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Selected topics on Wiener index*

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Abstract

The Wiener index is defined as the sum of distances between all unordered pairs of vertices in a graph. It is one of the most recognized and well-researched topological indices, which is on the other hand still a very active area of research. This work presents a natural continuation of the paper *Mathematical aspects of Wiener index* (Ars Math. Contemp., 2016) in which several interesting open questions on the topic were outlined. Here we collect answers gathered so far, give further insights on the topic of extremal values of Wiener index in different settings, and present further intriguing problems and conjectures.

Keywords: Graph distance, Wiener index, average distance, topological index, molecular descriptor, chemical graph theory.

Math. Subj. Class. (2020): 05C05, 05C12, 05C20, 05C92, 92E10

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1 Introduction

The *Wiener index*, $W(G)$, is a topological index of a connected graph, defined as the sum of the lengths of the shortest paths between all unordered pairs of vertices in the graph. In other words, for a connected graph

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

where $d(u,v)$ denotes the distance between vertices u and v in G. This graph invariant has been investigated by numerous authors (see e.g. [24, 26, 27, 52, 56, 81]) under a variety of other names like transmission, total status, sum of all distances, path number and Wiener number of a graph. Due to its basic character and applicability, it has arisen in diverse contexts, including efficiency of information, sociometry, mass transport, cryptography, theory of communication, molecular structure, complex network topology and many more.

The index was originally introduced in 1947 by Harold Wiener for the purpose of determining the approximation formula of the boiling point of paraffin [80]. The definition of Wiener index in terms of distances between vertices of a graph was first given by Hosoya [40].

The *transmission* (also called the *distance*) of $u \in V(G)$ is $t_G(u) = \sum_{v \in V(G)} d_G(u,v)$. Thus the Wiener index can be expressed as

$$W(G) = \frac{1}{2} \sum_{v \in V(G)} t_G(v).$$

Another view on the Wiener index was presented in [3] as follows. Suppose that $\{t_G(u) \,|\, u \in V(G\} = \{d_1, d_2, \ldots, d_k\}$. Assume in addition that G contains t_i vertices whose transmission is d_i, $1 \leq i \leq k$. Then the Wiener index of G can be expressed as

$$W(G) = \frac{1}{2} \sum_{i=1}^{k} t_i d_i.$$

We therefore say that the *Wiener dimension* $\dim_W(G)$ of G is k. That is, the Wiener dimension of a graph is the number of different transmissions of its vertices.

Fundamental properties regarding extremal values of Wiener index are already a part of the folklore. In [30] and later in many subsequent papers (e.g. [36, 37]) it was shown that for trees on n vertices, the maximum Wiener index is obtained for the path P_n, and the minimum for the star S_n. Thus, for every tree T on n vertices, it holds

$$(n-1)^2 = W(S_n) \leq W(T) \leq W(P_n) = \binom{n+1}{3}.$$

Since the distance between any two distinct vertices is at least one, we have that among all graphs on n vertices K_n has the smallest Wiener index. In general, removing (resp. adding) of an edge from a connected graph results in increased (resp. decreased) Wiener index, which leads to the observation that Wiener index of a connected graph is less than or equal to the Wiener index of its spanning tree. Therefore, for any connected graph G on n vertices, it holds

$$\binom{n}{2} = W(K_n) \leq W(G) \leq W(P_n) = \binom{n+1}{3}.$$

Despite extensive literature on the Wiener index, many interesting and basic questions remain open. In our previous survey [56] we have exposed some of them that mainly pertain to extremal values of Wiener index in different settings. In this paper we continue with summarizing knowledge accumulated since then, and integrate some new conjectures, problems and ideas for possible future work.

2 Minimum Wiener index for chemical graphs

The *degree* $\deg_G(v)$ of a vertex $v \in V(G)$ in a graph G is $|N_G(v)|$, where $N_G(v)$ denotes the neighborhood of v in G. The *maximum degree* of a graph G, $\max_{v\in V(G)} \deg_G(v)$, is denoted by $\Delta(G)$, and the *minimum degree*, $\min_{v\in V(G)} \deg_G(v)$, is denoted by $\delta(G)$.

Since every atom has a certain valency, chemists are often interested in graphs with restricted degrees, which correspond to valencies. Particularly interesting is the class of *chemical graphs*, i.e. graphs for which the degrees of its vertices do not exceed 4. In [60] the authors addressed an "overlooked" problem of determining the minimum value of Wiener index and corresponding extremal graphs among chemical graphs with prescribed number of vertices. Note that the upper bound for this class of graphs is attained by paths.

Problem 2.1. Find all the chemical graphs G on n vertices with the minimum value of Wiener index.

Inserting of an edge in a graph decreases the Wiener index, thus one would expect that its minimum in the class of chemical graphs is attained by 4-regular graphs. Using a computer it was verified that for $n \in \{1, 2, \dots, 5\}$ minimum is attained for K_n. Extremal graphs in cases $n = 6, 7$ are presented in Figure 1. Observe that the first two graphs in this figure are circulant graphs $C_6(1, 2)$ and $C_7(1, 2)$, respectively, and they are vertex-transitive. There are 1929 simple connected graphs on 8 vertices and the minimum Wiener index value is 40, which is attained by only 6 graphs depicted in Figure 2. Note that the first three graphs, which are the circulant graph $C_8(1, 2)$, the Cartesian product $K_4 \square P_2$ and the complete bipartite graph $K_{4,4} = C_8(1, 3)$, respectively, are vertex-transitive. The above cases support the following conjecture.

Conjecture 2.2. *Every chemical graph G on $n \geq 5$ vertices with the minimum value of Wiener index is 4-regular.*

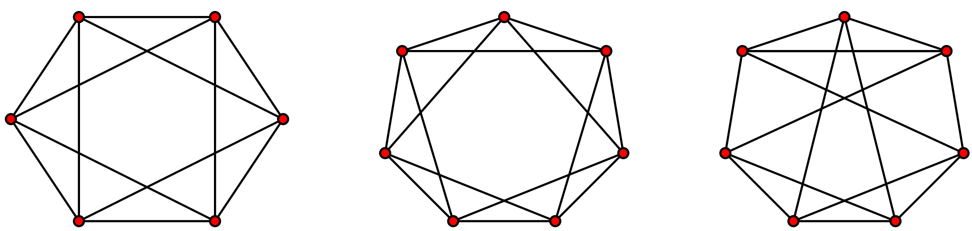

Figure 1: Extremal graphs for $n = 6$ and $n = 7$.

Although computer results indicate the above conjecture to be true, the problem seems to be far from tractable. In [60] it is shown that a chemical graph with the minimum value of Wiener index has at most 3 vertices of degree smaller than 4. In fact, a more general statement holds.

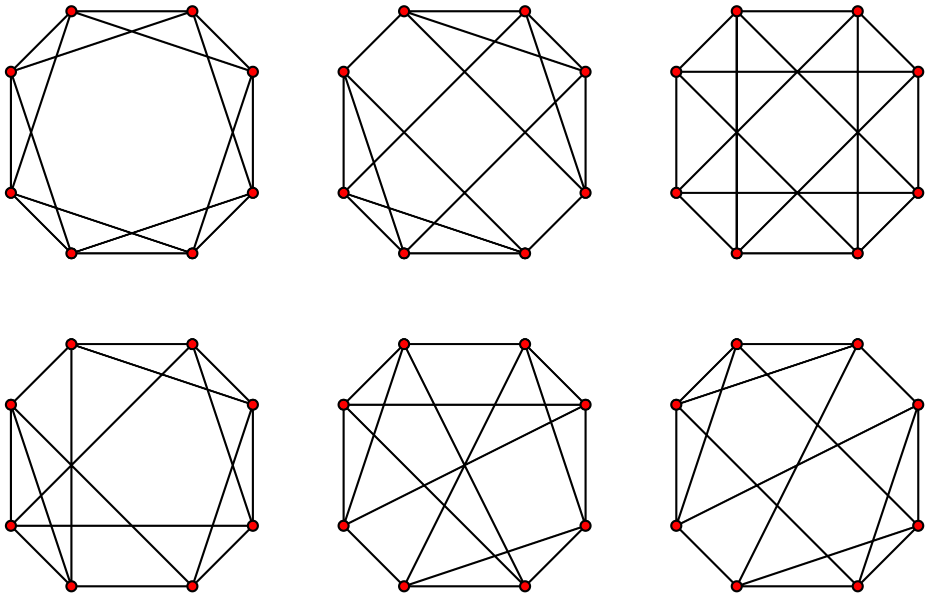

Figure 2: Extremal graphs for $n = 8$.

Observation 2.3. If G is a graph on n vertices with maximum degree Δ, $n \geq \Delta + 1$, and with the minimum possible value of Wiener index, then G contains at most $\Delta - 1$ vertices whose degree is strictly smaller than Δ, and these vertices induce a clique.

3 Prescribed degrees

As mentioned earlier, among n-vertex graphs with minimum degree at least 1, the maximum Wiener index is attained by P_n. But when restricting to minimum degree at least 2, the extremal graph is different. Observe that with the reasonable assumptions $\Delta \geq 2$ and $\delta \leq n - 1$, the following holds:

- $W(P_n) = \max\{W(G);\ G$ has maximum degree at most Δ and n vertices$\}$,
- $W(K_n) = \min\{W(G);\ G$ has minimum degree at least δ and n vertices$\}$.

Analogous reasons motivate the following two problems from [56].

Problem 3.1. What is the maximum Wiener index among n-vertex graphs with minimum degree at least δ?

Problem 3.2. What is the minimum Wiener index among n-vertex graphs with maximum degree at most Δ?

Both problems are still on the list of unsolved problems, but several results were obtained under additional requirements. Fischermann et al. [33], and independently Jelen and Trisch [44, 45] solved Problem 3.2 for trees. In addition, they determined the trees which maximize the Wiener index among all trees of given order whose vertices are either end-vertices or of maximum degree Δ.

Stevanović [73] solved Problem 3.1 for trees (where $\delta = 1$) under the assumption that the maximum degree is precisely Δ. Let $T_{n,\Delta}$ be the tree on n vertices obtained by taking a path on $n - \Delta + 1$ vertices and joining new $\Delta - 1$ vertices to one end-vertex of the path, see Figure 3.

Theorem 3.3. *For every n-vertex graph G with maximum degree $\Delta \geq 2$ it holds that $W(G) \leq W(T_{n,\Delta})$ with equality if and only if G is $T_{n,\Delta}$.*

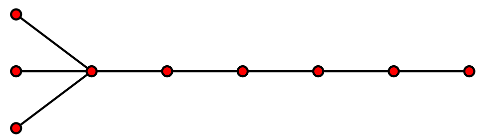

Figure 3: Graph $T_{9,4}$.

Dong and Zhou [29] determined the maximum Wiener index of unicyclic graphs with fixed maximum degree and they characterized the unique extremal graph.

Lin [62] characterized trees with the maximal Wiener index in the class of trees of order n with exactly k vertices of maximum degree, and proposed analogous problem for the minimum. The solution of this problem was recently presented by Božović et al. in [13]. The same authors considered a similar problem with a predetermined value of the maximum degree, i.e. they obtained the maximal value of Wiener index in the class of trees of order n with exactly k vertices of a given maximum degree and showed that the corresponding maximal trees are caterpillars with certain properties.

Recently Alochukwu and Dankelmann [4] obtained the following asymptotically sharp upper bound in terms of given minimum and maximum degree.

Theorem 3.4. *Let G be a graph of order n, minimum degree δ and maximum degree Δ. Then $W(G) \leq \binom{n-\Delta+\delta}{2}\frac{n+2\Delta}{\delta+1} + 2n(n-1)$, and this bound is sharp apart from an additive constant.*

Another interesting class of graphs with restrictions on degrees is the class of *regular graphs*, i.e. graphs for which $\Delta(G) = \delta(G)$. In general, introducing edges in a graph decreases the Wiener index, but in the class of r-regular graphs on n vertices the number of edges is fixed, therefore the following conjecture from [54] seems to be reasonable. The *diameter*, $\mathrm{diam}(G)$, of a graph G is the maximum distance between all pairs of vertices, i.e. $\mathrm{diam}(G) = \max\{d(u, v) |\ u, v \in V(G)\}$.

Conjecture 3.5. *Among all r-regular graphs on n vertices, the maximum Wiener index is attained by a graph with the maximum possible diameter.*

The above conjecture can be supported by the fact that in the case of trees, where the number of edges is fixed as well, the maximum Wiener index is attained by P_n which has the largest diameter. In fact, Chen et al. [18] recently proved that the conjecture is valid for $r = 3$. More precisely, they proved a conjecture from [54], that cubic graphs of the form L_n, presented in Figure 4, have maximum Wiener index among all cubic graphs of order n.

The minimum Wiener index in the class of trees is attained by S_n, which has the smallest diameter. A similar claim may hold for regular graphs [54].

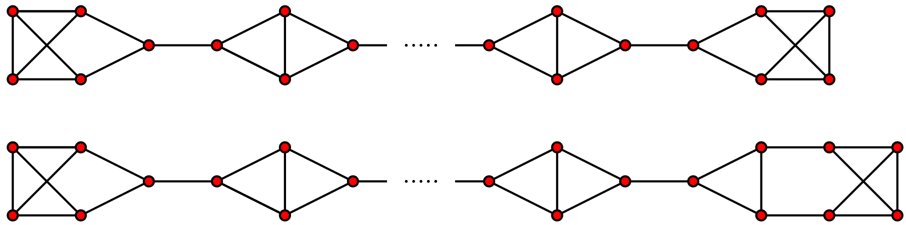

Figure 4: Graphs L_{4k+2} (above) and L_{4k+4} (below).

Conjecture 3.6. *Among all r-regular graphs on n vertices, the minimum Wiener index is attained by a graph with the minimum possible diameter.*

Finally, the following problem from [60] is of a special interest.

Problem 3.7. Find all k-regular graphs on n vertices with the smallest value of Wiener index.

As observed in [60], Problem 3.7 is surprisingly related to the cages and the following famous degree-diameter problem (see [66] for details).

Problem 3.8 (The degree-diameter problem)**.** Given positive integers d and k, find the largest possible number $n(d, k)$ of vertices in a graph of maximum degree d and diameter k.

Computer results in [60] (see also [65]) showed that among graphs with the minimum Wiener index there are graphs achieving $n(k, d)$ for pairs (k, d) from $\{(3, 2), (3, 3), (4, 2)\}$. There might appear graphs achieving $n(k, d)$ also for higher values of diameter d, but for those we could not search the space of k-regular graphs of order n exhaustively. Anyway, for higher diameters the graphs achieving $n(k, d)$ do not need to be those with the smallest Wiener index. Among extremal graphs found by a computer, $n(3, 2)$ and $n(3, 3)$ are realized by the well-known Petersen graph and the Flower snark J_5. Interestingly, there appears also the Heawood graph, which is the Cage$(3, 6)$, i.e., the smallest graph of degree 3 and girth 6, see [31].

The following conjectures were proposed in [60] (probably, it suffices to choose $n_k = k + 1$ therein).

Conjecture 3.9 (The even case conjecture)**.** *Let $k \geq 3$, and let n be large enough with respect to k, say $n \geq n_k$. Suppose that G is a graph on n vertices with the maximum degree k, and with the smallest possible value of Wiener index. If kn is even, then G is k-regular.*

Conjecture 3.10 (The odd case conjecture)**.** *Let $k \geq 3$, and let n be large enough with respect to k, say $n \geq n_k$. Suppose that G is a graph on n vertices with the maximum degree k, and with the smallest possible value of Wiener index. If kn is odd, then G has a unique vertex of degree smaller than k and in that case this smaller degree is $k - 1$.*

4 Wiener index of digraphs

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*. If uv is an arc in D, we say that

u *dominates* v. The *out-degree* $d^+(u)$ of a vertex $u \in V(D)$ is the number of its *out-neighbors*, i.e. the vertices, dominated by u. A *(directed) path* in D is a sequence of vertices $v_0, v_1, \ldots, v_k$ such that $v_{i-1}v_i$ is an arc of D for each $i \in \{1, 2, \ldots, k\}$, and by adding the arc v_kv_0 we obtain a *directed cycle*. An orientation of a graph G is said to be *acyclic* if it has no directed cycles. The *distance* $d(u, v)$ between vertices $u, v \in V(D)$ is the length of a shortest path from u to v. Notice that $d(u, v)$ is usually distinct from $d(v, u)$.

Early studies of Wiener index of digraphs were limited to *strongly connected* digraphs, i.e. digraphs in which a directed path between every pair of vertices exists. However, in the studies of real directed networks it is possible that there is no directed path connecting some pairs of vertices, thus the convention $d(u, v) = 0$ is used if there is no directed path from u to v [11, 12]. Under this assumption, in analogy to graphs, the Wiener index $W(D)$ of a digraph D is defined as the sum of all distances, where each ordered pair of vertices is taken into account. Hence,

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

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 a graph G. If an orientation of G achieves the minimum Wiener index $W_{\min}(G)$, we call this orientation a *minimum Wiener index orientation* of G.

Problem 4.1. For a given graph G find $W_{\max}(G)$ and $W_{\min}(G)$.

In [58] there was posed a question if it is NP-hard to find an orientation of a given graph which maximizes the Wiener index. Dankelmann [19] answered it affirmatively. Plesník [69] proved that finding a strongly connected orientation of a given graph G that minimizes the Wiener index is NP-hard too, but the case for non-necessarily strongly connected digraphs is unsolved [58] in general. However, it can be decided in polynomial time if a given graph with m edges has an orientation for which the Wiener index is precisely m (note that it cannot be less).

Problem 4.2. What is the complexity of finding $W_{\min}(G)$ for an input graph G?

The following conjecture from [58] remains unsolved as well, but it is known to hold for bipartite graphs, unicyclic graphs, the Petersen graph and prisms.

Conjecture 4.3. *For every graph G, the value $W_{\min}(G)$ is achieved by some acyclic orientation of G.*

In [67, 69] Plesník and Moon found strongly connected tournaments (orientations of K_n) with the maximum and the second maximum Wiener index. In [57] it was shown that the same tournaments solve the problem if we drop out the requirement that the digraph should be strongly connected. In the same paper oriented Θ-graphs are studied. By $\Theta_{a,b,c}$ we denote a graph obtained when two distinct vertices u_1 and u_2 are connected by three internally vertex-disjoint paths of lengths $a + 1$, $b + 1$ and $c + 1$, respectively, where $a \ge b \ge c$ and $b \ge 1$ (see Figure 5 where a non-strongly connected orientation of $\Theta_{3,2,1}$ is depicted). Although intuitively one may expect that $W_{\max}$ is attained for some strongly connected orientation, this is not the case. Namely, in [57] it is shown that the orientation of $\Theta_{a,b,c}$ which achieves the maximum Wiener index is not strongly connected if $c \ge 1$.

For strongly connected orientations of $\Theta_{a,b,c}$, it was shown that the maximum Wiener index is achieved by the one in which the union of the u_1, u_2-paths of lengths $a + 1$ and $b + 1$ forms a directed cycle. Li and Wu [61] confirmed the conjecture from [57], that the same holds if we drop the assumption that orientations are strongly connected.

Theorem 4.4. *Let $a \geq b \geq c$. Then $W_{\max}(\Theta_{a,b,c})$ is attained by an orientation of $\Theta_{a,b,c}$ in which the union of the paths of lengths $a + 1$ and $b + 1$ forms a directed cycle.*

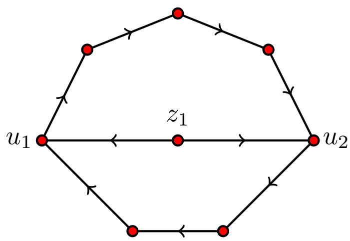

Figure 5: An orientation of $\Theta_{3,2,1}$.

However, the following conjecture remains open.

Conjecture 4.5. *Let G be a 2-connected chordal graph. Then $W_{\max}(G)$ is attained by an orientation which is strongly connected.*

Among digraphs on n vertices, the directed cycle $\overrightarrow{C}_n$ (in which all edges are directed in the same way, say clockwise) achieves the maximum Wiener index. In [55] digraphs with the second maximum Wiener index were investigated. In [58] the Wiener theorem was generalized to directed graphs, as well as a relation between the Wiener index and betweenness centrality.

An orientation of a graph G is called *k-coloring-induced*, if it is obtained from a proper k-coloring of G such that each edge is oriented from the end-vertex with the bigger color to the end-vertex with the smaller color. In [58] it was proved that graphs with at most one cycle and prisms attain the minimum Wiener index for k-coloring-induced orientation with k being the chromatic number $\chi(G)$. The same holds for bipartite graphs, complete graphs, Petersen graph and others. These observations lead to the conjecture that $W_{\min}(G)$ of an arbitrary graph is achieved for a $\chi(G)$-coloring-induced orientation, which Fang and Gao [32] showed to be false. They expressed the Wiener index of a digraph D as $W(D) = \sum_{u\in V(D)} w(u)$ where $w(u) = \sum_{v\in V(D)} d(u, v)$, and defined the notion of Wiener increment. For $u \in V(D)$ the *Wiener increment of u* is defined as $\Delta w(u) = w(u) - d^+(u)$. The *Wiener increment of D*, $\Delta W(D)$, is the sum of Wiener increments of all vertices of D. Fang and Gao observed that the comparison of Wiener indices of two different orientations of a graph is equal to the comparison of their Wiener increments. Using this observation they found that for the graph G in Figure 6, $W_{\min}(G)$ cannot be achieved for any $\chi(G)$-coloring-induced orientation of G, and this is not the only counterexample. Moreover, their investigations lead them to pose the following two conjectures.

Conjecture 4.6. *For any given constant $k \geq 3$, there exists a 3-colorable graph G such that any minimum Wiener index orientation of G has a directed path of length k.*

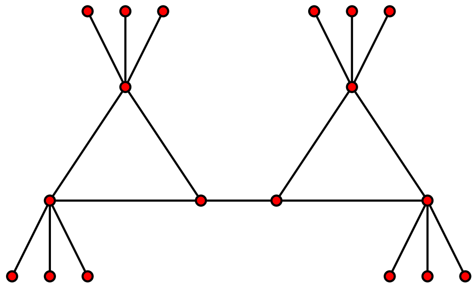

Figure 6: A graph G, for which $W_{\min}(G)$ is not achieved for any $\chi(G)$-coloring-induced orientation of G.

Conjecture 4.7. *For any given constant $k \geq 3$, there exists a 3-colorable graph G such that $W_{\min}(G)$ cannot be achieved by any k-coloring-induced orientation.*

Figure 7: A no-zig-zag path (left) and a zig-zag path (right) on six vertices.

In [58] orientations of trees with the maximum Wiener index were considered. An orientation of a tree is called *zig-zag* if there is a subpath in which edges change the orientation twice. If an orientation is not zig-zag, it is *no-zig-zag*, see Figure 7. A different view on no-zig-zag trees can be described as follows. A vertex v in a directed tree T is *core*, if for every vertex u of T there exists either a directed path from u to v or a directed path from v to u, see Figure 8. 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.

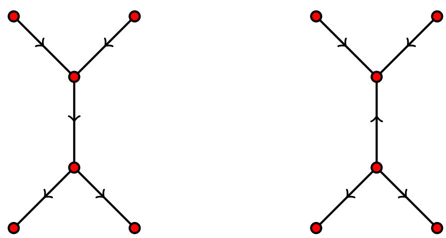

Figure 8: The graph on the left-hand side has two core vertices, while the right-hand side one has no core vertex.

In [58] the following conjecture was proposed.

Conjecture 4.8. *Let T be a tree. Then every orientation of T achieving the maximum Wiener index is no-zig-zag (i.e. has a core vertex).*

It was supported by showing that it holds for trees on at most 10 vertices, subdivision of stars, and trees constructed from two stars whose central vertices are connected by a path. Furthermore, since it is reasonable to expect that an orientation of a tree maximizing the Wiener index also maximizes the number of pairs of vertices (u, v) between which there exists a path, Conjecture 4.8 is supported also by a result of Henning and Oellermann [39]. They proved that if T is a tree and D is an orientation of T that maximizes the number of ordered pairs (u, v) of vertices of D for which there exists a (u, v)-path in D, then D contains a core vertex. However, Li and Wu [61] constructed a tree of order 85 contradicting Conjecture 4.8. Independently, Dankelmann [19] found an infinite family of counter-examples. For $k \in \mathbb{N}$, where k is a multiple of 3, let T_k be the tree obtained from a path of order k with vertices $w_1, w_2, \dots, w_k$, by connecting vertices $u_1, u_2, \dots, u_{k^2/9}$ to w_1, connecting x_1 from the path $x_1x_2x_3x_4x_5$ to w_2, and a single vertex y_1 to w_3. Now let D_k be the orientation of T_k such the edges of the path $w_1w_2 \dots w_k$ are oriented towards w_k, each edge u_iw_1 is oriented towards w_1, the edges of the path $x_1x_2x_3x_4x_5$ are oriented towards x_5, and the edge y_1w_3 is oriented towards w_3, see Figure 9 for an example. Observe that the edges of the (x_5, y_1)-path change their direction twice as the path is traversed, thus D_k is a zig-zag orientation. Dankelmann proved that if k is sufficiently large, then D_k and its converse (i.e., a digraph obtained by reversing the direction of every arc in D_k) are the only orientations of T_k that maximize the Wiener index, which contradicts Conjecture 4.8.

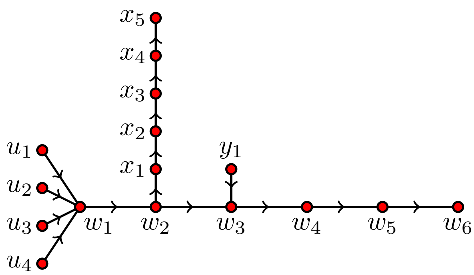

Figure 9: A no-zig-zag tree T_6.

The Cartesian product $P_m \Box P_n$ of paths on m and n vertices, respectively, is called the *grid* and is denoted by $G_{m,n}$. If $m = 2$, it is a called the ladder graph L_n. Kraner Šumenjak et al. [75] proved a conjecture from [59] by showing that the maximum Wiener index of a digraph whose underlying graph is L_n is $(8n^3 + 3n^2 - 5n + 6)/3$, and is obtained for the orientation presented in Figure 10. In addition, they proved a lower bound for $W_{\max}(G \Box H)$ for general graphs G and H, and posed a question regarding its sharpness. Let $\tau(G) = \sum_{x \in V(G)} \sigma(x)$, where $\sigma(x)$ denotes the number of vertices $x' \in V(G)$ for which there is a path from x to x' in G.

Theorem 4.9. *For any graphs G and H,*

$$W_{\max}(G \Box H) \geq W_{\max}(G)\tau(H) + W_{\max}(H)|V(G)|^2.$$

Problem 4.10. Is the bound given in Theorem 4.9 sharp? Find a sharp lower bound.

Another problem from [75] concerns a comparison of the maximum Wiener index of an orientation of G with the Wiener index of the undirected graph G.

Problem 4.11. Find functions f and g so that $f(W(G)) \leq W_{\max}(G) \leq g(W(G))$ for all graphs G. In particular, can f and g be linear functions?

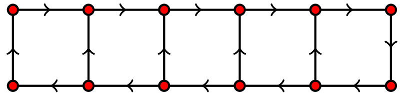

Figure 10: An orientation of the ladder $P_6 \Box P_2$ with the maximum Wiener index.

Note that the orientation of L_n in Figure 10 is obtained when all layers isomorphic to one factor are directed paths directed in the same way, except one which is a directed path directed in the opposite way. Kraner Šumenjak et al. considered the following natural generalization of this orientation to general grids. 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 the left graph in Figure 11.

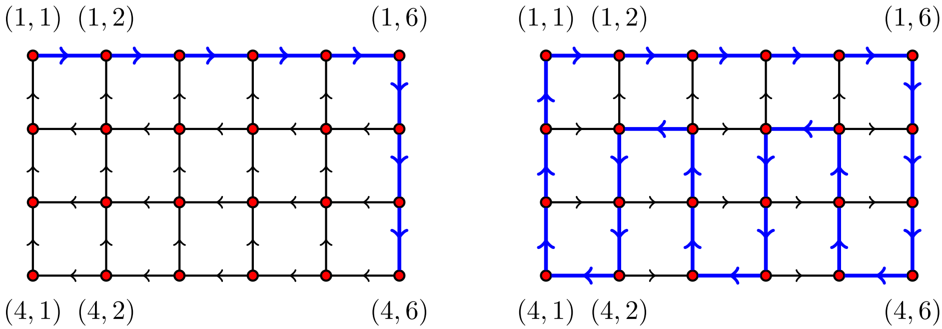

Figure 11: Two orientations, $D_{4,6}$ (left) and $C_{4,6}$ (right), of $P_4 \Box P_6$.

The authors of [75] conjectured that for every $m, n \geq 2$, it holds $W_{\max}(G_{m,n}) = W(D_{m,n})$. However, it turns out that a comb-like orientation has significantly bigger Wiener index. 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 the right graph in Figure 11. Moreover, the other edges are directed in such a way that they do not shorten directed blue path starting at the vertex $(1, 1)$. Of course, $C_{m,n}$ exists only if n is even. In [53] it was shown that if $n \geq 4$ is even, and $m \geq 3$, then $W(C_{m,n}) > W(D_{m,n})$, and further observations led the authors to the following problem.

Problem 4.12. Find the biggest possible constant c, such that $W_{\max}(G_{m,n}) \geq c(mn)^3 + o\big((mn)^3\big)$.

To sum up, the following is still open.

Problem 4.13. Find an orientation of $G_{m,n}$ with the maximum Wiener index.

The authors think the above problem might be difficult as the extremal graphs in the cases $m = 3$ and $n \in \{4, 5, 6\}$ do not have any obvious simple property, but they are strongly connected. Thus they ask the following.

Question 4.14. Let $M_{m,n}$ be an orientation of $G_{m,n}$ with the maximum Wiener index. Is $M_{m,n}$ strongly connected?

5 Maximum Winer index of graphs with prescribed diameter

Recall that the *eccentricity* of a vertex in a connected graph G is the maximum distance between this vertex and any other vertex of G, and the maximum eccentricity is the graph *diameter*. Similarly, the *radius* of G, denoted by $\mathrm{rad}(G)$, is the minimum graph eccentricity. In 1984 Plesník identified graphs as well as digraphs with a given diameter that minimize the Wiener index (see also [14] for a recent alternative proof), and posed the opposite problem regarding the maximum [69].

Problem 5.1. What is the maximum Wiener index among graphs of order n and diameter d?

In general this question remains unsolved, but there has been progress and important results were obtained. First, Wang and Guo [79] determined the trees with maximum Wiener index among trees of order n and diameter d for some special values of d, $2 \leq d \leq 4$ or $n-3 \leq d \leq n-1$. Mukwembi and Vetrík [68] independently considered trees with the diameter up to 6 and gave asymptotically sharp upper bounds.

DeLaViña and Waller [22] posed a conjecture with additional restrictions in Problem 5.1.

Conjecture 5.2. *Let G be a graph with diameter $d > 2$ and order $2d+1$. Then $W(G) \leq W(C_{2d+1})$, where C_{2d+1} denotes the cycle of length $2d+1$.*

Sun et al. [76] considered general small-diameter and large-diameter graphs. They observed that if G is a graph on n vertices with diameter equal to 2, then the maximum Wiener index is attained by the star S_n. For diameter 3 they proposed a conjecture, that the extremal graph is isomorphic to K_n^c, which is a graph of order n that consists of a complete graph on c vertices and has the rest of the vertices attached to these c vertices as uniformly as possible (meaning that each of the c vertices of the complete graph has either $\lfloor (n-c)/c \rfloor$ or $\lceil (n-c)/c \rceil$ pendant vertices attached, see Figure 12 where K_4^{15} is depicted.

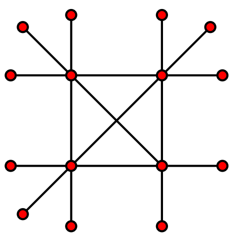

Figure 12: The graph K_4^{15}.

Conjecture 5.3. *Let G be a graph on n vertices with diameter equal to 3. Then $W(G) \leq W(K_n^c)$ where $c = \left\lfloor \sqrt{\frac{n^2}{2(n-1)}} \right\rfloor$ or $c = \left\lceil \sqrt{\frac{n^2}{2(n-1)}} \right\rceil$.*

To explain the results pertaining to trees and a conjecure on general graphs with diameter 4, we need the following definition. Let $k = \lfloor \sqrt{n-1} \rfloor$. For $k^2 + k \geq n-1$ we denote by T_n the rooted tree on n vertices in which the root has degree k, $n-k^2-1$ of its neighbours are of degree $k+1$ and the rest of them of degree k. When $k^2+k \leq n-1$ let T_n' denote the rooted tree on n vertices in which the root has degree $k+1$, $n-k^2-k-1$

of its neighbours are of degree $k+1$ and the rest of them of degree k. Wang and Guo [79] gave a complete description of trees with diameter 4 that maximize the Wiener index.

Theorem 5.4. *Let T be a tree on n vertices with diameter 4 and let $k = \lfloor \sqrt{n-1} \rfloor$. Then the following holds:*

- *if $k^2 + k > n-1$, then $W(T) \leq W(T_n)$, with equality holding only when $T \cong T_n$;*
- *if $k^2 + k < n-1$, then $W(T) \leq W(T'_n)$, with equality holding only when $T \cong T'_n$;*
- *if $k^2 + k = n-1$, then $W(T) \leq W(T_n) = W(T'_n)$, with equality holding only when $T \cong T_n$ or $T \cong T'_n$.*

The authors of [76] suspect that the extremal graphs from the theorem above are extremal also for general graphs.

Conjecture 5.5. *The trees T_n and T'_n remain the unique optima in the class of graphs of diameter 4 on n vertices as it is described in* Theorem 5.4 *with the only exception of $n = 9$, in which case C_9 is also an optimal graph.*

An interested reader is referred to [76] for computer results supporting Conjectures 5.2, 5.3 and 5.5. The role of extremal graphs in the case of large-diameter graphs play the so called *double brooms* $D(n, a, b)$, i.e. graphs consisting of a path on $n - a - b$ vertices together with a leaves adjacent to one of its end-vertices and b leaves adjacent to the other end-vertex (see Figure 13 for an example).

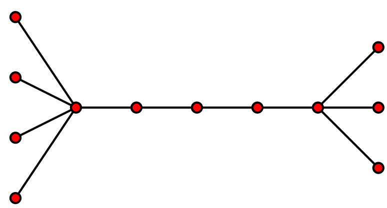

Figure 13: Double broom $D(12, 4, 3)$.

Theorem 5.6. *Let G be a graph of order n and diameter $n - c$, where $c \geq 1$ is a constant and n is large enough relative to c. Then $W(G) \leq W(D(n, \lfloor (c+1)/2 \rfloor, \lceil (c+1)/2 \rceil))$ with equality if and only if $G \cong D(n, \lfloor (c+1)/2 \rfloor, \lceil (c+1)/2 \rceil)$.*

Further details on diameters $n-3$ and $n-4$ can be found in [76]. A different approach to Problem 5.1 was recently used by Cambie [14] who gave asymptotically sharp upper bounds for Wiener index. As the main first step towards the proof of his result he constructed an almost extremal graph, in which there are many pairs of vertices which are of distance d from each other. This is achieved by having many subtrees with many leaves, and, when the diameter is even, combining them into one tree. When the diameter is odd, a central clique is used so that the distance between leaves of different subtrees are of distance d. Now if we take two vertices at random, the probability that both vertices are leaves is large since the number of leaves is large. Similarly, since we have many subtrees, the probability that both leaves are in different subtrees is large. Hence the probability that two vertices are at maximal distance is large, implying that the average distance is close to d. The above is a foundation of the following asymptotic solution to the problem of Plesník.

Theorem 5.7. *There exist positive constants c_1 and c_2 such that for any $d \geq 3$ the following holds. The maximum Wiener index among all graphs of diameter d and order n is between $d - c_1 \frac{d^{3/2}}{\sqrt{n}}$ and $d - c_2 \frac{d^{3/2}}{\sqrt{n}}$, i.e. it is of the form $d - \Theta\left(\frac{d^{3/2}}{\sqrt{n}}\right)$.*

In addition, Cambie [14] gives slightly stronger upper bound for trees, by which he extends a result of Mukwembi and Vetrík [68]. Moreover, the results he obtained lead him to the following question.

Question 5.8. For even d and large n, are the graphs of order n and diameter d with the largest Wiener index all trees?

Digraphs were considered in [14] as well, where the problem of Plesník is solved exactly if the order is large comparing to the diameter. For the sake of completeness we also mention that trees of order n and diameter d with the minimum Wiener index were presented in [63].

Having in mind the close relationship between the diameter and the radius of a connected graph, $\operatorname{rad}(G) \leq \operatorname{diam}(G) \leq 2\operatorname{rad}(G)$, it is natural to consider the above problems with radius instead of diameter. Chen et al. [17] posed the following question.

Problem 5.9. What is the maximum Wiener index among graphs of order n and radius r?

They succeeded to characterize graphs with the maximum Wiener index among all graphs of order n with radius 2. Das and Nadjafi-Arani [21] gave an upper bound on Wiener index of trees and graphs in terms of number of vertices n and radius r. In addition, they presented an upper bound on the Wiener index in terms of order, radius and maximum degree of trees and of graphs. The authors concluded that these results are not enough to solve Problem 5.9. Stevanović et al. [74] provide examples obtained by computer experiments, which suggest that a simple characterization of the structure of trees with maximum Wiener index among trees with a given number of vertices and radius will probably be out of our reach in some foreseeable future.

Analogous problem for the minimum Wiener index was posed by You and Liu [84].

Problem 5.10. What is the minimum Wiener index among all graphs of order n and radius r?

If $r \in \{1, 2\}$, the extremal graphs attaining the minimum total distance among all graphs of order n are easily characterized: they are complete graphs when $r = 1$, complete graphs minus a maximum matching when $r = 2$ and n is even, and complete graphs minus a maximum matching and an additional edge adjacent to the vertex not in the maximum matching, when $r = 2$ and n is odd.

A conjecture for $n \geq 3$ was posed by Chen et al. [17]. The notation $G_{n,r,s}$, where n, r and s are positive integers such that $n \geq 2r$, $r \geq 3$, and $n - 2r + 1 \geq s \geq 1$, stands for the graph obtained in the following way: let v_1, v_2, v_3 and v_4 be four consecutive vertices on a $2r$-cycle. Replace v_2 with a clique of order s, replace v_3 with a clique of order $n-2r+2-s$, join each vertex of one clique to all vertices of the other clique, join v_1 to all vertices of K_s, and join v_4 to all vertices of $K_{n-2r+2-s}$. Notice that the resulting graph has n vertices and radius r, and $W(G_{n,r,s}) = W(G_{n,r,s'})$ for any $s, s' \in \{1, \dots, r-1\}$.

Conjecture 5.11. *Let n and r be two positive integers with $n \geq 2r$ and $r \geq 3$. For any graph G of order n with radius r, $W(G) \geq W(G_{n,r,1})$. Equality is attained if and only if $G = G_{n,r,s}$ for $s \in \{1, \dots, r-1\}$.*

Cambie showed that the hypercube Q_3 is a counterexample to the above conjecture, so it does not hold when n is small, but he demonstrated that the conjecture is true asymptotically, i.e. if the order is sufficiently large compared to the radius [15].

Theorem 5.12. *For any $r \geq 3$, there exists a value $n_1(r)$ such that for all $n \geq n_1(r)$ it holds that any graph G of order n with radius r satisfies $W(G) \geq W(G_{n,r,1})$. Equality holds if and only if $G = G_{n,r,s}$ for $s \in \{1, \ldots, r-1\}$.*

We refer to [15] for an analog of this result for directed graphs, and to [69] for a characterization of digraphs of given order and diameter with the minimum Wiener index.

6 Šoltés problem and its relaxed variations

An interesting question regarding the Wiener index is to study how Wiener index is affected by small changes in a graph. Clearly, by removing an edge Wiener index is increased. On the other hand, the effect of deleting a vertex is far from obvious, and it was first studied by Šoltés. In his paper from 1991, Šoltés posed the following problem [71].

Problem 6.1. Find all graphs G in which the equality $W(G) = W(G - v)$ holds for all $v \in V(G)$.

Therefore, if for a vertex v in a graph G it holds that $W(G) = W(G - v)$, we say that v satisfies the *Šoltés property* in G, and a graph in which every vertex satisfies the Šoltés property is referred to as a *Šoltés graph*. The only known Šoltés graph so far is the cycle on 11 vertices. The above problem appears to be difficult, thus in subsequent studies relaxed variations were considered. The authors of [50] showed that the class of graphs for which the Wiener index does not change when a particular vertex is removed is rich, even when restricted to unicyclic graphs with fixed length of the cycle. More precisely:

- there is a unicyclic graph G on n vertices containing a vertex v with $W(G) = W(G-v)$ if and only if $n \geq 9$;
- there is a unicyclic graph G with a cycle of length c and a vertex satisfying the Šoltés property if and only if $c \geq 5$;
- for every graph G there are infinitely many graphs H such that G is an induced subgraph of H and $W(H) = W(H - v)$ for some $v \in V(H) \setminus V(G)$.

If a vertex v has degree 1 in G, then clearly $W(G) > W(G - v)$. In the construction of the above mentioned infinite class of graphs G with a vertex v satisfying the Šoltés property the vertex v is of degree 2. In [49] the authors extended their research to graphs in which v is of arbitrary degree. They showed that for a fixed positive integer $k \geq 2$ there exist infinitely many graphs G with a vertex v such that $\deg_G(v) = k$ and $W(G) = W(G-v)$. Moreover, if $n \geq 7$, there exists an n-vertex graph G with a vertex v so that $\deg_G(v) = n - 2$ or $\deg_G(v) = n - 1$, and $W(G) = W(G - v)$. By proving the next theorem they showed that dense graphs cannot be a solution of Problem 6.1.

Theorem 6.2. *If G is an n-vertex graph for which $\delta(G) \geq n/2$, then $W(G) \neq W(G - v)$ for every $v \in V(G)$.*

In the results above, removal of one vertex only was considered. So the authors proposed the study of graphs G in which a given number of vertices satisfying the Šoltés property exist [49, 51].

Problem 6.3. For a given k, find (infinitely many) graphs G for which $W(G) = W(G - v_1) = W(G - v_2) = \cdots = W(G - v_k)$ for some distinct vertices $v_1, \dots, v_k$ in G.

This problem was considered by Bok et al. [9, 10] who showed the existence of:

- infinitely many *cactus graphs* (i.e. graphs in which every edge belongs to at most one cycle) with exactly k cycles of length at least 7 that contain exactly $2k$ vertices satisfying the Šoltés property; and
- infinitely many cactus graphs with exactly k cycles of length $c \in \{5, 6\}$ that contain exactly k vertices satisfying the Šoltés property.

In addition, they proved that G contains no vertex with the Šoltés property if the length of the longest cycle in G is at most 4. Another infinite family of graphs satisfying the condition from Problem 6.3 was constructed by Hu et al. [43]. Furthermore, Hu et al. settled another problem from [49, 51] by proving that for any $k \geq 2$, there exist infinitely many graphs G such that $W(G) = W(G - \{v_1, v_2, \dots, v_k\})$ for some distinct vertices $v_1, v_2, \dots, v_k \in V(G)$.

Akhmejanova et. al [1] considered a relaxation of the original Šoltés problem from another point of view. They asked for graphs with a large proportion of vertices satisfying the Šoltés property. More precisely, they defined the function $\Delta_v(G) = W(G) - W(G - v)$. Then

$$\frac{|\{v \in V(G); \Delta_v(G) = 0\}|}{|V(G)|}$$

is the proportion of vertices satisfying the Šoltés property. So Akhmejanova et. al asked the following.

Problem 6.4. For a fixed $\alpha \in (0, 1]$ construct an infinite series S of graphs such that for all $G = (V(G), E(G))$ from S the following holds:

$$\frac{|\{v \in V(G); \Delta_v(G) = 0\}|}{|V(G)|} \geq \alpha.$$

Note that a solution to this problem for $\alpha = 1$ would give an infinite series of solutions to Problem 6.1. The authors noted that a slight modification of a construction from [9] yields an infinite series of graphs with the proportion of vertices satisfying the Šoltés property tending to $\frac{1}{3}$, and improved this constant by finding another two constructions. The first construction contains many 11-cycles as induced subgraphs: given $k \in \mathbb{N}, k > 1$, they defined a graph $B(k)$ on $5k + 6$ vertices by taking two vertices and connecting them with k distinct paths of length 6 and one path of length 5. It turns out that for $B(k)$ the proportion of vertices satisfying the Šoltés property equals $\frac{2k}{5k+6}$, thus this proportion tends to $\frac{2}{5}$ as k tends to infinity. Another construction of so called lily-shaped graphs involves graphs that are not 2-connected and whose proportion tends to $\frac{1}{2}$, see [1] for details. Furthermore, the authors found a graph with the proportion $\frac{2}{3}$ and expect that there exist an infinite series of graphs with a proportion $\alpha > \frac{1}{2}$, or perhaps even α tending to 1. Furthermore, they propose the following problems.

Problem 6.5. For a fixed $z \in \mathbb{Z}$, find all graphs G, for which the equality $W(G) - W(G - v) = z$ holds for all vertices v.

Problem 6.6. For a fixed $z \in \mathbb{Z}$ and $\alpha \in (0, 1]$, construct an infinite series S of graphs such that for all $G = (V(G), E(G))$ from S the following inequality takes place:

$$\frac{|\{v \in V(G); \Delta_v(G) = z\}|}{|V(G)|} \geq \alpha.$$

In [49, 51] the problem of finding k-regular connected graphs G other than C_{11} for which the equality $W(G) = W(G - v)$ holds for at least one vertex $v \in V(G)$ was posed. The answer is affirmative, see Figure 14 for 3-regular and 4-regular graphs with 4 and 2, respectively, (blue) vertices satisfying the Šoltés property. Using computer software and counting cubic graphs of orders $n \leq 26$, Bašić et al. [5] found that cubic graphs of order 12 or less do not contain Šoltés vertices. Cubic graphs with two Šoltés vertices first appear at the order 14 (there are three such graphs), and examples with three and four Šoltés vertices appear at the order 16. Moreover, they proved the following.

Theorem 6.7. *There exist infinitely many cubic* 2*-connected graphs which contain two Šoltés vertices.*

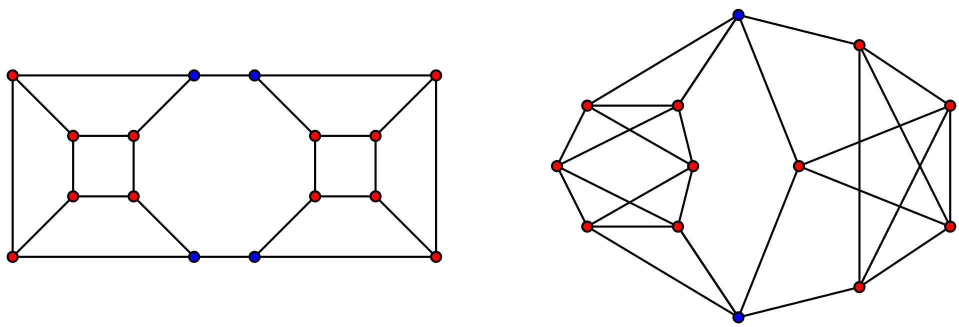

Figure 14: Regular graphs with blue vertices satisfying the Šoltés property.

In the same paper, graphs where the ratio between the number of Šoltés vertices and the order of the graph is at least α are called α-Šoltés graphs. So Problem 6.1 asks to find all 1-Šoltés graphs. The authors believe the solution to this problem should be graphs having all vertices of the same degree.

Conjecture 6.8. *If G is a Šoltés graph, then it is regular.*

For a general regular graph G, the values $W(G - u)$ and $W(G - v)$ might be significantly different for two different vertices u and v from G. It may happen that removal of one vertex increases the Wiener index, while removal of the other vertex descreases it. However, $W(G - u)$ and $W(G - v)$ are equal if vertices u and v belong to the same vertex orbit. This led the authors to believe the following.

Conjecture 6.9. *If G is a Šoltés graph, then G is vertex-transitive.*

Further, the authors report that a computer search on publicly available collections of vertex-transitive graphs did not reveal any 1-Šoltés graphs. All examples of $\frac{1}{3}$-Šoltés graphs are obtained by truncating certain cubic vertex-transitive graphs, and there are no Šoltés graphs among vertex-transitive graphs with less than 48 vertices. Recall that if v is a vertex of degree 3 adjacent to u_1, u_2 and u_3, then by *truncation* of v we mean the replacement of v by a triangle $v_1v_2v_3$, where v_i is adjacent to u_i, and by truncation of a cubic graph we mean the truncation of all its vertices. Therefore it is reasonable to consider the following conjectures and a problem.

Conjecture 6.10. *If G is a Šoltés graph, then G is a Cayley graph.*

Problem 6.11. Find an infinite family of cubic vertex-transitive graphs $\{G_i\}_{i=1}^{\infty}$, such that the truncation of G_i is a $\frac{1}{3}$-Šoltés graph for all $i \geq 1$.

Conjecture 6.12. *The cycle on eleven vertices is the only Šoltés graph.*

7 Wiener index of signed graphs

A *signed graph* is a pair (G, σ) where G is a graph and σ is a function from $E(G)$ to $\{-1, 1\}$, called a *signature function* (also called *signing* in the literature). A path P is a uv*-path* if its end-vertices are u and v. If P is a path in G and σ is a signature function of G then the notation $\sigma(P)$ stands for the sum $\sum_{e \in P} \sigma(e)$. For $u, v \in V(G)$ the *signed distance* $d_{G,\sigma}(u, v)$ equals $\min_P |\sigma(P)|$ where the minimum ranges over all uv-paths P. Spiro [72] recently introduced the Wiener index $W_\sigma(G)$ of the signed graph (G, σ) as

$$W_\sigma(G) = \sum_{\{u,v\} \subseteq V(G)} d_{G,\sigma}(u, v).$$

If σ is a constant function, then $d_{G,\sigma}(u, v) = d(u, v)$, and therefore $W_\sigma(G) = W(G)$. In particular, if $W(G) = W(G - v)$ for all $v \in V(G)$, then there exists a (constant) signature function σ of G such that $W_\sigma(G) = W_\sigma(G - v)$. In this sense the problem of finding signed graphs (G, σ) with $W_\sigma(G) = W_\sigma(G - v)$ can be viewed as a relaxation of Šoltés problem. Note that in the signed setting, it is possible to have $W_\sigma(G) = 0$. Spiro used this fact to provide many examples of signed graphs satisfying $W_\sigma(G) = W_\sigma(G - v)$ for all $v \in V(G)$, and even with $W_\sigma(G) = W_\sigma(G - S)$ for any set S of size less than some value k. To present his results, a signature function σ of a graph G is called k*-canceling* if for any set $S \subseteq V(G)$ of size less than k, we have $W_\sigma(G - S) = 0$. A graph G is k*-canceling* if there exists a k-canceling signature function σ of G, and graphs with $W_\sigma(G) = 0$ are simply referred to as *canceling graphs*. For instance, a complete graph K_n is k-canceling if $n \geq 2k + 4$. Furthermore, he proved the following.

Proposition 7.1. *Let G' be a bipartite graph with partite sets U and V, where $|U|, |V| \geq k + 2$, and minimum degree at least $k + 1$. Let G be the graph obtained from G' by adding every edge between two vertices of U and every edge between two vertices of V. Then G is k-canceling.*

Another family of examples is obtained from the blowups of odd cycles: if G is a graph on $\{v_1, \ldots, v_t\}$, then the $\{n_1, \ldots, n_t\}$*-blowup* of G is defined to be the t-partite graph on sets $V_1, \ldots V_t$ with $|V_i| = n_i$ and with $u \in V_i$ and $w \in V_j$ adjacent if and only if v_i, v_j are adjacent in G.

Proposition 7.2. *Let G be the $(n_1, \ldots, n_{2t+1})$-blowup of a cycle C_{2t+1} with $t \geq 1$. If $n_i \geq 2k$ for all i, then G is k-canceling.*

Furthermore, the following holds.

Theorem 7.3. *If n is sufficiently large and G is an n-vertex graph with minimum degree at least $\frac{2n}{3}$, then there exists a signature function σ of G such that $W_\sigma(G) = W_\sigma(G - v) = 0$ for all $v \in V(G)$.*

For necessary conditions for a graph to be canceling and several interesting open questions we refer to [72]. One of the conjectures pertains to the well known fact that in the class of n-vertex trees the star S_n and the path P_n are extremal graphs for the Wiener index. Let (T, σ) be a signed n-vertex tree and let $+$ be the constant signature function that assigns $+1$ to every edge of P_n. Then the fact that $W_\sigma(T) \leq W_+(P_n)$ follows from the result for the classical Wiener index since $W_+(P_n) = W(P_n)$. It remains to prove the lower bound.

Conjecture 7.4. *If (T, σ) is a signed n-vertex tree, then*

$$W_\alpha(P_n) \leq W_\sigma(T),$$

where α is the alternating signature function which assigns the first edge of the path $+1$, the second -1, the third $+1$, and so on.

Another possible direction for future study according to Spiro is the *minimum signed Wiener index* $W_*(G) = \min_\sigma(G)$, where the minimum ranges over all signature functions σ of G. Note that this concept is analogous to the minimum digraph Wiener index of all orientations of a graph G presented in Section 4. Spiro proposed a conjecture in which double stars appear as extremal graphs; a *double star* is a tree T in which there exist vertices $x, y \in V(T)$ such that every edge of T has at least one of the vertices x, y as an end-vertex. Note that by this definition a star is also a double star.

Conjecture 7.5. *If T is an n-vertex tree, then*

$$W_*(P_n) \leq W_*(T) \leq \max_{D \in \mathcal{D}} W_*(D),$$

where $\mathcal{D}$ is the set of all n-vertex double stars.

The conjecture was verified for $n \leq 9$, and noted that it is false if one considers stars instead of double stars. We refer to [72] for more interesting questions related to the presented topic.

8 Variable Wiener index vs. variable Szeged index

For an edge uv in a graph, let $n_v(u)$ denote the number of vertices strictly closer to u than v, and analogously, let $n_u(v)$ be the number of vertices strictly closer to v than u. In his original paper [80] Wiener observed that the Wiener index of a tree can be computed as the sum of products $n_v(u) \cdot n_u(v)$ over all edges uv in the tree, but this is not the case in general graphs, owing to the fact that shortest paths are typically not unique. By relaxing the condition that the graph is a tree, the Szeged index of a graph G was defined in [34, 46] as

$$\mathrm{Sz}(G) = \sum_{uv \in E(G)} n_v(u) \cdot n_u(v).$$

Klavžar et al. [47] proved that $\mathrm{Sz}(G) \geq W(G)$ for every graph G, and in [25] all graphs for which the equality holds were classified.

Theorem 8.1. *For every graph G we have $\mathrm{Sz}(G) \geq W(G)$, and equality holds if and only if every block of G is a complete graph.*

The *variable Wiener index* (also known as the *generalized Wiener index*) of a graph G is defined as

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

and the *variable Szeged index* of a graph G is

$$\mathrm{Sz}^\alpha(G) = \sum_{uv \in E(G)} \left(n_v(u) \cdot n_u(v)\right)^\alpha .$$

Note that in [38] the quantity $\sum_{uv \in E(T)} \left(n_v(u) \cdot n_u(v)\right)^\alpha$ was named as the *variable Wiener index for trees*, but referring to it as the *variable Szeged index* seems to be more natural. By Theorem 8.1, for trees it holds $W(T) = \mathrm{Sz}(T)$. Using Karamata's inequality Hriňáková et al. [42] proved the following statement.

Theorem 8.2. *Let T be a tree on n vertices. Then*

(1) $W^\alpha(T) \leq \mathrm{Sz}^\alpha(T)$ *if* $\alpha > 1$,

(2) $W^\alpha(T) \geq \mathrm{Sz}^\alpha(T)$ *if* $0 \leq \alpha < 1$.

Moreover, equalities hold if and only if $n = 2$.

In the case when $\alpha > 1$, they extended this result to the class of bipartite graphs.

Theorem 8.3. *Let G be a bipartite graph on n vertices and $\alpha > 1$. Then $W^\alpha(G) \leq \mathrm{Sz}^\alpha(G)$ with equality if and only if $n = 2$.*

If G is a complete graph, we have $\mathrm{Sz}^\alpha(G) = \binom{|V(G)|}{2} = W^\alpha(G)$ for every α. Note that α is non-negative in the above results. If $\alpha < 0$ then for non-complete graphs we have the following strict inequality [42].

Proposition 8.4. *Let G be a non-complete graph. Then for every $\alpha < 0$ we have $\mathrm{Sz}^\alpha(G) < W^\alpha(G)$.*

Based on Theorem 8.2 and examples provided in [42], Hriňáková et al. proposed the following conjecture.

Conjecture 8.5. *For every non-complete graph G there is a constant $\alpha_G \in (0,1]$ such that*

$$\begin{aligned} \mathrm{Sz}^\alpha(G) &> W^\alpha(G), \text{ if } \alpha > \alpha_G, \\ \mathrm{Sz}^\alpha(G) &= W^\alpha(G), \text{ if } \alpha = \alpha_G, \\ \mathrm{Sz}^\alpha(G) &< W^\alpha(G), \text{ if } 0 \leq \alpha < \alpha_G. \end{aligned}$$

In other words, the conjecture states that for any non-complete graph there is a critical exponent in $(0,1]$, below which the variable Wiener index is larger and above which the variable Szeged index is larger. As seen above, this holds for trees. However, Cambie and Haslegrave [16] found infinitely many counterexamples by constructing a family of graphs $G_{k,\ell}$ as follows: take a complete graph K_k, remove a k-cycle from it, and connect all its vertices with one end-vertex of a path of length l, see Figure 15 where $G_{8,3}$ is depicted. By fixing a connected non-complete graph G, $h(\alpha) = Sz^{\alpha}(G) - W^{\alpha}(G)$ is a continuous function with $h(0) < 0$ and $h(1) \geq 0$, which by intermediate value theorem implies that there is at least one value of α for which $h(\alpha) = 0$, and at least one such value lies in $(0, 1]$. Therefore Conjecture 8.5 is equivalent to α being unique, which is not the case for many graphs of the form $G_{k,\ell}$. It turns out that if k is reasonably large, then there exist some corresponding values of ℓ having three values of α for which $Sz^{\alpha}(G_{k,\ell}) - W^{\alpha}(G_{k,\ell})$ equals 0.

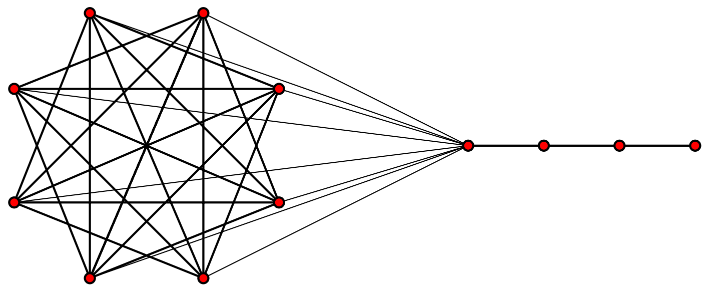

Figure 15: The graph $G_{k,\ell}$ for $k = 8$ and $\ell = 3$.

On the other hand, the authors found further families of graphs for which the statement in Conjecture 8.5 does hold. In fact, they showed its validity for almost all graphs.

Theorem 8.6. Conjecture 8.5 *holds for*

- *block graphs,*
- *edge-transitive graphs,*
- *bipartite graphs,*
- *graphs with diameter* 2*,*
- *graphs with diameter* 3*,* n *vertices and at most* $\frac{1}{2}\binom{n}{2}$ *edges,*
- *graphs with* n *vertices and* m *edges whenever* $m \leq \frac{1}{4}(n^{4/3} - n^{1/3})$.

They also proved that Conjecture 8.5 holds for almost all random graphs in 2 models of random graphs, see [16] for more detailed explanation. Anyway, it is an open problem if there exist graphs G, other than complete ones, for which $|\{\alpha; Sz^{\alpha}(G) - W^{\alpha}(G) = 0\}|$ is larger than 3. So we have the following problem.

Problem 8.7. Let $\mathcal{G}$ be the class of graphs which contain at least one block which is not complete. Is $|\{\alpha; Sz^{\alpha}(G) - W^{\alpha}(G) = 0\}|$ bounded for $G \in \mathcal{G}$? If so, what is its maximum value?

By showing that for every graph G, the sequence $(n_v(u) \cdot n_u(v))_{uv \in E(G)}$ majorizes the sequence $(d(u, v))_{u,v \in V(G)}$, Cambie and Haslegrave proved that a weaker version of Conjecture 8.5 holds. Using a different approach the same result was independently obtained by Kovijanić Vukićević and Bulatović [78].

Theorem 8.8. *For every non-complete graph G and $\alpha > 1$, we have $\mathrm{Sz}^{\alpha}(G) > W^{\alpha}(G)$.*

We conclude this section with the following question.

Question 8.9. Does Conjecture 8.5 hold for triangle-free graphs?

9 Wiener index of apex graphs

An *apex graph* is a graph that becomes planar by removal of a single vertex. Along these lines a graph G is called an *apex tree* if it contains a vertex x such that $G - x$ is a tree. Furthemore, a graph G is called an *ℓ-apex tree* if there exists a vertex subset $A \subset V(G)$ of cardinality ℓ such that $G - A$ is a tree and there is no other subset of smaller cardinality with this property [82, 83].

In [82] extremal values of (additively and multiplicatively) weighted Harary indices of apex and ℓ-apex trees were studied. Extremal values of some other topological indices of ℓ-apex trees were recently explored in [2] and [48]. In the later authors studied the generalized Wiener index and derived the following result in which $K_\ell + T$ denotes the join of a complete graph K_ℓ and a tree T on $n - \ell$ vertices.

Theorem 9.1. *Let G be an ℓ-apex tree on n vertices, where $\ell \geq 1$ and $n \geq \ell + 2$, and let $\alpha \neq 0$. Then, the following two claims hold:*

- *If $\alpha > 0$ then $W^{\alpha}(G)$ has the minimum value if and only if $G = K_\ell + T$, where T is any tree on $n - \ell$ vertices;*
- *If $\alpha < 0$ then $W^{\alpha}(G)$ has the maximum value if and only if $G = K_\ell + T$, where T is any tree on $n - \ell$ vertices.*

Moreover, in the extremal case

$$W^{\alpha}(G) = (n^2 - 2n\ell - 3n + \ell^2 + 3\ell + 2)\, 2^{\alpha-1} + (2n\ell + 2n - \ell^2 - 3\ell - 2)\, 2^{-1}.$$

Observe that for $\alpha = 1$ the invariant W^{α} is the Wiener index, and by Theorem 9.1 the extremal value is

$$W(G) = (2n^2 - 2n\ell - 4n + \ell^2 + 3\ell + 2)\, 2^{-1}.$$

Recall that a *dumbbell graph* is a graph comprised of two disjoint cliques connected by a path. More precisely, a dumbbell graph $D_c(a, b)$ is a graph obtained from a path $P_c = v_1 v_2 \cdots v_c$ and disjoint complete graphs K_a and K_b by connecting v_1 to a vertex of K_a and connecting v_c to a vertex of K_b, see Figure 16 for $D_5(3, 4)$. The order of so constructed graph is $a + b + c$. Note that without loss of generality, we can always assume that $a, b \neq 2$.

Theorem 9.2. *Let G be an apex tree on $n \geq 3$ vertices, and let $\alpha \neq 0$.*

- *If $\alpha > 0$ then $W^{\alpha}(G)$ has the maximum value if and only if $G = D_{n-4}(3, 1)$;*
- *If $\alpha < 0$ then $W^{\alpha}(G)$ has the minimum value if and only if $G = D_{n-4}(3, 1)$.*

Moreover, in the extremal case

$$W^{\alpha}(G) = 1 + \sum_{i=1}^{n-2} (n - i) i^{\alpha}.$$

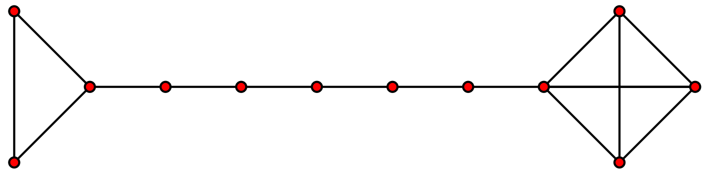

Figure 16: The graph $D_5(3,4)$.

In [48] the following conjecture was proposed.

Conjecture 9.3. *Let G be an ℓ-apex tree on n vertices, where $\ell \geq 3$ and $n \geq \ell + 1$, such that G has maximum Wiener index. Then G is the balanced dumbbell graph, i.e. $G \cong D_c(a,b)$, where $a = \lceil \ell/2 \rceil$, $b = \lfloor \ell/2 \rfloor$, and $c = n - \ell$.*

10 Wiener index of line graphs

The *line graph* $L(G)$ of a graph G is defined as a graph whose vertex set coincides with the set of edges of G and two vertices of $L(G)$ are adjacent if and only if the corresponding edges are incident in G. Higher iterations of the line graph are defined recursively.

$$L^k(G) = \begin{cases} G & \text{for } k = 0, \\ L(L^{k-1}(G)) & \text{for } k > 0. \end{cases}$$

Van Rooij and Wilf [77] showed that for the sequence

$$G, L(G), L(L(G)), L(L(L(G))), \ldots$$

only four options are possible. If G is a cycle graph, then $L(G)$ and each subsequent graph in this sequence is isomorphic to G itself. If G is a claw $K_{1,3}$, then $L(G) = C_3$ and consequently the same holds for all subsequent graphs in the sequence. For a path we have $L(P_n) = P_{n-1}$, $L^2(P_n) = P_{n-2}$, $\ldots$, $L^{n-1}(P_n) = P_1$ and $L^k(P_n)$ is an empty graph if $k \geq n$. In all the remaining cases the order of the graphs in the sequence increases without bound.

The following problem was proposed by Gutman [35].

Problem 10.1. Find an n-vertex graph G whose line graph $L(G)$ has maximum Wiener index.

Supported by a result from [20], we pose the following conjecture (see also [56]).

Conjecture 10.2. *Among all graphs G on n vertices, $W(L(G))$ attains maximum for some dumbbell graph on n vertices.*

Similar conjecture was proposed for bipartite graphs [56]. Let us call a graph a *barbell* graph if it is comprised of two disjoint complete bipartite graphs connected by a path.

Conjecture 10.3. *Let n be large. Among all bipartite graphs G on n vertices, $W(L(G))$ attains maximum for some barbell graph on n vertices.*

A related question we pose is the following.

Problem 10.4. For given n and k, find graphs G on n vertices with the extremal value of $W(L^k(G))$.

Dobrynin and Mel'nikov [27] proposed to estimate the extremal values for the ratio $\frac{W(L^k(G))}{W(G)}$, for a graph G on n vertices and explicitly stated the case $k = 1$ as a problem. The minimum value was given in [54].

Theorem 10.5. *Among all connected graphs on n vertices, the fraction $\frac{W(L(G))}{W(G)}$ is minimum for the star S_n, in which case $\frac{W(L(G))}{W(G)} = \frac{n-2}{2(n-1)}$.*

The problem was recently solved also for the maximal value [70] .

Theorem 10.6. *For a graph G on n vertices it holds that $\frac{W(L(G))}{W(G)} \leq \binom{n-1}{2}$ with equality if and only if $G = K_n$.*

For $k > 1$ the problem remains open.

Problem 10.7. Find n-vertex graphs G with extremal values of $\frac{W(L^k(G))}{W(G)}$ for $k \geq 2$.

Note that the line graph of K_n has the greatest number of vertices, and restricting to bipartite graphs, the (almost) balanced complete bipartite graphs have line graphs with most vertices, so $K_{\lfloor n/2 \rfloor, \lceil n/2 \rceil}$ could be the graph attaining maximal value in this class of graphs. It is expected that the minimum value should be attained by P_n, since this is the only graph whose line graph decreases in size, see a conjecture from [56].

Conjecture 10.8. *Let $k \geq 2$ and let n be large. Among all graphs G on n vertices, $\frac{W(L^k(G))}{W(G)}$ attains the maximum for K_n, and it attains the minimum for P_n.*

The above conjecture is supported by a result from [41], where it was proved that among all trees on n vertices the path P_n has the smallest value of this ratio for $k \geq 3$, and it was conjectured that the same holds also in the case $k = 2$. Another related problem is the following.

Problem 10.9. For various ℓ and k find the extremal graphs for the ratio $\frac{W(L^k(G))}{W(L^l(G))}$.

11 Graphs with prescribed number of blocks

A graph is *non-separable* if it is connected and has no cut-vertices, i.e. either it is 2-connected or it is K_2. A *block* of G is a maximal non-separable subgraph of G. As known, the n-path P_n, which has $n - 1$ blocks, has the maximum Wiener index in the class of graphs on n vertices, and among graphs on n vertices that have just one block, the n-cycle has the largest Wiener index. The ordering of trees with respect to decreasing Wiener index is known up to the 17th maximum Wiener index [23, 64], and the increasing ordering up to the 15th maximum Wiener index [28].

Bessy et al. [8] studied the ordering of n-vertex graphs with just one block (i.e. 2-vertex connected graphs) with respect to decreasing Wiener index. Let $1 \leq p \leq q \leq n-p-q+1$ and $q > 1$. The notation $H_{n,p,q}$ stands for the graph on n vertices comprised of three internally disjoint paths with the same end-vertices, where the first path has length p, the second one has length q, and the last one has length $n - p - q + 1$. Obviously $H_{n,1,2}$ is a graph obtained from C_n by introducing a new edge connecting two vertices at distance two on the cycle, and $H_{n,2,2}$ is a graph that is obtained from a 4-cycle by connecting opposite vertices by a path of length $n-3$, see Figure 17.

In [8] it was shown that among graphs on n vertices that have just one block, $H_{n,1,2}$ has the second largest Wiener index if $n \neq 6$. If $n \geq 11$, the third extremal graph is $H_{n,2,2}$. The authors also give conjectures on the graphs with 4th and 5th greatest Wiener index in the class of 2-connected graphs. Let $H^+_{n,2,2}$ be the graph obtained from $H_{n,2,2}$ by inserting an edge between two vertices that are at distance 1 from the vertices of degree 3, see the third graph in Figure 17. Then $H^+_{n,2,2}$ has Wiener index exactly 1 less than $H_{n,2,2}$, so it is the fourth 2-connected graph by decreasing Wiener index for $n = 9$ and $n \geq 11$, but it may not be unique. However, the following can be true.

Conjecture 11.1. *For n large enough, $H^+_{n,2,2}$ is the graph with the 4th largest Wiener index among blocks on n vertices.*

Conjecture 11.2. *For n large enough, $H_{n,1,3}$ is the graph with the 5th largest Wiener index among blocks on n vertices.*

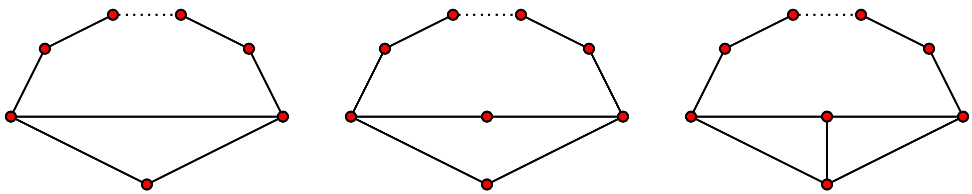

Figure 17: Graphs $H_{n,1,2}$, $H_{n,2,2}$ and $H^+_{n,2,2}$.

Bessy et al. [7] studied a general problem of finding the maximum possible value of Wiener index among graphs on n vertices with fixed number of blocks. They showed that among all graphs on n vertices which have $p \geq 2$ blocks, the maximum Wiener index is attained by a graph comprised of two cycles joined by a path, where one or both cycles can be replaced by a single edge. To be more specific, we need the following notation.

If G is a connected graph and v is a cut-vertex that partitions G into subgraphs G_1 and G_2, i.e., $G = G_1 \cup G_2$ and $G_1 \cap G_2 = \{v\}$, then we write $G = G_1 \circ_v G_2$. For simplicity reasons, by C_2 we mean the complete graph K_2.

Theorem 11.3. *Let n and p be numbers such that $n > p > 1$. Among all graphs on n vertices with p blocks, the maximum Wiener index is attained by the graph $C_a \circ_u P_{p-1} \circ_v C_b$ for some integers $a \geq 2$ and $b \geq 2$, where $a + b = n - p + 3$, and u and v are distinct end-vertices of P_{p-1}.*

Note that C_a or C_b can also be edges, and then we obtain $C_{n-p+1} \circ_u P_p$, which is a graph composed of one cycle with an attached path, or P_n if both C_a and C_b are edges.

In [6] the authors provide further details by determining the sizes of a and b in the extremal graphs for each n and p. Roughly speaking, if n is bigger than $5p-7$, then the extremal graph is obtained for $a = 2$, i.e. the graph is a path glued to a cycle. For values $n = 5p-8$ and $5p-7$, there is more than one extremal graph. And when $n < 5p-8$, the extremal graph is again unique with a and b being equal or almost equal depending on the congruence of $n-p$ modulo 4.

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