point, heat of evaporation, heat of formation, surface tension, vapor pressure, partition coefficients etc.) of organic compounds representing G. Wiener index is currently a widely used topological index (see, for example, [9]) and has applications in modern drug design [5]. For more information about Wiener index in chemistry and in mathematics, see [6], [2] and [3].

In this paper, for any graph G, we obtain a sharp lower bound for $W(G)$ in terms of the order, size and diameter of G.

2 Lower bound for $W(G)$

Let $S_2(G)$ be the set of all 2-subsets of $V(G)$ (that is, the set of all unordered pairs of distinct vertices of G). We can then equivalently define $W(G)$ as

$$W(G) = \sum_{\{u,v\} \in S_2(G)} d(u, v). \tag{1}$$

Let $P = u_0 u_1 \ldots u_d$ be a diametral path of G, so that $d(u_0, u_d) = d$, the diameter of G. We partition $S_2(G)$ into disjoint sets X, Y and Z defined as follows:

$$X = \{\{u, v\} \in S_2(G)| \quad \text{both } u, v \in P\},$$
$$Y = \{\{u, v\} \in S_2(G)| \quad \text{none of } u \text{ and } v \text{ is in } P\}, \quad \text{and}$$
$$Z = \{\{u, v\} \in S_2(G)| \quad \text{one of } u \text{ and } v \text{ alone is in } P\}.$$

It follows that

$$|X| = \frac{d(d+1)}{2}; \quad |Y| = \frac{(n-d-1)(n-d-2)}{2}; \quad |Z| = (n-d-1)(d+1).$$

From (1), we have

$$W(G) = \sum_{\{u,v\} \in S_2(G)} \left(2 + (d(u,v) - 2)\right)$$

$$= \sum_{\{u,v\} \in S_2(G)} 2 + \sum_{\{u,v\} \in S_2(G)} \left(d(u,v) - 2\right) \tag{2}$$

$$= n(n-1) + \sum_{\substack{\{u,v\} \in S_2(G) \\ d(u,v)=1}} \left(d(u,v) - 2\right) + \sum_{\substack{\{u,v\} \in S_2(G) \\ d(u,v) \geq 2}} \left(d(u,v) - 2\right)$$

(since $|S_2(G)| = n(n-1)/2$)

$$= \left(n(n-1) - m\right) + \sum_{\substack{\{u,v\} \in S_2(G) \\ d(u,v) \geq 2}} \left(d(u,v) - 2\right)$$

$$\geq \left(n(n-1) - m\right) + \sum_{\substack{\{u,v\} \in X \cup Z \\ d(u,v) \geq 2}} \left(d(u,v) - 2\right). \tag{3}$$

For $0 \leq k \leq (d-1)$ in X, there are $(d-k)$ pairs $\{u,v\}$ with $d(u,v) = 1+k$. Hence

$$\sum_{\substack{\{u,v\} \in X \\ d(u,v) \geq 2}} \left(d(u,v) - 2\right) = (d-2)1 + (d-3)2 + \cdots + 1(d-2)$$

$$= \frac{d(d-1)(d-2)}{6}. \tag{4}$$

We next obtain a lower bound for the summation term on the right hand side of equation (3). We first assume that $d \geq 5$. Fix one vertex w in $V(G) \setminus V(P)$, where $V(P)$ is the set of vertices of P. Then, by triangle inequality, we have

$$d(u_i, w) + d(w, u_{d-i}) \geq d(u_i, u_{d-i}) = d - 2i, \tag{5}$$
$$\text{for} \quad 0 \leq i < (d-3)/2.$$

Therefore, for each of the $(n - d - 1)$ choices of w, we have

$$\sum_{d(u_i,w) \geq 2} \left(d(u_i, w) - 2\right)$$

$$\geq \sum_{i=0}^{d} \left(d(u_i, w) - 2\right) \geq \sum_{i=o}^{\lfloor \frac{d-3}{2} \rfloor} \left(d(u_i, w) + d(u_{d-i}, w) - 4\right) \tag{6}$$

$$\geq \sum_{i=o}^{\lfloor \frac{d-3}{2} \rfloor} (d - 2i - 4). \tag{7}$$

Since each summand on the right side of (6) is nonnegative, so is each summand on the right side of (7). Hence the term on the right side of (6) is

$$\geq \begin{cases} (d-4) + (d-6) + \cdots + 5 + 3 + 1 & \text{if } d \text{ is odd, and} \\ (d-4) + (d-6) + \cdots + 2 & \text{if } d \text{ is even.} \end{cases}$$

$$= \begin{cases} (\frac{d-3}{2})^2 & \text{if } d \text{ is odd, and} \\ \frac{(d-2)(d-4)}{4} & \text{if } d \text{ is even.} \end{cases}$$

Thus, for each fixed $w \in V(G) \setminus V(P)$ we have

$$\sum_{(u,\,w)\in Z} (d(u,\,w) - 2) = \begin{cases} (\frac{d-3}{2})^2 & \text{if } d \text{ is odd, and} \\ \frac{(d-2)(d-4)}{4} & \text{if } d \text{ is even.} \end{cases}$$

In conclusion, for $d \geq 5$, we have

$$W(G) \geq \begin{cases} (n(n-1) - m + \frac{d(d-1)(d-2)}{6} + \frac{(n-d-1)(d-3)^2}{4}, & \text{if } n \text{ is odd,} \\ (n(n-1) - m) + \frac{d(d-1)(d-2)}{2} + \frac{(n-d-1)(d-2)(d-4)}{4}, & \text{if } n \text{ is even.} \end{cases}$$

We now consider the cases when $d = 2$, 3 and 4. If $d = 2$, $d(u, v) = 1$ or 2. Hence from (2), we get

$$W(G) = n(n-1) + \sum_{d(u,\,v)=1} (1 - 2)$$

$$= n(n-1) - m. \tag{8}$$

Now consider the case when $d = 3$. Then $d(u, v) = 1, 2$ or 3. Hence from (2) we get

$$W(G) = n(n-1) - m + \sum_{d(u,\,v)=3} (d(u,\,v) - 2)$$

$$\geq n(n-1) - m + 1,$$

as there is at least one pair with $d(u, v) = 3$. If $d = 3$, $\dfrac{d(d-1)(d-2)}{6} = 1$. Hence we have

$$W(G) \geq n(n-1) - m + \frac{d(d-1)(d-2)}{6}.$$

Finally if $d = 4$, we have

$$W(G) \geq n(n-1) - m + \sum_{d(u,\,v)=3} (d(u,\,v) - 2)$$

$$+ \sum_{d(u,\,v)=4} (d(u,\,v) - 2)$$

$$\geq n(n-1) - m + 2 + 2.$$
$$\text{(since } d(u_0,\,u_d) = d = 4,\ d(u_0,\,u_3) = 2 = d(u_1,\,u_4))$$

Hence

$$W(G) \geq n(n-1) - m + \frac{d(d-1)(d-2)}{6}.$$
$$\left(\text{as } \tfrac{d(d-1)(d-2)}{6} = 4 \text{ in this case.}\right)$$

To conclude, we have proved the following result:

Theorem 1:
If G is any graph of order n, size (= number of edges) m, and $d \geq 2$, then

$$W(G) \geq \begin{cases} n(n-1) - m + \frac{d(d-1)(d-2)}{6} + \frac{(n-d-1)(d-3)^2}{4}, & \text{if } n \text{ is odd.} \\ n(n-1) - m + \frac{d(d-1)(d-2)}{6} + \frac{(n-d-1)(d-2)(d-4)}{4}, & \text{if } n \text{ is even.} \end{cases}$$
$$\text{(9)}$$

Remark 1:
Let the maximum degree of G be Δ. The Moore bound (see for example [7]) gives an upper bound for n in terms of Δ and the diameter d:

$$n \leq \begin{cases} 1 + \Delta \frac{(\Delta-1)^d - 1}{\Delta - 2} & \text{if } \Delta > 2 \\ 2d + 1 & \text{if } \Delta = 2 \end{cases} \qquad (10)$$

From (10), a lower bound for d in terms of n and Δ can be obtained and if this is used in (9), a lower bound for $W(G)$ can be obtained in terms of n, m and Δ.

Remark 2:
If G is planar and if d is known to be bounded by a constant then we can compute the exact value of d in time $O(n)$ as shown in [4]. In turn, this implies that the lower bound on $W(G)$ in (9) can be computed in time $O(n)$ if G is planar.

We observe that the lower bound given in Theorem 1 is sharp. The graph $C_3 \,\square\, K_2$ and the Petersen graph attain the bound. It is easy to

check that the lower bound is also attained for the following families of graphs G:

1. G is a path.

2. G is a star with even number of vertices.

3. For any even d, take G to be the graph of Fig. 1.

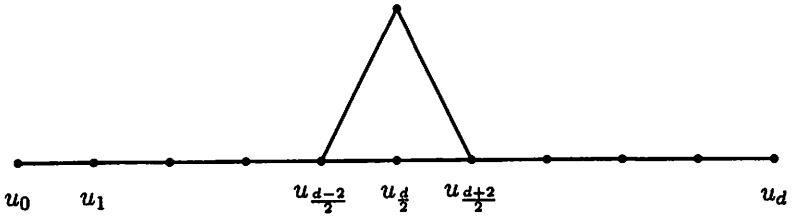4. For any odd d, take G to be the graph of Fig. 2

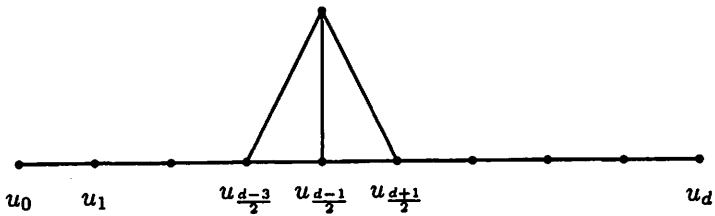Figure 1: A family of graphs with d specified as even.

Figure 2: A family of graphs with d specified as odd.

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