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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.

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 [18] 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 [17]. 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 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,

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

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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 [18], 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. □

3. Wiener index vs. betweenness centrality

White and Borgatti [19] 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 $\sigma_{u,v} \neq 0$.