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# On maximum Wiener index of directed grids

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#### Abstract

This paper is devoted to Wiener index of directed graphs, more precisely of directed grids. The grid  $G_{m,n}$  is the Cartesian product  $P_m \square P_n$  of paths on m and n vertices, and in a particular case when m=2, it is a called the ladder graph  $L_n$ . Kraner Šumenjak et al. in 2021 proved that the maximum Wiener index of a digraph, which is obtained by orienting the edges of  $L_n$ , is obtained when all layers isomorphic to one factor are directed paths directed in the same way except one (corresponding to an endvertex of the other factor) which is a directed path directed in the opposite way. Then they conjectured that the natural generalization of this orientation to  $G_{m,n}$  will attain the maximum Wiener index among all orientations of  $G_{m,n}$ . In this paper we disprove the conjecture by showing that a comb-like orientation of  $G_{m,n}$  has significantly bigger Wiener index.

Keywords: Wiener index, topological graph theory, graph distance.

Math. Subj. Class.:

#### Introduction 1

Let G be a graph. Its Wiener index, W(G), is the sum of distances between all pairs of vertices of G. Thus.

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

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Wiener index was introduced by Wiener [28] in 1947 for its correlation with the boiling point of alkanes, and afterwards it became popular among chemists. By graph theorists it has been considered later under various names, see [10, 13, 24]. More about this invariant can be found in [6, 7, 15, 17, 29]. Wiener index is also tightly related to the average distance, for which  $\mu(G) = W(G)/\binom{n}{2}$ , see [4, 9], and also [11] for a brief survey.

Wiener index of directed graphs. Let D be a directed graph (a digraph). A (directed) path in D is a sequence of vertices  $v_0, v_1, \ldots, v_t$  such that  $v_{i-1}v_i$  is an arc of D, where  $1 \le i \le t$ . The distance  $d_D(u, v)$  is the length of a shortest path from u to v, and if there is no such path, we set

$$d_D(u,v) = 0. (1.1)$$

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 different ways. For instance, Botafogo et al. [3] defined it as the number of vertices in the analyzed network, while Bonchev [1, 2] assumed the condition (1.1). We adopt the latter in this paper.

Denote  $w_D(u) = \sum_{v \in V(D)} d_D(u, v)$ . Wiener index of D, W(D), is the sum of all distances in D, where each ordered pair of vertices has to be taken into account. Hence,

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

The study of Wiener index of digraphs was initiated by Harary [13], who applied it to sociometric problems. Strict lower bound for the Wiener index of digraphs was found by Ng and Teh [20]. Wiener index of digraphs was considered also indirectly, through the study of the average distance, see [5, 8].

Wiener theorem for directed trees. In [28], 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.

We have shown an analogous statement for directed trees assuming the condition (1.1) in [18]. 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)|. A directed tree is a digraph whose underlying graph is a tree. We have the following.

**Theorem 1.1.** Let T be a directed tree. Then

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

Wiener index vs. betweenness centrality. Additional motivation for using (1.1) arises from betweenness certality in complex networks. White and Borgatti [27] generalized Freeman's geodesic centrality measures for betweenness on graphs to the case of digraphs in the following way. Let P(D) denote the set of ordered pairs (u,v) of distinct vertices u and v such that there exists a directed path from u to v in D. Furthermore,  $\sigma_{u,v}$  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. The (directed) betweenness centrality B(x) of a vertex x in a digraph D is defined as

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

Note that  $\sigma_{u,v} \neq 0$  as  $(u,v) \in P$ .

Gutman and Škrekovski [25] 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.

In [18] we extended the above relation to directed graphs.

**Theorem 1.2.** For any digraph D of order n

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

**Maximum and minimum orientations.** For a graph G, let  $W_{\text{max}}(G)$  and  $W_{\text{min}}(G)$  be the maximum and the minimum, respectively, Wiener index among all digraphs obtained by orienting the edges of G. The following problem was posed in [16].

**Problem 1.3.** For a graph G, find  $W_{\max}(G)$  and  $W_{\min}(G)$ .

Plesník [22] proved that finding a strongly connected orientation of a given graph G that minimizes the Wiener index is NP-hard, but the case for non-necessarily strongly connected digraphs is unsolved [18].

**Problem 1.4.** What is the complexity of finding  $W_{\text{max}}(G)$  (resp.  $W_{\text{min}}(G)$ )?

If the graph is from some specific class, e.g. ladders, then we know these values directly. However for general grids we have no such a strucutral theorem and the complexity is unkown.

Let  $K_n$  be the complete graph on n vertices. In [19, 22] Plesník and Moon solved Problem 1.3 for  $W_{\max}(K_n)$  under an additional assumption that the extremal graph is strongly connected. In [16] it was shown that the results of Plesník and Moon hold also without the additional assumption (i.e., assuming the condition (1.1)). One may expect that when G is 2-connected,  $W_{\max}(G)$  is attained for some strongly connected orientation. This was disproved in [16] using some  $\Theta$ -graphs  $\Theta_{a,b,1}$ . More about this topic can be found in [5, 14, 16, 18].

Let  $P_n$  be a directed path on n vertices. Then  $W(P_n) = \binom{n+1}{3} = \frac{1}{6}n^3 + O(n^2)$ . Now suppose that G is a graph on n vertices which has a Hamiltonian path H. Direct all edges of H in one direction and direct remaining edges of G in the opposite way. Let  $D_H$  be the resulting directed graph. Then the orientation of H is a directed path P and if  $d_P(u,v)>0$  then  $d_P(u,v)=d_{D_H}(u,v)$  since the arcs obtained by directing edges not in H cannot be used as "shortcuts". Consequently,  $W_{\max}(G)\geq W(P_n)=\frac{1}{6}n^3+O(n^2)$ . This gives a simple lower bound for  $W_{\max}(G)$  if G has a Hamiltonian path.

Wiener index of directed grids. In this paper we consider Wiener index of directed grids. The  $m \times n$  grid  $G_{m,n}$  is the Cartesian product  $P_m \square P_n$  of paths on m and n vertices. If m=2, the grid is called the ladder graph  $L_n$ . Kraner Šumenjak et al. [26] proved that the maximum Wiener index of a digraph whose underlying graph is  $L_n$  is  $(8n^3 + 3n^2 - 5n + 6)/3$ . Moreover, the optimal orientation of  $L_n$  is attained for orientation presented in Figure 1.

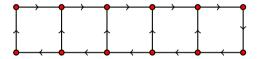


Figure 1: An orientation of the ladder  $P_2 \square P_6$  with the maximum Wiener index.

Let  $D_{m,n}$  be the orientation of  $G_{m,n}$  with all  $P_m$ -layers oriented up except the last  $P_m$ -layer which is oriented down, and all  $P_n$ -layers oriented to the left except the first  $P_n$ -layer which is oriented to the right, see Figure 3. The following conjecture was stated in [26].

**Conjecture 1.5.** For every 
$$m, n \geq 2$$
, we have  $W_{\max}(G_{m,n}) = W(D_{m,n})$ .

The conjecture naturally generalizes the result for m=2, but in this paper we show that it is not true if  $m\geq 3$ . Let  $C_{m,n}$  be an orientation of  $G_{m,n}$  in which the top  $P_n$ -layer is directed to the right and this layer is completed to a directed Hamiltonian cycle C in a zig-zag way as shown by blue arrows on Figure 2. Moreover, the other edges are directed in such a way that they do not shorten directed blue path starting at vertex (1,1). Of course,  $C_{m,n}$  exists only if n is even. We show that if n is even  $n\geq 4$  and  $m\geq 3$ , then  $W(C_{m,n})>W(D_{m,n})$ . To do this, we calculate  $W(C_{m,n})$  and  $W(D_{m,n})$ .

# 2 Wiener indices of $C_{m,n}$ and $D_{m,n}$

We start with calculating the Wiener index of a comb-like orientation of a grid.

**Theorem 2.1.** Let n be even and  $m, n \geq 4$ . Then

$$W(C_{m,n}) = \frac{1}{12}(2m^3n^3 + 2m^3n^2 + 2m^3n + 4m^3 + 4m^2n^3 - 3m^2n^2 - m^2n - 6m^2 - 2mn^3 + 4mn^2 - 2mn - 16m + 24n^2 - 72n + 72 + \beta)$$

where  $\beta = 3n - 6$  if m is odd and  $\beta = 0$  if m is even.

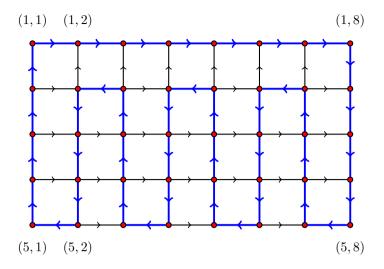


Figure 2: A comb orientation of the grid  $G_{5,8}$ .

*Proof.* We denote the vertices of  $C_{m,n}$  as in Figure 2. In the calculation we use  $\sum_{i=1}^k i = \frac{1}{2}(k^2+k)$  and  $\sum_{i=1}^k i^2 = \frac{1}{6}(2k^3+3k^2+k)$ . However, we need also to evaluate the following two sums. First,

$$\sum_{i=1}^{k/2} (1+2+\cdots+2i) = \sum_{i=1}^{k/2} \left(\frac{1}{2} \left((2i)^2+2i\right)\right) = \sum_{i=1}^{k/2} (2i^2+i) = \frac{1}{24} (2k^3+9k^2+10k).$$

Second.

$$\sum_{2 \le r, s \le m} |r - s| = 2 \sum_{2 \le r < s \le m} (s - r) = 2 ((m - 2)1 + (m - 3)2 + \dots + 1(m - 2))$$
$$= 2 \sum_{i=1}^{m-2} (m - 1 - i)i = \frac{1}{3} (m^3 - 3m^2 + 2m).$$

We divide all distances in  $C_{m,n}$  into 7 groups.

**1.** Distances from (1,k) to all vertices of  $C_{m,n}$ . Recall that  $C_{m,n}$  contains a Hamiltonian cycle C with some chords. Using these chords one cannot shorten the distance from (1,k) to (x,y), where  $2 \le x \le m$  and  $1 \le y \le n$ . Only the distances to  $(1,\ell)$ , where  $\ell < k$ , can be shortened. Hence, the sum of distances from (1,k) equals  $\binom{mn}{2} - \Delta_k$ , where  $\Delta_k$  sums the shortenings of k-1 distances on C, those from (1,k) to  $(1,\ell)$ ,  $1 \le \ell < k$ . Observe that each pair (1,k),  $(1,\ell)$ ,  $1 \le \ell < k$ , contributes to  $\Delta_k$  by the number of vertices which are avoided when using the edge  $(2,\ell)(1,\ell)$  instead of the directed blue path from  $(2,\ell)$  to  $(1,\ell)$ . Obviously,  $\Delta_1 = \Delta_2 = 0$ , but  $\Delta_3 = 2m-2$ ,  $\Delta_4 = (2m-2) + 2m$ ,

etc. For  $\Delta = \sum_{k=1}^{n} \Delta_k$  we have

$$\begin{split} \Delta = & [(2m-2)] + [(2m-2) + 2m] + [(2m-2) + 2m + (4m-2)] + \dots \\ & + [(2m-2) + 2m + \dots + ((n-2)m-2) + (n-2)m] \\ = & (n-2)(m+m-2) + (n-3)(2m) + \dots + 2((n-3)m+m-2) + 1(n-2)m \\ = & (n-2)1m + \dots + 1(n-2)m + (m-2)(n-2) + \dots + (m-2)2 \\ = & m \sum_{i=1}^{n-2} (n-1-i)i + (m-2)2 \sum_{i=1}^{n/2-1} (\frac{n}{2}-i) \\ = & m(n-1) \sum_{i=1}^{n-2} i - m \sum_{i=1}^{n-2} i^2 + 2(m-2) \sum_{i=1}^{n/2-1} i \\ = & \frac{1}{12} (2mn^3 - 3mn^2 - 2mn - 6n^2 + 12n). \end{split}$$

So the sum of distances considered in this case is

$$W_1 = n \binom{mn}{2} - \Delta = \frac{1}{12} (6m^2n^3 - 2mn^3 - 3mn^2 + 2mn + 6n^2 - 12n).$$

**2.** Distances from (k,t) to  $(1,\ell)$ , where  $2 \le k \le m$  and  $1 \le \ell < t \le n$ . Here the distances

$$\begin{array}{llll} \text{to } (1,1) \text{ are } & m+(m+1)+\cdots+(m-1)n & = \binom{(m-1)n+1}{2}-\binom{m}{2} \\ \text{to } (1,2) \text{ are } & 2+3+\cdots+((m-1)(n-2)+1) & = \binom{(m-1)(n-2)+2}{2}-1 \\ \text{to } (1,3) \text{ are } & m+(m+1)+\cdots+(m-1)(n-2) & = \binom{(m-1)(n-2)+1}{2}-\binom{m}{2} \\ \text{to } (1,4) \text{ are } & 2+3+\cdots+(m-1)(n-4)+1 & = \binom{(m-1)(n-4)+2}{2}-1 \\ & & \vdots \\ \text{to } (1,n-2) \text{ are } & 2+3+\cdots+((m-1)2+1) & = \binom{(m-1)2+2}{2}-1 \\ \text{to } (1,n-1) \text{ are } & m+(m+1)+\cdots+(m-1)2 & = \binom{(m-1)2+1}{2}-\binom{m}{2} \\ \text{to } (1,n) \text{ are } & 0. \end{array}$$

And their sum is

$$\begin{split} W_2 &= \sum_{i=1}^{n/2} \binom{(m-1)2i+1}{2} - \sum_{i=1}^{n/2} \binom{m}{2} + \sum_{i=1}^{n/2-1} \binom{(m-1)2i+2}{2} - \sum_{i=1}^{n/2-1} 1 \\ &= \frac{1}{12} (2m^2n^3 + m^2n - 4mn^3 + 6mn^2 - 11mn + 2n^3 - 6n^2 + 10n). \end{split}$$

**3.** Distances from (k,t) to  $(1,\ell)$ , where  $2 \le k \le m$  and  $1 \le t = \ell \le n$ . Here the distances

to 
$$(1, \ell)$$
 for odd  $\ell$  are 
$$1 + 2 + \dots + (m-1) = {m \choose 2}$$
 to  $(1, \ell)$  for even  $\ell < n$  are 
$$1 + 4 + 5 + \dots + (m+1) = {m+2 \choose 2} - 5$$
 to  $(1, \ell)$  for  $\ell = n$  are 
$$(m+1) + (m+2) + \dots + (2m-1) = {2m \choose 2} - {m+1 \choose 2}$$

And their sum is

$$W_3 = \left(\frac{n}{2} - 1\right) \left(\binom{m}{2} + \binom{m+2}{2} - 5\right) + \binom{m}{2} + \binom{2m}{2} - \binom{m+1}{2}$$
$$= \frac{1}{12} (6m^2n + 12m^2 + 6mn - 36m - 24n + 48).$$

**4.** Distances from (k,t) to  $(1,\ell)$ , where  $2 \le k \le m$  and  $1 \le t < \ell \le n$ . In this case when t is odd or k=2 then the shortest path is

$$(k,t), (k-1,t), \ldots, (1,t), (1,t+1), \ldots, (1,\ell).$$

On the other hand if t is even and  $k \ge 3$  then the shortest path is

$$(k,t),(k,t+1),(k-1,t+1),\ldots,(1,t+1),(1,t+2),\ldots,(1,\ell).$$

So the sum of distances

for 
$$\ell - t = 1$$
 is  $(n-1)(2+3+\cdots+m) = (n-1)\binom{m+1}{2} - \binom{2}{2}$  for  $\ell - t = 2$  is  $(n-2)(3+4+\cdots+(m+1)) = (n-2)\binom{m+2}{2} - \binom{3}{2}$   $\vdots$  for  $\ell - t = n-1$  is  $1(n+(n+1)+\cdots+(n+m-2)) = 1\binom{n+m-1}{2} - \binom{n}{2}$ .

And the sum of distances considered in this case is

$$W_4 = \sum_{i=1}^{n-1} (n-i) \left( \binom{m+i}{2} - \binom{1+i}{2} \right)$$
$$= \frac{1}{12} (3m^2n^2 - 3m^2n + 2mn^3 - 3mn^2 + mn - 2n^3 + 2n).$$

So, we are done with this case.

It remains to consider the distances between the vertices (r,t) and  $(s,\ell)$  where  $2 \le r, s \le m$  and  $1 \le t, \ell \le n$ . Let P be the subpath of the Hamiltonian cycle C in  $C_{m,n}$  starting at (2,n) and terminating at (2,1). We say that (r,t) preceds  $(s,\ell)$  if (r,t) preceds  $(s,\ell)$  on P.

**5.** Distances from (r,t) to  $(s,\ell)$ , where  $2 \le r,s \le m$  and  $1 \le t,\ell \le n$  when (r,t) preceds  $(s,\ell)$  on P.

In this case the distance from (r,t) to  $(s,\ell)$  equals the distance of these vertices on P. Hence,

$$W_5 = \sum_{i=1}^{(m-1)n} {i \choose 2} = \frac{1}{12} (2m^3n^3 - 6m^2n^3 + 6mn^3 - 2mn - 2n^3 + 2n).$$

**6.** Distances from (r,t) to  $(s,\ell)$ , where  $2 \le r, s \le m$  and  $1 \le t = \ell \le n$  when  $(s,\ell)$  preceds (r,t) on P. Since both (r,t) and  $(s,\ell)$  are in the same column, see Figure 2, we have r < s if t is odd and r > s if t is even.

First assume that t = 1. Then r < s and the shortest path from (r, t) to  $(s, \ell)$  is

$$(r,1), (r,2), (r+1,2), \ldots, (m,2), (m,1), (m-1,1), \ldots, (s,1)$$

with length 1 + (m - r) + 1 + (m - s) = 2m + 2 - r - s. Hence the sum of considered distances in the first column is

$$\Delta_1 = \sum_{2 \le r < s \le m} (2m + 2 - r - s) = {m - 1 \choose 2} (2m + 2) - \sum_{2 \le r < s \le m} (r + s)$$
$$= {m - 1 \choose 2} (2m + 2) - (m - 2) \sum_{i=2}^{m} i = \frac{1}{12} (6m^3 - 18m^2 + 12m).$$

Now let t=n. We argue similarly. In this case r>s and the shortest path from (r,t) to  $(s,\ell)$  is

$$(r,n), (r+1,n), \ldots, (m,n), (m,n-1)(m-1,n-1), \ldots, (s,n-1), (s,n)$$

with length (m-r)+1+(m-s)+1=2m+2-r-s. Hence the sum of considered distances in the n-th column is

$$\Delta_n = \sum_{2 \le r \le s \le m} (2m + 2 - r - s) = \Delta_1 = \frac{1}{12} (6m^3 - 18m^2 + 12m).$$

Now let m be odd and  $2 \le t \le n-1$ . First assume that t is odd. Then r < s and the shortest path from (r,t) to  $(s,\ell)$  either uses the column t-1 or t+1. Hence, the shortest path is one of the following two

$$(r,t), (r,t+1), \ldots, (m,t+1), (m,t), (m-1,t), \ldots, (s,t)$$
 with length  $2m+2-r-s$ ,  $(r,t), (r-1,t), \ldots, (2,t), (2,t-1), \ldots, (s,t-1), (s,t)$  with length  $r+s+2$ .

Hence the distance from (r,t) to  $(s,\ell)$  is  $\min\{2m+2-r-s,r+s+2\}$ . Let us split the distances according to the value of r. Observe that if r=2 then the second path is the shortest one, while if s=m (i.e., in the last column) then the first path is the shortest one.

These summands are symmetric with respect to the diagonal formed by values m. Therefore using the formula derived in the beginning of this proof we get

$$\Delta_t = \frac{m-1}{2}m + 2\left(\frac{m-1}{2}\left(1+2+\dots+(m-1)\right) - \sum_{i=1}^{(m-1)/2}\left(1+2+\dots+2i\right)\right)$$
$$= \frac{1}{12}(4m^3 - 9m^2 + 2m + 3).$$

Now assume that t is even, so that r > s. Again, the shortest path is one of the following two

$$(r,t),(r,t+1),\ldots,(2,t+1),(2,t),\ldots,(s,t)$$
 with length  $r+s+2,$   $(r,t),\ldots,(m,t),(m,t-1),\ldots,(s,t-1),(s,t)$  with length  $2m+2-r-s$ .

Hence the distance from (r,t) to (s,t) is again  $\min\{2m+2-r-s,r+s+2\}$ , and we get the same formula as in the case when t is odd.

Now let m be even and  $2 \le t \le n-1$ . We already know that regardless of the parity of t it holds

$$d((r,t),(s,t)) = \min\{2m+2-r-s,r+s+2\}.$$

Nevertheless, assume that t is odd and split the distances according to the value of r.

Again the summands are symmetric with respect to the diagonal formed by values m. Therefore using the formula derived in the beginning of this proof we get

$$\Delta_t = \frac{m-2}{2}m + 2\left(\frac{m-2}{2}\left(1+2+\dots+(m-1)\right) - \sum_{i=1}^{(m-2)/2}\left(1+2+\dots+2i\right)\right)$$
$$= \frac{1}{12}(4m^3 - 9m^2 + 2m).$$

And since for even t we get the same distances,  $\Delta_t$  does not depend on the parity of t though it depends on the parity of m.

Hence, the contribution of considered pairs to  $W(D_{m,n})$  is

$$W_6 = 2\Delta_1 + (n-2)\Delta_2 = \frac{1}{12}(4m^3n + 4m^3 - 9m^2n - 18m^2 + 2mn + 20m + \beta)$$

where  $\beta = 3(n-2)$  if m is odd and  $\beta = 0$  if m is even.

**7.** Distances from (r,t) to  $(s,\ell)$ , where  $2 \le r, s \le m$  and  $1 \le t < \ell \le n$ . Obviously, in this case  $(s,\ell)$  preceds (r,t) on P. Using the paths  $(m,q), (m-1,q), \ldots, (2,q)$  for odd q,  $(2,q), (3,q), \ldots, (m,q)$  for even q, and for  $2 the paths <math>(p,1), (p,2), \ldots, (p,n)$  which exist if  $m \ge 4$ , one can see that the distance from (r,t) to  $(s,\ell)$  in  $D_{m,n}$  equals the distance from (r,t) to  $(s,\ell)$  in the underlying graph. The only exceptions occure when r=s=2 or r=s=m. If r=s=2 then the distance from (r,t) to  $(s,\ell)$  is  $\ell-t+2$  except the case when  $\ell=t+1$  and  $\ell$  is odd, in which case the distance is 1. On the other hand if r=s=m then the distance from (r,t) to  $(s,\ell)$  is  $\ell-t+2$  except the case when

 $\ell=t+1$  and t is even, in which case the distance is 1 again. So for any parity of t, two distances between the layers t and  $\ell$  exceed the corresponding distance in the underlying graph by 2, except the case when  $\ell=t+1$ , when only one distance between the layers t and  $\ell$  exceeds the corresponding distance in the underlying graph by 2. Using the formula from the beginning of the proof, the sum of all distances from the vertices of  $\{(r,t)\}_{r=2}^m$  to the vertices of  $\{(s,\ell)\}_{s=2}^m$  is

$$\Delta_{t,\ell} = \sum_{2 \le r,s \le m} |r - s| + \sum_{2 \le r,s \le m} (\ell - t) + 4 - \delta$$
$$= \frac{1}{3} (m^3 - 3m^2 + 2m) + (m - 1)^2 (\ell - t) + 4 - \delta,$$

where  $\delta=2$  if  $\ell=t+1$  and  $\delta=0$  otherwise. Consequently, the contribution of considered distances is

$$W_7 = \sum_{t=1}^{n-1} \left( \sum_{\ell=t+1}^{n} \left( \frac{1}{3} (m^3 - 3m^2 + 2m) + (m-1)^2 (\ell - t) + 4 \right) - 2 \right)$$

$$= \frac{n(n-1)}{2} \frac{1}{3} (m^3 - 3m^2 + 2m) + (m-1)^2 \sum_{i=1}^{n-1} (n-i)i + \frac{n(n-1)}{2} 4 - 2(n-1)i + \frac{1}{2} (2m^3 n^2 - 2m^3 n + 2m^2 n^3 - 6m^2 n^2 + 4m^2 n - 4mn^3 + 4mn^2 + 2n^3 + 24n^2 - 50n + 24 \right).$$

Now  $W(C_{m,n}) = \sum_{i=1}^{7} W_i$ .

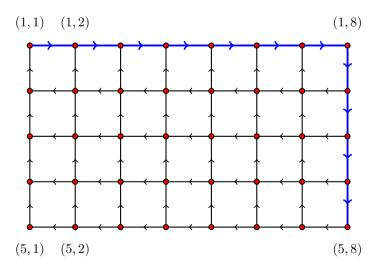


Figure 3: The orientation  $D_{m,n}$  of the grid  $G_{5,8}$  from Conjecture 1.5.

In [26], the authors did not evaluate the Wiener index of  $D_{m,n}$ . In order to be able to compare the Wiener indices of  $C_{m,n}$  and  $D_{m,n}$ , we prove the following statement.

**Theorem 2.2.** We have

$$W(D_{m,n}) = \frac{1}{12}(10m^3n^2 + 10m^2n^3 - 6m^3n - 24m^2n^2 - 6mn^3 + 4m^3 + 14m^2n + 14mn^2 + 4n^3 - 12mn - 4m - 4n).$$

*Proof.* We denote the vertices of  $G=D_{m,n}$  as in Figure 3. Let  $(x,y)\in V(G)$ . We describe specific subgraphs of G with respect to (x,y) and we describe a formula for calculating distances from (x,y) to the vertices of the specific subgraph. Let H be a subgraph of G which is an orientation of  $P_r\square P_s$ . Of course,  $r\leq m$  and  $s\leq n$ . Moreover, let H has a vertex (a,b) in its corner, such that for every  $(u,v)\in V(H)$  we have  $d_G((x,y),(u,v))=d_G((x,y),(a,b))+d_G((a,b),(u,v))$ . I.e., the corner vertex (a,b) is on a shortest path from (x,y) to every vertex of H. Finally, let the distance from (a,b) to vertices of H are the same in H as in the underlying graph. We denote the graph H by Q(a,b,c,d), where (c,d) is a corner of H opposite to (a,b). Obviously, |a-c|=r-1 and |b-d|=s-1. Denote  $t=d_G((x,y),(a,b))$ . Then the sum of distances from (x,y) to the vertices of H is

$$B(t,r,s) = t + \dots + (t+r-1) + (t+1) + \dots + (t+r) + \dots + (t+s-1) + \dots + (t+s+r-2)$$
$$= {t+r+s \choose 3} - {t+r \choose 3} - {t+s \choose 3} + {t \choose 3}.$$

We divide the vertices of G into three groups,  $S_1$ ,  $S_2$  and  $S_3$ , and for each group  $S_i$ ,  $1 \le i \le 3$ , we calculate the contribution of vertices of  $S_i$  to W(G), i.e., we calculate  $\sum_{u \in S_i} w_G(u)$ . However, our calculation is not so detailed as in the proof of Theorem 2.1. The reason is that when we find that the formulae do not split into cases (like the parity of m in Theorem 2.1), then the resulting formula is a polynomial which is of at most 3rd order in both m and n. Hence, its 16 coefficients can be calculated using a system of linear equations for small m and n ( $2 \le m, n \le 5$ ), for which  $W(D_{m,n})$  can be calculated by a computer. (In fact, the resulting polynomial was checked on a much wider range of m and n.)

1.  $S_1 = \{(1, a); 1 \le a \le n\}$ . Let  $1 \le a \le n$ . Observe that G contains Q(2, n, m, 1). So considering first the distances to the vertices of  $S_1$  and then to the vertices of Q(2, n, m, 1) we get

$$w_G(1,a) = 1 + 2 + \dots + (n-a) + (2(n-a)+3) + (2(n-a)+4) + \dots + (2(n-a)+a+1)$$

$$+B(n-a+1,m-1,n) = \binom{n-a+1}{2} + \binom{2n-a+2}{2} - \binom{2n-2a+3}{2}$$

$$+\binom{2n+m-a}{3} - \binom{n+m-a}{3} - \binom{2n-a+1}{3} + \binom{n+1-a}{3},$$

which gives

$$W_1 = \sum_{a=1}^{n} w_G(1, a) = \frac{1}{12} (6m^2n^2 + 12mn^3 - 18mn^2 - 4n^3 + 12n^2 - 8n).$$

**2.**  $S_2 = \{(a,n); \ 2 \le a \le m\}$ . Let  $2 \le a \le m$ . Then the distances to (x,y), where  $1 \le x \le m$  and  $1 \le y \le n-1$ , are the same in G as in the underlying graph. So considering first the distances to vertices of  $S_2 \cup \{(1,n)\}$  and then to the other vertices we get

$$w_G(a,n) = 1 + 2 + \dots + (m-a) + (a+1) + (a+2) + \dots + (2a-1)$$

$$+ (n-1) \sum_{s=1}^{m} |s-a| + m \sum_{i=1}^{m-1} i$$

$$= {m-a+1 \choose 2} + {2a \choose 2} - {a+1 \choose 2} + (n-1) \sum_{s=1}^{m} |s-a| + m {n \choose 2},$$

which gives

$$W_2 = \sum_{n=2}^{m} w_G(a,n) = \frac{1}{12} (4m^3n + 6m^2n^2 + 4m^3 - 12m^2n - 6mn^2 + 8mn - 4m).$$

3.  $S_3 = \{(a,b); \ 2 \le a \le m; \ 1 \le b \le n-1\}$ . Let  $2 \le a \le m$  and  $1 \le b \le n-1$ . Now we consider first the distances to the vertices of Q(a,b,1,1), second the distances to (1,i) where  $b < i \le n$ , then the distances to vertices of Q(2,n,a,b+1), and finally the distances to the vertices of Q(a+1,n,m,1). We get

$$w_{G}(a,b) = B(0,a,b) + a + (a+1) + \dots + (a+(n-b)-1)$$

$$+ B(a+n-b,a-1,n-b) + B(2a+n-b-1,m-a,n)$$

$$= \binom{a+b}{3} - \binom{a}{3} - \binom{b}{3} + \binom{n+a-b}{2} - \binom{a}{2} + \binom{2n+2a-2b-1}{3}$$

$$- \binom{n+2a-b-1}{3} - \binom{2n+a-2b}{3} + \binom{n+a-b}{3} + \binom{2n+m+a-b-1}{3}$$

$$- \binom{n+m+a-b-1}{3} - \binom{2n+2a-b-1}{3} + \binom{n+2a-b-1}{3},$$

which gives

$$\begin{split} \sum_{a=2}^{m} w_G(a,b) &= \binom{m+b+1}{4} - \binom{b+2}{4} - \binom{m+1}{4} - (m-1) \binom{b}{3} \\ &+ \binom{n+m-b+1}{3} - \binom{n-b+2}{3} - \binom{m+1}{3} \\ &+ \sum_{i=1}^{m} \binom{2n-2b-1+2i}{3} - \binom{2n-2b+1}{3} - \binom{2n+m-2b+1}{4} + \binom{2n-2b+2}{4} \\ &+ \binom{n+m-b+1}{4} - \binom{n-b+2}{4} + \binom{2n-2m-b}{4} - \binom{2n+m-b+1}{4} \\ &- \binom{n+2m-b}{4} + \binom{n+m-b+1}{4} - \sum_{i=1}^{m} \binom{2n-b-1+2i}{3} + \binom{2n-b+1}{3}, \end{split}$$

and consequently

$$W_3 = \sum_{b=1}^{n-1} \sum_{a=2}^{m} w_G(a, b) = \frac{1}{12} (10m^3n^2 + 10m^2n^3 - 10m^3n - 36m^2n^2 - 18mn^3 + 26m^2n + 38mn^2 + 8n^3 - 20mn - 12n^2 + 4n).$$

Now 
$$W(D_{m,n}) = \sum_{i=1}^{3} W_i$$
.

# 3 Comparing Wiener indices

By Theorems 2.1 and 2.2, in variables m and n the polynomial  $W(C_{m,n})$  is of 6th order while  $W(D_{m,n})$  is only of 5th order. Therefore, for big m and n we have  $W(C_{m,n}) > W(D_{m,n})$ . In the next proof we show that  $W(C_{m,n}) > W(D_{m,n})$  for all m and n for which  $C_{m,n}$  exists.

**Theorem 3.1.** Let  $m \geq 3$  and let n be even,  $n \geq 4$ . Then  $W(C_{m,n}) > W(D_{m,n})$ .

*Proof.* Observe that 3n-6>0 if  $n\geq 4$ . Moreover, part 7 of the proof of Theorem 2.1 is the only one in which we assume m>3. If m>3 then the distances considered there are the shortest ones, that is as in the underlying graph, with a few exceptions. In these exceptions the distances are second shortest, i.e. increased by 2, since the graph is bipartite. In the same cases the distances are not shortest possible if m=3 and they are not shortest even in some other cases. Therefore for all  $m\geq 3$  and even  $n\geq 4$  the expression in Theorem 2.1 without  $\beta$  is a lower bound for  $W(C_{m,n})$ . Hence

$$12\Big(W(C_{m,n}) - W(D_{m,n})\Big) \ge 2m^3n^3 - 8m^3n^2 - 6m^2n^3 + 8m^3n + 21m^2n^2 + 4mn^3$$
$$-15m^2n - 10mn^2 - 4n^3 - 6m^2 + 10mn + 24n^2 - 12m - 68n + 72$$
$$= 2(m-3)^3(n-3)^3 + 10(m-3)^3(n-3)^2 + 12(m-3)^2(n-3)^3$$
$$+14(m-3)^3(n-3) + 57(m-3)^2(n-3)^2 + 22(m-3)(n-3)^3$$
$$+6(m-3)^3 + 75(m-3)^2(n-3) + 98(m-3)(n-3)^2 + 8(n-3)^3$$
$$+30(m-3)^2 + 130(m-3)(n-3) + 39(n-3)^2 + 54(m-3) + 61(n-3) + 30 > 0,$$

since  $m, n \geq 3$  and all the coefficients are positive.

By Theorem 2.2, we have  $W(D_{m,n}) = W(D_{n,m})$ . This is not the case of  $W(C_{m,n})$ . If both m and n are even and m < n, which of  $W(C_{m,n})$  and  $W(C_{n,m})$  is bigger? The next statement answers this question.

**Theorem 3.2.** If both m and n are even and  $4 \le m < n$  then  $W(C_{m,n}) > W(C_{n,m})$ .

Proof. By Theorem 2.1

$$12(W(C_{m,n}) - W(C_{n,m})) = -2m^3n^2 + 2m^2n^3 + 4m^3n - 4mn^3 - 5m^2n + 5mn^2 + 4m^3 - 4n^3 - 30m^2 + 30n^2 + 56m - 56n$$
$$= (n-m)[2m^2n^2 - 4mn(m+n) - 4m^2 - 4n^2 + mn + 30(m+n) - 56].$$
(3.1)

Denote by  $\Delta$  the long expression in brackets of (3.1). If  $m, n \geq 6$  then

$$m^{2}n^{2} - 4m^{2}n - 4m^{2} = m^{2}(n^{2} - 4n - 4) > 0$$
  

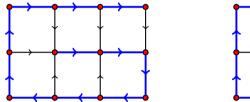
$$m^{2}n^{2} - 4mn^{2} - 4n^{2} = n^{2}(m^{2} - 4m - 4) > 0$$
  

$$mn + 30(m + n) - 56 > 0,$$

and so  $\Delta > 0$ . On the other hand if m = 4 then

$$\Delta = 32n^2 - 64n - 16n^2 - 64 - 4n^2 + 4n + 120 + 30n - 56 = 12n^2 - 30n > 0$$
 as well. Hence, if  $m \ge 4$  then  $\Delta > 0$  and consequently  $W(C_{m,n}) > W(C_{n,m})$ .

## 4 Concluding remarks and possible further work



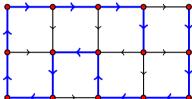


Figure 4: Grids  $G_{3,4}$  and  $G_{3,5}$  with optimal orientations  $M_{3,4}$  and  $M_{3,5}$ , respectively, Hamiltonian paths are thick.

Let  $C_q$  be a directed cycle on q vertices. Then  $W(C_q) = q\binom{q}{2} = \frac{1}{2}q^3 + O(q^2)$ . It is known that if G is a directed graph on q vertices then  $W(G) \leq W(C_q)$ . Thus, we have the following observation.

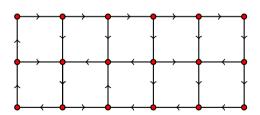


Figure 5: Gird  $G_{3,6}$  with the optimal orientation  $M_{3,6}$ .

**Observation 4.1.** Among all orientations of  $G_{m,n}$ , where  $m \geq 3$  and  $n \geq 4$  is even,  $W(C_{m,n})$  has the best possible order, i.e.  $W(C_{m,n}) = \Theta(W_{\max}(G_{m,n}))$ .

Observe that this is not the case of  $D_{m,n}$  if  $cn \leq m \leq n$  for a constant c. Even if both m and n are odd, it is easy to find an orientation of the grid in which the Wiener index has the correct order. Just take a Hamiltonian path H of the grid G, and construct  $G_H$  as decsribed in the Introduction.

By Theorem 2.1, if  $c_1n \leq m \leq c_2m$  where  $c_1$  and  $c_2$  are constants, then for q=mn we have  $W(C_{m,n})=\frac{1}{6}q^3+o(q^3)$ . Here the leading term has multiplier as the leading term for  $W(P_q)$ . But if m is a constant, we have a better bound. In such a case  $W(C_{m,n})=\frac{1}{6}(1+\frac{2}{m}-\frac{1}{m^2})q^3+O(q^2)$  and for m=3 the Wiener index is probably even higher. Anyway,  $C_{3,n}$  is not the orientation of  $G_{3,n}$  with the biggest Wiener index at least if  $n\in\{4,6\}$ . The orientations  $M_{3,n}$  of  $G_{3,n}$ ,  $4\leq n\leq 6$ , with the biggest Wiener index are in Figures 4 and 5. They were found by a computer and  $W(M_{3,4})=578$ ,  $W(M_{3,5})=1116$ ,  $W(M_{3,6})=1928$ . Just to compare let us mention that  $W(C_{3,4})=538$ ,  $W(C_{3,6})=1740$ ,  $W(D_{3,4})=516$ ,  $W(D_{3,5})=968$ ,  $W(D_{3,6})=1626$ . In  $M_{3,4}$  and  $M_{3,5}$ , thick lines form a Hamiltonian path such that all arcs not in this path are directed oppositely. However,  $M_{3,6}$  does not have such a path. Although  $W(M_{3,k})>W(C_{3,k})$  for  $k\in\{4,6\}$ , it can be true that  $\lim_{m,n\to\infty}W_{\max}(G_{m,n})/W(C_{m,n})=1$  for even n. Hence, we have the following problem.

**Problem 4.2.** Find the biggest possible constant c, such that  $W_{\max}(G_{m,n}) \ge c(mn)^3 + o((mn)^3)$ .

Of course, the main problem is the following one.

**Problem 4.3.** Find an orientation of  $G_{m,n}$  with the maximum Wiener index.

The above problem may be difficult. The extremal graphs  $M_{3,4}$ ,  $M_{3,5}$  and  $M_{3,6}$  do not have any obvious simple property, but they are at least strongly connected. Therefore, we conclude the paper with the following question.

**Question 4.4.** Let  $M_{m,n}$  be an orientation of  $G_{m,n}$  with the maximum Wiener index. Is  $M_{m,n}$  strongly connected?

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