A Note on Wiener Indices of Unicyclic Graphs

Zhibin Du and Bo Zhou*

Department of Mathematics, South China Normal University, Guangzhou 510631, P. R. China

Abstract. The Wiener index of a connected graph is defined as the sum of all distances between unordered pairs of vertices. We determine the unicyclic graphs of given order, cycle length and number of pendent vertices with minimum Wiener index.

Keywords: Wiener index, distance, unicyclic graphs, pendent vertices

1 Introduction

The topological indices are numbers associated with chemical structures via their hydrogen–depleted graphs, which have been often used in modeling of structure–property relationships.

The Wiener index (often also called the Wiener number) is one of the oldest topological indices [13, 9], and it has been studied extensively [3, 4, 7, 8]. For recent results on Wiener index, see, e.g., [1, 5, 12, 14].

Let G be a connected graph with vertex set $V(G)$. For $u, v \in V(G)$, let $d_G(u, v)$ be the distance between vertices u and v in G. Evidently, $d_G(u, u) = 0$. The Wiener index of G is defined as

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

Burns and Entringer [2] and Moon [11] determined the trees of given order and number of pendent vertices (vertices of degree one) with minimum

*Correspondence to B. Zhou; e-mail: zhoubo@scnu.edu.cn

Wiener index. Gutman et al. [10] gave a relation related to the Wiener indices of unicyclic graphs (connected graph with a unique cycle) and some of its subgraphs, which seems to be the first result on the Wiener index of unicyclic graphs. Recently, we determined in [6] the unicyclic graphs of given order, cycle length and diameter with minimum Wiener index.

In this note, we determine the unicyclic graphs of given order, cycle length and number of pendent vertices with minimum Wiener index.

2 Preliminaries

For a graph G with $u \in V(G)$, let $d_G(u)$ be the degree of u in G. Let P_s be a path on s vertices. For a vertex v of the graph G, $G - v$ denotes the graph resulting from G by deleting v (and edges incident with it). For a edge subset E_1 of the graph G (the complement of G, respectively), $G - E_1$ ($G + E_1$, respectively) denotes the graph resulting from G by deleting (adding, respectively) the edges in E_1.

Let n, m and p be integers with $m \geq 3$, $p \geq 2$ and $m+p \leq n$. For integer a with $0 \leq a \leq n-m-p$, let $k(a) = \left\lfloor \frac{n-m-a}{p} \right\rfloor$ and $s = n - m - a - pk(a)$, and let $U_{n,m,p}(a)$ be the unicyclic graph obtained from the cycle $C_m = v_0v_1 \dots v_{m-1}v_0$ by attaching the path P_a at an end vertex to v_0, and then attaching to the other end vertex of the path the end vertices of $p - s$ paths with $k(a)$ vertices, and s paths with $k(a) + 1$ vertices (if $a = 0$, then these p paths are attached to v_0).

Lemma 2.1. *Let n, m and p be integers with $m \geq 3$, $p \geq 2$ and $m+p \leq n$. Let $\gamma = \gamma(n, m, p) = \max\left\{\left\lfloor \frac{n-2}{p+1} \right\rfloor + 2 - m, 0\right\}$. Then $W(U_{n,m,p}(a))$ with $0 \leq a \leq n-m-p$ is minimum if and only if $a = \gamma$ or $\gamma - 1$ if $\gamma \geq 1$ and $\frac{n-1}{p+1}$ is not an integer, and $a = \gamma$ otherwise.*

Proof. For $1 \leq a \leq n-m-p$, suppose that u is the vertex outside the cycle such that $d_G(u, v_0) = a$, where $G = U_{n,m,p}(a)$. Let $u_1, u_2, u_3, \dots, u_{d_G(u)}$ be the neighbors of u, where u_1 lies on the path between v_0 and u ($u_1 = v_0$ if $a = 1$), u_2 is an end vertex of one path with $k(a)$ vertices attached to u. It is easily seen that $U_{n,m,p}(a-1) \cong G - \{uu_3, \dots, uu_{d_G(u)}\} + \{u_1u_3, \dots, u_1u_{d_G(u)}\}$, and thus

$$\begin{aligned} & W(U_{n,m,p}(a-1)) - W(U_{n,m,p}(a)) \\ = \; & (n-m-a-k(a))[k(a) - (m+a-2)]. \end{aligned}$$

Obviously, $n - m - a - k(a) \geq k(a) > 0$, thus $W(U_{n,m,p}(a-1)) \geq$

$W(U_{n,m,p}(a))$ if and only if $k(a) \geq m + a - 2$, and $W(U_{n,m,p}(a-1)) = W(U_{n,m,p}(a))$ if and only if $k(a) = m + a - 2$.

Suppose that $k(1) \geq m - 1$. Then there is a maximum integer $a \geq 1$ with $k(a) \geq m + a - 2$ such that $W(U_{n,m,p}(a))$ is minimum. Such an a is denoted by a_0.

Suppose that $k(a) \geq m + a - 2$. Let $a' = \left\lfloor \frac{n-2}{p+1} \right\rfloor + 2 - m$. Let $t = n - 2 - (p+1)\left\lfloor \frac{n-2}{p+1} \right\rfloor$, where $0 \leq t \leq p$. For any integer a'' with $a' < a'' \leq n - m - p$, it is easily seen that $k(a'') - (m + a'' - 2) = \left\lfloor \frac{t-i}{p} \right\rfloor - i < 0$, and then $k(a'') < m + a'' - 2$ where $i = a'' - a'$. Note that $k(a') \geq m + a' - 2$. Thus, $a_0 = a' = \left\lfloor \frac{n-2}{p+1} \right\rfloor + 2 - m$.

If $\frac{n-1}{p+1}$ is not an integer, then $0 \leq t \leq p-1$, $k(a_0) = m + a_0 - 2$, and thus $W(U_{n,m,p}(a_0)) = W(U_{n,m,p}(a_0 - 1))$ for $a_0 \geq 1$. If $\frac{n-1}{p+1}$ is an integer, then $t = p$, $k(a_0) > m + a_0 - 2$ and thus $W(U_{n,m,p}(a_0)) < W(U_{n,m,p}(a_0 - 1))$ for $a_0 \geq 1$.

If $k(1) < m + 1 - 2 = m - 1$, then $W(U_{n,m,p}(0)) < W(U_{n,m,p}(1)) < \cdots < W(U_{n,m,p}(n - m - p))$. Now the result follows easily. □

3 Result

For integers n, m and p with $m \geq 3$, $p \geq 0$ and $m+p \leq n$, let $\mathcal{U}(n,m,p)$ be the set of unicyclic graphs with n vertices, cycle length m and p pendent vertices. The cases $p = 0, 1$ are trivial. We assume that $p \geq 2$. We will determine graphs in $\mathcal{U}(n,m,p)$ with minimum Wiener index.

Let G be a unicyclic graph with n vertices and let $C_m = v_0 v_1 \ldots v_{m-1} v_0$ be its unique cycle. Then $G - E(C_m)$ consists of m trees $T_0, T_1, \ldots, T_{m-1}$, where $v_i \in V(T_i)$ for $i = 0, 1, \ldots, m-1$. If $d_G(v_i) \geq 3$, then the components of $T_i - v_i$ are called the branches of G at v_i, each containing a neighbor of v_i in T_i. Let $v_{i_1}, \ldots, v_{i_{d_G(v_i)-2}}$ be the neighbors of v_i in T_i.

Lemma 3.1. *Let G be a unicyclic graph and $C_m = v_0 v_1 \ldots v_{m-1} v_0$ be its unique cycle. Suppose that $d_G(v_i), d_G(v_j) \geq 3$, where $0 \leq i, j \leq m-1$ and $i \neq j$. Let $G' = G - \left\{v_j v_{j_1}, \ldots, v_j v_{j_{d_G(v_j)-2}}\right\} + \left\{v_i v_{j_1}, \ldots, v_i v_{j_{d_G(v_j)-2}}\right\}$ and $G'' = G - \left\{v_i v_{i_1}, \ldots, v_i v_{i_{d_G(v_i)-2}}\right\} + \left\{v_j v_{i_1}, \ldots, v_j v_{i_{d_G(v_i)-2}}\right\}$. Then $W(G) > \min\{W(G'), W(G'')\}$.*

Proof. Let n_i be the number of vertices of $T_i - v_i$ for $i = 0, 1, \ldots, m-1$. Note that for $u \in V(T_i)$ and $v \in V(T_j)$ with $i \neq j$, $d_G(u,v) = d_G(u, v_i) +$

$d_G(v_i, v_j) + d_G(v, v_j)$. It is easily seen that

$$W(G') - W(G) = n_j \sum_{\substack{0 \le k \le m-1 \\ k \ne j}} n_k \left[d_G(v_k, v_i) - d_G(v_k, v_j)\right].$$

If $W(G') \ge W(G)$, then $\sum_{\substack{0 \le k \le m-1 \\ k \ne j}} n_k \left[d_G(v_k, v_j) - d_G(v_k, v_i)\right] \le 0$, and thus

$$\begin{aligned} & W(G'') - W(G) \\ = \; & n_i \sum_{\substack{0 \le k \le m-1 \\ k \ne i}} n_k \left[d_G(v_k, v_j) - d_G(v_k, v_i)\right] \\ = \; & n_i \sum_{\substack{0 \le k \le m-1 \\ k \ne j}} n_k [d_G(v_k, v_j) - d_G(v_k, v_i)] - n_i(n_i + n_j) d_G(v_i, v_j) \\ \le \; & -n_i(n_i + n_j) d_G(v_i, v_j) < 0. \end{aligned}$$

The result follows. □

Let G be a connected graph of the form in Fig. 1, where Q_1, Q_2, M_1 and M_2 are vertex-disjoint graphs, $|V(Q_1)|$, $|V(Q_2)|$, $|V(M_1)|$, $|V(M_2)| \ge 1$, and u and v are connected by a path of length $i \ge 1$, u (resp. v) is adjacent to at least one vertex in M_1 and Q_1 (resp. M_2 and Q_2).

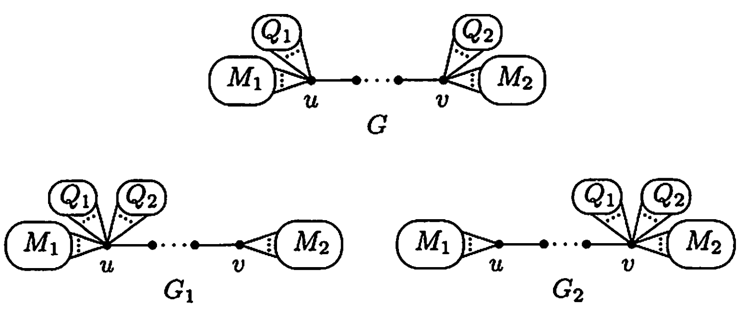

Fig. 1. The graphs G, G_1 and G_2

Lemma 3.2. *Let G, G_1 and G_2 be the three graphs in Fig. 1. Then $W(G) > \min\{W(G_1), W(G_2)\}$.*

Proof. It is easily seen that

$$W(G_1) - W(G) = i \cdot |V(Q_2)| \cdot [|V(M_2)| - (|V(M_1)| + |V(Q_1)|)].$$

If $W(G_1) \geq W(G)$, then $|V(M_1)| \leq |V(M_2)| - |V(Q_1)|$, and thus

$$\begin{aligned} W(G_2) - W(G) &= i \cdot |V(Q_1)| \cdot [|V(M_1)| - (|V(M_2)| + |V(Q_2)|)] \\ &\leq i \cdot |V(Q_1)| \cdot [(|V(M_2)| - |V(Q_1)|) \\ &\quad -(|V(M_2)| + |V(Q_2)|)] \\ &= -i \cdot |V(Q_1)|(|V(Q_1)| + |V(Q_2)|) < 0. \end{aligned}$$

The result follows. □

For a unicyclic graph G whose unique cycle is C_m, let $V_1(G) = \{x \in V(C_m) : d_G(x) \geq 3\}$ and $V_2(G) = \{x \in V(G) \setminus V(C_m) : d_G(x) \geq 3\}$.

Lemma 3.3. *Let G be a graph with minimum Wiener index in $\mathcal{U}(n, m, p)$, where $m \geq 3$, $p \geq 2$ and $m + p \leq n$. Then $|V_2(G)| = 0$ or 1.*

Proof. Let $C_m = v_0 v_1 \ldots v_{m-1} v_0$ be the unique cycle of G. By Lemma 3.1, we have $|V_1(G)| = 1$, say $V_1(G) = \{v_0\}$.

Suppose that a branch B' of G at v_0 contains two vertices, say x and y, in $V_2(G)$. Choose x and y such that $d_G(x, y)$ is as small as possible and let P be the unique path in G joining x to y. If $d_G(x, y) > 1$, then vertices on P except x and y all have degree two. Let x_1 (resp. y_1) be any neighbor of x (resp. y) outside P. Using Lemma 3.2 by setting $u = x$, $v = y$, M_1 (resp. M_2) to be the component of $G - x$ (resp. $G - y$) containing x_1 (resp. y_1), Q_1 (resp. Q_2) to be the graph consisting of all the components of $G - x$ (resp. $G - y$) not containing x_1 and y (resp. y_1 and x), then we get a graph $G' \in \mathcal{U}(n, m, p)$, such that $W(G') < W(G)$, a contradiction. Thus, for any branch B of G at v_0, $|V_2(G) \cap V(B)| = 0$ or 1. If $|V_2(G) \cap V(B)| = 0$ for any branch B, then $|V_2(G)| = 0$.

Now suppose that for some branch B_1 of G at v_0, $|V_2(G) \cap V(B_1)| = 1$, say $V_2(G) \cap V(B_1) = \{u_0\}$.

Suppose that $d_G(v_0) > 3$. Let Q be the unique path in G joining u_0 to v_0. Let u_1 be any neighbor of u_0 outside Q. Applying Lemma 3.2 by setting $u = u_0$, $v = v_0$, M_1 to be the component of $G - u_0$ containing u_1, M_2 to be $C_m - v_0$, Q_1 to be all the components of $G - u_0$ not containing u_1 and v_0, Q_2 to be all branches of G at v_0 not containing u_0, we may get a graph $G'' \in \mathcal{U}(n, m, p)$, such that $W(G'') < W(G)$, a contradiction. Thus, $d_G(v_0) = 3$, i.e., B_1 is the unique branch of G at v_0, then $|V_2(G)| = |V_2(G) \cap V(B_1)| = 1$. □

Now we prove the main result.

Theorem 3.1. *Let n, m and p be integers with $n \geq 6$, $m \geq 3$, $p \geq 2$ and $m+p \leq n$. Let $\gamma = \gamma(n,m,p) = \max\left\{\left\lfloor \frac{n-2}{p+1} \right\rfloor + 2 - m, 0\right\}$. Then $U_{n,m,p}(\gamma)$ and $U_{n,m,p}(\gamma - 1)$ if $\gamma \geq 1$ and $\frac{n-1}{p+1}$ is not an integer, and $U_{n,m,p}(\gamma)$ otherwise are the unique graphs in $\mathcal{U}(n,m,p)$ with minimum Wiener index.*

Proof. Suppose that G is a graph with minimum Wiener index in $\mathcal{U}(n,m,p)$. Let $C_m = v_0v_1 \ldots v_{m-1}v_0$ be its unique cycle. By Lemma 3.3, we have $|V_1(G)| = 1$, say $V_1(G) = \{v_0\}$, and $|V_2(G)| = 0$ or 1.

Let $v' = v_0$ if $|V_2(G)| = 0$ and let v' be the only vertex in $V_2(G)$ if $|V_2(G)| = 1$. It is easily seen that all the components consisting of vertices outside the cycle of $G - v'$ are paths. Suppose that there are two such paths (attached to v' in G), say P_s and P_t, such that $t \geq s + 2$ and $s \geq 1$. Let u (resp. v) be the pendent vertex of G in P_s (resp. P_t). For $G' = (G - v) + \{uv\} \in \mathcal{U}(n,m,p)$,

$$\begin{aligned} W(G') - W(G) &= -(t-1)(n-t-1) + s(n-s-2) \\ &= (t-s-1)(t+s+1-n) < 0, \end{aligned}$$

and thus $W(G') < W(G)$, a contradiction. We have $G = U_{n,m,p}(0)$ if $|V_2(G)| = 0$, and $G = U_{n,m,p}(a)$ with some $a \geq 1$ if $|V_2(G)| = 1$. Now by Lemma 2.1, the result follows. □

Example. If $n = 6$, then the possible cases in Theorem 3.1 are $(m,p) = (3,2)$, $(m,p) = (3,3)$ and $(m,p) = (4,2)$, for which $U_{6,3,2}(0)$, $U_{6,3,3}(0)$ and $U_{6,4,2}(0)$ are the unique extremal graphs with Wiener indices 27, 24 and 26, respectively. If $n = 8$, $m = 3$ and $p = 2$, then $U_{8,3,2}(1)$ and $U_{8,3,2}(0)$ are the unique extremal graphs with Wiener index 66.

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