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Detour Index of Hexagonal Chains

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Abstract

Detour index of a connected graph is defined as the sum of the lengths of the longest paths between all pairs of its vertices. We derive expression for the detour index of hexagonal chains, the molecular graphs of unbranched catacondensed benzenoids, using which we show that the linear hexagonal chain has the minimum, while the zig-zag hexagonal chain has the maximum detour index.

1 Introduction

The detour index, defined as the sum of the lengths of the longest paths between all pairs of vertices of a molecular graph, is a counterpart of the well-known Wiener index, defined as the sum of the lengths of the shortest paths between all pairs of vertices. The detour index was first considered by Amić and Trinajstić [1], while its potential for use in quantitative structure-activity relationship studies has been investigated by Lukovits [6], who showed that the product of the Wiener and detour indices yields good correlations for selected size-dependent molecular properties, such as the boiling points of alkanes. Trinajstić et al. [13] confirmed Lukovits' finding that the product of the Wiener and detour indices correlates well with the boiling point on the set of 76 lowest alkanes and cycloalkanes, and this was further confirmed by Rücker and Rücker [12] on a large combined sample of acyclic, monocyclic and polycyclic alkanes.

Theoretical properties of the detour index have been much less studied than that of the Wiener index. While the detour and the Wiener index coincide for trees, in which there is a unique path between any two vertices, the situation changes drastically for cyclic structures. The reason is that the problem of finding a longest path in an arbitrary graph is NP-hard [4], meaning that there cannot exist a polynomial time algorithm to calculate its detour index unless P=NP (which is one of the Millenium Prize Problem [3]). Two of the exponential time algorithms were described by Lukovits and Razinger [7] and Rücker and Rücker [12]. The detour indices were calculated for a few special classes of molecular graphs, such as fused bicyclic structures (Lukovits and Rücker [7]), bridge and chain graphs (Mansour and Schork [8]), nanostar dendrimers (Karbasioun and Ashrafi [5]) and certain nanotubes (Ashrafi et al. [2]). The degeneracy of the detour index was studied by Randić et al. [11]. The extremal values of the detour index of unicyclic graphs were studied by Zhou and Cai [14] and by Qi and Zhou [9, 10].

It is interesting that the detour index of molecular graphs having a Hamiltonian cycle that contains all the vertices, in which, therefore, longest paths may have maximum possible length, has not been studied so far. As prominent examples of such molecular graphs, we study here the detour index of hexagonal chains, the molecular graphs of unbranched catacondensed benzenoids. In Section 2 we introduce an auxiliary representation of hexagonal chains with strings. We describe the structure of longest paths in hexagonal chains in Section 3 and express the detour index of a hexagonal chain in terms of its string representation. Based on this expression, we show in Section 4 that the linear hexagonal chain has the minimum detour index, while the zig-zag hexagonal chain has the maximum detour index.

The rest of this section contains necessary notation and definitions. The vertex and the edge sets of a simple graph G are denoted by $V(G)$ and $E(G)$, respectively. Unless otherwise notes, it is assumed that all graphs are connected. For a set $S \subset V(G)$, $G - S$ represents the graph obtained from G by deleting vertices in S and their incident edges. The set $S \subset V(G)$ is a *vertex cut* if $G - S$ has more connected components than G. For vertices $u, v \in V(G)$, the detour distance $d^*(u, v)$ is defined as the length of the longest path between u and v in G if $u \neq v$ and as $d^*(u, v) = 0$ if $u = v$. The sum

$$D^*(G) = \sum_{u,v \in V(G)} d^*(u, v),$$

where the summation goes over all pairs of vertices of G, is the *detour index* of G.

2 Encoding of hexagonal chains

Definition 1 *Let $n > 0$ be an integer and let $\{H_i\}_{i=1}^n$ be a set of n mutually disjoint hexagons. For $i = 1, \ldots, n$, let $u_i, v_i, w_i, t_i \in V(H_i)$ be distinct vertices such that $\{u_i, v_i\}, \{w_i, t_i\} \in E(H_i)$. The graph*

$$H \equiv H(\{H_i\}_{i=1}^n; \{u_i, v_i, w_i, t_i\}_{i=1}^n),$$

obtained from the union of $H_1, \ldots, H_n$ by identifying the vertex w_i with the vertex u_{i+1} and the vertex t_i with the vertex v_{i+1} for $i = 1, \ldots, n-1$, is called a hexagonal chain of length n. The set of all hexagonal chains of length n is denoted by HC_n.

Figure 1: A hexagonal chain of length 6.

An example of a hexagonal chain of length 6 is given in Fig. 1.

In order to simplify calculation of the detour index of a hexagonal chain $H \in HC_n$, we will represent H by a ternary string of length n in the alphabet $\{F, R, L\}$. Connect the centers of successive hexagons $H_1, \ldots, H_n$ of H with vectors $v_2, \ldots, v_n$ such that v_i connects the centers of H_{i-1} and H_i for $i = 2, \ldots, n$. Then for $i = 2, \ldots, n-1$, let

$$s_i = \begin{cases} F, & \text{if } v_{i+1} \text{ and } v_i \text{ are parallel,} \\ R, & \text{if } v_{i+1} \text{ makes a right turn after } v_i, \\ L, & \text{if } v_{i+1} \text{ makes a left turn after } v_i. \end{cases}$$

This way, each hexagon H_i is encoded by the symbol $s_i \in \{F, R, L\}$, indicating its relation with the previous and the next hexagon in the chain. Since this encoding cannot be defined for the first and the last hexagon in the chain, we let $s_1 = s_n = F$ by convention.

The process of encoding a hexagonal chain by ternary string is illustrated in Fig. 2.

For expressing the detour index, it will be helpful to use one more representation of H by a $\{-1, 0, 1\}$-sequence $(I_i)_{i=1}^n$, defined in the following way:

$$I_i = \begin{cases} 0, & \text{if } s_i = F, \\ 1, & \text{if } s_i = R, \\ -1, & \text{if } s_i = L. \end{cases}$$

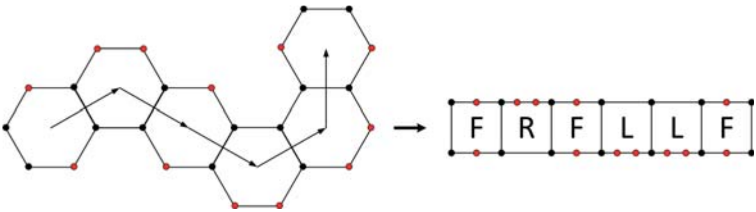

Figure 2: Encoding of a hexagonal chain by ternary string.

In the sequel we will use both of these encodings to represent a hexagonal chain H. We also introduce following notation for the vertices of the hexagonal chain H: from left to right, the vertices of degree three from the upper layer will be denoted as $a_1, \ldots, a_{n-1}$, while vertices of degree three from the lower layer will be denoted as $b_1, \ldots, b_{n-1}$. We extend this notation with a_0 and b_0 to denote the vertices of the edge opposite to a_1b_1 in H_1, and with a_n and b_n to denote the vertices of the edge opposite to $a_{n-1}b_{n-1}$ in H_n. The remaining two vertices of degree two in each hexagon H_i, $1 \leq i \leq n$, will be denoted in the following way:

(i) if H_i is of type F, the degree two vertex from the upper layer will be denoted by c_i and that from the lower layer will be denoted by d_i;

(ii) if H_i is of type R, the degree two vertices from the upper layer will be denoted by c_i and d_i (from left to right);

(iii) if H_i is of type L, the degree two vertices from the lower layer will be denoted by c_i and d_i (from left to right).

The process of labelling the vertices of a hexagonal chain is illustrated in Fig. 3.

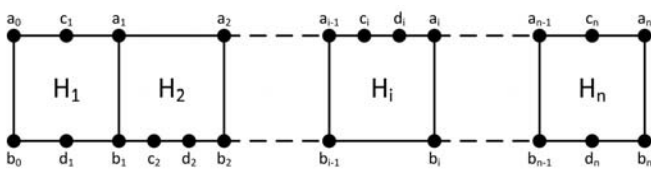

Figure 3: Vertex labels in a hexagonal chain.

For $1 \leq i \leq j \leq n$, let $H_{i,j}$ be a subgraph of H induced by the vertex set $\cup_{k=i}^{j} V(H_k)$. Two vertices $u, v \in H$ form a *close pair* if there exists i such that $u \in V(H_i)$ and

$v \in V(H_i)$. Otherwise, they form a *distant pair* and we say that u is left of v (denoting it by $u \prec v$) if there are i and j such that $u \in V(H_i)$, $v \in V(H_j)$ and $i < j$. In addition, the close pair $\{a_i, b_i\}$, $0 \le i \le n$, will be called a *vertical pair*.

Further, we let $V_i = \{a_i, b_i, c_i, d_i\}$ for $1 \le i \le n$. Note that $V_i \cap V_j = \emptyset$ for $i \ne j$, and that $V(H) = \{a_0, b_0\} \cup (\cup_{i=1}^{n} V_i)$.

3 Structure of the longest paths

We describe here structure of the longest paths between pairs of vertices of a hexagonal chain H, divided into three subsections, corresponding to vertical pairs, close pairs and distant pairs of vertices. We start off with a simple, but useful result.

Lemma 2 *Let G be a connected graph and let P be a simple path in G with $u \in V(G)$ as one endpoint of P. If $v \in V(G)$ does not belong to P or if v is the other endpoint of P, then all vertices from $P \setminus \{u, v\}$ belong to the same component in $G - \{u, v\}$.*

Proof. All edges from P, except its pendant edges, are present in $G - \{u, v\}$. Then, since $P - \{u, v\}$ contains a path between any two vertices from $P \setminus \{u, v\}$, we conclude that they belong to the same component of $G - \{u, v\}$ they all belong to the same component. ■

3.1 Detour distance between vertices of vertical pairs

Consider the vertical pair $\{a_i, b_i\}$ for some $0 \le i \le n$. The set $\{a_i, b_i\}$ is a vertex cut in H and so by Lemma 2, the longest path between a_i and b_i belongs either to the left or to the right component of $H - \{a_i, b_i\}$. Since both of these components are Hamiltonian with the left one having $4i$, and the right one having $4(n - i)$ vertices, it follows that

$$d^*(a_i, b_i) = 1 + 4 \max(i, n - i). \tag{1}$$

Note that $d^*(a_i, b_i)$ does not depend on the structure of H, but only on n and i. If we denote $X(H) = \sum_{i=0}^{n} d^*(a_i, b_i)$, then from (1) we have

$$\begin{aligned} X(H) &= (n+1) + 4 \sum_{i=0}^{n} \max(i, n-i) \\ &= n + 1 + 4 \left(\sum_{i=0}^{\lfloor n/2 \rfloor} (n - i) + \sum_{i=\lfloor n/2 \rfloor + 1}^{n} i \right) \end{aligned}$$

$$\begin{aligned} &= 4(n - \lfloor n/2 \rfloor)(\lfloor n/2 \rfloor + 1) + (2n+1)(n+1) \\ &= 3n^2 + 5n + \frac{3 - (-1)^n}{2} \end{aligned} \tag{2}$$

where we used $\lfloor n/2 \rfloor = \frac{n}{2} - \frac{1-(-1)^n}{4}$.

3.2 Detour distance between vertices of other close pairs

For $0 \leq i \leq n$, let $Y(H_i)$ denote the sum of detour distances between pairs of vertices in H_i, not counting its vertical pairs. In order to indicate whether H_i is a middle hexagon in H, we will use the indicator

$$M_i^n = \begin{cases} 1, & \text{if } n \text{ is odd and } i = \frac{n+1}{2}, \\ 0, & \text{otherwise.} \end{cases}$$

Theorem 3 *For $H \in HC_n$ and $1 \leq i \leq n$*

$$Y(H_i) = \begin{cases} 28n + 21 + 24\max(i-1, n-i) + 4M_i^n, & \text{if } H_i \text{ is of type } R \text{ or } L, \\ 24n + 25 + 28\max(i-1, n-i) + 4M_i^n, & \text{if } H_i \text{ is of type } F. \end{cases} \tag{3}$$

Proof. The proof is divided in cases based on the type of hexagon H_i.

Case I: H_i is of type R. It holds

$$d^*(a_{i-1}, c_i) = d^*(c_i, d_i) = d^*(d_i, a_i) = d^*(b_{i-1}, b_i) = 4n + 1,$$

since H contains a Hamiltonian path between each of these pairs of vertices. From Lemma 2 we further get

$$d^*(a_{i-1}, d_i) = d^*(c_i, a_i) = 4n \quad \text{and} \quad d^*(a_{i-1}, a_i) = 4n - 1.$$

Let us calculate $d^*(b_{i-1}, a_i)$. Since $H - \{b_{i-1}, a_i\}$ consists of two components, from Lemma 2 follows that the longest path between b_{i-1} and a_i fully belongs to one of these components. The longest path in the left component has length $4(i-1)+4$, while that in the right component has length $4(n-i)+2$ and, because of factor 4, the detour distance depends on $\max(i-1, n-i)$. Analogous argument holds for the detour distance between b_i and a_{i-1}, so that

$$d^*(b_{i-1}, a_i) + d^*(a_{i-1}, b_i) = 2 \cdot 4\max(i-1, n-i) + 2 + 4$$

if H_i is not the middle hexagon of H. If H_i is the middle hexagon, the longest path will be of length $4\max(i-1, n-i) + 3$ in both cases, so that we have

$$d^*(b_{i-1}, a_i) + d^*(a_{i-1}, b_i) = 8\max(i-1, n-i) + 6 + 2M_i^n.$$

The same argument shows that

$$d^*(b_{i-1},c_i)+d^*(b_i,d_i)=8\max(i-1,n-i)+6+2M_i^n$$

and

$$d^*(b_{i-1},d_i)+d^*(b_i,c_i)=8\max(i-1,n-i)+6,$$

yielding the expression for $Y(H_i)$.

Case II: H_i is of type L. The argument from previous case holds also for a type L hexagon by symmetry.

Case III: H_i is of type F. Due to the existence of a Hamiltonian path between each of the following pairs of vertices, we have

$$d^*(a_{i-1},c_i)=d^*(c_i,a_i)=d^*(b_{i-1},d_i)=d^*(d_i,b_i)=4n+1$$

and from Lemma 2 we further get

$$d^*(a_{i-1},a_i)=d^*(b_{i-1},b_i)=4n.$$

Similar argument as in Case I shows that

$$\begin{aligned}
d^*(b_{i-1},c_i)+d^*(b_i,c_i)=d^*(a_{i-1},d_i)+d^*(a_i,d_i) &= 8\max(i-1,n-i)+6+2M_i^n,\\
d^*(a_{i-1},b_i)+d^*(b_{i-1},a_i) &= 8\max(i-1,n-i)+6,\\
d^*(c_i,d_i) &= 4\max(i-1,n-i)+3.
\end{aligned}$$

The expression for $Y(H_i)$ follows by summing all these detour distances. ■

Let $Y(H)=\sum_{i=1}^{n}Y(H_i)$. The sum $X(H)+Y(H)$ gives the sum of detour distances between all close vertex pairs in H. Using the fact that $I_i^2=1$ when H_i is of type R and L and $I_i^2=0$ if H_i is of type F, the expression (3) may be written more compactly as

$$\begin{aligned}
Y(H_i) &= 24n+4nI_i^2+25-4I_i^2+28\max(i-1,n-i)-4I_i^2\max(i-1,n-i)+4M_i^n\\
&= 24n+25+28\max(i-1,n-i)+4I_i^2\min(i-1,n-i)+4M_i^n.
\end{aligned}$$

From this and the fact that $\sum_{i=1}^{n}4M_i^n=2(1-(-1)^n)$, we get

$$\begin{aligned}
Y(H) &= 24n^2+25n+28\sum_{i=1}^{n}\max(i-1,n-i)+4\sum_{i=1}^{n}I_i^2\min(i-1,n-i)+\sum_{i=1}^{n}4M_i^n\\
&= 38n^2+11n+28\lfloor n/2\rfloor(n-\lfloor n/2\rfloor)+2(1-(-1)^n)+4\sum_{i=1}^{n}I_i^2\min(i-1,n-i)\\
&= 45n^2+11n-\frac{3-3(-1)^n}{2}+4\sum_{i=1}^{n}I_i^2\min(i-1,n-i) \qquad (4)
\end{aligned}$$

3.3 Detour distance between vertices of distant pairs

Define function $p : V(H) \setminus \{a_0, b_0\} \to V(H)$ as follows: if $u \in V_i$ for $1 \leq i \leq n$ set

$$p(u) = \begin{cases} a_{i-1}, & \text{if } u \text{ belongs to the lower layer of } H, \\ b_{i-1}, & \text{if } u \text{ belongs to the upper layer of } H. \end{cases}$$

The following theorem describes detour distance between distant pair of vertices in H in terms of detour distances within smaller hexagonal chains.

Theorem 4 *Let $u, v \in V(H)$, $H \in HC_n$, be a distant pair of vertices such that $u \prec v$. If $v \in V_i$ then*

$$d_H^*(u, v) = d_{H_{1,i-1}}^*(u, p(v)) + d_{H_{i,n}}^*(p(v), v).$$

Proof. Without loss of generality, assume that v belongs to the upper layer, so that $p(v) = b_{i-1}$. The set $\{a_{i-1}, b_{i-1}\}$ is a vertex cut in H with u and v in different components of $H - \{a_{i-1}, b_{i-1}\}$, so that at least one of a_{i-1} and b_{i-1} belongs to the longest path between u and v. Let x be the vertex from $\{a_{i-1}, b_{i-1}\}$ which appears later on the longest path from u to v (provided that both a_{i-1} and b_{i-1} belong to it), so that

$$d_H^*(u, v) = d_{H_{1,i-1}}^*(u, x) + d_{H_{i,n}}^*(x, v). \tag{5}$$

We show that it must be $x = p(v) = b_{i-1}$, for which the conclusion stems directly from (5), as the choice of $x = a_{i-1}$ cannot lead to longer longest path between u and v.

Namely, in case $x = a_{i-1}$ the longest path between a_{i-1} and v in $H_{i,n}$ cannot contain b_{i-1}, due to the choice of x, so that $d_{H_{i,n}}^*(a_{i-1}, v) = d_{H_{i,n}}(a_{i-1}, v)$, where $d_{H_{i,n}}(a_{i-1}, v)$ denotes the standard distance, i.e., the length of the shortest path between a_{i-1} and v. Since $p(v)$ and a_{i-1} are adjacent and rightmost in $H_{1,i-1}$, it follows that

$$d_{H_{1,i-1}}^*(u, p(v)) \geq d_{H_{1,i-1}}^*(u, a_{i-1}) - 1.$$

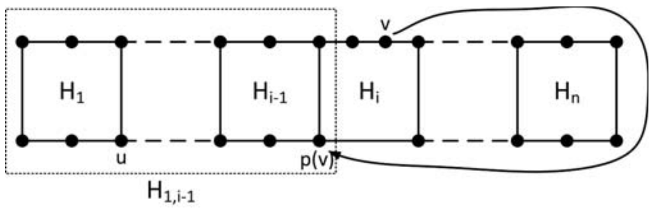

Figure 4: Part of the longest path from u to v contained within $H_{i,n}$.

On the other hand, if $i < n$ then $d_H(a_{i-1}, v) \leq 3$ since both a_{i-1} and v belong to the upper layer of H_i, while $d^*_{H_{i,n}}(p(v), v) > 4(n-i)+1 \geq 5$ since the longest path from $p(v)$ to v contains vertices from the last hexagon (see Figure 4). If $i = n$, then H_i is of type F and v is either c_n or a_n. In both cases, it is straightforward to check that $d^*_{H_{i,n}}(p(v), v) \geq d_H(a_{i-1}, v) + 1$. Therefore

$$d^*_{H_{1,i-1}}(u, p(v)) + d^*_{H_{i,n}}(p(v), v) \geq d^*_{H_{1,i-1}}(u, a_{i-1}) + d_H(a_{i-1}, v)$$

showing that $x = a_{i-1}$ cannot lead to longer longest path between u and v in H. Hence, $p(v) = b_{i-1}$ belongs to the longest path between u and v, and it comes after a_{i-1}, in case that a_{i-1} also belongs to this longest path. ■

The value $d^*_{H_{i,n}}(p(v), v)$ can be easily calculated using Figure 4 and previous discussion on close pairs of vertices. Table 1 shows the values $d^*_{H_{i,n}}(p(v), v)$ for $v \in V_i$, depending on the type of the hexagon H_i.

Type of H_i	$v = a_i$	$v = b_i$	$v = c_i$	$v = d_i$
F	$4(n-i)+3$	$4(n-i)+3$	$4(n-i)+4$	$4(n-i)+4$
R	$4(n-i)+2$	$4(n-i)+4$	$4(n-i)+4$	$4(n-i)+3$
L	$4(n-i)+4$	$4(n-i)+2$	$4(n-i)+4$	$4(n-i)+3$

Table 1: The values of $d^*_{H_{i,n}}(p(v), v)$.

For $H \in HC_n$ and $1 \leq i \leq n$ we introduce the following notation

$$D^a_i = \sum_{u \in H_{1,i},\ u \neq b_i} d^*_{H_{1,i}}(a_i, u) \qquad \text{and} \qquad D^b_i = \sum_{u \in H_{1,i},\ u \neq a_i} d^*_{H_{1,i}}(b_i, u).$$

The following theorem gives a recurrent formula for D^a_i and D^b_i.

Theorem 5 *For $1 \leq i \leq n$ holds*

$$D^a_i = \begin{cases} 28i - 12 + D^b_{i-1}, & \textit{if } H_i \textit{ is of type } F, \\ 28i - 12 + D^a_{i-1}, & \textit{if } H_i \textit{ is of type } R, \\ 32i - 18 + D^b_{i-1}, & \textit{if } H_i \textit{ is of type } L, \end{cases}$$

and

$$D^b_i = \begin{cases} 28i - 12 + D^a_{i-1}, & \textit{if } H_i \textit{ is of type } F, \\ 32i - 18 + D^a_{i-1}, & \textit{if } H_i \textit{ is of type } R, \\ 28i - 12 + D^b_{i-1}, & \textit{if } H_i \textit{ is of type } L, \end{cases}$$

where $D^a_0 = D^b_0 = 0$.

Proof. For $i = 1$, the formulas can be easily checked as H_1 is a hexagon of type F.

Let us suppose $i > 1$. From the definition we have

$$D_i^a = d^*_{H_{1,i}}(a_i, a_{i-1}) + d^*_{H_{1,i}}(a_i, b_{i-1}) + d^*_{H_{1,i}}(a_i, c_i) + d^*_{H_{1,i}}(a_i, d_i) + \sum_{u \in H_{1,i},\ u \prec a_i} d^*_{H_{1,i}}(a_i, u).$$

Assume that H_i is a hexagon of type F. From the discussion of close pairs of vertices, it follows that

$d^*_{H_{1,i}}(a_i, a_{i-1}) + d^*_{H_{1,i}}(a_i, b_{i-1}) + d^*_{H_{1,i}}(a_i, c_i) + d^*_{H_{1,i}}(a_i, d_i) = 4i + 4i - 1 + 4i + 1 + 4i = 16i.$

Let $u \in H$ be an arbitrary vertex satisfying $u \prec a_i$. As in the proof of Theorem 4, we conclude that at least one of vertices a_{i-1} and b_{i-1} occurs on the longest path from u to a_i. If a_{i-1} appears later than b_{i-1} on the path, then $d^*_{H_{1,i}}(a_i, u) = 2 + d^*_{H_{1,i-1}}(a_{i-1}, u)$, otherwise $d^*_{H_{1,i}}(a_i, u) = 3 + d^*_{H_{1,i-1}}(b_{i-1}, u)$. From $|d^*_{H_{1,i-1}}(a_{i-1}, u) - d^*_{H_{1,i-1}}(b_{i-1}, u)| \le 1$ it follows that it is optimal to choose $d^*_{H_{1,i}}(a_i, u) = 3 + d^*_{H_{1,i-1}}(b_{i-1}, u)$, so that

$$\sum_{u \in H_{1,i},\ u \prec a_i} d^*_{H_{1,i}}(a_i, u) = \sum_{u \in H_{1,i},\ u \prec a_i} 3 + \sum_{u \in H_{1,i-1},\ u \neq a_i} d^*_{H_{1,i-1}}(b_{i-1}, u) = 3 \cdot 4(i-1) + D^b_{i-1}.$$

Combining these results we get $D_i^a = 28i - 12 + D^b_{i-1}$. The cases when H_i is of type R (so that the longest path goes through a_{i-1}) and when H_i is of type L (so that the longest path goes through b_{i-1}) are discussed similarly. The recurrent formula for D_i^b follows from that for D_i^a by symmetry. ■

Corollary 6 *For* $1 \le i \le n$

$$\begin{aligned} D_i^a + D_i^b &= D^a_{i-1} + D^b_{i-1} + 56i - 24 + (4i-6)I_i{}^2 + I_i(D^a_{i-1} - D^b_{i-1}) && (6)\\ D_i^a - D_i^b &= (I_i{}^2 - 1)(D^a_{i-1} - D^b_{i-1}) - (4i-6)I_i. && (7) \end{aligned}$$

Proof. Follows directly from Theorem 5 using the fact that $I_i^2 = 1$ when H_i is of type R or L and $I_i^2 = 0$ when H_i is of type F. ■

Further, for $u \in V(H)$ denote

$$d^*_H(u) = \sum_{v \in H,\ v \prec u} d^*_H(u, v),$$

and for $1 \le i \le n$ denote

$$Z(H_i) = \sum_{u \in V_i} d^*_H(u).$$

Evidently, $Z(H) = \sum_{i=1}^{n} Z(H_i)$ represents the sum of detour distances between all distant pairs of vertices in H. From Theorem 4, Table 1 and the fact that there exists $4(i-1)$ nodes in H left to any $u \in H_i$, we get

$$Z_i(H) = \begin{cases} 4(i-1)(16(n-i)+14) + 2D_{i-1}^a + 2D_{i-1}^b, & \text{if } H_i \text{ is of type } F, \\ 4(i-1)(16(n-i)+13) + D_{i-1}^a + 3D_{i-1}^b, & \text{if } H_i \text{ is of type } R, \\ 4(i-1)(16(n-i)+13) + 3D_{i-1}^a + D_{i-1}^b, & \text{if } H_i \text{ is of type } L. \end{cases}$$

This formula can be written more compactly using the indicator sequence I_i:

$$\begin{aligned} Z_i(H) &= 4(i-1)(16(n-i)+14-I_i{}^2) + (2-I_i)D_{i-1}^a + (2+I_i)D_{i-1}^b \\ &= 4(i-1)(16(n-i)+14) + 2(D_{i-1}^a + D_{i-1}^b) - I_i(D_{i-1}^a - D_{i-1}^b) - 4(i-1)I_i^2 \quad (8) \end{aligned}$$

In order to simplify the expression for $Z_i(H)$, we will focus on the term $D_{i-1}^a + D_{i-1}^b$. Since $D_0^a + D_0^b = 0$, from the recurrent formula (6) one easily obtains by induction that

$$D_{i-1}^a + D_{i-1}^b = 56\frac{(i-1)i}{2} - 24(i-1) + \sum_{j=1}^{i-1}(4j-6)I_j{}^2 + \sum_{j=1}^{i-1} I_j(D_{j-1}^a - D_{j-1}^b). \quad (9)$$

Combining (8) and (9), we obtain

$$\begin{aligned} Z_i(H) &= \underbrace{8(i-1)(8n-i+1)}_{\text{Denote this by } Z_i'(H)} \\ &+ \underbrace{2\sum_{j=1}^{i-1}(4j-6)I_j{}^2 - 4(i-1)I_i^2}_{\text{Denote this by } Z_i''(H)} \\ &+ \underbrace{2\sum_{j=1}^{i-1} I_j(D_{j-1}^a - D_{j-1}^b) - I_i(D_{i-1}^a - D_{i-1}^b)}_{\text{Denote this by } Z_i'''(H)}, \end{aligned}$$

so that $Z(H) = \sum_{i=1}^{n} Z_i'(H) + \sum_{i=1}^{n} Z_i''(H) + \sum_{i=1}^{n} Z_i'''(H)$. The first sum equals to

$$\sum_{i=1}^{n} Z_i'(H) = 64n\sum_{i=1}^{n-1} i - 8\sum_{i=1}^{n-1} i^2 = \frac{4n(n-1)(22n+1)}{3}.$$

Rearranging the terms, we evaluate the remaining two sums

$$\begin{aligned} \sum_{i=1}^{n} Z_i''(H) &= 2\sum_{i=1}^{n}\sum_{j=1}^{i-1}(4j-6)I_j{}^2 - \sum_{i=1}^{n} 4(i-1)I_i{}^2 \\ &= 2\sum_{j=1}^{n}\sum_{i=j+1}^{n}(4j-6)I_j{}^2 - \sum_{i=1}^{n} 4(i-1)I_i{}^2 \end{aligned}$$

$$
\begin{aligned}
&= 2\sum_{j=1}^{n}(n-j)(4j-6){I_j}^2 - \sum_{i=1}^{n}4(i-1){I_i}^2 \\
&= \sum_{i=1}^{n}(2(n-i)(4i-6)-4(i-1)){I_i}^2, \\
\sum_{i=1}^{n} Z_i'''(H) &= \sum_{i=1}^{n}(2(n-i)-1)I_i(D_{i-1}^a - D_{i-1}^b),
\end{aligned}
$$

which gives

$$
Z(H) = \frac{4n(n-1)(22n+1)}{3} + \sum_{i=1}^{n}(2(n-i)-1)I_i(D_{i-1}^a - D_{i-1}^b + (4i-6)I_i) - 2\sum_{i=1}^{n}{I_i}^2. \quad (10)
$$

Finally, from $D^*(H) = X(H) + Y(H) + Z(H)$ by combining (2), (4) and (10) and the fact that $I_1 = I_n = 0$, we obtain

Theorem 7 *The detour index of a hexagonal chain $H \in HC_n$ is equal to*

$$
\begin{aligned}
D^*(H) &= \frac{88n^3 + 60n^2 + 44n}{3} + (-1)^n + 2\sum_{i=2}^{n-1}{I_i}^2(2\min(i-1, n-i) - 1) + \\
&\quad \sum_{i=2}^{n-1}(2(n-i)-1)I_i(D_{i-1}^a - D_{i-1}^b + (4i-6)I_i). \qquad (11)
\end{aligned}
$$

Note that this theorem yields a straightforward linear time algorithm for calculating the detour index of H, since the values of the indicator sequence I_i stem from the structure of the hexagonal chain, while the differences $D_{i-1}^a - D_{i-1}^b$ can be calculated iteratively for $i = 1, \ldots, n-2$ from (7).

4 Extremal values of the detour index

We now characterize hexagonal chains in HC_n with extremal values of the detour index. We will rely on the following

Lemma 8 *If $H \in HC_n$, then for all $2 \le i \le n$ holds $|D_i^a - D_i^b| \le 4i - 6$ with equality if and only if H_i is of type R or L.*

Proof. By induction on i. For $i = 2$, the statement trivially holds. Supposing that the statement holds $i-1$, from the recurrent formula (7) we have that either $|D_i^a - D_i^b| = 4i-6$ if $I_i = \pm 1$ or $|D_i^a - D_i^b| = |D_{i-1}^a - D_{i-1}^b|$ if $I_i = 0$. In the latter case, by the inductive hypothesis $|D_{i-1}^a - D_{i-1}^b| \le 4(i-1) - 6 < 4i - 6$. ∎

From the recurent formula (7) and the proof of the Lemma 8 we can obtain explicit value of $D^a_{i-1} - D^b_{i-1}$:

$$D^a_i - D^b_i = (-1)^{i-j+1} I_j (4j-6)$$

where j is the largest index less than i with $I_j \neq 0$ (if no such j exists, then $D^a_i - D^b_i = 0$). Let $1 < t_1 < t_2 < \ldots < t_m < n$ be the indices of hexagons of types R or L. The formula (11) can also be rewritten without D^a_i and D^b_i:

$$\begin{aligned} D^*(H) &= \frac{88n^3 + 60n^2 + 44n}{3} + (-1)^n + \\ &\quad 4\sum_{i=1}^{m} \left(\min(t_i - 1, n - t_i) + 2t_i n - 2t_i^2 - 3n + 2t_i\right) + \\ &\quad \sum_{i=2}^{m} (2(n-i)-1)(-1)^{t_i - t_{i-1}} I_{t_i} I_{t_i - 1}(4t_{i-1} - 6). \end{aligned}$$

Let $H^n_F \in HC_n$ be the linear chain represented by the string $FF\ldots F$, i.e., with $I_i = 0$ for all $1 \leq i \leq n$. The minimum value of the detour index among hexagonal chains is given in the following theorem.

Theorem 9 *Let $H \in HC_n$. Then*

$$D^*(H) \geq \frac{88n^3 + 60n^2 + 44n}{3} + (-1)^n \tag{12}$$

with equality if and only if H is isomorphic to H^n_F.

Proof. The first part of the formula (11) is equal for all hexagonal chains in HC_n.

Next, since $2\min(i-1, n-i) - 1 > 0$ for $2 \leq i \leq n-1$, we have

$$2\sum_{i=2}^{n-1} {I_i}^2 (2\min(i-1, n-i) - 1) \geq 0$$

with equality if and only if $I_i = 0$ for all $2 \leq i \leq n-1$.

In the second sum, for $2 \leq i \leq n$ holds $2(n-i) - 1 > 0$. If $I_i \neq 0$ then by Lemma 8 follows

$$\begin{aligned} I_i\left(D^a_{i-1} - D^b_{i-1} + (4i-6)I_i\right) &= 4i - 6 + I_i(D^a_{i-1} - D^b_{i-1}) \\ &\geq 4i - 6 - |D^a_{i-1} - D^b_{i-1}| \\ &\geq 4i - 6 - (4(i-1) - 6) > 0. \end{aligned}$$

Therefore, for the second sum holds

$$\sum_{i=2}^{n-1}(2(n-i)-1)I_i(D_{i-1}^a - D_{i-1}^b + (4i-6)I_i) \geq 0$$

with equality if and only if $I_i = 0$ for all $2 \leq i \leq n-1$.

In conclusion, inequality (12) holds for every hexagonal chain H, while equality holds if and only if $I_i = 0$ for all $2 \leq i \leq n-1$, i.e., if and only if $H \cong H_F^n$. ■

Next, let $H_{RL}^n, H_{RL}^n \in HC_n$ be isomorphic hexagonal chains represented by ternary strings $FRLRL \dots F$ and $FLRLR \dots F$, respectively. The maximum value of the detour index among hexagonal chains is given in the following theorem.

Theorem 10 *Let $H \in HC_n$. Then*

$$D^*(H) \leq 32n^3 + n^2 - 64n - 46 + \frac{1+(-1)^n}{2}$$

with equality if and only if H is isomorphic to H_{RL}^n or H_{LR}^n.

Proof. From the proof of Theorem 9 we know that the sum $\sum_{i=2}^{n-1} I_i{}^2(2\min(i-1, n-i)-1)$ from (11) attains the maximum value if and only if $I_i \neq 0$ for all $2 \leq i \leq n-1$.

Since $D_1^a - D_1^b = 0$, the second sum in (11) can be rewritten as

$$2(2n-5) + \sum_{i=3}^{n-1}(2(n-i)-1)I_i(D_{i-1}^a - D_{i-1}^b + (4i-6)I_i).$$

For $3 \leq i \leq n-1$, we have

$$\begin{aligned} I_i(D_{i-1}^a - D_{i-1}^b + (4i-6)I_i) &\leq |4i-6+I_i(D_{i-1}^a - D_{i-1}^b)| && (13)\\ &\leq 4i-6+|D_{i-1}^a - D_{i-1}^b| && (14)\\ &\leq 4i-6+4(i-1)-6 = 8(i-2) && (15)\end{aligned}$$

where we used Lemma 8 in (15). We know that $I_i(D_{i-1}^a - D_{i-1}^b + (4i-6)I_i) \geq 0$ from the proof of Theorem 9 and that equality holds in (13) if and only if $I_i \neq 0$. Further, equality holds in (14) if and only if $I_i(D_{i-1}^a - D_{i-1}^b) \geq 0$. For $I_i \neq 0$ from (7) we have

$$I_i(D_{i-1}^a - D_{i-1}^b) > 0 \Leftrightarrow -I_i I_{i-1}(4(i-1)-6) > 0 \Leftrightarrow I_i = -I_{i-1}.$$

Finally, equality in (15) holds if and only if $I_i \neq 0$ by Lemma 8.

Therefore, $D^*(H)$ achieves its maximum value if and only if $I_i = (-1)^i$ for all $2 \le i \le n$ or $I_i = (-1)^{i+1}$ for all $2 \le i \le n$, i.e., if and only if H is isomorphic to either H^n_{RL} or H^n_{LR}. For these two hexagonal chains we have

$$\begin{aligned} 2\sum_{i=2}^{n-1} I_i^{\,2}(2\min(i-1,n-i)-1) &= 4(\sum_{i=2}^{\lfloor n/2\rfloor}(i-1) + \sum_{i=\lfloor n/2\rfloor+1}^{n-1}(n-i)) - 2(n-2) \\ &= n^2 - 4n + 4 + \frac{1-(-1)^n}{2} \end{aligned}$$

and

$$\begin{aligned} \sum_{i=3}^{n-1}(2(n-i)-1)I_i(D^a_{i-1} - D^b_{i-1} + (4i-6)I_i) &= 8(2n-5)\sum_{i=3}^{n-1}(i-2) - 16\sum_{i=3}^{n-1}(i-2)^2 \\ &= \frac{8n^3 - 60n^2 + 160n - 150}{3}. \end{aligned}$$

Substituting these two expressions in (11) we get

$$D^*(H^n_{RL}) = 32n^3 + n^2 - 64n - 46 + \frac{1+(-1)^n}{2}. \qquad \blacksquare$$

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