MATCH
Communications in Mathematical and in Computer Chemistry

MATCH Commun. Math. Comput. Chem. **64** (2010) 727-742

ISSN 0340 - 6253

Wiener Number of Directed Graphs and Its Relation to the Oriented Network Design Problem

Igor Pesek[1], Maja Rotovnik[1], Damir Vukičević[2] and Janez Žerovnik[1,3]

[1]IMFM, Jadranska 19, SI-1000 Ljubljana, Slovenia

[2]Department of Mathematics, University of Split, Croatia

[3]FME, University of Ljubljana, Aškerčeva 6, SI-1000 Ljubljana, Slovenia

e-mails: igor.pesek@uni-mb.si, maja.rotovnik@imfm.uni-lj.si, vukicevic@pmfst.hr, janez.zerovnik@imfm.uni-lj.si

(Received March 31, 2009)

ABSTRACT

The modified Wiener number on trees has been defined recently as a sum of modified edge contributions, which are simply the number of shortest paths traversing the edge to the power of α. We study digraphs with minimal value for one possible modification of the Wiener number for directed graphs. For this generalization. For digraphs with unique shortest paths we provide minimal digraphs for $\alpha \leq 0$ and $\alpha \geq 1$, and give some partial results for $\alpha \in (0, 1)$.

1 Introduction

The modified Wiener number on trees has been defined recently as a sum of modified edge contributions, which are simply the number of shortest paths traversing the edge

to the power of α [7]. It is known that the extremal graphs for the modified Wiener number are the star graph and the path. More precisely, for positive α, the star graph is maximal and the path is minimal, and for negative α, the star graph is minimal and the path is maximal. Wiener number [16] is probably the most popular topological invariant in chemical graph theory [11, 12]. For our discussion it is relevant to mention that the Wiener number of a tree can be computed as a sum of edge contributions. On trees, the edge contribution is simply the number of shortest paths traversing it. On general graphs, the edge contribution is equivalent to the sum of shortest paths contributions. If there are more than one shortest path between two vertices, then the contribution is usually assumed to be split evenly among all shortest paths, see for example [10]. While there are several studies on the Wiener number of weighted graphs, there seems to be no generalization(s) to directed graphs (or, digraphs). In the undirected case, the Wiener number is usually defined as the sum of all distances, hence analogous natural definition for directed graphs is again the sum of all distances. Of course, each ordered pair of vertices has to be taken into account. In analogy to the undirected case we propose some possible modifications of the Wiener number for directed graphs. One of the generalizations appears to be equivalent to the cost of certain optical network and the directed graphs with extremal Wiener number appear to be optimal networks [1].
The rest of this paper is organized as follows. In the first section we define the problem, then we present some properties of extremal cases and finally give some results for directed graphs with cycles.

2 Modifications of the Wiener number of undirected graphs

A large number of modifications and extensions of the Wiener number was considered in the chemical literature; an extensive bibliography on this matter can be found in the reviews [4, 5]. One of the newest such modifications was put forward by Nikolić, Trinajstić and Randić [9]. This idea was generalized in [7] where a class of modified Wiener indices was defined, with the original Wiener number and the Nikolić-Trinajstić-Randić index as special cases.

Usually, the Wiener number of a graph is defined as the sum of all distances in a graph.

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

In the paper [6] by Gutman et al., the following modification is proposed:

$$W_\alpha\left(G\right)=\sum_{u,v\in V(G)} d_G\left(u,v\right)^\alpha,\ \ \alpha\neq 0.$$

It was already known to Wiener that on a tree, the invariant can also be computed by summing up the edge contributions, where the contribution of each edge $e=uv$ is the number of vertices closer to the vertex u times the number of vertices closer to the vertex v. Formally,

$$W\left(G\right)=\sum_{uv\in E(G)} n_G\left(u,v\right)n_G\left(v,u\right).$$

where $n_G\left(u,v\right)$ is the number of vertices closer to vertex u than to vertex v and $n_G\left(v,u\right)$ is the number of vertices closer to vertex v than to vertex u.
The modified Wiener indices [14, 8, 15, 13, 3] are defined as

$$W_\alpha\left(G\right)=\sum_{uv\in E(G)} n_G\left(u,v\right)^\alpha n_G\left(v,u\right)^\alpha.$$

On trees, the last expression is equivalent to $\sum_{e\in E(G)}\omega(e)^\alpha$, where $\omega(e)$ is the edge weight that equals the number of shortest paths in G that traverse e.

Here we propose a generalization of this concept to directed graphs and give some preliminary results on digraphs with minimal value of the invariant which we call $Cost_\alpha$ due to analogy with an optimization problem in design of communication networks on optical fibres [1]. One of the most popular applications of graph theory in computer science is the design of interconnection networks. A desirable network is usually optimal with respect to the value of one (or more) graph invariants, for example it has small diameter, small average distance, small routing costs, or allows uniform distribution of traffic, etc. As the Wiener number can be seen as the total communication load of a graph it is natural that it has already been considered in this context [2, 18]. Here we mention close relationship to the Oriented network design problem that arises in the design of optical networks. In such networks, the traffic requests are routed along a set of containers of fixed capacity, where each container connects two nodes of the network. The cost of the network is defined as the sum of arc contributions where the arc contribution is a certain power ($w(e)^\alpha$, $0 < \alpha < 1$) of the number of paths (of the routing) traversing the arc. While the problem given in [1] asks simply for optimal networks, it may also be of interest to find extremal cases for given number of nodes and given number of arcs.

3 Basic definitions

A directed graph or shortly digraph G is given by a set of vertices $V = V(G)$ and a set of ordered pairs of vertices $E = E(G)$ called directed edges or arcs. The number of nodes of G is denoted by $n = n(G)$ and the number of arcs is denoted by $m = m(G)$. A (directed) path in G is a sequence of vertices $v_0, v_1, \ldots, v_i, \ldots, v_n$ such that $v_{i-1}v_i$ is an arc of G for all i. G is strongly connected if there is a directed path from u to v for any pair of vertices u, v. The distance $d(u,v)$ is the length of a shortest path from u to v. In digraphs, in general $d(u,v) = d(v,u)$ does not hold. We will assume that the graphs are strongly connected, i.e. $d(u,v) < \infty$ and $d(v,u) < \infty$ for all pairs u, v.

Furthermore, we will also assume that the graphs have the USP property (USP stands for unique shortest paths), i.e. each two vertices are connected by a unique shortest path. In other words, in all graphs studied here there will be exactly one shortest path between any pair of vertices. We assume that the reader is familiar with basic notions of graph theory, see for example [17].

If we approach the problem as an optimization problem, we need to define the cost of a graph:

$$Cost_\alpha(G) = \sum w_\alpha(e),$$

where the sum runs over all edges of G, $w_\alpha(e) = [w(e)]^\alpha$ and $w(e)$ stands for the number of shortest paths that use e.

4 Extremal cases

In this section we will examine extremal cases when $\alpha < 0$ and $\alpha > 1$. Let us define T_n as graph depicted on Figure 1.

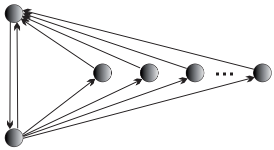

Figure 1: Graph T_n

4.1 Cases when $\alpha \to \infty$

Lemma 1. *Let $G_n \neq K_n$ be any USP-graph with n vertices. Then,*

$$\lim_{\alpha\to\infty} Cost_\alpha (G_n) = \infty.$$

Proof. Note that there are $n(n-1)$ shortest paths and less then $n(n-1)$ edges. Hence, there is at least one edge e such that $w(e) \geq 2$. □

Therefore, in other words:

Proposition 2. *K_n is the cheapest USP-graph with n vertices according to the function $Cost_\alpha$ when α tends to infinity.*

Lemma 3. *Let $G_n \neq T_n$ be any USP-graph with $n > 3$ vertices. Then, there is no edge such that $w(e) \geq (n-1)\cdot(n-2)+1$.*

Proof. Suppose to the contrary that there is such edge u_1u_2. Denote remaining vertices by $v_1, ..., v_{n-2}$. Note that the shortest paths from u_2 to u_1; from v_i to u_1, $i = 1, ..., n-2$; and from u_2 to v_i, $i = 1, ..., n-2$ can not contain edge u_1u_2. Hence, all other shortest paths contain this edge. It follows that no two vertices v_i and v_j are adjacent, $i, j = 1, ..., n-2$. Also, it follows that there are no arcs u_1v_i and v_iu_2, $i = 1, ..., n-2$. Since each v_i has in-degree and out-degree at least one, it follows that v_iu_1 and u_2v_i are arcs for each $i = 1, ..., n-2$. Finally, u_2u_1 has to be arc of G_n, because n is USP-graph, but then $G_n = T_n$, which is a contradiction. □

It directly follows:

Proposition 4. *T_n is the most expensive USP-graph with n vertices according to the function $Cost_\alpha$ when α tends to infinity. More formally,*

$$\lim_{\alpha\to\infty} \frac{Cost_\alpha(G_n)}{Cost_\alpha(T_n)} = 0$$

for each USP-graph G_n with n vertices.

4.2 Cases when $\alpha = 1$

Note that $Cost_1$ is the number of edges covered by shortest paths. It can be easily seen that:

Proposition 5. *For each USP-graph $G_n \neq K_n, C_n$ with n vertices, we have: $Cost_1(K_n) < Cost_1(G_n) < Cost_1(C_n)$.*

Proof. Denote by $l(u,v)$ length of the shortest path from u to v. We have:

$$Cost_1(G_n) = \sum_{u,v\in V(G_n)} l(u,v) > \sum_{u,v\in V(G_n)} 1 = Cost_1(K_n).$$

$$\begin{aligned} Cost_1(G_n) &= \sum_{u,v\in V(G_n)} l(u,v) = \frac{1}{2}\sum_{u,v\in V(G_n)} (l(u,v)+l(v,u)) \\ &< \frac{1}{2}\sum_{u,v\in V(G_n)} n = \frac{1}{2}n\cdot n\cdot(n-1) = Cost_1(C_n). \end{aligned}$$

This proves the proposition. □

4.3 Cases when $\alpha \leq 0$

Proposition 6. *K_n is the most expensive USP-graph with n vertices according to the function $Cost_\alpha$, for each $\alpha \leq 0$.*

Proof. Let $G_n \neq K_n$ be any USP-graph with n vertices. Then,

$$\begin{aligned} Cost_\alpha(G_n) &= \sum_{e\in E(G_n)} w_\alpha(e) \leq \sum_{e\in E(G_n)} 1 = \\ &= |E(G_n)| < n\cdot(n-1) = Cost_\alpha(K_n). \end{aligned}$$

□

Proposition 7. *C_n is the cheapest USP-graph with n vertices according to the function $Cost_\alpha$ for each $\alpha \leq 0$.*

Proof. For $\alpha = 0$, $w(e)^\alpha = 1$, therefore $Cost_\alpha(C_n) = n$ and $Cost_\alpha(G_n) \geq |V(G)| = n$. Let us consider the case when $\alpha < 0$. Denote edges of digraph G_n with $e_1, ..., e_k$ and the number of times edge e_i is part of the shortest path with $x_1, ..., x_k$. Denote $x = x_1 + ... + x_k$. It holds $x_1^\alpha + ... + x_k^\alpha \geq k \cdot \left(\frac{x}{k}\right)^\alpha$, because of the concavity. Note that k is minimized when G_n is cycle and x is maximized in the same case. Hence, $\frac{x}{k}$ is also maximized for the cycles and and then $k \cdot \left(\frac{x}{k}\right)^\alpha$ is minimized for the cycle. □

5 Results for digraphs with $0 < \alpha < 1$

For a later reference let us define

$$f_\alpha(x) = (x+1) \cdot \left(\frac{1}{2}x(2n-1-x)\right)^\alpha$$

Furthermore, let

$$Cost_\alpha\left(R, r, k\right)$$

denote the cost of communication in graph R where each pair of vertices of R has a path and a distinguished vertex $r \in R$ has additional k paths to each of other vertices in R.

Lemma 8. *Let G be a graph depicted on Figure 2 with n vertices, a segment R with $n-k$ vertices and a loop of length $k+1$ rooted at the vertex r of R. Then the cost of the graph G is*

$$\begin{aligned} Cost_\alpha\left(G\right) &= Cost_\alpha\left(R, r, k\right) + (k+1)\left(\frac{1}{2}k(2n-k-1)\right)^\alpha = \\ &= Cost_\alpha\left(R, r, k\right) + f_\alpha\left(k\right). \end{aligned}$$

Proof. Let e be an arbitrary arc on the cycle. There are $k+1$ paths of length 1, $k+1$ paths of length 2, ... and $k+1$ paths of length k around the cycle that connect nodes of the cycle. The edge e appears on exactly one path of length one, two paths of length 2 ... and k paths of length k. In total, the edge is used by $\frac{k(k+1)}{2}$ paths.

Each vertex in the segment R has to communicate with each of the vertices on the cycle and similarly each vertex on the cycle has to communicate with segment R; we can split

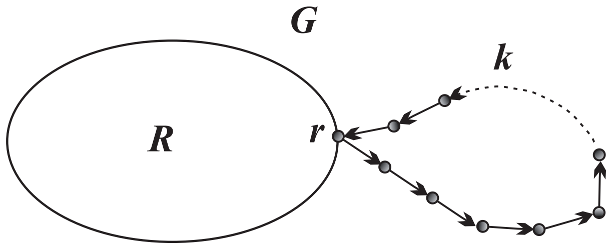

Figure 2: Graph with the cycle of length $k+1$

this communication in two parts. First part is the path between vertex r and vertices on the cycle, each such pair gives another shortest path that uses e. So the number of paths on the edge equals to $\left(k(n-k-1)+\frac{k(k+1)}{2}\right)^{\alpha}=\left(\frac{1}{2}k(2n-k-1)\right)^{\alpha}$, and the cost of the cycle of length $k+1$ is $f_{\alpha}(k)=(k+1)\left(\frac{1}{2}k(2n-k-1)\right)^{\alpha}$.

Second part is cost from all vertices in the segment R to vertex r. Since we have to communicate in both directions with vertices on the cycle, we need k paths from r to any other vertex of R. Finally, the paths between pairs of vertices of R have to be taken into account, and a set of shortest paths between each pair of vertices is needed to realize this. Clearly, the paths inside R contribute to weights of edges of G exactly $Cost_{\alpha}(R,r,k)$. $\square$

Lemma 9. *Let G and G' be graphs depicted on Figure 3 with n vertices, and two segments R_1 and R_2. Let the two segments together have $n-k$ vertices. Then*

$$Cost_{\alpha}(G) \quad \geq \quad Cost_{\alpha}(G').$$

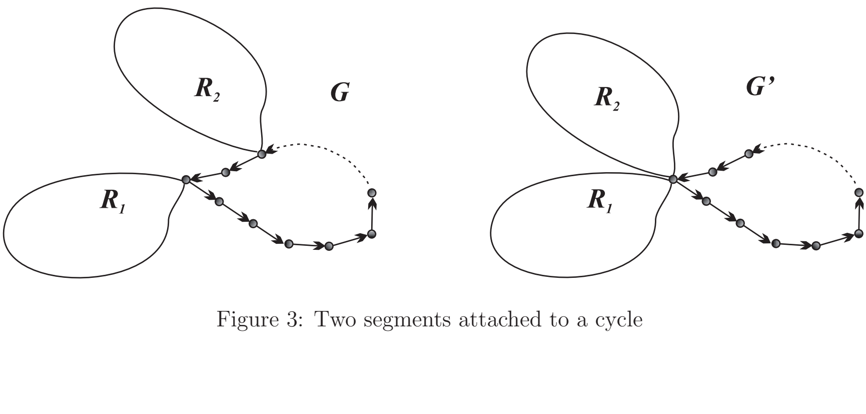

Figure 3: Two segments attached to a cycle

Proof. The cost of the network G' is given by $Cost_\alpha(G') = Cost_\alpha(R) + f_\alpha(k) = Cost_\alpha(R_1) + Cost_\alpha(R_2) + f_\alpha(k)$, where the $Cost_\alpha(R)$ can be seen as a sum of arc contributions of the two segments, $Cost_\alpha(R_1) + Cost_\alpha(R_2)$. Clearly, all the paths between vertices of the two segments avoid the loop in G', hence their cost is included in $Cost_\alpha(R)$.

On the other hand, in G any pair of vertices from different segments needs, in addition, one turn around the loop for the two shortest paths in both directions, $C(R_1, R_2) = |n(R_1)||n(R_2)| > 0$. Hence the arcs on the loop have additional weight $C(R_1, R_2)$, and as

$$\omega'(e)^\alpha < \omega(e)^\alpha = (\omega'(e) + C(R_1, R_2))^\alpha,$$

the cost of the loop L in the graph G is larger than the cost of the loop in G'. Consequently,

$$\begin{aligned} Cost_\alpha(G) &= Cost_\alpha(R_1) + Cost_\alpha(R_2) + Cost_\alpha(L) \\ &> Cost_\alpha(G') = Cost_\alpha(R_1) + Cost_\alpha(R_2) + f_\alpha(k). \end{aligned}$$

□

Lemma 10. *Let $G = G(k_1, k_2)$ be a graph depicted on Figure 4 with n vertices, a segment R with $n - k$ vertices and two loops rooted at the vertex r of R of lengths $k_1 + 1$, $k_2 + 1$ and $k = k_1 + k_2$. Then*

$$Cost_\alpha(G) = Cost_\alpha(R, r, k) + f_\alpha(k_1) + f_\alpha(k_2).$$

Proof. Goes along the same lines as the proof of Lemma 8. We omit the details. □

Let $G(R, x, k)$ be the graph with a segment R on $n - k$ vertices, and with two cycles of lengths $x + 1$ and $k - x + 1$ attached to a fixed vertex r of R (see Figure 4). We will assume that $x + 1$ is the length of the shorter cycle, i.e $x < k - x$.

Lemma 11. *Let R be any digraph, let $k \geq 4$ and let $1 \leq x_1 \leq k - x_1 \leq k - 1 < \frac{n}{2}$. Then*

$$Cost_\alpha\left(G\left(R, x_1, k\right)\right) \geq Cost_\alpha\left(G\left(R, x_1 + 1, k\right)\right),$$

for every $\alpha \in (0, 1]$.

Proof. Denote edges as on the Figure 4 and the number of shortest paths passing through the edge e on the shorter cycle by $c\left(R, k, x, e\right)$ and let $c\left(R, k, x, f\right)$ be the number of shortest paths passing through the edge f on the longer cycle. Denote by $s = n - k$ the number of vertices in R and let $x_2 = x_1 + 1$.

Note that the contribution of each edge in $E(R)$ is the same in both cases, hence:

$$\begin{aligned} &Cost_\alpha(G(R, x_1, k)) - Cost_\alpha(G(R, x_2, k)) = \\ &= \sum_{i=1}^{x_1+1} (c(R, k, x_1, e_i))^\alpha + \sum_{i=1}^{k-x_1+1} (c(R, k, x_1, f_i))^\alpha \\ &- \sum_{i=1}^{x_2+1} (c(R, k, x_2, e_i))^\alpha - \sum_{i=1}^{k-x_2+1} (c(R, k, x_2, f_i))^\alpha . \end{aligned} \tag{1}$$

Further, note that:

$$c(R, k, x_1, e_i) = (s + k - x_1) \cdot x_1 + \frac{x_1 \cdot (x_1 - 1)}{2},$$

where the first summand corresponds to the paths that have

1. one end-vertex in the cycle of length $x_1 + 1$
2. other end-vertex in the cycle of length $k - x_1 + 1$ or in $R \backslash \{r\}$

and the second summand corresponds to the number of paths that have both end-vertices on the cycle of length $x_1 + 1$ with the exception of r.

Analogously:

$$c(R, k, x_2, e_i) = (s + k - x_2) \cdot x_2 + \frac{x_2 \cdot (x_2 - 1)}{2};$$

$$c(R, k, x_1, f_i) = (s + x_1) \cdot (k - x_1) + \frac{(k - x_1) \cdot (k - x_1 - 1)}{2};$$

$$c(R, k, x_2, f_i) = (s + x_2) \cdot (k - x_2) + \frac{(k - x_2) \cdot (k - x_2 - 1)}{2}.$$

Substituting this in (1), one gets:

$$
\begin{aligned}
&Cost_\alpha\left(G\left(R,x_1,k\right)\right)-Cost_\alpha\left(G\left(R,x_2,k\right)\right)=\\
&=\left[(s+k-x_1)\cdot x_1+\frac{x_1\cdot(x_1-1)}{2}\right]^\alpha\cdot(x_1+1)\\
&+\left[(s+x_1)\cdot(k-x_1)+\frac{(k-x_1)\cdot(k-x_1-1)}{2}\right]^\alpha\cdot(k-x_1+1)\\
&-\left[(s+k-x_2)\cdot x_2+\frac{x_2\cdot(x_2-1)}{2}\right]^\alpha\cdot(x_2+1)\\
&-\left[(s+x_2)\cdot(k-x_2)+\frac{(k-x_2)\cdot(k-x_2-1)}{2}\right]^\alpha\cdot(k-x_2+1)=\\
&=f_\alpha(x_1)+f_\alpha(k-x_1)-f_\alpha(x_2)-f_\alpha(k-x_2)
\end{aligned}
$$

We have to prove that

$$f_\alpha(x_1)+f_\alpha(k-x_1)>f_\alpha(x_2)+f_\alpha(k-x_2).$$

It is sufficient to show that $f_\alpha(x)$ is increasing convex function for all $x\in(1,\frac{n}{2})$. To prove that we have to calculate first and second derivative of $f_\alpha(x)$:

$$f'_\alpha(x)=2^{-\alpha}\left(x\left(2n-x-1\right)\right)^\alpha\left(1+\frac{\alpha\left(2n-2x-1\right)\left(1+x\right)}{x\left(2n-x-1\right)}\right)$$

$$
\begin{aligned}
f''_\alpha(x)=2^{-\alpha}\alpha\left(x\left(2n-x-1\right)\right)^\alpha\Bigg(&\frac{4n^2(x-1)+n\left(4-8x^2\right)}{x^2\left(1-2n+x\right)^2}\\
&+\frac{\alpha(x+1)\left(1-2n+2x\right)^2+(1+x)(2x^2-1)}{x^2\left(1-2n+x\right)^2}\Bigg).
\end{aligned}
$$

Both derivatives are positive for $x\in(1,\frac{n}{2})$, hence lemma is proved. □

Remark: the statement of Lemma 11 does not hold for some examples with $k>\frac{n}{2}$ ($n=7$, $k=6$, $x_1=2$, $x_2=4$, $\alpha=0.01$). It seems obvious that the bound for k depends on α, but we were not able to find an explicit relationship.

Lemma 12. *Let* $G(x,\alpha)=(\frac{1}{2}x\left(2n-x-1\right))^\alpha$. *Then for* $0<\alpha_1<\alpha_2$ *and* $1\le x_1<x_2\le n-1$, $\frac{G(x_1,\alpha_2)}{G(x_2,\alpha_2)}<\frac{G(x_1,\alpha_1)}{G(x_2,\alpha_1)}$.

Proof. Note that for $1\le x_1<x_2\le n-1$ we have $x_1\left(2n-x_1-1\right)<x_2\left(2n-x_2-1\right)$, so

$$C=\frac{x_1\left(2n-x_1-1\right)}{x_2\left(2n-x_2-1\right)}<1$$

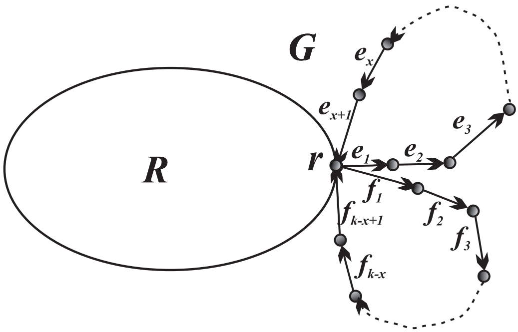

Figure 4: Graph with two cycles rooted at r

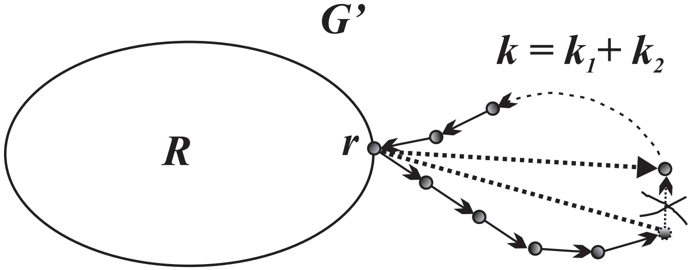

Figure 5: Dividing the cycle

and for $0 < \alpha_1 < \alpha_2$,

$$C^{\alpha_2} < C^{\alpha_1}.$$

As $\frac{G(x_1,\alpha_2)}{G(x_2,\alpha_2)} = C^{\alpha_2}$ and $\frac{G(x_1,\alpha_1)}{G(x_2,\alpha_1)} = C^{\alpha_1}$, the claim follows. $\square$

Proposition 13. *Let the function $F(\alpha)$ be defined as*

$$F(\alpha) = Cost_\alpha\left(G'\right) - Cost_\alpha\left(G\right), \tag{2}$$

where the graphs G and G' are depicted on Figure 2 and on Figure 5. Then $F(\alpha) = 0$ has exactly one root on $[0, 1]$.

Proof. Recall from Lemma 8 that $Cost_\alpha(G) = Cost_\alpha\left(R, r, k\right) + f_\alpha\left(k\right)$ and from Lemma 10 that $Cost_\alpha(G') = Cost_\alpha\left(R, r, k\right) + f_\alpha\left(k_1\right) + f_\alpha(k_2)$. Hence using $k = k_1 + k_2$ we can write

$$F(\alpha) = f_\alpha(k_1) + f_\alpha(k_2) - f_\alpha(k)\ . \tag{3}$$

Observe

$$F(0) = k_1 + 1 + k - k_1 + 1 - k - 1 = 1 > 0$$

and, because $(k - k_1)$ and k_1 are positive and $(4 + 3k - 4n)$ is negative as $n \geq k + 1$,

$$F(1) = \frac{1}{2}(k - k_1)k_1(4 + 3k - 4n) < 0.$$

Function $F(\alpha)$ is continuous and its values at the ends of interval have different sign, therefore there must exist at least one α, for which $F(\alpha) = 0$. Let us denote it as α_0. So we know that for α_0 it holds

$$f_{\alpha_0}(k) = f_{\alpha_0}(k_1) + f_{\alpha_0}(k_2). \tag{4}$$

We will show that $f_\alpha(k) < f_\alpha(k_1) + f_\alpha(k_2)$ for $\alpha < \alpha_0$ and $f_\alpha(k) > f_\alpha(k_1) + f_\alpha(k_2)$ for $\alpha > \alpha_0$.

Let us rewrite $f_\alpha(k)$ as

$$f_\alpha(k) = (k + 1)G(k, \alpha), \tag{5}$$

where $G(x, \alpha) = (\frac{1}{2}x\,(2n - x - 1))^\alpha$.

Substituting (5) in (4) we have

$$(k + 1)G(k, \alpha_0) = (k_1 + 1)G(k_1, \alpha_0) + (k_2 + 1)G(k_2, \alpha_0).$$

Dividing the last equation by $G(k, \alpha_0)$ one gets

$$k + 1 = (k_1 + 1)\frac{G(k_1, \alpha_0)}{G(k, \alpha_0)} + (k_2 + 1)\frac{G(k_2, \alpha_0)}{G(k, \alpha_0)}.$$

Let $\alpha > \alpha_0$. Then from Lemma 12 we know $\frac{G(k_1,\alpha)}{G(k,\alpha)} < \frac{G(k_1,\alpha_0)}{G(k,\alpha_0)}$ and $\frac{G(k_2,\alpha)}{G(k,\alpha)} < \frac{G(k_2,\alpha_0)}{G(k,\alpha_0)}$, therefore

$$k + 1 > (k_1 + 1)\frac{G(k_1, \alpha)}{G(k, \alpha)} + (k_2 + 1)\frac{G(k_2, \alpha)}{G(k, \alpha)}$$

and, multiplying by $G(k, \alpha)$,

$$f_\alpha(k) > f_\alpha(k_1) + f_\alpha(k_2).$$

Hence $F(\alpha) \neq 0$ for all $\alpha > \alpha_0$.

Analogously, $f_\alpha(k) < f_\alpha(k_1) + f_\alpha(k_2)$, and therefore $F(\alpha) \neq 0$ for all $\alpha < \alpha_0$. $\square$

Theorem 14. *Let G be a graph depicted on Figure 2 with n vertices, a segment R with $n-k$ vertices and a loop of length $k+1$ rooted at the vertex r of R. Let G' be a graph depicted on Figure 5 which is obtained from G by replacing the arc opposite to the vertex r with two arcs meeting at r. There is a constant $0 < \alpha_2 < 1$ such that*

$$\begin{aligned} Cost_\alpha(G) &< Cost_\alpha(G') \text{ for all } \alpha, 0 \leq \alpha < \alpha_2 \text{ and} \\ Cost_\alpha(G) &> Cost_\alpha(G') \text{ for all } \alpha, \alpha_2 < \alpha \leq 1. \end{aligned}$$

Proof. By Proposition 13 $F(\alpha) = Cost_\alpha(G') - Cost_\alpha(G)$ has exactly one root on interval [0,1], $F(\alpha_2) = 0$. Furthermore, for $0 \leq \alpha < \alpha_2$, $F(\alpha) > 0$ and for $\alpha_2 < \alpha \leq 1$, $F(\alpha) < 0$. □

6 Conclusion

For $\alpha \leq 0$ we have provided a complete answer about digraphs with minimal value of the proposed invariant by showing that the cycle C_n is minimal among USP-graphs, i.e graphs with unique shortest paths.

For positive α, the question is more involved. While it was proven that K_n is the minimal USP-graph for $\alpha \geq 1$, our results for $\alpha \in (0,1)$ only give some intuition about possible extremal digraphs. It remains an open problem to find the minimal digraphs for these values of α.

Furthermore, it would be of interest to study the extremal general digraphs without somewhat artificial assumption that the shortest paths must be unique.

Acknowledgement. The authors wish to thank to the anonymous referee for careful reading of the manuscript and for many constructive remarks including spotting an error in original proof of Proposition 13. Partial support of Slovenian Research Agency ARRS, Croatian Ministry of Science and Education (grant numbers 177-0000000-0884 and 037-0000000-2779) and bilateral Slovenian-Croatian project (Mathematical modeling and experimental research in analytical, environmental and food chemistry) is gratefully acknowledged.

References

[1] J. S. Choplin, J. Galtier, S. Perennes, Optimal concave costs in the sdh context, Technical Report 5201, INRIA Rapport de Recherche, May 2004.

[2] B. Elenbogen, J. F. Fink, Distance distributions for graphs modeling computer networks, *Discrete Appl. Math.* **155** (2007) 2612–2624.

[3] M. Gorše, J. Žerovnik, A remark on modified Wiener indices, *MATCH Commun. Math. Comput. Chem.* **50** (2004) 109–116.

[4] I. Gutman, S. Klavžar, B. Mohar (Eds.), Fifty years of the Wiener index, *MATCH Commun. Math. Comput. Chem.* **35** (1997) 1–259.

[5] I. Gutman, S. Klavžar, B. Mohar (Eds.), Special issue on the Wiener index, *Discr. Appl. Math.* **80** (1997) 1–115.

[6] I. Gutman, D. Vidović, L. Popović, On graph representation of organic molecules Cayley's plerograms vs. his kenograms, *J. Chem. Soc. Faraday Trans.* **94** (1998) 857–860.

[7] I. Gutman, D. Vukičević, J. Žerovnik, A class of modified Wiener indices, *Croat. Chem. Acta* **77** (2004) 103–109.

[8] I. Gutman, J. Žerovnik, Corroborating a modification of the Wiener index, *Croat. Chem. Acta* **75** (2002) 603–612.

[9] S. Nikolić, N. Trinajstić, M. Randić, Wiener index revisited, *Chem. Phys. Lett.* **333** (2001) 319–321.

[10] T. Pisanski, J. Žerovnik, Weights on edges of chemical graphs determined by paths, *J. Chem. Inf. Comput. Sci.* **34** (1994) 395–397.

[11] R. Todeschini, V. Consonni, *Handbook of Molecular Descriptors*, Wiley–VCH, Weinheim, 2000.

[12] N. Trinajstić, *Chemical Graph Theory*, CRC Press, Boca Raton, 1992.

[13] D. Vukičević, Distinction between modifications of Wiener indices, *MATCH Commun. Math. Comput. Chem.* **47** (2003) 87–105.

[14] D. Vukičević, I. Gutman, Note on a class of modified Wiener indices, *MATCH Commun. Math. Comput. Chem.* **47** (2003) 107–117.

[15] D. Vukičević, J. Žerovnik, New indices based on the modified Wiener indices, *MATCH Commun. Math. Comput. Chem.* **47** (2003) 119–132.

[16] H. Wiener, Structural determination of paraffin boiling points, *J. Am. Chem. Soc.* **69** (1947) 17–20.

[17] R. Wilson, J. Watkins, *Graphs, An Introductionary Approach*, Wiley, New York, 1990.

[18] B. Zmazek, J. Žerovnik, Estimating the traffic on weighted cactus networks in linear time, in E. Banissi (Ed.), *Ninth International Conference on Information Visualization, London*, IEEE Computer Society, 2005, pp. 536–541.