Wiener Index and Remoteness in Triangulations and Quadrangulations

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Let G be a connected graph. The Wiener index of a connected graph is the sum of the distances between all unordered pairs of vertices. We provide asymptotic formulas for the maximum Wiener index of simple triangulations and quadrangulations with given connectivity, as the order increases, and make conjectures for the extremal triangulations and quadrangulations based on computational evidence. If $\overline{\sigma}(v)$ denotes the arithmetic mean of the distances from v to all other vertices of G, then the remoteness of G is defined as the largest value of $\overline{\sigma}(v)$ over all vertices v of G. We give sharp upper bounds on the remoteness of simple triangulations and quadrangulations of given order and connectivity.

Keywords: distance, Wiener index, average distance, planar graph, triangulation, quadrangulation, connectivity, remoteness

1 Definitions and Selected Results on the Wiener Index

Let G be a connected graph. The Wiener index $W(G)$ of G is the sum of the distances between all unordered pairs of distinct vertices, i. e.,

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

where $d_G(u,v)$ is the usual distance between vertices u and v, i.e., the minimum number of edges on a (u,v)-path in G. The Wiener index was first studied by the chemist Wiener [41], who observed that it relates well to the boiling point of certain alkanes. Several other applications in chemistry were found subsequently, see for example [35].

The systematic study of the mathematical properties of the Wiener index began with the classical papers by Doyle and Graver [18], Entringer, Jackson and Snyder [19] and Plesník [34]. Several bounds on the Wiener index and closely related parameters, such as transmission or routing cost (defined as the sum of the distances between all ordered pairs of vertices), average distance or mean distance (both are defined

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as the arithmetic mean of the distances between all unordered pairs of distinct vertices) have been proved since.

The most basic upper bound on $W(G)$ states that if G is a connected graph of order n, then

$$W(G) \leq \frac{(n-1)n(n+1)}{6}, \tag{1}$$

which is attained only by paths (see [18] [34], [30]). Many sharp or asymptotically sharp bounds on $W(G)$ in terms of other graph parameters are known, for example minimum degree ([4], [11], [28]), connectivity ([14], [21]), edge-connectivity ([12], [13]) and maximum degree [20]. For recent results on the Wiener index see, for example, [17], [23], [25], [26], [27] [29], [33], [39], [38] and [40].

Entringer et al. [19] found that among trees on the same number of vertices, the star minimizes and the path maximizes the Wiener index (see also [30] problem 6.23). Fischermann, Hoffmann, Rautenbach, Székely and Volkmann [20] (see also [24]) characterized binary trees with minimum and maximum Wiener index.

The notation we use in this paper is as follows. If G is a graph, then we denote its vertex set and edge set by $V(G)$ and $E(G)$. By $n(G)$ and $m(G)$ we mean the *order* and *size* of G, defined as $|V(G)|$ and $|E(G)|$, respectively. The *eccentricity* $e(v)$ of a vertex v is the distance to a vertex farthest from v, i.e., $e(v) = \max_{u \in V(G)} d_G(v,u)$. The largest and the smallest of the eccentricities of the vertices of G are the *diameter* and the *radius* of G, respectively. The *neighborhood* of a vertex v of G is the set of vertices adjacent to v, it is denoted by $N_G(v)$, and the cardinality $|N_G(v)|$ is the *degree* of v, which we denote by $\deg_G(v)$. If i is an integer with $0 \leq i \leq e(v)$, then $N_i(v)$ denotes the set of all vertices at distance exactly i from v, and we write $n_i(v)$ for $|N_i(v)|$. If there is no danger of confusion, we often omit the subscript G or the argument G or v. If $A, B \subseteq V(G)$, then $m(A,B)$ denotes the number of edges that join a vertex in A to a vertex in B, and $G[A]$ denotes the subgraph of G induced by A. If w is a vertex of G and $A \subseteq V(G)$, then a (w,A)-*fan* is a set of $|A|$ paths from w to A, where any two paths have only w in common. If G is connected and not complete, then the *connectivity* of G, $\kappa(G)$, is the smallest number of vertices whose deletion renders G disconnected. The (not necessarily simple) plane graph G is a *triangulation* (resp. *quadrangulation*) if every face is a triangle (resp. 4-cycle). A *simple triangulation* (resp. *simple quadrangulation*) is a triangulation (resp. quadrangulation) whose underlying graph is simple. i.e. has no multiple edges. The graph H is a *minor* of the graph G, if H can be obtained from a subgraph of G by edge-contractions.

By C_n, K_n and $\overline{K_n}$ we mean the cycle, the complete graph, and the edgeless graph on n vertices, respectively. If G and H are graphs then $G + H$ denotes the graph obtained from the union of G and H by adding edges joining every vertex of G to every vertex of H.

2 Summary of the Results in this Paper

Another natural class of study for extremal Wiener index is planar graphs. However, as the maximum Wiener index of graphs (1) is attained by a path, it makes sense to consider more restricted classes of planar graphs, like simple triangulations and quadrangulations. Che and Collins [8], and the authors of the present paper [9] investigated independently the maximum Wiener index of triangulations and presented the same simple triangulation of order n (see Figures 5, 6, 7) with Wiener index

$$W(T_n) = \frac{1}{3}\binom{n+2}{3} - \frac{1}{3}\left\lfloor \frac{n+2}{3} \right\rfloor = \begin{cases} \frac{n^3}{18} + \frac{n^2}{6} & \text{if } n = 3k \\ \frac{n^3}{18} + \frac{n^2}{6} - \frac{2}{9} & \text{if } n = 3k+1 \\ \frac{n^3}{18} + \frac{n^2}{6} - \frac{1}{9} & \text{if } n = 3k+2, \end{cases} \tag{2}$$

which they conjectured to be optimal. (Note that this sequence is present in the On-Line Encyclopedia of Integer Sequences [37] under A014125, which is the bisection of A001400. The displayed closed form is due to Bruno Berseli [37].) We [9] announced that this conjecture is asymptotically true before the paper [8] was submitted. Che and Collins [8] verified this conjecture for simple triangulations of order not exceeding 10. Using computer, we verified this conjecture for simple triangulations of order not exceeding 18, see Table 1 in [10], an earlier version of this paper. Very recently, Debarun Ghosh, Ervin Győri, Addisu Paulos, Nika Salia, Oscar Zamora verified this conjecture [22].

In this paper we prove a *generalization* of this conjecture *asymptotically*. Note that every simple triangulation is 3-connected, but a simple triangulation cannot be 6-connected because of the number of edges. Our main theorem (Theorem 2) proves that for any $3 \leq \kappa \leq 5$, the Wiener index of any κ-connected simple triangulation of order n is at most $\frac{1}{6\kappa}n^3 + O(n^{5/2})$. We also prove in Theorem 3 that for any $2 \leq \kappa \leq 3$, the Wiener index of any κ-connected simple quadrangulation of order n is at most $\frac{1}{6\kappa}n^3 + O(n^{5/2})$.

We provide constructions matching the upper bounds of Theorems 2 and 3 for the maximum Wiener index of triangulations and quadrangulations of given connectivity. We do more, as we exhibit triangulations and quadrangulations following patterns by the residue of the order n modulo κ, which we conjecture as realizers of the maximum Wiener index. Our conjectures are based on extensive computations. We detail next these conjectures.

We constructed 4-connected simple triangulations with Wiener index

$$W(T_n^4) = \begin{cases} \frac{n^3}{24} + \frac{n^2}{4} + \frac{n}{3} - 2 & \text{if } n = 4k+2 \\ \frac{n^3}{24} + \frac{n^2}{4} + \frac{5n}{24} - 1 & \text{if } n = 4k+3 \\ \frac{n^3}{24} + \frac{n^2}{4} + \frac{n}{3} - 2 & \text{if } n = 4k \\ \frac{n^3}{24} + \frac{n^2}{4} + \frac{5n}{24} - \frac{3}{2} & \text{if } n = 4k+1, \end{cases} \tag{3}$$

see Figures 8, 9, 10, 11. This proves that Theorem 2 is also asymptotically tight for $\kappa = 4$. Furthermore, we conjecture that the repetition of the obvious pattern in these figures provide the extremal triangulations. Using computer, we verified this conjecture for simple triangulations of order not exceeding 22, see Table 2.

We constructed 5-connected simple triangulations with Wiener index

$$W(T_n^5) = \begin{cases} \frac{n^3}{30} + \frac{3n^2}{10} - \frac{23n}{15} + \frac{168}{5} & \text{if } n = 5k+2 \\ \frac{n^3}{30} + \frac{3n^2}{10} - \frac{23n}{15} + 31 & \text{if } n = 5k+3 \\ \frac{n^3}{30} + \frac{3n^2}{10} - \frac{23n}{15} + \frac{161}{5} & \text{if } n = 5k+4 \\ \frac{n^3}{30} + \frac{3n^2}{10} - \frac{23n}{15} + 32 & \text{if } n = 5k \\ \frac{n^3}{30} + \frac{3n^2}{10} - \frac{23n}{15} + \frac{156}{5} & \text{if } n = 5k+1, \end{cases} \tag{4}$$

see Figures 12, 13, 15, 16, 17. This proves that Theorem 2 is also asymptotically tight for $\kappa = 5$. Furthermore, we conjecture that the repetition of the obvious pattern in these figures provide the extremal triangulations. We arrived to these conjectures using computer and also guesswork regarding the pattern. Therefore these conjectures for the 5-connected case are less supported with computational evidence than other conjectures in this paper, as we were able to do the computation only up to the order 32, see Table 3. The issue is that the pattern slowly develops, and orders following the same pattern differ by 5—therefore we do not have sufficiently many data points to have a very convincing conjecture.

We are indebted to Paul Kainen, who after hearing about our triangulation results, asked whether we can prove similar results for simple quadrangulations. Recall that any simple quadrangulation is 2-connected, but no simple quadrangulation is 4-connected. We conjecture that the maximum Wiener index of a simple quadrangulation of order n is

$$W(Q_n) = \begin{cases} \frac{n^3}{12} + \frac{7n}{6} - 2 & \text{if } n = 2k \\ \frac{n^3}{12} + \frac{11n}{12} - 1 & \text{if } n = 2k+1, \end{cases} \tag{5}$$

based on Figures 18, 19. Furthermore, we conjecture that the repetition of the obvious pattern in these figures provide the extremal quadrangulations. Using computer, we verified this conjecture for simple quadrangulations of order not exceeding 20, see Table 4.

We conjecture that the maximum Wiener index of a 3-connected simple quadrangulation of order n is

$$W(Q_n^3) = \begin{cases} \frac{n^3}{18} + \frac{n^2}{3} - \frac{17n}{6} + \frac{206}{9} & \text{if } n = 3k+14 \\ \frac{n^3}{18} + \frac{n^2}{3} - \frac{17n}{6} + 20 & \text{if } n = 3k+15 \\ \frac{n^3}{18} + \frac{n^2}{3} - \frac{17n}{6} + \frac{184}{9} & \text{if } n = 3k+16, \end{cases} \tag{6}$$

based on Figures 20, 21, 22. Furthermore, we conjecture that the repetition of the obvious pattern in these figures provide the extremal quadrangulations. Using computer, we verified this conjecture for simple quadrangulations of order not exceeding 28, see Table 5.

Section 5 contains the conjectures stated so far in the form of drawings for some fixed order, but with emphasis on the general pattern: the red colored part is the repeated pattern. Even more, we conjecture based on computational evidence that those drawings not only provide the maximum Wiener index, but for sufficiently large n they are unique with this property.

We remark here that the result of [22] described by formula (2) does not hold for *non-simple* triangulations. For the construction of non-simple triangulations with asymptotically larger Wiener indices, see Figure 1. In fact, we conjecture that these constructions are optimal for non-simple triangulations. The non-simple quadrangulation on Figure 2 has a larger Wiener index than conjectured best simple quadrangulation on Figure 18, but difference is not in the leading term. For the rest of the paper, under the terms triangulation and quadrangulation we will always understand simple triangulation and quadrangulation.

Che and Collins noted [8] that the *minimum* Wiener index of a triangulation of order n is a trivial problem, as Euler's formula determines the number of edges, and there are constructions, in which every pair of vertices are at most distance two. The situation is analogous for quadrangulations. For minimizers, see Figure 3.

There is second research direction of this paper, in addition to the Wiener index. We give bounds on the total distance $\sigma(v)$ and the average distance $\overline{\sigma}(v)$ of a vertex v, defined as the sum and the average, respectively, of the distances from v to all other vertices. Bounds on $\sigma(v)$ were obtained, for example, in

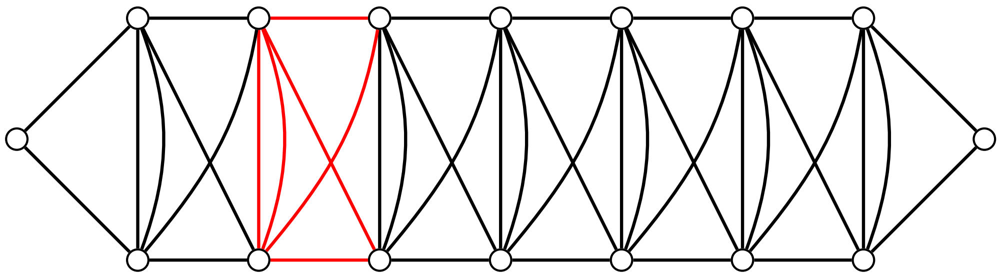

Fig. 1: A non-simple triangulation with larger Wiener index. $W(T'_n) = \frac{n^3}{12} + \frac{2n}{3} - 1$ for even n.

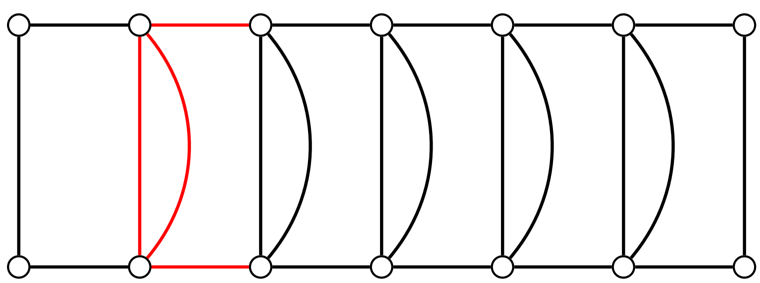

Fig. 2: A non-simple quadrangulation with larger Wiener index. $W(Q'_n) = \frac{n^3}{12} + \frac{n^2}{4} - \frac{n}{3}$ for even n. For this sequence, see A131423 [37].

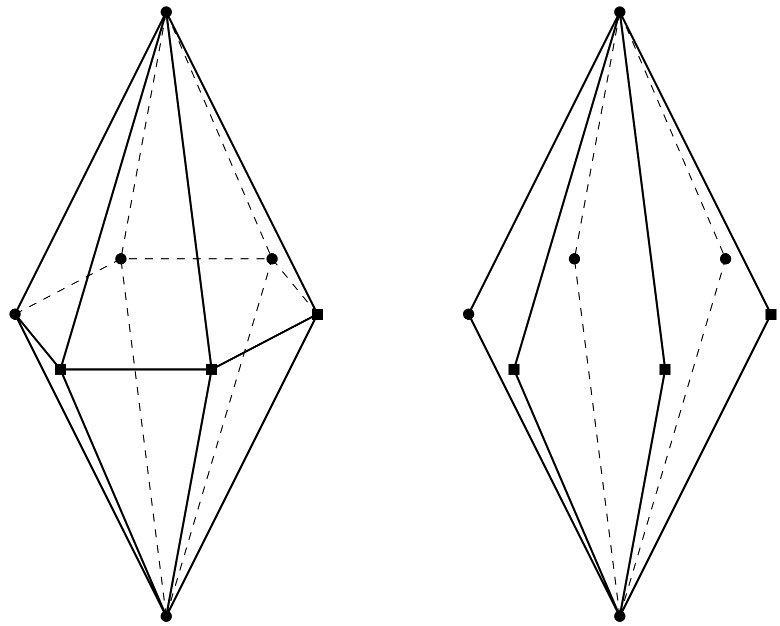

Fig. 3: Minimizers for the Wiener index of simple triangulations and quadrangulations.

[3] [19] and [43]. Of particular interest is the maximum value over all $v \in V(G)$ of $\overline{\sigma}(v)$ in a graph G, usually referred to as the *remoteness* $\rho(G)$, of G. It was shown by Zelinka [43] and, independently, by Aouchiche and Hansen [2] that the remoteness is at most $\frac{n}{2}$. For graphs of given minimum degree δ these bounds were improved in [15] by a factor of about $\frac{3}{\delta+1}$. For more recent results on remoteness see, for example, [16], and [42].

In this paper we give sharp upper bounds on remoteness of triangulations and quadrangulations with given connectivity in Corollary 1 and Proposition 2. The bounds are sharp in Proposition 2 and Corollary 1 by Figures 5 through 12 and Figures 14 through 22. It is not difficult to compute the distances on those figures from the black vertex to the remaining vertices and show that the sum of distances from the black vertex meets the upper bound for remoteness. Details will be provided in the Ph.D. dissertation of the third author. Our results show that the maximum remoteness among triangulations and quadrangulations of prescribed connectivity κ is achieved on those ones that are conjectured to maximize the Wiener index, *except for 5-connected triangulations of order* $n = 5k + 3$. There are, however, lots of different realizations of the maximum of remoteness in all classes that we investigate, except among quadrangulations.

3 Upper Bounds on the Remoteness of Triangulations and Quadrangulations

In this section we present bounds on the remoteness of triangulations and quadrangulations. A sharp upper bound on the remoteness of a triangulation of given order was given by Che and Collins [8]. We give corresponding bounds for 4-connected and 5-connected triangulations, as well as for 2-connected and 3-connected quadrangulations.

We begin by stating a sharp bound on the distance of an arbitrary vertex in a κ-connected graph of given order due to Favaron, Kouider and Mahéo [21], from which we will derive some of our bounds.

Proposition 1. [21] *Let G be a κ-connected graph of order n, and x an arbitrary vertex of G. Then*

$$\sigma(x) \leq \left\lfloor \frac{n+\kappa-1}{\kappa} \right\rfloor \left(n-1-\frac{\kappa}{2}\left\lfloor \frac{n-1}{\kappa} \right\rfloor \right).$$

Every simple triangulation is 3-connected, and every simple quadrangulation is 2-connected. Proposition 1 yields thus the following sharp bounds for the remoteness of 3-connected and 4-connected triangulations and 2-connected quadrangulations.

Corollary 1. *(a)* [8] *If G is a simple triangulation of order n, then*

$$\rho(G) \leq \frac{n+2}{6} + \varepsilon_n,$$

where $\varepsilon_n = 0$ if $n \equiv 1 \pmod 3$, and $\varepsilon_n = \frac{1}{3(n-1)}$ if $n \equiv 0, 2 \pmod 3$.
(b) If G is a 4-connected triangulation of order n, then

$$\rho(G) \leq \frac{n+3}{8} + \varepsilon_n,$$

where $\varepsilon_n = 0$ if $n \equiv 1 \pmod 4$, $\varepsilon_n = \frac{3}{8(n-1)}$ if $n \equiv 0, 2 \pmod 4$, and $\varepsilon_n = \frac{1}{2(n-1)}$ if $n \equiv 3 \pmod 4$.
(c) If G is a simple quadrangulation of order n, then

$$\rho(G) \leq \frac{n+1}{4} + \varepsilon_n,$$

where $\varepsilon_n = 0$ if $n \equiv 1 \pmod 2$, and $\varepsilon_n = \frac{1}{4(n-1)}$ if $n \equiv 0 \pmod 2$. □

Proposition 1 also yields good bounds for the remoteness of 5-connected triangulations and 3-connected quadrangulations. These bounds are however not sharp for all values of n. In order to obtain sharp bounds we need some additional terminology and results from [1].

Let v be a fixed vertex of a connected plane graph and $i \in \mathbb{N}$ with $i < e(v)$. We say that a vertex $w \in N_i(v)$ is *active* if it has a neighbor in $N_{i+1}(v)$.

Lemma 1. [1] *Let G be a 3-connected plane graph, v a vertex of G and $i \in \mathbb{N}$ with $1 \leq i \leq e(v)-1$. For every active vertex $w \in N_i(v)$ there exist two other active vertices $w', w'' \in N_i(v)$ such that w and w' share a face of G, and w and w'' also share a face of G.*

Lemma 2. *(a) Let G be a 5-connected simple triangulation, v a vertex of G and $d = e_G(v)$. If $n_{d-1}(v) = 5$, then $n_d(v) = 1$.*
(b) Let G be a 3-connected simple quadrangulation, v a vertex of G and $d = e_G(v)$. If $n_{d-1}(v) = 3$, then $n_d(v) = 1$. If $n_{d-2}(v) = 3$ and $n_{d-1}(v) = 4$, then $n_d(v) > 1$.

Proof: (a) Assume that G is a 5-connected simple triangulation, v is a vertex of G, and $n_{d-1} = 5$, where d is the eccentricity of v. This implies that N_{d-1} is a minimum cutset of G. Hence, since G is a triangulation, N_{d-1} induces a cycle C of length 5. We first show that

$$\text{the vertices in } N_d \text{ are all inside } C \text{, or all outside } C. \tag{7}$$

Suppose not. Then there exist vertices $a, b \in N_d$ such that a is inside C, and b is outside C. Since G is 5-connected, there exist a (v, N_{d-1})-fan F_v, an (a, N_{d-1})-fan F_a, and a (b, N_{d-1})-fan F_b. Any two of these three fans share only the vertices of N_{d-1}. Indeed, other than vertices in N_{d-1}, fan F_v contains only vertices in $\bigcup_{i=0}^{d-1} N_i$, while fan F_a contains only vertices in $N_{d-1} \cup N_d$ that are inside C, while fan F_b contains only vertices in $N_{d-1} \cup N_d$ that are outside C. Now contracting the edges in $F_a - N_{d-1}$, the edges in $F_b - N_{d-1}$, and the edges in $F_v - N_{d-1}$ to three single vertices yields a graph that contains $3K_1 + C_5$ as a subgraph. Hence G contains $3K_1 + C_5$ as a minor. Contracting three consecutive vertices of the 5-cycle shows that this implies that G contains $K_3 + 3K_1$ as a minor, which contradicts the planarity of G. This contradiction proves (7).

By (7) we may assume that all vertices of N_d are inside the cycle C. Since every vertex of N_d is adjacent to some vertex of N_{d-1}, the subgraph $G[N_d]$ is outerplanar. Hence

$$m(G[N_d]) \leq \begin{cases} 0 & \text{if } n_d = 1, \\ 1 & \text{if } n_d = 2, \\ 2n_d - 3 & \text{if } n_d \geq 3. \end{cases} \tag{8}$$

We now bound the sum of the degrees of the vertices in N_d. Let H be the plane graph obtained from $G[N_{d-1} \cup N_d]$ by adding a new vertex z in the outer face of C and joining it to all five vertices of C. Then H has order $n(H) = 1 + n_{d-1} + n_d = n_d + 6$. Since H is a plane graph we have $m(H) \leq 3n(H) - 6 \leq 3n_d + 12$. At least 10 edges of H are incident with z or belong to C, and are thus not incident with any vertex of N_d, so they don't contribute to the sum of the degrees of vertices in N_d. Since the edges of $G[N_d]$ contribute two to the sum of the degrees of vertices in N_d, we have

$$\sum_{x \in N_d} \deg_G(x) \leq (m(H) - 10) + m(G[N_d]) \leq \begin{cases} (3n_d + 2) + 0 & \text{if } n_d = 1, \\ (3n_d + 2) + 1 & \text{if } n_d = 2, \\ (3n_d + 2) + (2n_d - 3) & \text{if } n_d \geq 3. \end{cases}$$

It is easy to verify that this implies $\sum_{x \in N_d} \deg_G(x) < 5n_d$ whenever $n_d > 1$. But since G is 5-connected, every vertex of G has degree at least five. Hence we conclude that $n_d = 1$, which proves (a).

(b) Let G be a 3-connected simple quadrangulation, v a vertex of G, and $d = e(v)$.
To prove the first statement assume that $n_{d-1} = 3$. Let $N_{d-1}(v) = \{w, w', w''\}$. Since G is a quadrangulation and thus bipartite, the set $\{w, w, w''\}$ is independent in G. Since G is 3-connected, the vertices w, w', w'' have a neighbor in N_d and are thus active. By Lemma 1, w and w' share a face, and so do w and w'', as well as w' and w''. Hence we can add edges ww', ww'' and ww'' to G to obtain a plane graph (but not a quadrangulation). Let C be the cycle consisting of the edges $ww', w'w'', w''w$. A proof similar to that in (a) shows that the vertices of N_d are all inside C, or all outside C. Without loss of generality we assume the former. We now bound the sum of the degrees of the vertices in N_d.
Let H be the plane graph obtained from $G[N_{d-1} \cup N_d] + E(C)$ by adding a new vertex z in the outer face of C and joining it to all three vertices of C. Since G is a quadrangulation, the only faces of H of length

three are the six faces that have one of the three edges of C on their boundary. Let H' be the plane graph $H - E(C) = G[N_{d-1} \cup N_d]$. Then $n(H') = n_{d-1} + n_d + 1 = n_d + 4$ and, since H' has only faces of length at least four, $m(H') \leq 2n(H') - 4 = 2n_d + 4$.
Exactly three edges of H are incident with z and are thus not incident with any vertex of N_d. Since G is bipartite, $G[N_d]$ contains no edges. Hence

$$\sum_{x \in N_d} \deg_G(x) = (m(H') - 3) \leq 2n_d + 1.$$

This implies $\sum_{x \in N_d} \deg_G(x) < 3n_d$ whenever $n_d > 1$. But since G is 3-connected, every vertex of G has degree at least three. Hence we conclude that $n_d = 1$, which proves the first statement of (b).
To prove the second statement of (b) assume that $n_{d-2} = 3$ and $n_{d-1} = 4$. Suppose to the contrary that $n_d = 1$. Let $N_{d-2} = \{w, w', w''\}$. The same arguments as in the proof of the first statement of (b) show that we can add the edges $ww', ww'', w'w''$ to G to obtain a plane graph, such that these three edges form a cycle C, and that the vertices in $N_{d-1} \cup N_d$ are either all inside C or all outside C, without loss of generality we assume the former. Let H be the plane graph obtained from $G[N_{d-2} \cup N_{d-1} \cup N_d] + E(C)$ by adding a new vertex z in the outer face of C and joining it to all three vertices of C. Since G is a quadrangulation, the only faces of H of length three are the six faces that have one of the three edges of C on their boundary. Let H' be the plane graph $H - E(C) = G[N_{d-2} \cup N_{d-1} \cup N_d]$. Then $n(H') = n_{d-2} + n_{d-1} + n_d + 1 = 9$ and, since H' has only faces of length at least four, $m(H') \leq 2n(H') - 4 = 14$. Exactly three edges of H' are incident with z and thus not incident with vertices in N_{d-1}. Since G is bipartite, no edge joins two vertices of N_{d-1}, and so we have $\sum_{x \in N_{d-1}} \deg_G(x) \leq 11 < 3n_{d-1}$. Therefore, N_{d-1} contains a vertex of degree less than three in G, which contradicts G being 3-connected. The second statement of (b) follows. $\square$

For the remaining proof of this section we define the function F which assigns to a finite sequence $X = (x_0, x_1, \ldots, x_k)$ of integers the value $F(X) = \sum_{i=0}^{k} i x_i$. So if v is a vertex of eccentricity d in a connected graph G, then $\sigma(v) = \sum_{i=0}^{d} i n_i(v) = F(n_0, n_1, \ldots, n_d)$.

Proposition 2. *(a) Let G be a 5-connected triangulation of order n. Then*

$$\rho(G) \leq \frac{n+4}{10} + \varepsilon_n,$$

where $\varepsilon_n = -\frac{3}{5(n-1)}$ if $n \equiv 0 \pmod 5$, $\varepsilon_n = -\frac{1}{n-1}$ if $n \equiv 1 \pmod 5$, $\varepsilon_n = \frac{2}{5(n-1)}$ if $n \equiv 2 \pmod 5$, and $\varepsilon_n = -\frac{2}{5(n-1)}$ if $n \equiv 3, 4 \pmod 5$.
(b) If G is a 3-connected quadrangulation of order n, then

$$\rho(G) \leq \frac{n+2}{6} + \varepsilon_n,$$

where $\varepsilon_n = -\frac{5}{3(n-1)}$ if $n \equiv 0 \pmod 3$, $\varepsilon_n = -\frac{1}{n-1}$ if $n \equiv 1 \pmod 3$, and $\varepsilon_n = \frac{1}{3(n-1)}$ if $n \equiv 2 \pmod 3$.

Proof:
(a) It suffices to show that for an arbitrary vertex v of G we have

$$\sigma(v) \leq \frac{n^2 + 3n}{10} + \varepsilon'_n,$$

where $\varepsilon'_n = -10$ if $n \equiv 0 \pmod 5$, $\varepsilon'_n = -14$ if $n \equiv 1 \pmod 5$, $\varepsilon'_n = 0$ if $n \equiv 2 \pmod 5$, and $\varepsilon'_n = -8$ if $n \equiv 3, 4 \pmod 5$.
Fix $v \in V(G)$ and let $d = e(v)$. Then

$$\sigma(v) = \sum_{i=0}^{d} i n_i = F(n_0, n_1, \ldots, n_d).$$

All n_i are positive integers, $n_0 = 1$ and $\sum_{i=0}^{d} n_i = n$. Since G is 5-connected we also have $n_i \geq 5$ for all $i \in \{1, 2, \ldots, d-1\}$. To bound $F(n_0, n_1, \ldots, n_d)$ from above we assume that n is fixed, and that $d' \in \mathbb{N}$ and $X_{max}(n) = (n'_0, n'_1, \ldots, n'_{d'})$ maximise the function F among all integers d and sequences X that satisfy these constraints. We first note that $n'_1 = n'_2 = \cdots = n'_{d-1} = 5$. Indeed, if $n'_i > 5$ for some i with $1 \leq i \leq d' - 1$, then decreasing n'_i by 1 and increasing n'_{i+1} by 1 yields a new sequence X' that satisfies the above constraints and for which $F(X') = F(X_{max}(n)) + 1$, contradicting the choice of $X_{max}(n)$. Also, if $n'_{d'} > 5$, then decreasing $n'_{d'}$ by 1, appending a new entry $n'_{d'+1} = 1$ at the end and increasing d' by 1 yields a sequence that satisfies the requirement but whose F-value is greater, again a contradiction to the choice of $X_{max}(n)$. Therefore, if q and r are positive integers with $1 \leq r \leq 5$ such that $n - 1 = 5q + r$, then the unique sequence maximising F subject to the above constraints is

$$X_{max}(n) = (1, 5, 5, \ldots, 5, r),$$

where the entry 5 appears exactly q times. If $r \neq 1$, then it is easy to see that the unique sequence with the second largest F-value satisfying the constraints is the sequence

$$X'_{max}(n) = (1, 5, 5, \ldots, 5, 6, r - 1),$$

where the entry 5 appears exactly $q - 1$ times.

CASE 1: $n \equiv 2 \pmod 5$.
Then $F(n_0, n_1, \ldots, n_d) \leq F(X_{max}(n)) = \frac{1}{10}(n^2 + 3n)$, as desired.

CASE 2: $n \equiv 0, 1, 3, 4 \pmod 5$.
Then $(n_0, n_1, \ldots, n_d) \neq X_{max}(n)$ since otherwise, if $(n_0, n_1, \ldots, n_d) = X_{max}(n)$, then $n_{d-1} = 5$ and $n_d = r \neq 1$, contradicting Lemma 2(a). Therefore, $F(n_0, n_1, \ldots, n_d) \leq F(X'_{max}(n))$, and a simple calculation shows that $F(X'_{max})(n)$ is the claimed upper bound on $\sigma(v)$.
(b) The proof of (b) is analogous to that of (a), with only two differences: The condition $n_i \geq 5$ for all $i \in \{1, 2, \ldots, d-1\}$ in (a) is replaced by $n_i \geq 3$ for all $i \in \{1, 2, \ldots, d-1\}$. Also, Lemma 2(b) implies that for $n \equiv 1, 2 \pmod 3$ we have $(n_0, n_1, \ldots, n_d) \neq X_{max}(n)$ and so $F(n_0, n_1, \ldots, n_d) \leq F(X_{max}(n)')$, while for $n \equiv 0 \pmod 3$ Lemma 2(b) implies that $(n_0, n_1, \ldots, n_d) \neq X_{max}(n), X_{max}(n)'$ and thus $F(n_0, n_1, \ldots, n_d) < F(X_{max}(n)')$. □

4 Upper Bounds on the Wiener Index of Triangulations and Quadrangulations

In this section we present asymptotically sharp upper bounds on the Wiener index of simple triangulations and simple quadrangulations, and improved bounds for simple 4-connected and 5-connected triangulations as well as simple 3-connected quadrangulations.

In the statements and proofs of our results we use the following notation. If S is a separating cycle of a plane graph G, then we denote the set of vertices inside S by A, and the set of vertices outside S by B. We often use S also for the set of vertices on this cycle, and we further let $a := |A|$, $b := |B|$ and $s := |S|$. The following separator theorem by Miller is an important tool for the proof of our bounds.

Theorem 1. ([32]) *If G is a 2-connected plane graph of order n whose faces have length at most ℓ, then G has a separating cycle S of length at most $2\sqrt{2\lfloor \ell/2 \rfloor n}$, such that $a, b \leq \frac{2}{3}n$.*

We now define a plane graph which will be used in the proof of the main result of this section.

Definition 1. *For $p \in \mathbb{N}$ with $p \geq 3$ let F_p be the plane graph constructed as follows. Let $C = u_0, u_1, \ldots, u_{p-1}, u_0$ be a cycle of length p. Inside C we add a cycle $C' = v_0, v_1, \ldots, v_{2p-1}v_0$ of length $2p$ and edges u_iv_{2i-1}, u_iv_{2i}, u_iv_{2i+1} for $i = 0, 1, \ldots, p-1$, with indices taken modulo p for the u_i and modulo $2p$ for the v_i. Inside C' we add a cycle $C'' = w_0, w_1, \ldots, w_{2p-1}, w_0$ of length $2p$ and edges v_iw_i, v_iw_{i+1} for $i = 0, 1, \ldots, 2p-1$, with all indices taken modulo $2p$. Inside C'' we add a new vertex z and join it to every vertex of C''. The graph F_4 is shown in Figure 4.*
We define F_p' to be a plane graph with the same vertex and edge set as F_p, but with the cycle C' outside the cycle C, the cycle C'' outside the cycle C', and z lying in the unbounded face whose boundary is C''.

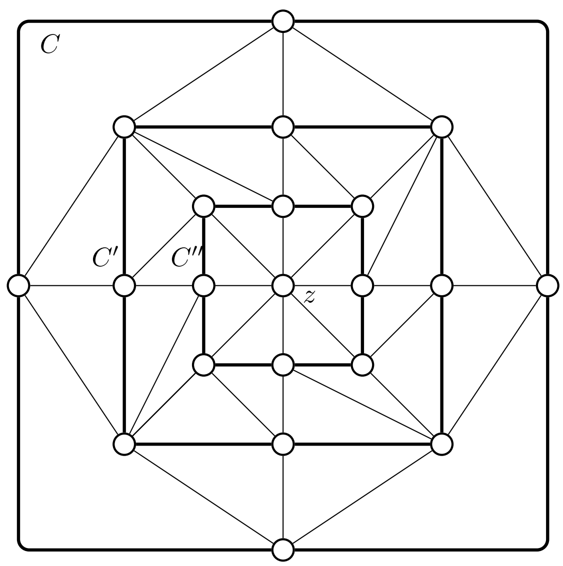

Fig. 4: The graph F_p for $p = 4$. The p-cycle C and $2p$-cycles C' and C'' drawn with thick lines.

Lemma 3. *Let F_p be the graph defined in Definition 1 above.*
(a) $\kappa(F_p) \geq 5$ for $p \geq 3$.
(b) If $u \in V(F_p)$ and $M \subseteq V(C)$ with $|M| \leq 5$, then F_p contains a (u, M)-fan.
(c) If $M_1, M_2 \subseteq V(C)$ are two sets with $|M_1| = |M_2| \leq 5$, then F_p contains a set of $|M_1|$ disjoint paths from M_1 to M_2.

Proof: (a) It is easy to verify that any two vertices of F_p are joined by five internally disjoint paths, hence F_p is 5-connected.
(b) and (c) follow directly from F_p being 5-connected. □

Theorem 2. *Let $\kappa \in \{3,4,5\}$. Then there exists a constant D such that*

$$W(G) \le \frac{1}{6\kappa}n^3 + Dn^{5/2}$$

for every κ-connected simple triangulation of order n.

Proof: Our proof is by induction on n. Define $D := \max\{D_1, D_2\}$, where D_1 is the smallest real x for which the inequality $W(G) \le \frac{1}{6\kappa}n^3 + xn^{5/2}$ holds for all κ-connected simple triangulations G of order at most 10^4, and D_2 is the smallest real x for which $8.1 + 0.76x \le x$ holds. We prove by induction on n that for all simple triangulations G of order n,

$$W(G) \le \frac{1}{6\kappa}n^3 + Dn^{5/2}, \tag{9}$$

Now (9) holds for all $n \le 10^4$ by the choice of D. Let $n > 10^4$. By our induction hypothesis we may assume that (9) holds for all graphs of order less than n.

Since G is 2-connected, it follows by Theorem 1 that G contains a separating cycle $S = t_0t_1\dots t_{s-1}t_0$ with $a, b \le \frac{2}{3}n$, where A, B, a, b, s are as in Theorem 1 and above it. Let H be the simple triangulation obtained from the plane graph $G - A$ as follows. We first delete all edges between non-consecutive vertices of S that run inside the cycle S. Inside S we insert the graph F_s by identifying the cycles S and C, specifically $t_i \in S$ with $u_i \in V(F_s)$ for $i = 0, 1, \dots, s-1$. Clearly, H is a simple triangulation of order $b + 5s + 1$. Similarly let K be the simple triangulation of order $a + 5s + 1$ obtained from the plane graph $G - B$ by deleting all edges between non-consecutive vertices of S that run outside the cycle S and inserting F'_s (a copy of F_s) into the unbounded face, bounded by the vertices of S, by identifying $t_i \in S$ with $u_i \in V(F'_s)$ for $i = 0, 1, \dots, s-1$.

For an illustration, see Figure 4. We claim that

$$H \text{ and } K \text{ are } \kappa\text{-connected.} \tag{10}$$

We prove (10) only for H, the proof for K is analogous. Let u, v be two arbitrary vertices of H. It suffices to show that there exist κ internally disjoint (u, v)-paths in H. First assume that both, u and v, are in $V(F_s)$, then it follows from Lemma 3(a) and $\kappa \le 5$ that there are κ internally disjoint (u, v)-paths in F_s, and thus in H. Now assume that exactly one of the two vertices, say u, is in $V(F_s)$. Fix a vertex $w \in A$. It follows from the κ-connectedness of G that in G there exist κ internally disjoint (w, v)-paths $P_1, P_2, \dots, P_\kappa$. For $i = 1, 2, \dots, \kappa$ let w_i be the last vertex of P_i on C, and let P'_i be the (w_i, v)-section of P_i. By Lemma 3(b), F_s contains a $(u, \{w_1, \dots, w_\kappa\})$-fan F. Then F together with $P'_1, \dots, P'_\kappa$ yields a collection of κ internally disjoint (u, v)-paths in H. Finally assume that both, u and v, are not in $V(F_s)$. Then it follows from the κ-connectedness of G that there exists internally disjoint (u, v)-paths $P_1, P_2, \dots, P_\kappa$ in G. If none of these contains a vertex in $V(F_s)$, then $P_1, P_2, \dots, P_\kappa$ form a collection of κ internally disjoint (u, v)-paths in H. If some of the paths, $P_1, \dots, P_k$ say, contain a vertex of $V(F_s)$, then let a_i and a'_i be the first and last vertex, respectively, of P_i in $V(F_s)$. Let $M = \{a_1, \dots, a_k\}$

and $M' = \{a'_1, \ldots, a'_k\}$. By Lemma 3(c), F_s contains k disjoint paths $Q_1, \ldots, Q_k$ from M to M'. Then the (u, a_i)-sections and the (a'_i, v)-sections of the paths P_i together with $Q_1, \ldots, Q_k$ and the paths $P_{k+1}, \ldots, P_\kappa$ form a collection of κ internally disjoint (u, v)-paths in H. This proves (10).

The two graphs H and K have exactly the vertices in S in common. We now bound the Wiener index of G in terms of the Wiener indices of H and K, and the total distance of z in H and K.

$$\begin{aligned} W(G) &< \sum_{\{x,y\}\subseteq B\cup S} d_G(x,y) + \sum_{\{x,y\}\subseteq A\cup S} d_G(x,y) + \sum_{x\in A,\ y\in B} d_G(x,y) \\ &< \binom{n}{2}\frac{s}{2} + \sum_{\{x,y\}\subseteq B\cup V(F_s)} d_H(x,y) + \sum_{\{x,y\}\subseteq A\cup V(F_s)} d_K(x,y) + \sum_{x\in A,\ y\in B} \big(d_H(x,z) + d_K(z,y)\big). \end{aligned} \tag{11}$$

Indeed, for any two vertices x and y of G that are both in $B \cup S$, we have $d_G(x, y) \leq d_H(x, y) + \frac{s}{2}$ since a shortest (x, y)-path in H either contains only vertices in $B \cup S$, in which case it is also a path in G, or it contains vertices in $V(F_s) - S$, in which case replacing the segment between the first and last occurrence of a vertex in $V(F_s) - S$ in the path by a segment of the cycle S that contains at most $s/2$ vertices yields an (x, y)-path in G. Similarly, if x and y are both in $A \cup S$, then $d_G(x, y) \leq d_K(x, y) + \frac{s}{2}$. Finally, if $x \in A$ and $y \in B$, then we can obtain an (x, y)-path in G from the concatenation of an (x, z)-path in K and a (z, y)-path in H by replacing z with a segment of S containing at most $s/2$ vertices. This proves (11).

We now bound each of the terms in (11). Since H and K are κ-connected simple triangulations of order $b + 5s + 1$ and $a + 5s + 1$, respectively, we have by induction

$$\sum_{\{x,y\}\subseteq B\cup V(F_s)} d_H(x,y) = W(H) \leq \frac{1}{6\kappa}(b+5s+1)^3 + D(b+5s+1)^{5/2}, \tag{12}$$

and

$$\sum_{\{x,y\}\subseteq A\cup V(F_s)} d_K(x,y) = W(K) \leq \frac{1}{6\kappa}(a+5s+1)^3 + D(a+5s+1)^{5/2}. \tag{13}$$

It follows from the bounds on remoteness in Corollary 1(a),(b) and Proposition 2 that $\sigma(v) \leq \frac{1}{2\kappa}n^2 + \frac{\kappa-2}{2\kappa}n + \frac{\kappa-3}{2\kappa}$ for every vertex v of a κ-connected triangulation of order n. Hence $\sigma(z, H) \leq \frac{1}{2\kappa}(a + 5s + 1)^2 + \frac{\kappa-2}{2\kappa}(a + 5s + 1) + \frac{\kappa-3}{2\kappa}$ and $\sigma(z, K) \leq \frac{1}{2\kappa}(b + 5s + 1)^2 + \frac{\kappa-2}{2\kappa}(b + 5s + 1) + \frac{\kappa-3}{2\kappa}$. Hence

$$\begin{aligned} \sum_{x\in A,\ y\in B} \big(d_H(x,z) + d_K(z,y)\big) &= b\sum_{x\in A} d_H(x,z) + a\sum_{y\in B} d_K(z,y) \\ &< b\,\sigma(z,H) + a\,\sigma(z,K) \\ &\leq \frac{b}{2\kappa}\big[(a+5s+1)^2 + (\kappa-2)(a+5s+1) + \kappa - 3\big] \\ &\quad + \frac{a}{2\kappa}\big[(b+5s+1)^2 + (\kappa-2)(b+5s+1) + \kappa - 3\big], \end{aligned}$$

and since $a < a + 5s + 1$ and $b < b + 5s + 1$,

$$\begin{aligned} \sum_{x\in A,\ y\in B} d_H(x,z) + d_K(z,y) &< \frac{1}{2\kappa}(a+5s+1)^2(b+5s+1) + \frac{1}{2\kappa}(a+5s+1)(b+5s+1)^2 \\ &\quad + \frac{\kappa-2}{\kappa}(a+5s+1)(b+5s+1) + \frac{\kappa-3}{2\kappa}(a+b). \end{aligned} \tag{14}$$

Hence we obtain from (11), (12), (13). and (14),

$$\begin{aligned}
W(G) &< \frac{1}{6\kappa}(a+5s+1)^3 + D(a+5s+1)^{5/2} + \frac{1}{6\kappa}(b+5s+1)^3 + D(b+5s+1)^{5/2} \\
&\quad + \frac{1}{2\kappa}(a+5s+1)^2(b+5s+1) + \frac{1}{2\kappa}(a+5s+1)(b+5s+1)^2 + \binom{n}{2}\frac{s}{2} \\
&\quad + \frac{\kappa-2}{\kappa}(a+5s+1)(b+5s+1) + \frac{\kappa-3}{2\kappa}(a+b) \\
&= \frac{1}{6\kappa}(a+b+10s+2)^3 + D\big[(a+5s+1)^{5/2} + (b+5s+1)^{5/2}\big] \\
&\quad + \frac{\kappa-2}{\kappa}(a+5s+1)(b+5s+1) + \frac{\kappa-3}{2\kappa}(a+b) + \binom{n}{2}\frac{s}{2}. \qquad (15)
\end{aligned}$$

We bound the terms of the right hand side of (15) separately. We make use of the facts that $a+b+s=n$, and that by Theorem 1 in conjunction with $n > 10^4$ we have $s \le 2^{3/2}n^{1/2} < 0.03n - 1$. We bound the first term of (15) by $(a+b+10s+2)^3 = (n+9s+2)^3 \le (n+9\cdot 2^{3/2}n^{1/2}+2)^2$. To bound the second term note that the real function $f(x) = x^{5/2}$ is concave up and that $a, b \le \frac{2}{3}n$ by Theorem 1, which implies that $(a+5s+1)^{5/2} + (b+5s+1)^{5/2}$ is maximised if $a = \frac{2}{3}n$ and $b = \frac{1}{3}n - s$ (or vice versa). Therefore, $(a+5s+1)^{5/2} + (b+5s+1)^{5/2} \le (\frac{2}{3}n+5s+1)^{5/2} + (\frac{1}{3}n+4s+1)^{5/2} \le (\frac{2}{3}n+0.15n)^{5/2} + (\frac{1}{3}n+0.12n)^{5/2} = \big((\frac{2}{3}+0.15)^{5/2} + (\frac{1}{3}+0.12)^{5/2}\big)n^{5/2} < 0.76n^{5/2}$. To bound the third term note that $\frac{\kappa-2}{\kappa} < 1$, $a+5s+1 < n$ and $b+5s+1 < n$, so $\frac{\kappa-2}{\kappa}(a+5s+1)(b+5s+1) < n^2$. To bound the fourth term note that $\frac{\kappa-3}{2\kappa} < 1$ and $a+b < n$, so $\frac{\kappa-3}{2\kappa}(a+b) < n$. Finally, $\binom{n}{2} < \frac{1}{2}n^2$, and so we bound the fifth term by $\binom{n}{2}\frac{s}{2} < 2^{-1/2}n^{5/2}$. In total we obtain from (15),

$$\begin{aligned}
W(G) &< \frac{1}{6\kappa}(n+9\cdot 2^{3/2}n^{1/2}+2)^3 + 0.76\,Dn^{5/2} + n^2 + n + 2^{-1/2}n^{5/2} \\
&= \frac{1}{6\kappa}n^3 + \big(\frac{13}{\kappa} + 0.76\,D + 1 + 2^{-1/2}\big)n^{5/2} + \frac{338}{\kappa}n^2 + \frac{8788}{3\kappa}n^{3/2}.
\end{aligned}$$

Since $n \ge 10^4$, we have $\frac{338}{\kappa}n^2 + \frac{8788}{3\kappa}n^{3/2} < 2n^{5/2}$. Also, $\frac{13}{\kappa} + 0.76\,D + 1 + 2^{-1/2} < 6.1 + 0.76\,D$, and so

$$\begin{aligned}
W(G) &< \frac{1}{6\kappa}n^3 + \big(8.1 + 0.76\,D\big)n^{5/2} \\
&\le \frac{1}{6\kappa}n^3 + Dn^{5/2}
\end{aligned}$$

since D satisfies $8.1 + 0.76\,D \le D$. The theorem follows. □

The following bound on the Wiener index of simple quadrangulations is proved in a similar way. The only difference is that a slightly modified version Q_p of the plane graph F_p is used in the proof. For an even p with $p \ge 4$ let Q_p be the plane graph obtained from a cycle $C = u_0, u_1, \ldots, u_{p-1}, u_0$ of length p, inside which we add a cycle $C' = v_0, v_1, \ldots, v_{p-1}, v_0$ of length p and edges u_iv_i for $i = 0, 1, \ldots, p-1$, inside which we add a vertex z and joint it to all v_i with i even. It is easy to verify that a 3-connected quadrangualation with the insertion of Q_p stays 3-connected. Apart from this difference, the proof of Theorem 3 follows closely that of Theorem 2, hence we omit the proof.

Theorem 3. *Let $\kappa \in \{2,3\}$. Then there exists a constant C such that*

$$W(G) \leq \frac{1}{6\kappa} n^3 + C n^{5/2}$$

for every κ-connected simple quadrangulation G of order n. □

The leading coefficients in the bounds in Theorems 2 and 3 are optimal. This is shown by the graphs in Figures 5, 6 and 7 for 3-connected triangulations, in Figures 8, 9, 10 and 11 for 4-connected triangulations, in Figures 12, 13, 15, 16 and 17 for 5-connected triangulations, in Figures 18 and 19 for 2-connected quadrangulations, and in Figures 20, 21 and 22 for 3-connected quadrangulations,

5 Computational Results and Conjectures

This section contains numerous figures and tables summarizing months of computer searches. None of this would have been possible without the help provided by Plantri, a program that generates triangulations and quadrangulation on numerous surfaces. For each category of problem (triangulations, 4-connected triangulations, 5-connected triangulations, quadrangulations and 3-connected quadrangulations) there is a table, which summarizes the largest Wiener index and remoteness found for a given order in that category, along with "Count", telling how many graphs attain the optimal value. Note that remoteness in this section is *not normalized* to keep the calculations in the domain of integers. In other words, in the Tables we show $(n-1)\rho(G)$ under the name of "Remoteness". Our Wiener index findings match those of [8] for triangulations. The number of isomorphism classes that our code searched matches the numbers in [5], [6], [7], [31], [36], verifying that the values that the search provides are in fact maximal. In each figure below, purple edges represent the repeating pattern and the black node marks a vertex which maximizes the remoteness. The computational evidence suggests that for sufficiently large order, the maximum Wiener index is uniquely realized in every category, while remoteness is not, except for quadrangulations.

5.1 Computational Results for Triangulations

Although the results of [22] made the Wiener index rows of Table 1 obsolete for $n \geq 9$, we still include it to show the multiplicity of maximizers up to $n = 8$ and the remoteness results.

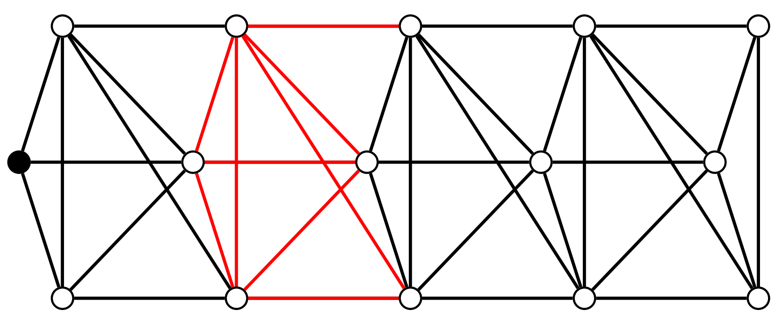

Fig. 5: A triangulation T_n on $n = 3k$ vertices, which maximizes the Wiener index [22] and the remoteness.

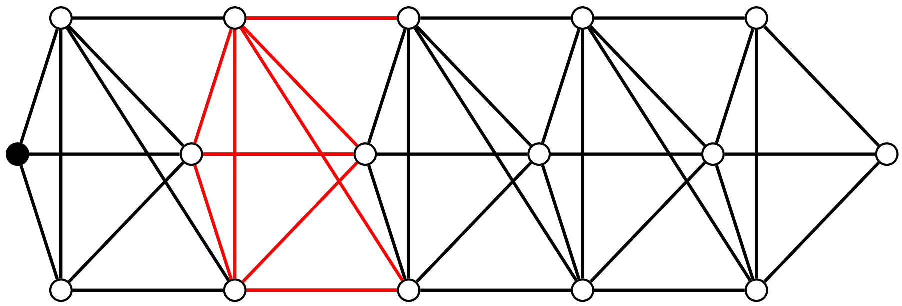

Fig. 6: A triangulation T_n on $n = 3k + 1$ vertices, which maximizes the Wiener index [22] and the remoteness.

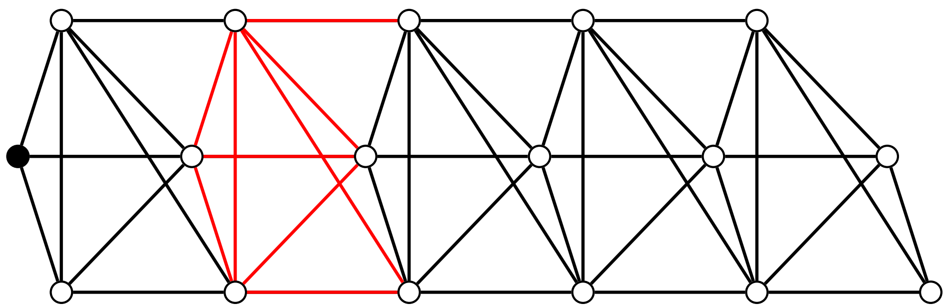

Fig. 7: A triangulation T_n on $n = 3k + 2$ vertices, which maximizes the Wiener index [22] and the remoteness.

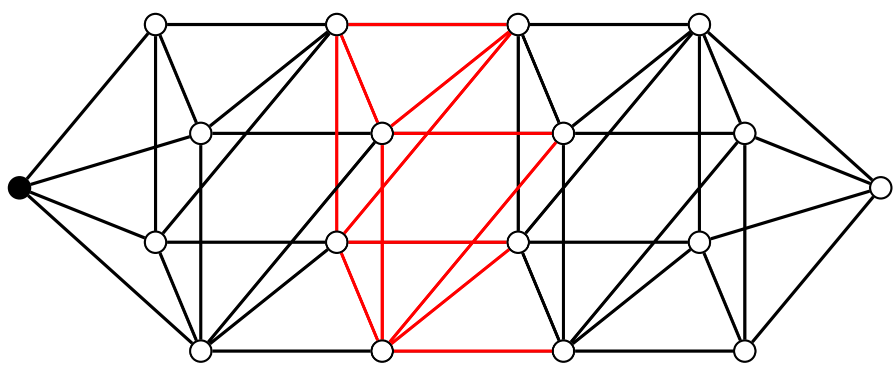

Fig. 8: A 4-connected triangulation T^4_n on $n = 4k + 2$ vertices, which maximizes the remoteness and is conjectured to maximize the Wiener index.

Order	Wiener index	Count	Remoteness	Count
4	6	1	3	1
5	11	1	5	1
6	18	2	7	1
7	27	5	9	4
8	39	2	12	2
9	54	1	15	4
10	72	1	18	17
11	94	1	22	7
12	120	1	26	25
13	150	1	30	107
14	185	1	35	35
15	225	1	40	171
16	270	1	45	743
17	321	1	51	217
18	378	1	57	1199

Tab. 1: A summary of the largest Wiener Index and remoteness among all triangulations on n vertices, and a count for how many isomorphism classes attain this value.

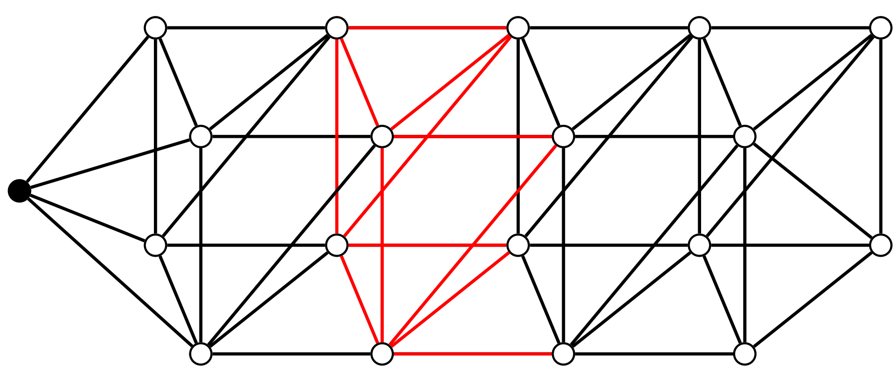

Fig. 9: A 4-connected triangulation T_n^4 on $n = 4k + 3$ vertices, which maximizes the remoteness and is conjectured to maximize the Wiener index.

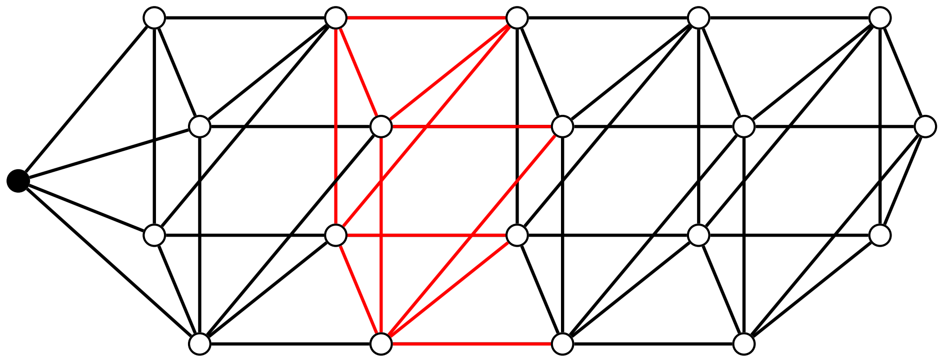

Fig. 10: A 4-connected triangulation T_n^4 on $n = 4k$ vertices, which maximizes the remoteness and is conjectured to maximize the Wiener index.

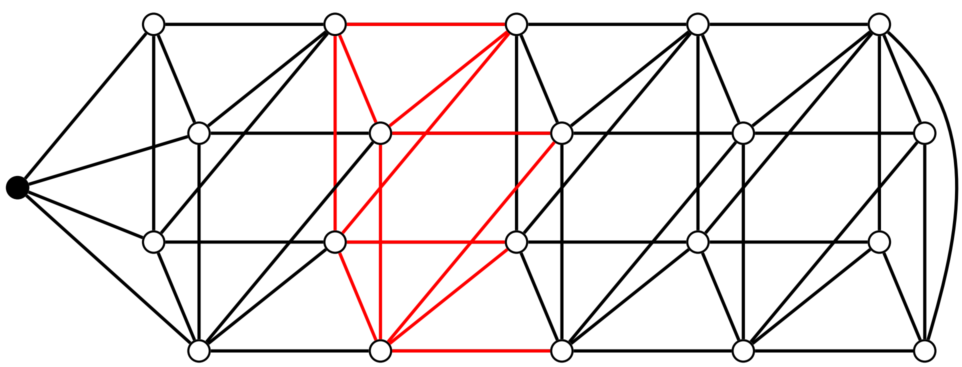

Fig. 11: A 4-connected triangulation T_n^4 on $n = 4k + 1$ vertices, which maximizes the remoteness and is conjectured to maximize the Wiener index.

Order	Wiener Index	Count	Remoteness	Count
6	18	1	6	1
7	27	1	8	1
8	38	2	10	2
9	51	4	12	4
10	68	1	15	4
11	87	1	18	6
12	110	1	21	16
13	135	1	24	50
14	166	1	28	24
15	199	1	32	66
16	238	1	36	186
17	279	1	40	653
18	328	1	45	250
19	379	1	50	879
20	438	1	55	2599
21	499	1	60	9429
22	570	1	66	3313

Tab. 2: A summary of the largest Wiener Index and remoteness among all 4-connected triangulations on n vertices, and a count for how many isomorphism classes attain this value.

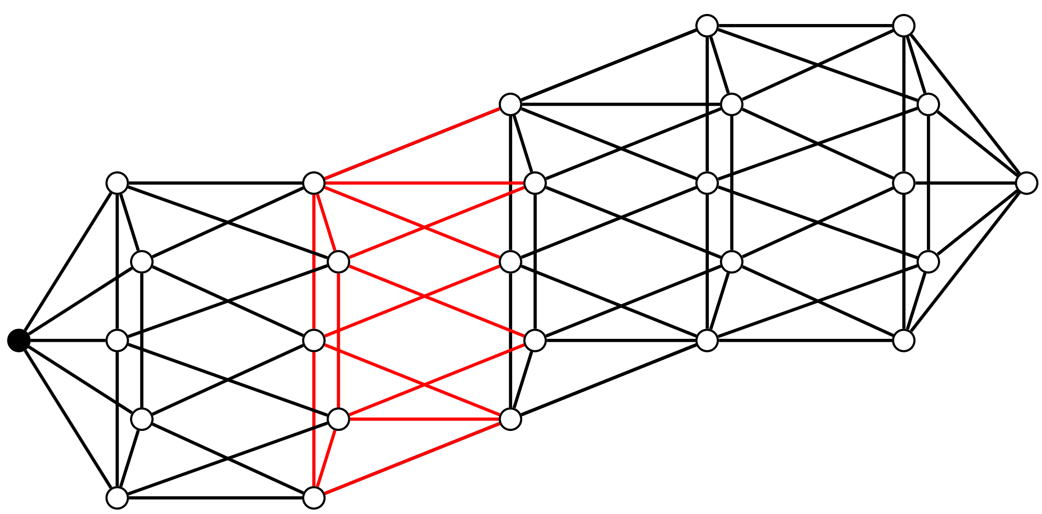

Fig. 12: A 5-connected triangulation T_n^5 on $n = 5k+2$ vertices, which maximizes the remoteness and is conjectured to maximize the Wiener Index.

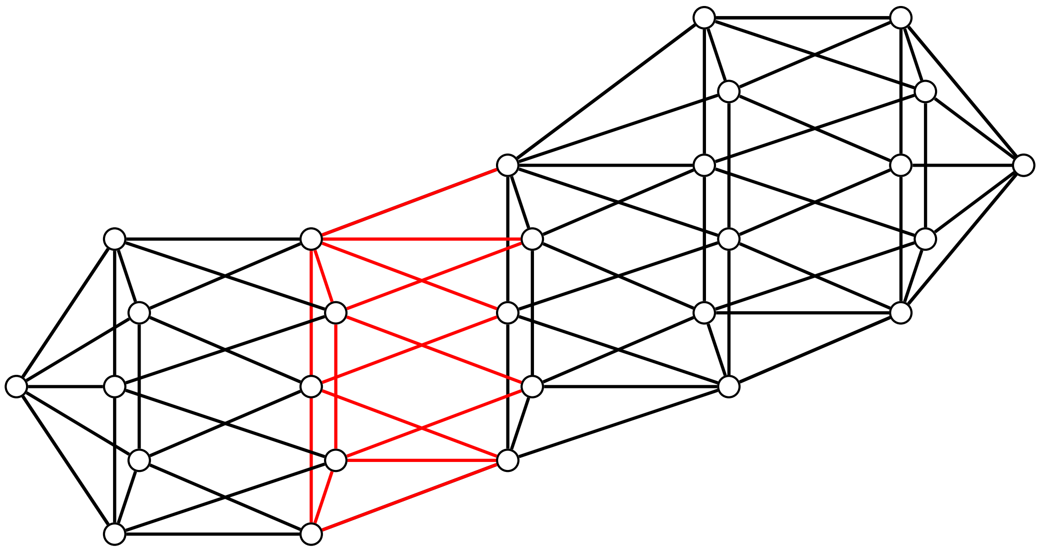

Fig. 13: A 5-connected triangulation T_n^5 on $n = 5k+3$ vertices, which is conjectured to maximize the Wiener Index.

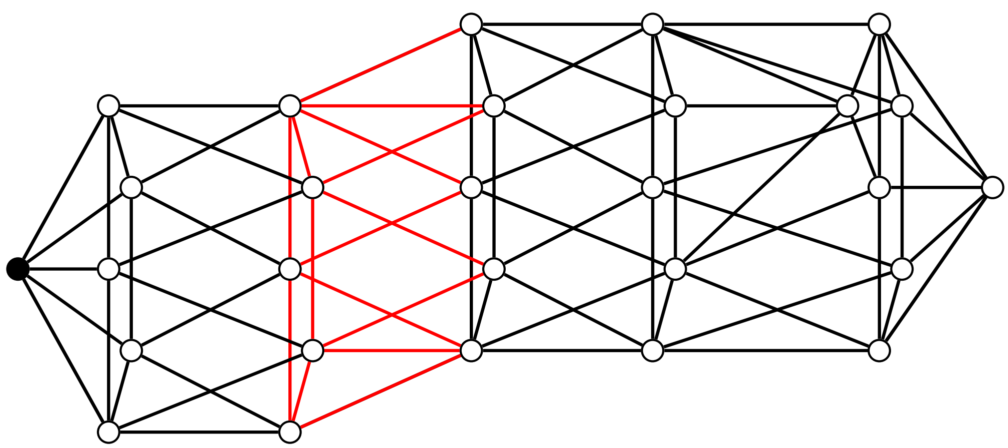

Fig. 14: A 5-connected triangulation T_n^5 on $n = 5k+3$ vertices which maximizes the remoteness.

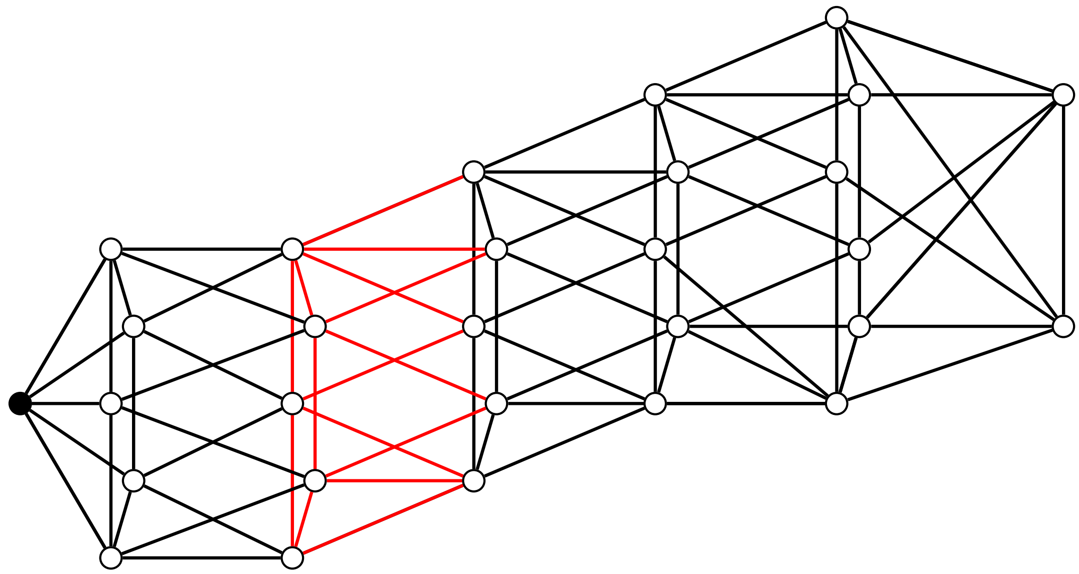

Fig. 15: A 5-connected triangulation T_n^5 on $n = 5k + 4$ vertices, which maximizes the remoteness and is conjectured to maximize the Wiener Index.

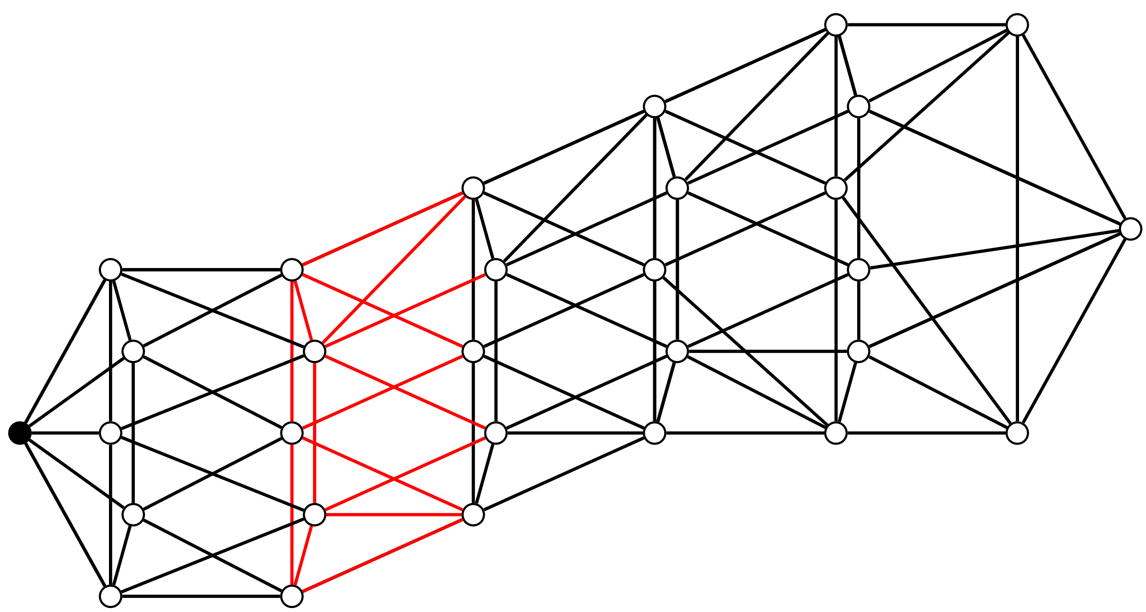

Fig. 16: A 5-connected triangulation T_n^5 on $n = 5k$ vertices, which maximizes the remoteness and is conjectured to maximize the Wiener Index.

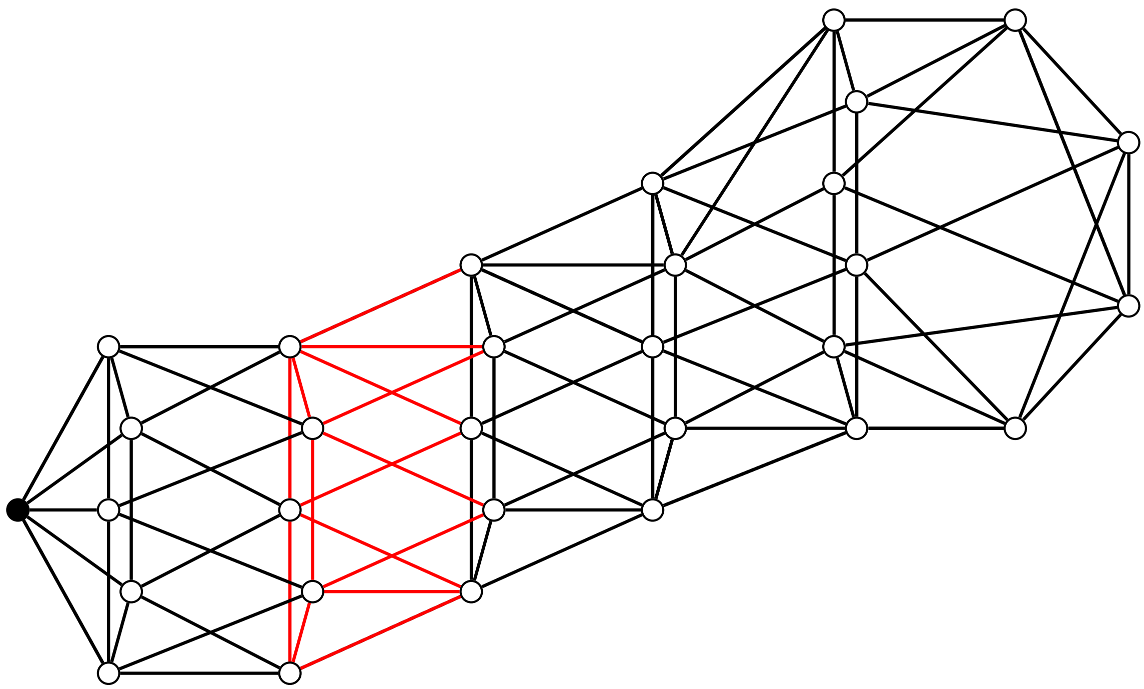

Fig. 17: A 5-connected triangulation T_n^5 on $n = 5k + 1$ vertices which maximizes the remoteness and is conjectured to maximize the Wiener index.

Order	Wiener index	Count	Remoteness	Count
12	108	1	18	1
13	—	0	—	0
14	159	1	23	1
15	189	1	26	1
16	222	2	29	1
17	259	1	34	1
18	300	1	37	1
19	342	1	41	2
20	391	1	45	4
21	444	1	49	9
22	500	2	55	4
23	560	1	59	11
24	630	1	64	36
25	702	1	69	66
26	780	1	74	193
27	867	1	81	39
28	955	1	86	240
29	1053	1	92	805
30	1156	1	98	1470
31	1265	1	104	4327
32	1384	1	112	763

Tab. 3: A summary of the largest Wiener Index and remoteness among all 5-connected triangulations on n vertices, and a count for how many isomorphism classes attain this value.

5.2 Computational Results for Quadrangulations

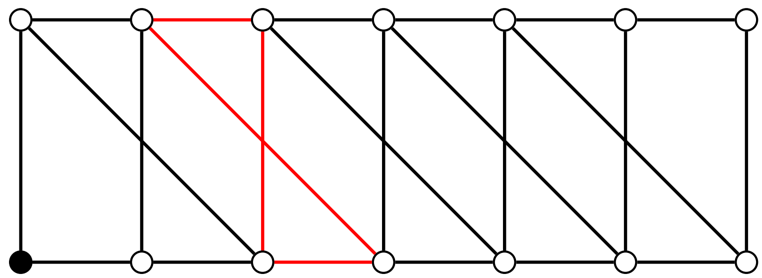

Fig. 18: A quadrangulation Q_n on $n = 2k$ vertices, which maximizes the remoteness and is conjectured to maximize the Wiener index.

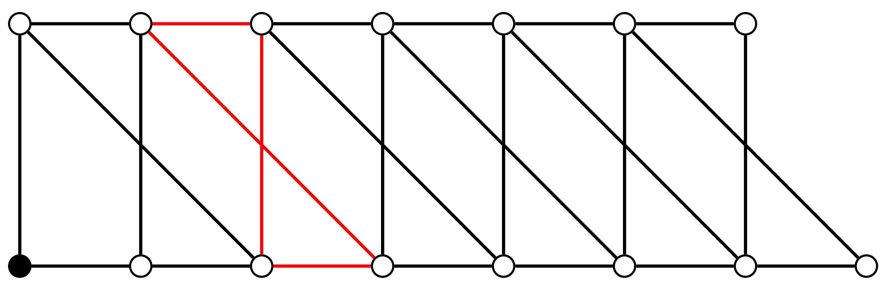

Fig. 19: A quadrangulation Q_n on $n = 2k + 1$ vertices, which maximizes the remoteness and is conjectured to maximize the Wiener index.

Order	Wiener Index	Count	Remoteness	Count
4	8	1	4	1
5	14	1	6	1
6	23	1	9	1
7	34	2	12	1
8	50	1	16	1
9	68	1	20	1
10	93	1	25	1
11	120	1	30	1
12	156	1	36	1
13	194	1	42	1
14	243	1	49	1
15	294	1	56	1
16	358	1	64	1
17	424	1	72	1
18	505	1	81	1
19	588	1	90	1
20	688	1	100	1

Tab. 4: A summary of the largest Wiener Index and remoteness among all quadrangulations on n vertices, and a count for how many isomorphism classes attain this value.

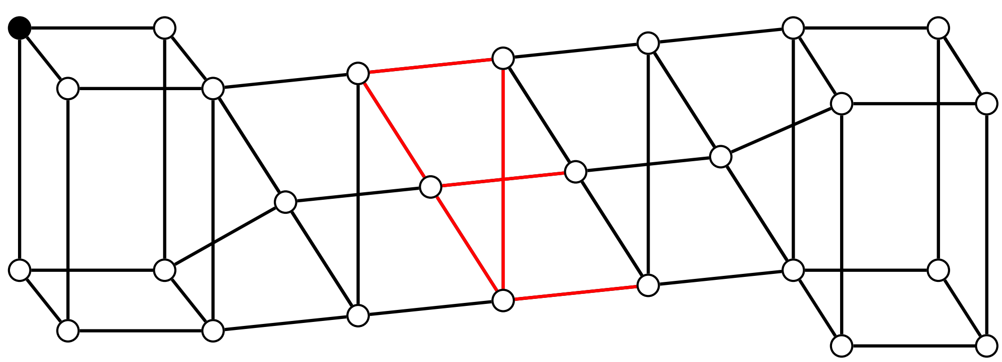

Fig. 20: A 3-connected quadrangulation Q_n^3 on $n = 3k + 14$ vertices, which maximizes the remoteness and is conjectured to maximize the Wiener index.

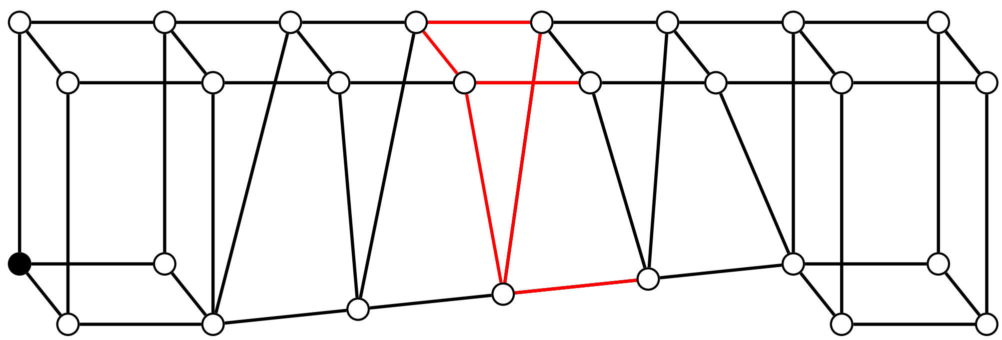

Fig. 21: A 3-connected quadrangulation Q_n^3 on $n = 3k + 15$ vertices, which maximizes the remoteness and is conjectured to maximize the Wiener index.

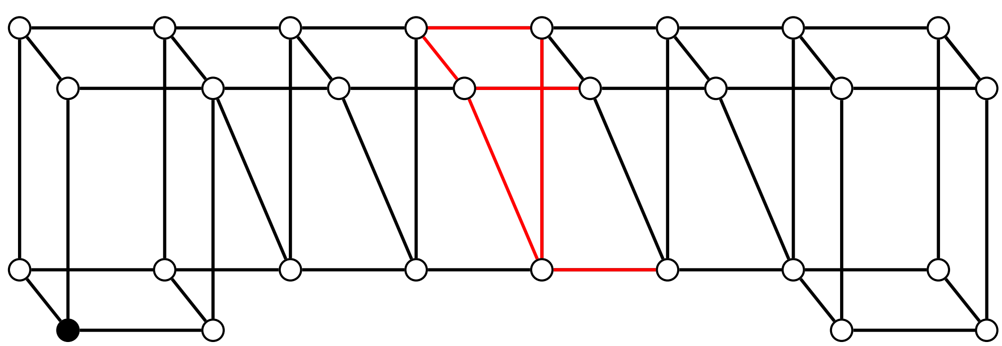

Fig. 22: A 3-connected quadrangulation Q_n^3 on $n = 3k + 16$ vertices which maximizes the remoteness and is conjectured to maximize the Wiener index.

Order	Wiener index	Count	Remoteness	Count
8	48	1	12	1
9	—	0	—	0
10	83	1	17	1
11	106	1	22	1
12	136	1	24	2
13	164	1	29	2
14	201	1	35	2
15	240	1	38	6
16	288	2	44	7
17	344	1	51	5
18	401	1	55	26
19	468	1	62	33
20	544	1	70	22
21	622	1	75	136
22	711	1	83	172
23	810	1	92	97
24	912	1	98	729
25	1026	1	107	923
26	1151	1	117	505
27	1280	1	124	3930
28	1422	1	134	4959

Tab. 5: A summary of the largest Wiener Index and remoteness among all 3-connected quadrangulations on n vertices, and a count for how many isomorphism classes attain this value.

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