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Bicyclic graphs with minimal values of the detour index

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Abstract. We are looking for the graphs with minimal detour index in the class of connected bicyclic graphs. For the fixed number of vertices, we split the problem into two cases: bicyclic graphs without common edges between cycles and the complement of it. In both cases, we find graphs with minimal detour index.

1. Introduction

Topological indices are the numbers that reflect certain structural characteristics of organic molecules, obtained from the respective graphs. One of the oldest and the most completely analyzed is the Wiener index or the Wiener number.

Let $G = (V, E)$ be a simple connected graph. The distance between vertices $u, v \in V$ in G is the length of the shortest path between them denoted by $d(u, v)$ or $d_G(u, v)$. The Wiener index of the graph G is defined as

$$W(G) = \sum_{\{u,v\}\subseteq V(G)} d_G(u, v).$$

That is

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

where $D_G(u)$ is the sum $D_G(u) = \sum_{v\in V} d_G(u, v)$, for any vertex $u \in V$.

The Wiener index was first proposed by Harold Wiener [3] as an aid to determining the boiling point of paraffin. In particular, he mentions in his article that the boiling point t_B can be quite closely approximated by the formula

$$t_B = aw + bp + c,$$

where w is the Wiener index, p the polarity number and a, b and c are constants for a given isomeric group. Since then, it was observed that the Wiener index has a connection to a host of other properties of molecules

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(viewed as graphs). For more information about the Wiener index in chemistry and mathematics see [5] and [4], respectively.

Another topological index, called the *detour index*, is conceptually close to Wiener index, except that its definition refers to *the longest distance* instead of *the shortest distance* between two graph vertices. The detour index $\omega(G)$, where G denotes the underlying graph, has been introduced by Amić and Trinajstić [8] and by John [9] independently

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

where $l_G(u,v)$ is the length of the longest path between two vertices.

The length $l_G(u,v)$ of the longest path is also called *detour distance* between vertices $u, v \in V$ in G. When it is clear from a context which underlying graph G is assumed, we simply write $l(u,v)$ instead of $l_G(u,v)$. Also, we define

$$\omega(G) = \frac{1}{2}\sum_{u\in V} L_G(u)$$

where $L_G(u)$ is the sum $L_G(u) = \sum_{v\in V} l_G(u,v)$, for any vertex $u \in V$.
Recently, as for Wiener index, it's been presented significance of detour index in the structure-boiling point relation [6], [7].

The main goal of this paper is to find graphs with minimal detour index among the class of connected bicyclic graphs with n vertices. For the rest of paper, we treat exclusively connected type of graphs.

In the Section 2 we give review of important terminology and theory regarding main problem, mostly based on papers [1] and [2].

The case of bicyclic graphs without common edges between two cycles is treated in Section 3. We found, by Theorem 3, that the smallest detour index in the corresponding class is $n^2 + 2n - 7$. It is attained at so called $n-$vertex butterfly, that looks like two triangles having one vertex in common and all other $n - 5$ vertices are attached as pendent vertices to that common vertex (Figure 1).

The most interesting and consequently the most complex case, subject of Section 4, is about bicyclic graphs with common edges between two cycles. The central role in this section has a Theorem 4 which brings out an iterative procedure of converting given graph to the one with smaller detour index. According to our result, the smallest detour index for this class has the graph that looks like two glued triangles by one side, making a parallelogram, and all other $n - 4$ pendent vertices are attached to one of two common vertices of those triangles (Figure 3).

2. Preliminaries

Let $H = (V(H), E(H))$ be graph without pendent vertices and $V(H) = \{v_1, v_2, \ldots, v_n\}$. Let $T_1, T_2, \ldots, T_n$ be vertex disjoint trees such that H and T_i have exactly one vertex v_i in common, for $1 \le i \le n$. Such graph is denoted by $H(T_1, T_2, \ldots, T_n)$. Let S_n and P_n be the n-vertex star and path, respectively. Let C_n be a cycle graph with n vertices.

The next assertion is valid for arbitrary cyclic graph. Although the proof of the next lemma is almost the same as for similar assertion proved in paper by Zhou and Cai [1], as well as in [11], we include it to facilitate reading the rest of the paper.

Lemma 1. *Let $H = (V(H), E(H))$ be graph without pendent vertices and $G = H(T_1, T_2, \ldots, T_n)$. Then*

$$\omega(G) = \sum_{i=1}^{n} W(T_i) + \sum_{1\le i<j\le n} [|T_i| D_{T_j}(v_j) + |T_j| D_{T_i}(v_i) + |T_i||T_j| l_H(v_i, v_j)].$$

Proof. From the definition of detour index

$$\omega(G) = \sum_{\{x,y\}\subseteq V(G)} l_G(x, y) = \sum_{i=1}^{n} \sum_{\{x,y\}\subseteq V(T_i)} l_{T_i}(x, y) + \frac{1}{2} \sum_{i=1}^{n} \sum_{\substack{j=1\\ j\neq i}}^{n} \sum_{\substack{x\in V(T_i)\\ y\in V(T_j)}} l_G(x, y).$$

For each $1 \le i \le n$, it obviously follows that

$$\sum_{\{x,y\}\subseteq V(T_i)} l_{T_i}(x, y) = W(T_i).$$

On the other hand,

$$\begin{aligned}
&\frac{1}{2} \sum_{i=1}^{n} \sum_{\substack{j=1\\ j\neq i}}^{n} \sum_{\substack{x\in V(T_i)\\ y\in V(T_j)}} l_G(x, y) = \\
&= \sum_{1\le i<j\le n} \sum_{\substack{x\in V(T_i)\\ y\in V(T_j)}} \left[d_{T_i}(x, v_i) + l_H(v_i, v_j) + d_{T_j}(y, v_j) \right] \\
&= \sum_{1\le i<j\le n} \left[\sum_{x\in V(T_i)} d_{T_i}(x, v_i) \sum_{y\in V(T_j)} 1 + l_H(v_i, v_j) \sum_{\substack{x\in V(T_i)\\ y\in V(T_j)}} 1 + \sum_{y\in V(T_j)} d_{T_j}(y, v_j) \sum_{x\in V(T_i)} 1 \right] \\
&= \sum_{1\le i<j\le n} [|T_j| D_{T_i}(v_i) + |T_i||T_j| l_H(v_i, v_j) + |T_i| D_{T_j}(v_j)],
\end{aligned}$$

which completes the proof. □

We will also use the following lemmas.

Lemma 2. *[2] Let T be n-vertex tree different from n-vertex star S_n. Then*

$$(n-1)^2 = W(S_n) < W(T).$$

Lemma 3. *[1] Let T be n-vertex tree where $n \ge 3$ and $u \in V(T)$. Let x be the center of star S_n. Then*

$$n - 1 = D_{S_n}(x) \le D_T(u).$$

Equality holds exactly when $T = S_n$ and $u = x$.

Denote by $\mathcal{U}_{n,r}$ the class of unicyclic graphs with n vertices and cycle length r, where $3 \le r \le n$. Subclass of $\mathcal{U}_{n,r}$ where all $n - r$ pendent vertices are attached to a single vertex of the cycle C_r is denoted by $\mathcal{S}_{n,r}$. For fixed n and r, all graphs from $\mathcal{S}_{n,r}$ are isomorphic, so concrete instance of this class we denote by $S_{n,r}$.

Proposition 1. *[1] Among n-vertex unicyclic graphs, $S_{n,3}$ for $n \ge 3$ is the unique graph with the smallest detour index, which is equal to $n^2 - 3$.*

3. Bicyclic graphs with cycles without common edges

Let $\mathcal{B}_{n;k,m}$ be a class of bicyclic graphs with $n-$vertices, whose cycles have k and m vertices and don't have common edges. We are going to prove that the smallest detour index in $\bigcup_{3\leq k\leq m} \mathcal{B}_{n;k,m}$, for $n \geq 5$, has the so called n-vertex butterfly $B \in \mathcal{B}_{n;3,3}$, the graph presented in the next figure

Proof.

$$\begin{aligned}\omega(G) &= \sum_{\{u,v\}\subseteq V_1} l(u,v) + \sum_{\{u,v\}\subseteq V_2} l(u,v) + \sum_{u\in V_1\setminus\{a_1\},\, v\in V_2\setminus\{a_2\}} l(u,v)\\ &= \omega(G_1)+\omega(G_2)+\sum_{u\in V_1\setminus\{a_1\}}\sum_{v\in V_2\setminus\{a_2\}}(l(u,a^*)+l(a^*,v))\\ &= \omega(G_1)+\omega(G_2)+L_{G_1}(a_1)|V_2-1|+L_{G_2}(a_2)|V_1-1|.\end{aligned}$$

□

Theorem 3. *Let G be a n-vertex bicyclic graph whose cycles have no common edges and $n \geq 5$. Then*

$$\omega(G) \geq \omega(B) = n^2 + 2n - 7,$$

where B is the n−vertex butterfly (Figure 1).

Proof. Let G be an arbitrary bicyclic graph with n vertices whose cycles have no common edges. Then $G = G_1^{a_1} * G_2^{a_2}$ for some unicyclic graphs $G_1 \in \mathcal{U}_{n_1,p}$ and $G_2 \in \mathcal{U}_{n_2,q}$ such that $n = n_1 + n_2 - 1$. Due to previous theorem

$$\omega(G) = \omega(G_1) + \omega(G_2) + L_{G_1}(a_1)(n_2 - 1) + L_{G_2}(a_2)(n_1 - 1).$$

By Proposition 1 we have

$$\omega(G_1) \geq \omega(S_{n_1,3}) \text{ and } \omega(G_2) \geq \omega(S_{n_2,3}) \text{ with equalities if and only if } G_1 = S_{n_1,3} \text{ and } G_2 = S_{n_2,3}.$$

From Theorem 1 it follows

$$L_{G_1}(a_1) \geq n_1 + 1 \text{ and } L_{G_2}(a_2) \geq n_2 + 1,$$

with equalities if and only if a_1 and a_2 are vertices in $S_{n_1,3}$ and $S_{n_2,3}$ with $n_1 - 2$ and $n_2 - 2$ pendent vertices, respectivelly. Hence

$$\begin{aligned}\omega(G) &\geq \omega(S_{n_1,3}) + \omega(S_{n_2,3}) + (n_1+1)(n_2-1) + (n_2+1)(n_1-1)\\ &= n_1^2 - 3 + n_2^2 - 3 + 2n_1n_2 - 2 = n^2 + 2n - 7.\end{aligned}$$

We conclude that $\omega(G) = n^2 + 2n - 7$ if and only if $G_i = S_{n_i,3}$ and a_i has $n_i - 2$ pendent vertices, for $i = 1, 2$. In this case, G is actually B, the n-vertex butterfly. □

4. Bicyclic graphs with cycles with common edges

Denote by $\mathcal{E}_n(s, p_1, p_2)$, $s \geq p_1 \geq p_2 \geq 1$, $p_1 \geq 2$, the class of n−vertex bicyclic graphs, $n \geq 4$, whose cycles R_1, R_2 have at least one common edge, where

$$s = |E(R_1) \cap E(R_2)|,\ p_1 = |E(R_1) \setminus E(R_2)| \text{ and } p_2 = |E(R_2) \setminus E(R_1)|.$$

Described class is illustrated in the following figure

For $u \in B$, let g' be an $(u,b)-$path in G' with length $l_{G'}(u,b)$. There are two possibilities: $e' = (v_{s-2}, b) \notin g'$ or $e' = (v_{s-2}, b) \in g'$. Suppose that $e' = (v_{s-2}, b) \notin g'$. Then, $g = g' + (b, v_{s-1})$ is $(u, v_{s-1})-$path in G and so

$$l_G(u, v_{s-1}) \geq |g| = |g'| + 1 = l_{G'}(u,b) + 1 = l_{G'}(u, v_{s-1}).$$

If $e' = (v_{s-2}, b) \in g'$, replace the edge e' by (v_{s-2}, v_{s-1}). We obtain an $(u, v_{s-1})-$path in the graph G. Path $g = g' - (b, v_{s-2}) + (v_{s-2}, v_{s-1})$ doesn't pass across the vertex b and, since $u \in B$, it is not the longest $(u, v_{s-1})-$path. Hence,

$$l_G(u, v_{s-1}) > |g| = |g'| = l_{G'}(u,b) = l_{G'}(u, v_{s-1}) - 1.$$

That is

$$l_G(u, v_{s-1}) \geq l_{G'}(u, v_{s-1}).$$

It follows that

$$l_G(u, v_{s-1}) - l_{G'}(u, v_{s-1}) \geq 0, \quad \text{for } u \in B.$$

From this inequality we conclude that

$$\sum_{u \in T} [l_G(u, v_{s-1}) - l_{G'}(u, v_{s-1})] \geq \sum_{u \in A} [l_G(u, v_{s-1}) - l_{G'}(u, v_{s-1})] \tag{3}$$

Let $u \in A$ and let g be an $(u, v_{s-1})-$path with length $l_G(u, v_{s-1})$ such that g doesn't pass across b. Then $h = g + (v_{s-1}, b)$ is an $(u,b)-$path. We are going to prove that its length is $l_G(u,b)$. If opposite, there is an $(u,b)-$path $\tilde{h}$ in the graph G, such that $|\tilde{h}| > |h| = l_G(u, v_{s-1}) + 1$. Therefore $(v_{s-1}, b) \notin \tilde{h}$. So, $\tilde{h} + (b, v_{s-1})$ is $(u, v_{s-1})-$path with length $|\tilde{h}| + 1 > l_G(u, v_{s-1})$, that is not possible. Hence,

$$l_G(u,b) = l_G(u, v_{s-1}) + 1$$

We are going to show that for $u \in A$ the longest $(u,b)-$path in G' passes across the v_{s-2}.

Suppose opposite. Let g' be an $(u,b)-$path with length $l_{G'}(u,b)$ such that $v_{s-2} \notin g'$. Then, $g = g' + (b, v_{s-1})$ is $(u, v_{s-1})-$path in G. Since $u \in A$ in G there is the longest $(u, v_{s-1})-$path h such that $b \notin h$. Replacing the vertex v_{s-1} on the path h with the vertex b in G' we obtain an $(u,b)-$path h'. Then $|h'| = |h| \geq |g| > |g'| = l_{G'}(u,b)$, that is not possible. So, the longest $(u,b)-$path in G' passes across the v_{s-2}. Denote by $\tilde{g}$ one such path. Let $g = \tilde{g} - (b, v_{s-2}) + (v_{s-2}, v_{s-1})$. It follows that

$$l_G(u, v_{s-1}) \geq |g| = |\tilde{g}| = l_{G'}(u,b).$$

Hence,

$$l_{G'}(u, v_{s-1}) = 1 + l_{G'}(u,b) \leq 1 + l_G(u, v_{s-1}) \text{ and } l_G(u,b) = l_G(u, v_{s-1}) + 1 \geq l_{G'}(u,b) + 1.$$

Therefore,

$$l_G(u, v_{s-1}) - l_{G'}(u, v_{s-1}) \geq -1 \text{ for } u \in A, \tag{4}$$

$$l_G(u,b) - l_{G'}(u,b) \geq 1 \text{ for } u \in A. \tag{5}$$

Since $l_G(u,b) - l_{G'}(u,b) \geq 0$ for $u \in B$ we have that

$$\sum_{u \in T} [l_G(u,b) - l_{G'}(u,b)] \geq \sum_{u \in A} [l_G(u,b) - l_{G'}(u,b)]$$

and so from (1) - (3) we have

$$\omega(G) - \omega(G') \geq 2 + \sum_{u \in A} [l_G(u, v_{s-1}) - l_{G'}(u, v_{s-1})] + \sum_{u \in A} [l_G(u,b) - l_{G'}(u,b)]$$

Using (4) and (5) we finally conclude $\omega(G) - \omega(G') \geq 2$. □

Previous theorem introduces, in a subtle way, the procedure of iterative reducing cycles R_1 and R_2 by absorbing two vertices into one. Namely, every bicyclic graph with common edges between two cycles, could be isomorphically transformed into graph that belongs to class $\mathcal{E}_n(s, p_1, p_2)$, i.e. that middle path is the longest one. For example, two graphs in the following picture there are two isomorphic graphs that belong to $\mathcal{E}_4(2, 2, 1)$.

Theorem 5. *Let $G = D(T_1, T_2, T_3, T_4)$ such that $|T_2| \leq |T_4|$. For any fixed $i \in \{1, 2, 3\}$ let G' be a graph obtained from G removing all pendent vertices from the vertex v_i to the vertex v_4. Then $\omega(G) > \omega(G')$.*

Proof.

$$\begin{aligned}
\omega(G) - \omega(G') &= \sum_{\substack{t\in T_i \\ t\neq v_i}} \sum_{j\neq i} \sum_{u\in T_j} [l_G(t,u) - l_{G'}(t,u)] \\
&= \sum_{\substack{t\in T_i \\ t\neq v_i}} \sum_{j\neq i} \sum_{u\in T_j} [(1 + l_D(v_i, v_j) + l(v_j, u)) \\
&- \sum_{\substack{t\in T_i \\ t\neq v_i}} \sum_{j\neq i} \sum_{u\in T_j} (1 + l_D(v_4, v_j) + l(v_j, u))] \\
&= \sum_{\substack{t\in T_i \\ t\neq v_i}} \sum_{j\neq i} \sum_{u\in T_j} [l_D(v_i, v_j) - l_D(v_4, v_j)]
\end{aligned}$$

Due to (6), $l_D(v_i, v_j) - l_D(v_4, v_j) > 0$, so $\omega(G) > \omega(G')$.
□

5. Conlusions

In this paper we studied detour index of connected bicyclic graphs. The main goal was to find the graphs with minimal detour index in the defined class. The problem was separated into two cases: bicyclic graphs without and with common edges between two cycles.

In the first case, we realized that every connected bicyclic graph G, without common edges, is made by merging two vertices of unicyclic graphs G_1 and G_2 into single vertex, as described in Section 3. That observation helped us to find the graph, so called $n-$vertex butterfly $B_{n;3,3}$, with minimal detour index n^2+2n-7.

The second case, problem of bicyclic graphs with common edges, is mainly resolved in the Theorem 4. In that theorem we introduced iterative procedure of removing a common edge between two cycles and attaching to the specific node which resulted in getting a new graph with smaller detour index. Once we reduced the problem to the case of parallelogram with attached stars to the four parallelogram vertices, as showed in the Figure 6, then Theorem 5 resolves that the smallest detour index has the graph represented in the Figure 3.

For the future research, it might be worth trying of finding the exact values of detour index for some particular type of graphs. It looks that the case of bicyclic graphs without common edges or the case of bicyclic graphs with just one edge in common could be, with some lengthy algebraic calculations, finally resolved. If that is achieved, then some of the results of this paper would be easily obtained.

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