Maximum Detour Index of Unicyclic Graphs with Given Maximum Degree

Xuli Qi and Bo Zhou*
Department of Mathematics, South China Normal University,
Guangzhou 510631, P. R. China

Abstract

The detour index of a connected graph is defined as the sum of detour distances between all its unordered vertex pairs. We determine the maximum detour index of n-vertex unicyclic graphs with maximum degree Δ, and characterize the unique extremal graph, where $2 \le \Delta \le n-1$.

1 Introduction

Let G be a simple connected graph with vertex set $V(G)$. The detour distance between vertices u and v in the graph G is the length of a longest path between them, denoted by $l_G(u,v)$, see [2, 8]. Note that $l_G(u,u) = 0$ for any $u \in V(G)$. The detour index of the graph G is defined as [1, 4, 5]

$$\omega(G) = \sum_{\{u,v\} \subseteq V(G)} l_G(u,v).$$

The detour matrix of G is an $n \times n$ matrix whose (i,j)-element is $l_G(v_i, v_j)$ with $V(G) = \{v_1, v_2, \ldots, v_n\}$, see [1, 3, 4, 7]. Evidently, the detour index is equal to the half-sum of the (off-diagonal) elements of the detour matrix.

The detour index found applications in quantitative structure–property relationship and quantitative structure–activity relationship studies, see the work of Lukovits [5], Trinajstić *et al.* [12], Rücker and Rücker [11], and Nikolić et al. [9]; For example, it was found that the detour index in combination with the Wiener index is very efficient in structure–boiling point modeling of acyclic and cyclic saturated hydrocarbons. Lukovits and Razinger [6], Trinajstić *et al.* [13], and Rücker and Rücker [11] proposed

*Corresponding author. E-mail: zhoubo@scnu.edu.cn

methods for computing the detour distances and hence for computing the detour index.

Among others, Zhou and Cai [14] gave bounds for the detour index, and determined the n-vertex unicyclic graphs with the first several smallest and largest detour indices for $n \geq 5$. We determined in [10] the n-vertex unicyclic graphs whose vertices on the unique cycle all have degree at least three with the first several smallest and largest detour indices for $n \geq 7$.

In this paper, we determine the maximum detour index of n-vertex unicyclic graphs with maximum degree Δ, and characterize the unique extremal graph, where $2 \leq \Delta \leq n-1$.

2 Preliminaries

For a connected graph G with $u \in V(G)$, let $\omega_u(G) = \sum_{v \in V(G)} l_G(u, v)$.

The ordinary distance between vertices u and v in a graph G is the length (number of edges) of a shortest path between them, denoted by $d_G(u, v)$. Evidently, if there is a unique path connecting u and v, then $l_G(u, v) = d_G(u, v)$.

Let $|G| = |V(G)|$ for a graph G.

For a subset M of $V(G)$ ($E(G)$, respectively), $G - M$ denotes the graph obtained from G by deleting the vertices in M and their incident edges (the edges in M, respectively). For a subset of the edge set of the complement of G, $G + M$ denotes the graph obtained from G by adding the edges in M. In the case M is a single vertex $\{v\}$ (edge e, respectively), then $G - M$ is denoted by $G - v$ ($G - e$, respectively), and $G + \{e\}$ is denoted by $G + e$.

Let P_n be the path and the star on $n \geq 1$ vertices, and C_n the cycle on $n \geq 3$ vertices.

Let n and r be integers with $3 \leq r \leq n$. For integers a and b with $a \geq b \geq 0$ and $a + b = n - r$, let $Q_{n,r}(a, b)$ be the unicyclic graph obtained by attaching respectively a path P_a and a path P_b at one terminal vertex to two adjacent vertices of the cycle C_r. Let $\mathbb{Q}_{n,r} = \{Q_{n,r}(a, b) : a + b = n - r, a \geq b \geq 0\}$.

For positive integer n, let $\varepsilon_n = 1$ if n is odd and $\varepsilon_n = 0$ if n is even.

Lemma 1. [14] *(i) For $n \geq 3$, $\omega(C_n) = \frac{1}{8}n(3n^2 - 4n + \varepsilon_n)$.*
(ii) Let $Q_{n,r}(a, b) \in \mathbb{Q}_{n,r}$. Then $\omega(Q_{n,r}(a, b))$ is independent of the values of a and b, i.e., all graphs in $\mathbb{Q}_{n,r}$ have the same detour index.
(iii) C_n is the unique graph with the largest detour index among the n-vertex unicyclic graphs.

Lemma 2. *Let u be a cut vertex of a connected graph G such that $G - u$ consists of vertex-disjoint subgraphs G_1' and G_2'. Let G_i be the subgraph of*

G *induced by* $V(G_i') \cup \{u\}$, *where* $i = 1, 2$. *Then*

$$\omega(G) = \omega(G_1) + \omega(G_2) + (|G_2| - 1)\,\omega_u(G_1) + (|G_1| - 1)\,\omega_u(G_2).$$

Proof. It is easily seen that

$$\begin{aligned}
\omega(G) &= \sum_{\{x,y\}\subseteq V(G)} l_G(x,y) \\
&= \omega(G_1) + \omega(G_2) + \sum_{x\in V(G_1'),y\in V(G_2')} l_G(x,y) \\
&= \omega(G_1) + \omega(G_2) + \sum_{x\in V(G_1'),y\in V(G_2')} (l_G(x,u) + l_G(y,u)) \\
&= \omega(G_1) + \omega(G_2) + (|G_2| - 1)\,\omega_u(G_1) + (|G_1| - 1)\,\omega_u(G_2),
\end{aligned}$$

as desired. □

Lemma 3. *Let* H_1 *and* H_2 *be vertex-disjoint connected graphs with at least two vertices, and* $u \in V(H_1)$ *and* $v \in V(H_2)$. *Let* G_1 *be the graph obtained from* H_1 *and* H_2 *by joining* u *and* v *by a path of length* $r \geq 1$, *and* G_2 *the graph obtained from* H_1 *and* H_2 *by identifying* u *and* v, *which is denoted by* w, *and attaching a path* P_r *to* w. *Then* $\omega(G_1) > \omega(G_2)$.

Proof. For G_1, v is a cut vertex, and let $G_{11} = G_1 - (V(H_2) \setminus \{v\})$ and $G_{12} = H_2$. For G_2, w is a cut vertex, and let $G_{21} = G_2 - (V(H_2) \setminus \{w\})$ and $G_{22} = H_2$. Obviously, $\omega_u(H_1) = \omega_w(H_1)$, $G_{11} = G_{21}$, $G_{12} = G_{22}$ and $\omega_v(G_{12}) = \omega_w(G_{22})$. Thus $\omega_v(G_{11}) = \frac{1}{2}r(r+1) + r(|H_1| - 1) + \omega_u(H_1) > \frac{1}{2}r(r+1) + \omega_w(H_1) = \omega_w(G_{21})$. Then by Lemma 2, the result follows. □

Let $C_r(T_1, T_2, \ldots, T_r)$ be the unicyclic graph for which the vertices of its unique cycle C_r are labeled consecutively by $v_1, v_2, \ldots, v_r$, and $T_1, T_2, \ldots, T_r$ are vertex–disjoint trees such that T_i and C_r share exactly one common vertex v_i for $i = 1, 2, \ldots, r$. Then any n-vertex unicyclic graph G with a cycle on r vertices is of the form $C_r(T_1, T_2, \ldots, T_r)$ with $\sum_{i=1}^{r} |T_i| = n$.

Lemma 4. *For integers* i *and* j *with* $2 \leq i < j \leq r$, *let* $G_{a_i,a_j} = C_r(T_1, T_2, \ldots, T_r)$, *where* T_s *is the path* P_{a_s+1} *with a terminal vertex* v_s *for* $2 \leq s \leq r$, *all trees* T_l *with* $l \neq i, j$ *and* $1 \leq l \leq r$ *are fixed, and* T_1 *is nontrivial. For* a_i, $a_j \geq 1$, *let* $x \neq v_i$ *and* $y \neq v_j$ *be respectively terminal vertices of* T_i *and* T_j, *and* z *the neighbor of* y *in* T_j. *If* $\omega_x(G_{a_i,a_j}) \geq \omega_y(G_{a_i,a_j})$, *then* $\omega(G_{a_i+1,a_j-1}) > \omega(G_{a_i,a_j})$, *where* $G_{a_{i+1},a_{j-1}} = G_{a_i,a_j} - zy + xy$.

Proof. Since T_1 is nontrivial, we have $l_{G_{a_i,a_j}}(x,y) < n - 1$. Then

$$\omega(G_{a_i+1,a_j-1}) - \omega(G_{a_i,a_j})$$

$$
\begin{aligned}
&= \omega_y(G_{a_i+1,a_j-1}) - \omega_y(G_{a_i,a_j}) \\
&= \omega_x(G_{a_i+1,a_j-1}) + n - 2 - \omega_y(G_{a_i,a_j}) \\
&= \omega_x(G_{a_i,a_j}) + 1 - l_{G_{a_i,a_j}}(x,y) + n - 2 - \omega_y(G_{a_i,a_j}) \\
&= \omega_x(G_{a_i,a_j}) - \omega_y(G_{a_i,a_j}) + n - 1 - l_{G_{a_i,a_j}}(x,y) > 0.
\end{aligned}
$$

The result follows easily. □

Lemma 5. *For integers i and r with $2 \le i \le \lfloor \frac{r}{2} \rfloor + 1$ and $r \ge 3$, let $G_i(a,r) = C_r(T_1, T_2, \ldots, T_r)$, where T_i is the path P_{a+1} with a terminal vertex v_i, $T_j = P_1$ for $2 \le j \le r$ with $j \ne i$, and T_1 is fixed. For fixed $b = a + r \ge 4$, we have $\omega(G_i(a,r)) \le \omega(G_2(a,r))$ with equality if and only if $G_i(a,r) = G_2(a,r)$.*

Proof. Note that v_i is a cut vertex of $G_i(a,r)$. Let $G_1 = G_i(a,r) - (V(T_i) \setminus \{v_i\})$ and $G_2 = T_i$. By Lemma 2, we have

$$
\begin{aligned}
\omega(G_i(a,r)) &= \omega(G_1) + \omega(G_2) + a\,\omega_{v_i}(G_1) + (|G_1| - 1)\omega_{v_i}(G_2) \\
&= \omega(G_1) + \omega(P_{a+1}) + a\,\omega_{v_i}(G_1) + (|G_1| - 1)\omega_{v_i}(P_{a+1}) \\
&= \omega(G_1) + \omega(P_{a+1}) + \frac{1}{2}a(a+1)(|G_1| - 1) \\
&\quad + a[\omega_{v_i}(C_r) + (|T_1| - 1) l_{C_r}(v_1, v_i) + \omega_{v_1}(T_1)] \\
&\le \omega(G_1) + \omega(P_{a+1}) + \frac{1}{2}a(a+1)(|G_1| - 1) \\
&\quad + a[\omega_{v_2}(C_r) + (|T_1| - 1)(r-1) + \omega_{v_1}(T_1)]
\end{aligned}
$$

with equality if and only if $i = 2$, i.e., $G_i(a,r) = G_2(a,r)$. □

Lemma 6. *For any unicyclic graph H with $u \in V(H)$, let $H(a_1, a_2, \ldots, a_t)$ be the graph obtained from H by attaching $t \ge 2$ paths $P_{a_1}, P_{a_2}, \ldots, P_{a_t}$ to u, where $1 \le a_1 \le a_2 \le \cdots \le a_t$. For fixed $b = a_1 + a_2 + \cdots + a_t$, $\omega(H(a_1, a_2, \ldots, a_t)) \le \omega(H(1, \ldots, 1, b - t + 1))$ with equality if and only if $H(a_1, a_2, \ldots, a_t) = H(1, \ldots, 1, b - t + 1)$.*

Proof. Suppose that $G = H(a_1, a_2, \ldots, a_t)$ is a graph with maximum detour index satisfying the given condition. Suppose that there is some i such that $a_i \ge 2$ with $1 \le i \le t-1$. Let x, $y \ne u$ be respectively the terminal vertices of the path P_{a_i} and $P_{a_{i+1}}$, and z the neighbor of x in G. Let $G_1 = G - xz + xy = H(a_1, a_2, \ldots, a_i - 1, a_{i+1} + 1, \ldots, a_t)$ and $G_2 = G - xz + xu$. Then

$$
\begin{aligned}
\omega(G_1) - \omega(G) &= (\omega(G_1) - \omega(G_2)) + (\omega(G_2) - \omega(G)) \\
&= a_{i+1}(|G| - a_{i+1} - 2) - (a_i - 1)(|G| - a_i - 1)
\end{aligned}
$$

$$= (a_{i+1} - a_i + 1)(|G| - a_{i+1} - a_i - 1) > 0,$$

which implies that $\omega(G_1) > \omega(G)$, a contradiction. Thus $a_i = 1$ for $i = 1, 2, \ldots, t-1$, and $a_t = b - t + 1$, i.e., $G = H(1, 1, \ldots, 1, b - t + 1)$. □

A path P in a graph G is called a pendant path at u if u is a terminal vertex of P with degree at least three in G, the other terminal vertex is pendant, and all internal vertices on P (if exist) have degree two in G.

3 The detour index of unicyclic graphs with given maximum degree

Let $\mathbb{U}(n, \Delta)$ be the set of n-vertex unicyclic graphs with maximum degree Δ, where $2 \leq \Delta \leq n-1$. Let $U_{n,\Delta}$ be the graph obtained by attaching $\Delta - 2$ pendant vertices to one vertex on the cycle $C_{n-\Delta+2}$. In particular, $U_{n,2} = C_n$.

Theorem 1. *Let $G \in \mathbb{U}(n, \Delta)$ with $2 \leq \Delta \leq n-1$. Then*

$$\omega(G) \leq \begin{cases} \frac{1}{8}(3n^3 - 3n^2\Delta - 3n\Delta^2 + 3\Delta^3 \\ \quad +2n^2 + 20n\Delta - 14\Delta^2 - 27n + 13\Delta + 6) & \text{if } n - \Delta \text{ is odd} \\ \frac{1}{8}(3n^3 - 3n^2\Delta - 3n\Delta^2 + 3\Delta^3 \\ \quad +2n^2 + 20n\Delta - 14\Delta^2 - 28n + 12\Delta + 8) & \text{if } n - \Delta \text{ is even} \end{cases}$$

with equality if and only if $G = U_{n,\Delta}$.

Proof. If $\Delta = 2$, then $G = C_n$, the result follows from Lemma 1 (i).

Suppose that $\Delta \geq 3$. Let G be a graph with the maximum detour in $\mathbb{U}(n, \Delta)$. Let C_r be the unique cycle of G. Obviously, $G \neq C_n$.

Case 1. Some vertex, say v_1, on C_r is of degree Δ.

By Lemma 3, the vertices outside C_r are of degree one or two, and the vertices on C_r different from v_1 are of degree two or three. By Lemmas 4 and 5, there is at most one vertex on C_r different from v_1 with degree three, and this vertex (if exists) must be one neighbor of v_1, say v_2. Thus G is a graph obtainable from C_r by attaching $\Delta - 2$ paths to v_1 and attaching at most one path to v_2. Let P_{a+1} be a longest pendant path at v_1 with $a \geq 1$. Let $T_2 = P_{b+1}$ with $b \geq 0$. Let $x_1, x_2, \ldots, x_{\Delta-2}$ be the neighbors of v_1 outside C_r, where $x_{\Delta-2}$ lies on the pendant path P_{a+1} at v_1. Let z be the pendant vertex of the pendant path P_{b+1} at v_2 if $b \geq 1$ and $z = v_2$ if $b = 0$.

By Lemma 6, there is at most one pendant path at v_1 in G with length at least two. Suppose that there is such a pendant path. Then $a \geq 2$. Let y be the neighbor of $x_{\Delta-2}$ different from v_1. Let $G' = G - x_{\Delta-2}y + zy \in \mathbb{U}(n, \Delta)$.

There is a pendant path P_{a+b} at v_2 in G'. Note that v_1 is a cut vertex in G and G'. Let $G_1 = G - \{x_1, x_2, \ldots, x_{\Delta-3}\}$, $G_2 = G - (V(G_1) \setminus \{v_1\})$, $G'_1 = G' - \{x_1, x_2, \ldots, x_{\Delta-3}\}$ and $G'_2 = G' - (V(G'_1) \setminus \{v_1\})$. Obviously, $G_2 = G'_2$. By Lemma 1 (ii), we have $\omega(G_1) = \omega(G'_1)$. It is easily seen that $\omega_{v_1}(G'_1) - \omega_{v_1}(G_1) = (a-1)(r+b-2) > 0$. By Lemma 2, $\omega(G') > \omega(G)$, a contradiction. Thus there is no pendant path at v_1 with length at least two, i.e., v_1 has $\Delta - 2$ pendant neighbors in G.

Suppose that $b \geq 1$. Let $G'' = G - v_1v_2 + v_1z \in \mathbb{U}(n, \Delta)$. Note that v_1 is a cut vertex in G and G''. Let $G_{1'} = G - \{x_1, x_2, \ldots, x_{\Delta-2}\}$, $G_{2'} = G - (V(G_{1'}) \setminus \{v_1\})$, $G''_1 = G'' - \{x_1, x_2, \ldots, x_{\Delta-2}\}$ and $G''_2 = G'' - (V(G''_1) \setminus \{v_1\})$. Obviously, $G_{2'} = G''_2$. By Lemma 1 (iii), we have $\omega(G''_1) > \omega(G_{1'})$. By Lemma 1 (i), we have $\omega_{v_1}(C_r) = \frac{1}{4}(3r^2 - 4r + \varepsilon_r)$ and a similar expression for $\omega_{v_1}(C_{r+b})$, where C_{r+b} is the cycle of G''. Then it is easily seen that $\omega_{v_1}(G''_1) - \omega_{v_1}(G_{1'}) = \frac{1}{4}[b^2 + (2r-2)b + \varepsilon_{r+b} - \varepsilon_r] \geq \frac{1}{4}(1 + 2r - 2 - 1) = \frac{1}{2}(r-1) > 0$. By Lemma 2, $\omega(G'') > \omega(G)$, a contradiction. Thus $b = 0$.

By the above arguments, it follows that $r = n - \Delta + 2$, and then $G = U_{n,\Delta}$. By direct calculation,

$$\omega(U_{n,\Delta}) = \begin{cases} \frac{1}{8}(3n^3 - 3n^2\Delta - 3n\Delta^2 + 3\Delta^3 \\ \quad +2n^2 + 20n\Delta - 14\Delta^2 - 27n + 13\Delta + 6) & \text{if } n - \Delta \text{ is odd,} \\ \frac{1}{8}(3n^3 - 3n^2\Delta - 3n\Delta^2 + 3\Delta^3 \\ \quad +2n^2 + 20n\Delta - 14\Delta^2 - 28n + 12\Delta + 8) & \text{if } n - \Delta \text{ is even.} \end{cases}$$

Case 2. All vertices on the cycle C_r have degree smaller than Δ in G.

There is some vertex u of degree Δ outside C_r and $4 \leq \Delta \leq n-3$. Suppose without loss of generality that v_1 is the vertex on C_r that is nearest to u. By Lemma 3, the vertices outside C_r different from u are of degree one or two, and the vertices on C_r are of degree two or three. By Lemmas 4 and 5, there is at most one vertex on C_r different from v_1 with degree three, and this vertex (if exists) must be one neighbor of v_1, say v_2. Let P_{a+1} be a longest pendant path at u with $a \geq 1$. Let $T_2 = P_{b+1}$ with $b \geq 0$.

By Lemma 6, there is at most one pendant path at u in G with length at least two. Suppose that there is such a pendant path. Then $a \geq 2$. Let x be the neighbor of the pendant vertex of the pendant path P_{a+1} at u. Let $s = d_G(u, x)$. Then $s = a - 1 \geq 1$. Let $y_1, y_2, \ldots, y_{\Delta-2}$ be the pendant neighbors of u, and $y_{\Delta-1}$ the neighbor of u on the pendant path P_{a+1} at u. For $G^* = G - \{uy_1, uy_2, \ldots, uy_{\Delta-2}\} + \{xy_1, xy_2, \ldots, xy_{\Delta-2}\} \in \mathbb{U}(n, \Delta)$, we have

$$\begin{aligned} \omega(G^*) - \omega(G) &= (a-1)(\Delta-2)(n-\Delta-s) - s(\Delta-2) \\ &= s(\Delta-2)(n-\Delta-s-1) > 0, \end{aligned}$$

a contradiction. Thus there is no pendant path at u with length at least two, i.e., u has $\Delta - 1$ pendant neighbors in G.

Suppose that $b \geq 1$. Let z be the pendant vertex of P_{b+1}. Let $G^{**} = G - v_1v_2 + v_1z \in \mathbb{U}(n, \Delta)$. Note that v_1 is a cut vertex in G and G^{**}. Let G_{1*} and G_{2*} be the subgraphs of G induced by $V(T_1)$ and $V(C_r) \cup V(T_2)$, respectively. Let G_1^{**} and G_2^{**} be the subgraphs of G^{**} induced by $V(T_1)$ and $V(C_{r+b})$, respectively. Obviously, $G_{1*} = G_1^{**}$. By Lemma 1 (iii), we have $\omega(G_2^{**}) > \omega(G_{2*})$. It is easily seen by Lemma 1 (i) that $\omega_{v_1}(G_2^{**}) - \omega_{v_1}(G_{2*}) = \frac{1}{4}[b^2 + (2r-2)b + \varepsilon_{r+b} - \varepsilon_r] \geq \frac{1}{4}(1 + 2r - 2 - 1) = \frac{1}{2}(r-1) > 0$. By Lemma 2, $\omega(G^{**}) > \omega(G)$, a contradiction. Thus $b = 0$.

Suppose that $d_G(u, v_1) \geq 2$. Let w be the neighbor of u on the path connecting u and v_1. Let $t = d_G(w, v_1)$. Then $t \geq 1$. Let $G^{***} = G - v_1v_2 + wv_2 \in \mathbb{U}(n, \Delta)$. Note that w is a cut vertex in G and G^{***}. Let $G_{1**} = G - \{u, y_1, y_2, \ldots, y_{\Delta-1}\}$, $G_{2**} = G - (V(G_{1**}) \setminus \{w\})$, $G_1^{***} = G^{***} - \{u, y_1, y_2, \ldots, y_{\Delta-1}\}$ and $G_2^{***} = G^{***} - (V(G_1^{***}) \setminus \{w\})$. Obviously, $G_{2**} = G_2^{***}$. By Lemma 1 (iii), we have $\omega(G_1^{***}) > \omega(G_{1**})$. It is easily seen by Lemma 1 (i) that $\omega_w(G_1^{***}) - \omega_w(G_{1**}) = \frac{1}{4}[t^2 + (2r-2)t + \varepsilon_{r+t} - \varepsilon_r] \geq \frac{1}{4}(1 + 2r - 2 - 1) = \frac{1}{2}(r-1) > 0$. By Lemma 2, $\omega(G^{***}) > \omega(G)$, a contradiction. Thus $d_G(u, v_1) = 1$.

By the above arguments, it follows that $r = n - \Delta$, and then $G = U'_{n,\Delta}$, where $U'_{n,\Delta}$ is the graph obtained by attaching a star on Δ vertices at its center to one vertex on the cycle $C_{n-\Delta}$. By direct calculation,

$$\omega(U'_{n,\Delta}) = \begin{cases} \frac{1}{8}(3n^3 - 3n^2\Delta - 3n\Delta^2 + 3\Delta^3 \\ \quad -4n^2 + 16n\Delta - 4\Delta^2 - 7n - 7\Delta + 8) & \text{if } n - \Delta \text{ is odd,} \\ \frac{1}{8}(3n^3 - 3n^2\Delta - 3n\Delta^2 + 3\Delta^3 \\ \quad -4n^2 + 16n\Delta - 4\Delta^2 - 8n - 8\Delta + 8) & \text{if } n - \Delta \text{ is even.} \end{cases}$$

Combining Cases 1 and 2, we have $G = U_{n,\Delta}$ for $3 \leq \Delta \leq n-1$ or $U'_{n,\Delta}$ for $4 \leq \Delta \leq n-3$. If $4 \leq \Delta \leq n-3$, then it is easily seen that

$$\begin{aligned} & \omega(U_{n,\Delta}) - \omega(U'_{n,\Delta}) \\ = & \begin{cases} \frac{1}{8}[-10\Delta^2 + (4n+20)\Delta + 6n^2 - 20n - 2] & \text{if } n - \Delta \text{ is odd} \\ \frac{1}{8}[-10\Delta^2 + (4n+20)\Delta + 6n^2 - 20n] & \text{if } n - \Delta \text{ is even} \end{cases} \\ > & \ 0, \end{aligned}$$

and thus $\omega(U_{n,\Delta}) > \omega(U'_{n,\Delta})$. Therefore $G = U_{n,\Delta}$. The result follows. □

By Theorem 1, $U_{n,\Delta}$ is the unique graph with the maximum detour index among graphs in $\mathbb{U}(n, \Delta)$, where $2 \leq \Delta \leq n-1$.

Acknowledgement. This work was supported by the National Natural Science Foundation of China (no. 11071089).

References

[1] D. Amić, N. Trinajstić, On detour matrix, Croat. Chem. Acta 68 (1995) 53–62.

[2] G. Chartrand, H. Escuadro, P. Zhang, Detour distance in graphs, J. Combin. Math. Combin. Comput. 53 (2005) 75–94.

[3] F. Harary, Graph Theory, Addison–Wesley, Reading, MA, 1969, p. 203.

[4] O. Ivanciuc, A. T. Balaban, Design of topological indices. Part 8. Path matrices and derived molecular graph invariants, MATCH Commun. Math. Comput. Chem. 30 (1994) 141–152.

[5] I. Lukovits, The detour index, Croat. Chem. Acta 69 (1996) 873–882.

[6] I. Lukovits, M. Razinger, On calculation of the detour index, J. Chem. Inf. Comput. Sci. 37 (1997) 283–286.

[7] D. Janežić, A. Miličević, S. Nikolić, N. Trinajstić, Graph–Theoretical Matrices in Chemistry, Univ. Kragujevac, Kragujevac, 2007, pp. 81–86.

[8] S. F. Kapoor, H. V. Kronk, D. R. Lick, On detours in graphs, Canad. Math. Bull. 11 (1968) 195–201.

[9] S. Nikolić, N. Trinajstić, Z. Mihalić, The detour matrix and the detour index, in: J. Devillers, A. T. Balaban (Eds.), Topological Indices and Related Descriptors in QSAR and QSPR, Gordon and Breach, Amsterdam, 1999, pp. 279–306.

[10] X. Qi, B. Zhou, Detour index of a class of unicyclic graphs, Filomat 24 (no. 1) (2010) 29–40.

[11] G. Rücker, C. Rücker, Symmetry–aided computation of the detour matrix and the detour index, J. Chem. Inf. Comput. Sci. 38 (1998) 710–714.

[12] N. Trinajstić, S. Nikolić, B. Lučić, D. Amić, Z. Mihalić, The detour matrix in chemistry, J. Chem. Inf. Comput. Sci. 37 (1997) 631–638.

[13] N. Trinajstić, S. Nikolić, Z. Mihalić, On computing the molecular detour matrix, Int. J. Quantum Chem. 65 (1998) 415–419.

[14] B. Zhou, X. Cai, On detour index, MATCH Commun. Math. Comput. Chem. 63 (2010) 199–210.