MATCH Communications in Mathematical and in Computer Chemistry

A Note on Wiener Index

Seiichi Yamaguchi*

Department of Mathematics, Graduate School of Science, Osaka University, Toyonaka, Osaka 560-0034, Japan

(Received December 17, 2007)

Abstract

The Wiener index of a connected graph is equal to the sum of distances between all pairs of its vertices. In this paper, we find a lower bound for the Wiener index in terms of graph invariants.

1 Introduction

The Wiener index of a graph was introduced by H.Wiener([1]). He observed a relationship between the boiling point of paraffin and the Wiener index. For a vertex vof a connected graph G, let $d_i(v)$ be the number of vertices at distance i from v. Let $dds(v) = (d_0(v), d_1(v), \ldots, d_{n-1}(v))$. It is called the distance degree sequence of a vertex v. This paper gives a lower bound of W(G) in terms of graph invariants by considering the distance degree of vertices.

2 Results

2.1 Definitions

Given a connected simple graph G = (V, E), (|V| = n, |E| = m). The distance d(v, w) between two vertices v and w is the minimum length of the paths connecting them.

^{*} e-mail: s-yamaguchi@cr.math.sci.osaka-u.ac.jp

For an integer *i* and a vertex *v*, let $N_i(v) = \{w \in V \mid d(v, w) = i\}$, $d_i(v) = |N_i(v)|$, $(d_0(v) := 1)$. Then, $dds(v) = (d_0(v), d_1(v), d_2(v), \ldots, d_{n-1}(v))$ is called the distance degree sequence of a vertex *v*. We let $\Delta_i = \max_v \{d_i(v)\}$, and $\delta_i = \min_v \{d_i(v)\}$ $e(v) = \max_w \{d(v, w)\}$. The radius and the diameter of G (r = r(G) and d = d(G))are defined as follows, $r = r(G) = \min_v \{e(v)\}$, $d = d(G) = \max_v \{e(v)\}$, respectively. Write D_i for the number of unordered pairs of vetices whose distance is *i*.

A nondecreasing sequence $S: a_1, a_2, \ldots, a_n$ of nonnegative integers is called an eccentric sequence if there exists a connected graph G whose vertices can be labelled v_1, v_2, \ldots, v_n so that $e(v_i) = a_i$ for all i. The vertex connectivity of a connected graph G, denoted by $\kappa(G)$, is the minimum number of vertices whose removal can either disconnect G or reduce it to a 1-vertex graph. A graph G is k-connected if G is connected and $k \leq \kappa(G)$. Finally, the Wiener index of G, denoted by W(G), is defined as follows.

$$W(G) = \sum_{v,w \in V} d(v,w). \qquad (v \text{ and } w \text{ are unordered})$$

Observation 1. For any vertex $v \in V$,

$$\sum_{i=0}^{e(v)} d_i(v) = n \; .$$

Observation 2.

$$\sum_{v} d_i(v) = 2D_i \; .$$

Observation 3.

$$W(G) = \sum_{i=1}^d i D_i \; .$$

2.2 Lemmas

Lemma 1.

$$n\delta_i \le 2D_i \le n\Delta_i \qquad (1 \le i \le d)$$

Proof. This follows from, $2D_i = \sum_v d_i(v)$ (see Observation 2).

Lemma 2. ([8]) Let G be k-connected. Then, for any vertex $v \in V$,

$$k \le d_i(v). \qquad (1 \le i \le e(v) - 1)$$

Lemma 3. ([9])

Suppose a nondecreasing sequence a_1, a_2, \ldots, a_n $(n \ge 2)$ is eccentric. Let h is any integer with $a_1 < h \le a_n$, then $a_i = a_{i+1} = h$ for some i $(2 \le i \le n-1)$.

2.3 Result

Theorem. Let G be k-connected. Then the Wiener index of G is at least

$$\frac{nr}{2}\left(\frac{k(r-1)}{2}+1\right) + \frac{d-r}{2}\left(2d + (d-r-1)\left(dk-1-\frac{k(2d-2r-1)}{3}\right)\right)$$

Proof. From Lemma 3, there are at least two vertices v_1, v_2 such that $e(v_1) = e(v_2) = d$. And from Lemma 2, we have $d_i(v_1) \ge k$, $d_i(v_2) \ge k$, $(1 \le i \le d-1)$. Also, from Lemma 3, there are at least two vertices v_3, v_4 (distinct from v_1, v_2) such that $e(v_3) = e(v_4) = d-1$, and we have $d_i(v_3) \ge k$, $d_i(v_4) \ge k$ $(1 \le i \le (d-1)-1)$. And so on. Thus from Observation 2, we have

$$D_d \ge 1, \quad D_{d-1} \ge 1+k, \quad D_{d-2} \ge 1+2k, \dots$$

 $\dots, \quad D_{r+1} = D_{d-(d-r-1)} \ge 1+(d-r-1)k.$

Therefore

$$\sum_{i=r+1}^{d} i D_i = (r+1)D_{r+1} + \dots + dD_d$$

$$\geq (r+1)(1 + (d-r-1)k + \dots + (d-1)(1+k) + d)$$

$$= \sum_{i=0}^{d-r-1} (d-i)(1+ik) .$$

Thus

$$W(G) = \sum_{i=1}^{d} iD_i = \sum_{i=1}^{r-1} iD_i + rD_r + \sum_{i=r+1}^{d} iD_i$$

$$\geq \frac{nr}{2} \left(\frac{k(r-1)}{2} + 1\right) + \sum_{i=r+1}^{d} iD_i \quad \text{(since } D_r \ge \frac{n}{2})$$

$$= \frac{nr}{2} \left(\frac{k(r-1)}{2} + 1\right)$$

$$+ \frac{d-r}{2} \left(2d + (d-r-1)(dk-1 - \frac{k(2d-2r-1)}{3})\right)$$

Remark: The lower bound of this Theorem is attained, if G is an even cycle.

References

- H. Wiener, Structural determination of paraffin boiling points, J. Am. Chem. Soc. 69 (1947) 17–20.
- H. Wiener, Correlation of heats of isomerization, and differences in heats of vaporization of isomers, among the paraffin hydrocarbons, J. Am. Chem. Soc. 69 (1947) 2636–2638.
- [3] M. Randić, Characterization of atoms, molecules and classes of molecules based on paths enumerations, MATCH Commun. Math. Comput. Chem. 7 (1979) 5–64.
- [4] G. S. Bloom, J. W. Kennedy, L. V. Quintas, Distance degree regular Graphs, in: The Theory and Applications of Graphs, Kalamazoo, 1980, pp. 95–108.
- [5] H. B. Walikar, V. S, Shigehalli, H. S. Ramane, Bounds on the Wiener number of a graph, MATCH Commun. Math. Comput. Chem. 50 (2004) 117–132.
- [6] J. A. Bondy, U. S. R. Murty, Graph Theory with Applications, Elsevier, Amsterdam, 1976.
- [7] F. Buckley, F. Harary, *Distance in Graphs*, Addison–Wesley, Redwood City, 1990.
- [8] L. Caccetta, W. F. Smyth, Graphs of maximum diameter, *Discrete Math.* 102 (1992) 121–141.
- [9] L. Lesniak, Eccentric sequences in graphs, Period. Math. Hungar. 6 (1975) 287– 293.
- [10] H. Hosoya, Topological index. A newly proposed quantity characterizing the topological nature of structural isomers of saturated hydrocarbons, *Bull. Chem. Soc. Jpn.* 44 (1971) 2332–2339.
- [11] A. A. Dobrynin, R. Entringer, I. Gutman, Wiener index of trees: Theory and applications, Acta Appl. Math. 66 (2001) 211–249.