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Some remarks on Wiener index of oriented graphs

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Abstract

In this paper, we study the Wiener index (i.e., the total distance or the transmission number) of not necessarily strongly connected digraphs. In order to do so, if there is no directed path from u to v, we follow the convention $d(u,v) = 0$, which was independently introduced in several studies of directed networks. Under this assumption we naturally generalize the Wiener theorem, as well as a relation between the Wiener index and betweenness centrality to directed graphs. We formulate and study conjectures about orientations of undirected graphs which achieve the extremal values of Wiener index.

Keywords: Wiener index, average graph distance, total distance, directed graph, betweenness centrality, social networks

1 Introduction

The Wiener index of a graph G, $W(G)$, is defined as the sum of distances between all (unordered) pairs of vertices of G. This parameter was introduced by Wiener in 1947 [20] and it has become popular among chemists. By graph theorists it has been considered much later and it was studied under other names, including the *gross status* [12], the distance of a graph [8], and the transmission [18]. Many papers also deal with the *average distance*, defined as $\mu(G) = W(G)/\binom{n}{2}$, cf. [4, 7], see also [9] for a brief survey. The Wiener index is considered as one of the most applicable graph invariant. Beside the chemistry, there are many applications in communication, facility location, cryptology, architecture etc., where the Wiener index of the corresponding graph, or the average distance, is of great interest. New results

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related to the Wiener index of a graph are constantly being reported, while less attention has been devoted to the study of an analogous concept for digraphs, despite its application in sociometry, informetric studies etc.

A *directed graph* (a *digraph*) D is given by a set of vertices $V(D)$ and a set of ordered pairs of vertices $A(D)$ called *directed edges* or *arcs*. A *(directed) path* in D is a sequence of vertices $v_0, v_1, \ldots, v_n$ such that $v_{i-1}v_i$ is an arc of D for all i. The *distance* $d_D(u,v)$ between vertices $u, v \in V(D)$ is the length of a shortest path from u to v, and if there is no such path then we assume that

$$d_D(u,v) = 0. \tag{1}$$

For $u \in V(D)$, we will denote $w_D(u) = \sum_{v \in V(D)} d_D(u,v)$. We omit the index D when no confusion is likely.

In analogy to graphs, the Wiener index $W(D)$ of a digraph D is defined as the sum of all distances, where of course, each ordered pair of vertices has to be taken into account. More precisely,

$$W(D) = \sum_{(u,v) \in V(D) \times V(D)} d_D(u,v) = \sum_{u \in V(D)} w_D(u).$$

The first results on the Wiener index of digraphs are due to Harary [12], whose investigation was motivated by certain sociometric problems. Ng and Teh [15] found a strict lower bound for the Wiener index of digraphs. As in the case of graphs, the Wiener index of digraphs was considered indirectly also through the study of the *average* (or *mean*) *distance*, defined as $\mu(D) = W(D)/n(n-1)$, see [5, 6].

In real directed networks, there could be no path connecting some pairs of vertices. Strictly speaking, the distance between such a pair of vertices is infinite (thus the study of the Wiener index of digraphs in pure mathematical papers is usually limited to *strongly connected* digraphs, i.e. digraphs in which a directed path between every pair of vertices exists). However, for practical purposes, in the case when a directed path between two vertices does not exist, the distance between them can be defined in a different way. For instance, Botafogo et al. [3] defined it as the number of vertices in the analyzed network, while Bonchev [1, 2] assumed the condition (1).

Let $W_{\max}(G)$ and $W_{\min}(G)$ be the maximum possible and the minimum possible, respectively, Wiener index among all digraphs obtained by orienting the edges of G. In [13], the following problems where posed.

Problem 1. *For a given graph G find $W_{\max}(G)$ and $W_{\min}(G)$.*

Problem 2. *For a given graph G, what is the complexity of finding $W_{\max}(G)$ (resp. $W_{\min}(G)$)? Are these problems NP-hard?*

Transitive tournaments, i.e. acyclic orientations of complete graphs K_n, clearly yield the smallest possible Wiener index among all orientations of complete graphs. Hence, $W_{\min}(K_n) =$

$\binom{n}{2} = W(K_n)$. We remark that the above problems have already been considered for strongly connected orientations. Plesník [16] proved that finding a strongly connected orientation of a given graph G that minimizes the Wiener index is NP-hard. In [5] a lower bound for the minimum average distance taken over all strongly connected orientations of certain families of graphs was established. Regarding the problem of finding $W_{\max}(G)$, Plesník and Moon [14, 16] resolved it for complete graphs, under the assumption that the orientation is strongly connected.

In [13] we show that the above mentioned results of Plesník and Moon hold also for non-strongly connected orientations assuming the condition (1). One may expect that for a 2-connected graph G, $W_{\max}(G)$ is attained for some strongly connected orientation. This was disproved by Θ-graphs $\Theta_{a,b,1}$ for a and b fulfilling certain conditions, see [13].

In this paper we generalize the Wiener theorem to digraphs. We also show that a well known relation between the Wiener index and betweenness centrality naturally extends to directed graphs assuming the condition (1). We conclude the paper with conjectures about orientations of undirected graphs which achieve the extremal values of Wiener index. To support these conjectures, we present a couple of classes of graphs which satisfy them.

2 Wiener theorem for directed graphs

In [20], Wiener proved that for a tree T

$$W(T) = \sum_{e=ij \in E(T)} n_e(i) n_e(j),$$

where $n_e(i)$ and $n_e(j)$ are the orders of components of $T - ij$. The result is known as the Wiener theorem. In this section, we show an analogous statement for directed trees.

Let $T(a)$ denote the set of vertices x with the property that there exists a directed path from x to a. Similarly, let $S(a)$ denote the set of vertices x with the property that there exists a directed path from a to x. Note that $a \in S(a)$ and $a \in T(a)$. Let $t(a) = |T(a)|$ and $s(a) = |S(a)|$.

Now we give the counterpart of the Wiener theorem for *directed trees*, i.e. digraphs whose underlying graphs are trees.

Theorem 3. *Let T be a directed tree. Then*

$$W(T) = \sum_{ab \in A(T)} t(a)s(b).$$

Proof. If there exists a directed path between two vertices in T, then it is unique. Hence an arc ab contributes 1 to $W(T)$ for each pair of vertices for which the directed path between them contains ab. Since there are $t(a)s(b)$ such paths the result follows. $\square$

3 Wiener index vs. betweenness centrality

White and Borgatti [21] generalized Freeman's geodesic centrality measures for betweenness on graphs to the case of digraphs. The *(directed) betweenness centrality* $B(x)$ of a vertex x in a digraph D is defined as

$$B(x) = \sum_{\substack{u,v \in V(D)\setminus\{x\} \\ u \neq v}} \frac{\sigma_{u,v}(x)}{\sigma_{u,v}},$$

where $\sigma_{u,v}$ denotes the number of all shortest directed paths in D from u to v and $\sigma_{u,v}(x)$ stands for the number of all shortest directed paths from u to v passing through the vertex x. Note that in the definition of $B(x)$ we consider only such ordered pairs (u, v) for which there exists a directed u, v-path in D, i.e., for which $\sigma_{u,v} \neq 0$.

Gutman and Škrekovski [10] showed that for a connected graph G the following holds

$$W(G) = \sum_{x \in V(G)} B(x) + \binom{n}{2}.$$

This formula shows that the Wiener index is related to the *betweenness centrality* of a vertex $x \in V(G)$.

We extend the above relation to directed graphs. Let $P(D)$ denote the set of ordered pairs (u, v) such that there exists a directed path from u to v in D.

Theorem 4. *For any digraph D of order n*

$$W(D) = \sum_{x \in V(D)} B(x) + |P(D)|.$$

Proof. Let $(u, v) \in P(D)$. For every i, $1 \leq i \leq d(u, v) - 1$, denote

$$N_i(u, v) = \{x \in V(D) : d(u, x) = i \text{ and } d(x, v) = d(u, v) - i\}.$$

Then $\bigcup_{i=1}^{d(u,v)-1} N_i(u, v)$ contains exactly the internal vertices of shortest u, v-paths. Now choose j, $1 \leq j \leq d(u, v) - 1$. Since every shortest u, v-path contains exactly one vertex of $N_j(u, v)$ we have $\sum_{x \in N_j(u,v)} \sigma_{u,v}(x) = \sigma_{u,v}$. Hence,

$$\sum_{x \in N_j(u,v)} \frac{\sigma_{u,v}(x)}{\sigma_{u,v}} = 1,$$

which means that

$$\sum_{x \in V(D)\setminus\{u,v\}} \frac{\sigma_{u,v}(x)}{\sigma_{u,v}} = d(u, v) - 1,$$

since $\sigma_{u,v}(y) = 0$ for $x \in V(D) \setminus \bigcup_{i=1}^{d(u,v)-1} N_i(u,v)$.

Now we derive the desired relation:

$$\begin{aligned}
\sum_{x \in V(D)} B(x) &= \sum_{x \in V(D)} \sum_{\substack{(u,v) \in P(D) \\ u \neq v,\ x \notin \{u,v\}}} \frac{\sigma_{u,v}(x)}{\sigma_{u,v}} \\
&= \sum_{\substack{(u,v) \in P(D) \\ u \neq v}} \sum_{x \in V(D) \setminus \{u,v\}} \frac{\sigma_{u,v}(x)}{\sigma_{u,v}} \\
&= \sum_{\substack{(u,v) \in P(D) \\ u \neq v}} (d(u,v) - 1) \\
&= W(D) - |P(D)|.
\end{aligned}$$

□

Since in a strongly connected digraph there is a directed path between every ordered pair of vertices, we derive the following.

Corollary 5. *Let D be a strongly connected digraph of order n. Then,*

$$W(D) = \sum_{x \in V(D)} B(x) + 2\binom{n}{2}.$$

4 Orientations of trees with the maximum Wiener index

A vertex v in a directed tree T is *core* if for every vertex u of T, there exists a directed path in T from u to v or from v to u. Notice that then in each component C of $T - v$ all edges point in the direction towards v or all edges point in the direction from v. See Figure 1 for an example of a directed tree with two core vertices and a directed tree that does not contain any core vertex.

A different view of the very same notion can be described as follows. An orientation of a tree is called *no-zig-zag* if there is no subpath in which edges change the orientation twice. Note that a directed tree has a core vertex if and only if its orientation is no-zig-zag.

Conjecture 6. *Let T be a tree. Then, every orientation of T achieving the maximum Wiener index is no-zig-zag.*

This conjecture is true for all trees on at most 10 vertices, see [11]. In order to prove further results that support the conjecture, first recall a simple observation from [13].

Observation 7. *Let D be a digraph. Let D^- be obtained from D by reversing the orientation of all arcs of D. Then $W(D^-) = W(D)$.*

Using the following lemma we can prove Conjecture 6 for some classes of trees.

Lemma 8. *If D is an orientation of a tree T with the maximum Wiener index, then all paths of T whose internal vertices have degree two are directed paths in D.*

Proof. Let v be a vertex of degree two in T and let u_1 and u_2 be the two neighbors of v in T. Let D be an orientation of T with the maximum Wiener index. Split D at v, that is, replace v by v_1 and v_2, so that the arc originally incident with u_1 and v is now incident with u_1 and v_1, while the arc originally incident with u_2 and v is now incident with u_2 and v_2, and denote the resulting digraphs by D_1 and D_2. Then D is obtained from $D_1 \cup D_2$ by identifying v_1 with v_2. Suppose that both arcs adjacent with v are directed to (or that both are directed from) v in D. Then $W(D) = W(D_1) + W(D_2)$. Now, take D, reverse the orientation of all arcs of D_1, and denote the resulting digraph by D'. Since $d_D(u_1, u_2) = d_D(u_2, u_1) = 0$ while $d_{D'}(u_1, u_2) = 2$ or $d_{D'}(u_2, u_1) = 2$, we have $W(D') \geq W(D_1) + W(D_2) + 2$, a contradiction. □

We remark that Lemma 8 holds also for general graphs under the assumption that internal vertices of degree two of the paths are at the same time cut-vertices.

For the next result recall that a subdivision of a star is any tree with at most one vertex of degree 3 or greater.

Proposition 9. *Let T be a subdivision of a star. Then, every orientation of T achieving the maximum Wiener index is no-zig-zag.*

Proof. By Lemma 8, if D is an orientation of G with the maximum Wiener index, then all paths of G whose internal vertices have degree two, are directed paths in D. This implies that in a subdivision of a star, the central vertex is a core vertex. □

Theorem 10. *Let $T_{a,b,c}$ be a tree obtained from two stars $K_{1,a}$ and $K_{1,b}$, central vertices of which are connected by a path of length c, $c \geq 1$. Then, every orientation of $T_{a,b,c}$ achieving the maximum Wiener index is no-zig-zag.*

Proof. Let u_1 and u_2 be the central vertices of $K_{1,a}$ and $K_{1,b}$, respectively. Denote by P the u_1, u_2-path of length c in $T_{a,b,c}$. Let D be an orientation of $T_{a,b,c}$ with the maximum Wiener index. By Lemma 8, P is a directed path in D. By Observation 7, we may assume that P is directed from u_1 to u_2 in D. Let x be the number of arcs directed towards u_1 in D. Then the number of arcs directed from u_1 is $a - x + 1$ since one such arc is on P. Analogously, let y be the number of arcs directed from u_2 in D. Then the number of arcs directed towards u_2 is $b - y + 1$. Observe that u_2 is a core vertex if $x = a$. Analogously, u_1 is a core vertex if $y = b$. Hence, suppose that $x < a$ and $y < b$. We will show that in such a case there is an orientation D' of $T_{a,b,c}$ with $W(D') > W(D)$.

First suppose that $x < a - x$. Let z be a vertex of $K_{1,a}$ in $T_{a,b,c}$, such that zu_1 is an arc of D. Denote $\overline{w}(z) = \sum d_D(z, v)$, where the sum is taken over all vertices v of $T_{a,b,c}$ which are not in $K_{1,a}$. Reverse all arcs of $K_{1,a}$ in D and denote the resulting digraph by D'. Since $d_D(v_1, v_2) = d_{D'}(v_1, v_2)$ if none of v_1, v_2 are pendant vertices of $K_{1,a}$ and $d_D(v_1, v_2) = d_{D'}(v_2, v_1)$ if both v_1, v_2 are vertices of $K_{1,a}$, to find $W(D') - W(D)$ we need to consider pairs with one vertex being pendant in $K_{1,a}$ and the other not being in $K_{1,a}$. Hence, $W(D') - W(D) = [(a-x) - x] \cdot \overline{w}(z)$, and so $W(D') > W(D)$.

Now suppose that $y < b - y$. This case can be proved analogously as the case $x < a - x$, considering z being a vertex of $K_{1,b}$ such that u_2z is an arc of D, and defining $\overline{w}(z) = \sum d_D(v, z)$ where the sum is taken over all vertices v of $T_{a,b,c}$ which are not in $K_{1,b}$. Now if D' is obtained from D by reversing all arcs of $K_{1,b}$, then $W(D') - W(D) = [(b-y) - y] \cdot \overline{w}(z) > 0$. Hence, in what follows we assume $x \geq a - x$ and $y \geq b - y$.

Suppose that $y \geq x$. Reverse all arcs u_1z of $K_{1,a}$ and denote the resulting digraph by D'. Then $d_D(v_1, v_2) = d_{D'}(v_1, v_2)$ if neither v_1 nor v_2 is an out-neighbor of u_1 in $K_{1,a}$ in D. Let z be an out-neighbor in $K_{1,a}$ of u_1 in D. Then the sum of distances $d_D(v, z)$ taken over all vertices v of $T_{a,b,c}$ is exactly $2x + 1$, while the sum of distances $d_{D'}(z, v)$ is at least $3y + 2 + 1$. Hence, $W(D') - W(D) > (a - x)(3y - 2x) > 0$ since $x < a$ and $y > 0$ as $y \geq b - y$.

Finally, suppose that $x \geq y$. Reverse all arcs zu_2 of $K_{1,b}$ and denote the resulting digraph by D'. Analogously as above we get $W(D') - W(D) > (b - y)(3x - 2y) > 0$.

Consequently, either u_1 or u_2 is a core vertex of D. □

We remark that generalization of Proposition 10 to trees with at most two vertices of degree at least three seems to be rather technical.

5 Orientations of graphs with the minimum Wiener index

Another problem is to find an orientation of a graph that yields the minimum possible Wiener index. As already mentioned in the introduction, Plesník [16] proved that this problem is NP-hard for strongly connected orientations of graphs. However, one might consider the following conjecture.

Conjecture 11. *For every graph G, the value $W_{\min}(G)$ is achieved for some acyclic orientation of G.*

This is certainly true for bipartite graphs. Namely, by orienting all edges of such a graph G so that the corresponding arcs go from one bipartition to the other, we obtain a digraph D with $W(D) = |E(G)|$. As obviously $W_{\min}(G) \geq |E(G)|$, this case is established.

Now we turn our attention to graphs with higher chromatic number. Our next conjecture is motivated by the Gallai-Hasse-Roy-Vitaver theorem, which states that a number k is the smallest number of colors among all colorings of a graph G if and only if k is the largest number for which every orientation of G contains a simple directed path with k vertices. In other words, the chromatic number $\chi(G)$ is one plus the length of a longest path in a special orientation of the graph which minimizes the length of a longest path. The orientations for which the longest path has the minimum length always include at least one acyclic orientation.

A graph orientation is called *k-coloring-induced*, if it is obtained from some proper k-coloring such that each edge is oriented from the end-vertex with the bigger color to the end-vertex with the smaller color.

Conjecture 12. *$W_{\min}(G)$ is achieved for a $\chi(G)$-coloring-induced orientation.*

As mentioned above, Conjecture 12 holds for bipartite graphs and trivially it holds for complete graphs. By computer it was tested also for the Petersen graph.

If Conjecture 12 is not true in general, it may be satisfied at least for 3-colorable graphs. For such graphs we can use the following lemma.

Lemma 13. *Let G be a graph and let D be an orientation of G with arcs xu and uy. If d is the degree of u in G, then D contains at least $d-1$ directed paths of length two with the central vertex u.*

Proof. Let z be a neighbor of u in G, other than x and y (if such a vertex does not exist, the claim follows immediately). If $zu \in A(D)$ then z, u, y is a directed path of length two in D. If $uz \in A(D)$ then x, u, z is a directed path of length two. Together with the path x, u, y we obtain $d-1$ required directed paths. $\square$

With the help of Lemma 13 we are able to prove that some classes of graphs satisfy Conjecture 12.

Theorem 14. *Let G be a graph with at most one cycle. Then, $W_{\min}(G)$ is achieved for a $\chi(G)$-coloring-induced orientation.*

Proof. Since Conjecture 12 is true for bipartite graphs, we may assume that G has a cycle C of odd length ℓ. Let D be an orientation of G with the minimum Wiener index. Since D contains $|E(G)|$ paths of length 1, which are obviously shortest paths, we have $W(D) \geq |E(G)|$.

Since the length of C is odd, there must be three consecutive vertices x, u, y on C such that $xu, uy \in A(D)$. Let d be the degree of u in G. By Lemma 13, in D there are at least $d-1$ directed paths of length two with central vertex u. If $\ell \geq 5$, then all these paths of length two are shortest paths, which gives $W(D) \geq |E(G)| + 2(d-1)$. On the other hand if $\ell = 3$, then x, u, y is not necessarily a shortest path but all the remaining paths of length two with central vertex u are shortest paths as G contains only one cycle. Consequently, $W(D) \geq |E(G)| + 2(d-2)$.

Now color all the neighbors of u except x by 1, color u by 2 and x by 3. Then extend this partial coloring to a proper 3-coloring of G using only the colors 1 and 3. Observe that such an extension is possible since the length of the unique cycle C in G is odd. If we denote by D' the digraph induced by this coloring, then $W(D') = |E(G)| + 2(d-2)$ if $\ell = 3$, while $W(D') = |E(G)| + 2(d-1)$ if $\ell \geq 5$. $\square$

Observe that from the above proof we have that if G is a unicyclic graph in which the unique cycle has odd length l and if d^* is the minimum degree of a vertex of this unique cycle, then $W_{\min}(G) = |E(G)| + 2d^* - 4$ if $\ell = 3$, while $W_{\min}(G) = |E(G)| + 2d^* - 2$ if $\ell \geq 5$.

Theorem 15. *Let G be a graph of a prism. Then, $W_{\min}(G)$ is achieved for a $\chi(G)$-coloring-induced orientation.*

Proof. Let $V(G) = \{u_{i,j};$ where $0 \leq i \leq 1$ and $0 \leq j \leq \ell - 1\}$ and $E(G) = (\cup_{j=0}^{\ell-1} u_{0,j}u_{1,j}) \cup (\cup_{i=0}^{1}(\cup_{j=0}^{\ell-1} u_{i,j}u_{i,j+1}))$, where the addition in subscript is modulo ℓ. If ℓ is even then G is bipartite and Conjecture 12 is true. Thus, suppose that ℓ is odd. Let D be an orientation of G with the minimum Wiener index.

Since ℓ is odd, there is j_0 such that either $u_{0,j_0-1}, u_{0,j_0}, u_{0,j_0+1}$ or $u_{0,j_0+1}, u_{0,j_0}, u_{0,j_0-1}$ is a directed path of length 2. By Lemma 13, there are two paths of length 2 in D with central vertex u_{0,j_0}. Analogously, there is j_1 such that either $u_{1,j_1-1}, u_{1,j_1}, u_{1,j_1+1}$ or $u_{1,j_1+1}, u_{1,j_1}, u_{1,j_1-1}$ is a directed path of length 2. By Lemma 13, there are two paths of length 2 with central vertex u_{1,j_1}.

So there are four directed paths of length 2, one connecting $u_{0,.}$ with $u_{0,.}$, one connecting $u_{1,.}$ with $u_{1,.}$, and two connecting $u_{0,.}$ with $u_{1,.}$. Since the last two paths may connect identical pair of vertices, we consider only one of them. If $\ell \geq 5$, this gives $W(D) \geq |E(G)| + 6$ as all three paths of length 2 are shortest paths. On the other hand if $\ell = 3$, then we get $W(D) \geq |E(G)| + 2$.

Now color the vertices $u_{0,0}, u_{0,1}, u_{0,2}, u_{0,3}, \ldots, u_{0,\ell-2}, u_{0,\ell-1}$ by colors $1, 3, 1, 3, \ldots, 3, 2$, respectively; and color the vertices $u_{1,0}, u_{1,1}, u_{1,2}, u_{1,3}, \ldots, u_{1,\ell-2}, u_{1,\ell-1}$ by colors $2, 1, 3, 1, \ldots, 1, 3$, respectively. Observe that this coloring is proper. If we denote by D' the digraph induced by this coloring, then $W(D') = |E(G)| + 2$ if $\ell = 3$, while $W(D') = |E(G)| + 6$ if $\ell \geq 5$. $\square$

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Figures

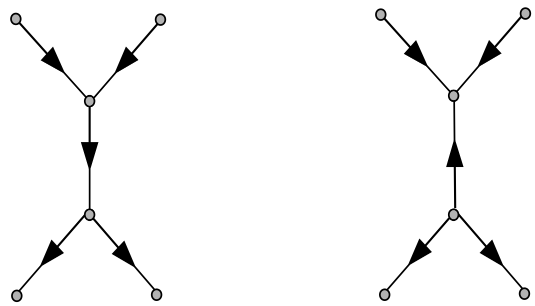

Figure 1: The graph on the left has two core vertices, while the right one has no core vertex.