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Maximizing Wiener index of graphs with fixed maximum degree

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Abstract

The Wiener index of a graph is the sum of all pairwise distances of vertices of the graph. Fischermann et al [5] characterized the trees which minimize the Wiener index among all trees with the maximum degree at most Δ. They also determined the trees which maximize the Wiener index, but in a much more restricted family of trees which have two distinct vertex degrees only.

In this note, we fully solve the latter problem and determine the trees which maximize the Wiener index among all graphs with the maximum degree Δ. We also determine all graphs whose Wiener index differs by less than $n - \Delta$ from the maximum value.

1 Introduction

The Wiener index is considered as one of the most applicable graph invariant, used as one of the topological indices for predicting physicochemical properties of organic compounds. Its many applications range from the one when the chemist H. Wiener in 1947 used it as a measure for the degree of molecular branching [10, 11] to a recent proposal to use it in

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the prediction of conformational switching in RNA structures [1, 2]. For a recent survey the reader may see [3], and for a more general introduction [6, 9].

In the drug design process, one wants to construct a chemical compound with certain properties, which are quantitatively represented via some topological indices of its molecular graph. The basic idea is to construct chemical compounds from the most common molecules so that the resulting compound has the expected Wiener index. However, before constructing too many different compounds, it may be helpful to a researcher to know in advance what are the extremal values of the Wiener index in a certain class of (molecular) graphs, and also what structural properties of a graph ensure that its Wiener index is close to the extremal values.

It is long known [4] that the path P_n has the maximum Wiener index among the connected graphs on n vertices, while the minimum Wiener index is attained by the star S_n among the trees with n vertices, and, of course, by the complete graph K_n among the connected graph on n vertices. However, as every atom has a certain valency, chemists are often interested in (molecular) graphs having bounded vertex degrees. Thus, it becomes plausible to study the extremal values of the Wiener index among graphs or trees with bounded maximum degree. The trees attaining the minimum Wiener index among trees with the maximum degree at most Δ have been determined by Fischermann et al. in [5] and, independently, by Jelen and Trisch in [7, 8]. Fischermann et al. [5] have also attacked the opposite problem and determined the trees which maximize the Wiener index, but in a much more restricted family of trees which have two distinct vertex degrees only.

We are interested here to find graphs which maximize the Wiener index and also to find graphs whose Wiener index is close to the maximum value. In order to better understand these graphs, we consider the set $\mathcal{G}_{n,\Delta}$, $\Delta \geq 2$, of connected graphs with n vertices having the fixed value of the maximum degree Δ. Otherwise, if we only bound the maximum degree by Δ, the maximum graphs will inevitably be the paths. Still, even with the requirement that a graph contains a vertex of degree Δ, the extremal graphs resemble a pathlike structure.

All graphs in this paper will be finite, simple and undirected, and we follow the standard graph-theoretic terminology, which may be found, for example, in [12]. For a simple graph G, let $d_G(u,v)$ denote the distance between vertices u and v in G. The *distance* $d_G(u)$ of a vertex u is defined as the sum of distances from u to all other vertices of G,

$$d_G(u) = \sum_{v \in V(G)} d_G(u,v).$$

The *Wiener index* W_G of a graph G is then defined as the sum of distances between all distinct pairs of its vertices,

$$W(G) = \frac{1}{2} \sum_{u \in V(G)} d_G(u) = \sum_{\{u,v\} \in \binom{V(G)}{2}} d_G(u,v),$$

where $\binom{V(G)}{2}$ denotes the set of all two element subsets of $V(G)$.

Definition 1 *Let $T_{n,\Delta}$ be the tree on n vertices obtained by taking a path $P_{n-\Delta+1}$ and an empty graph $\overline{K}_{\Delta-1}$, and joining one end-vertex of a path with every vertex of an empty graph.*

Let $T^*_{n,\Delta}$, $n \geq \Delta + 2$, be the tree obtained by taking $T_{n-1,\Delta}$ and attaching a pendent vertex to one of the leaves adjacent to a vertex of degree Δ in $T_{n-1,\Delta}$.

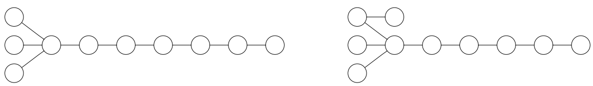

Figure 1: The trees $T_{10,4}$ and $T^*_{10,4}$.

The trees $T_{10,4}$ and $T^*_{10,4}$ are shown in Fig. 1. Further,

Definition 2 *Let $\mathcal{T}_{n,\Delta,m}$, $0 \leq m \leq \binom{\Delta-1}{2}$, be a set of graphs on n vertices obtained by taking a path $P_{n-\Delta+1}$ and any graph with $\Delta - 1$ vertices and m edges, and joining one end-vertex of a path with every vertex of a chosen graph.*

For a graph $G \in \mathcal{T}_{n,\Delta,m}$, the path $P_{n-\Delta+1}$ will be called the spine *of G. The end-vertex of the spine with degree Δ in G will be called the* atlas *of G, while the other end-vertex of the spine with degree 1 in G will be called the* distant leaf *of G.*

Note that $\mathcal{T}_{n,\Delta,0} = \{T_{n,\Delta}\}$.

Our main results are the following

Theorem 1 *For every graph $G \in \mathcal{G}_{n,\Delta}$, it holds that*

$$W(G) \leq W(T_{n,\Delta}),$$

with equality if and only if G is isomorphic to $T_{n,\Delta}$.

Theorem 2 *A graph $G \in \mathcal{G}_{n,\Delta}$ satisfies*

$$W(G) > W(T_{n,\Delta}) - (n - \Delta) \tag{1}$$

if and only if $G \in \mathcal{T}_{n,\Delta,m}$ for some $m < n - \Delta$ or $G \cong T^*_{n,3}$.

The proofs are given in Section 2, while in Section 3 we further discuss the ordering of graphs from $\mathcal{G}_{n,\Delta}$ by their Wiener index on a specific example.

2 The proofs

The small values of Δ in previous theorems represent degenerate cases for which their statements are obvious. Namely, as we work with connected graphs only, the case $\Delta = 1$ becomes possible only when $n = 2$. Similarly, for $\Delta = 2$ the only elements of $\mathcal{G}_{n,\Delta}$ are the path P_n and the cycle C_n.

Thus, we may assume that $\Delta \geq 3$ holds in the sequel. We start our proofs with a very simple lemma.

Lemma 3 *The diameter of a graph $G \in \mathcal{G}_{n,\Delta}$ is at most $n - \Delta + 1$.*

Proof. Let u be a vertex of degree Δ in G, and let P be a path of length $diam(G)$ in G. At least $\Delta - 2$ neighbors of u do not belong to P, since:

- if u belongs to P, then at most two neighbors of u belong to P as well;
- if u does not belong to P, then at most one neighbor of u belongs to P.

Thus, P contains at most $n - \Delta + 2$ vertices, and so, its length is at most $n - \Delta + 1$. ■

Lemma 4 *Let G be a graph in $\mathcal{G}_{n,\Delta}$. Then*

$$d_G(u) \leq \frac{(n - \Delta + 1)(n + \Delta - 2)}{2}$$

holds for any vertex u of G, with equality if and only if $G \in \mathcal{T}_{n,\Delta,m}$ for some m and u is a distant leaf of G.

Proof. Let $ecc(u)$ be the eccentricity of vertex u in G, i.e., the largest distance from u to all other vertices of G. Then the vertices on a path from u to (one of) its farthest vertices must lie at distances 1,2,. . . ,$ecc(u)$ from u, while the distance of the remaining vertices of G is at most $ecc(u)$. Thus,

$$\begin{aligned} d_G(u) &\leq (1 + 2 + \ldots + ecc(u)) + ecc(u)\,(n - 1 - ecc(u)) \\ &= ecc(u)\left(n - \frac{ecc(u)+1}{2}\right). \end{aligned}$$

The function $f(x) = x\left(n - \frac{x+1}{2}\right)$ is strictly increasing for $x < n - \frac{1}{2}$, and so, for $ecc(u) \leq diam(G) \leq n - \Delta + 1 < n - \frac{1}{2}$, it holds that

$$d_G(u) \leq f(ecc(u)) \leq f(n - \Delta + 1) = \frac{(n - \Delta + 1)(n + \Delta - 2)}{2}.$$

The equality holds if and only if $d_G(u) = f(ecc(u))$ and $ecc(u) = diam(G) = n - \Delta + 1$. Thus, there exists exactly one vertex at distance d from u for every $d = 1, 2, \ldots, ecc(u) - 1$, while all other vertices are at distance $ecc(u)$ from u. This shows that $G \in \mathcal{T}_{n,\Delta,m}$ with u being its distant leaf (where m is the number of edges in G among the vertices at distance $ecc(u)$ from u). ■

Taking u to be the distant leaf of $T_{n,\Delta}$ in the previous lemma, from $W(T_{n,\Delta}) = W(T_{n-1,\Delta}) + d_{T(n,\Delta)}(u)$, we get the following recurrence

$$W(T_{n,\Delta}) = W(T_{n-1,\Delta}) + \frac{(n - \Delta + 1)(n + \Delta - 2)}{2}. \tag{2}$$

By either solving this recurrence or by direct calculation, we get that

$$W(T_{n,\Delta}) = \binom{n - \Delta + 2}{3} + (\Delta - 1) \cdot \frac{(n - \Delta + 1)(n - \Delta + 2)}{2} + (\Delta - 1)(\Delta - 2).$$

Now, it is easy to see that the values $W(T_{n,\Delta})$ satisfy

$$W(P_n) = W(T_{n,2}) > W(T_{n,3}) > W(T_{n,4}) > \ldots > W(T_{n,n-1}) = W(S_n).$$

Proof of Theorem 1. Let G be a graph in $\mathcal{G}_{n,\Delta}$. Note first that removing an edge $\{u, v\}$ from G strictly increases its Wiener index: the distance between any pair of vertices does not decrease, while the distance between u and v strictly increases. Thus, for any spanning tree T of G it holds that

$$W(G) \leq W(T),$$

with equality if and only if $G = T$. As any graph in $\mathcal{G}_{n,\Delta}$ has a spanning tree with the same maximum degree Δ, we may thus in the sequel restrict our proof to such trees only.

We shall now prove the theorem by induction on n. For $n = \Delta + 1$, there exists only one tree with $\Delta + 1$ vertices and the maximum degree Δ: the star $K_{1,\Delta} \cong T_{\Delta+1,\Delta}$. Thus, the statement holds in this case.

Suppose now that $T_{n,\Delta}$, $n \geq \Delta + 1$, attains the maximum Wiener index in $\mathcal{G}_{n,\Delta}$ and let T be any tree in $\mathcal{G}_{n+1,\Delta}$.

The tree T contains a leaf q whose removal does not decrease the maximum degree of T. Otherwise, T would contain only one vertex of degree Δ and all leaves would be adjacent to that vertex, yielding that T would be isomorphic to a star, which is a contradiction with $n + 1 \geq \Delta + 2$.

Let p be the unique neighbor of q in T. For any vertex u of T it holds that

$$d_T(u, q) = d_{T-q}(u, p) + 1,$$

while the distance between all other pairs of vertices of $T - q$ remains intact. Thus, it holds that

$$\begin{aligned} W(T) &= \sum_{\{u,v\} \in \binom{V(T)}{2}} d_T(u, v) \\ &= \sum_{\{u,v\} \in \binom{V(T-q)}{2}} d_{T-q}(u, v) + \sum_{u \in V(T-q)} d_T(u, q) \\ &= W(T - q) + \sum_{u \in V(T-q)} (d_{T-q}(u, p) + 1) \\ &= W(T - q) + d_{T-q}(p) + n. \end{aligned}$$

From the inductive hypothesis it follows that

$$W(T - q) \leq W(T_{n,\Delta}) \tag{3}$$

and from Lemma 4 it follows that

$$d_{T-q}(p) \leq \frac{(n - \Delta + 1)(n + \Delta - 2)}{2}. \tag{4}$$

Thus,

$$W(T) \leq W(T_{n,\Delta}) + \frac{(n - \Delta + 1)(n + \Delta - 2)}{2} + n = W(T_{n+1,\Delta})$$

by (2).

The equality holds above if and only if the equality holds in (3) and (4). Then we have, by the inductive hypothesis, that $T - q \cong T_{n,\Delta}$ and that p is a distant leaf of $T_{n,\Delta}$. This shows that $T \cong T_{n+1,\Delta}$, and thus, $T_{n+1,\Delta}$ is the sole graph in $\mathcal{G}_{n+1,\Delta}$ that attains the maximum value of the Wiener index. ■

Lemma 5 *Let $G \in \mathcal{G}_{n,\Delta}$. If $\Delta < n-1$, then there exists a vertex u of G such that $G - u \in \mathcal{G}_{n-1,\Delta}$.*

Proof. Let v be a vertex of degree Δ in G and let T be a spanning tree of G containing all edges incident with v. Since $\Delta < n-1$, there exists a leaf u of T not adjacent to v. Then $G - u \in \mathcal{G}_{n-1,\Delta}$, as it contains a connected subgraph $T - u$ and v has degree Δ in $G - u$. ■

Proof of Theorem 2. Suppose first that $G \in \mathcal{T}_{n,\Delta,m}$ for some $m < n - \Delta$. The leaves adjacent to the vertex of degree Δ in $T_{n,\Delta}$ are all distance two apart from each other. However, m pairs of them are joined by edges in G, and so

$$W(G) = W(T_{n,\Delta}) - m > W(T_{n,\Delta}) - (n - \Delta).$$

Further, if $G \cong T^*_{n,3}$ (and so $\Delta = 3$) then it is easy to see that

$$W(T^*_{n,3}) = W(T_{n,3}) - (n-5) > W(T_{n,3}) - (n-3).$$

We will prove the opposite direction by induction on n for any fixed Δ. For $n = \Delta + 1$, we have that (1) implies that $W(G) = W(T_{n,\Delta})$ and it follows from Theorem 1 that $G \cong T_{n,\Delta} \in \mathcal{T}_{n,\Delta,0}$ in this case.

Suppose now that this direction has been proved for all connected graphs with less than n vertices for some $n > \Delta + 1$. Let $G \in \mathcal{G}_{n,\Delta}$ be a graph such that (1) holds. By Lemma 5, let u be the vertex of G such that $G - u \in \mathcal{G}_{n-1,\Delta}$. When u is removed from G, the distance between any two vertices of $G - u$ does not decrease, and so

$$W(G) \leq W(G-u) + d_G(u).$$

From Lemma 4, we have that

$$d_G(u) \leq \frac{(n-\Delta+1)(n+\Delta-2)}{2}.$$

If an equality holds above, then, by the same lemma, $G \in \mathcal{T}_{n,\Delta,m}$ for some m with u being its distant leaf. From the first part of this proof, it holds that $W(G) = W(T_{n,\Delta}) - m$ and then from (1) it follows that $m < n - \Delta$.

Thus, in the rest of the proof we may suppose that

$$d_G(u) \leq \frac{(n-\Delta+1)(n+\Delta-2)}{2} - 1.$$

Now, if $G - u$ does not belong to $\mathcal{T}_{n-1,\Delta,m}$ for any $m < (n-1) - \Delta$, then by the inductive hypothesis it holds that

$$W(G-u) \leq W(T_{n-1,\Delta}) - (n-1-\Delta).$$

Therefore,

$$\begin{aligned} W(G) &\leq W(G-u) + d_G(u) \\ &\leq W(T_{n-1,\Delta}) - (n-1-\Delta) + \left(\frac{(n-\Delta+1)(n+\Delta-2)}{2} - 1\right) \\ &\leq W(T_{n,\Delta}) - (n-\Delta), \end{aligned}$$

which is in contradiction with (1).

Next, suppose that $G - u$ belongs to $\mathcal{T}_{n-1,\Delta,m}$ for some $m < (n-1) - \Delta$, so that

$$W(G-u) = W(T_{n-1,\Delta}) - m \leq W(T_{n-1,\Delta}).$$

We divide the rest of the proof in two cases, depending on the type of neighbors of u.

First, if u is adjacent to a leaf adjacent to the atlas of $G - u$, then it is at distance at most 3 from other atlas neighbors, and at distances at most $2, 3, \ldots, n - \Delta + 1$ from the vertices in the spine of $G - u$. Thus,

$$\begin{aligned} d_G(u) &\leq 1 + (\Delta-2)\cdot 3 + [2 + 3 + \ldots + (n-\Delta+1)] \\ &= \frac{(n-\Delta)(n-\Delta+3)}{2} + 3\Delta - 5. \end{aligned}$$

The equality holds here if $m = 0$ and u has no other neighbors in G. Then

$$\begin{aligned} W(G) &\leq W(G-u) + d_G(u) \\ &\leq W(T_{n-1,\Delta}) + \frac{(n-\Delta)(n-\Delta+3)}{2} + 3\Delta - 5 \\ &= W(T_{n,\Delta}) - \frac{(n-\Delta+1)(n+\Delta-2)}{2} + \frac{(n-\Delta)(n-\Delta+3)}{2} + 3\Delta - 5 \\ &= W(T_{n,\Delta}) - n(\Delta-2) + (\Delta^2 - 4). \end{aligned} \tag{5}$$

If $\Delta = 3$ the above inequality (5) reads

$$W(G) \leq W(T_{n,3}) - (n-5).$$

The equality holds if and only if $G - u \cong T_{n-1,3}$ and u is a leaf in G, i.e., if and only if $G \cong T^*_{n,3}$. If the inequality is strict, then (1) implies that $W(G) = W(T_{n,3}) - (n-4)$. However, if u is adjacent to another vertex of $G - u$, then $d_G(u)$ becomes less than its upper bound by at least two, and in such case $W(G) \leq W(T_{n,3}) - (n-3)$, which is in contradiction with (1). Similarly, if $G - u \ncong T_{n-1,3}$, then it must hold that $W(G-u) = W(T_{n-1,3}) - 1$, and by the inductive hypothesis, $G - u$ belongs to $\mathcal{T}_{n-1,3,1}$. In that case, the distance from u to the other atlas neighbor becomes two instead of three, and thus, $d_G(u)$ becomes less than its upper bound by at least one, so that we again obtain $W(G) \leq W(T_{n,3}) - (n-3)$, a contradiction with (1).

Further, for $4 \leq \Delta \leq n-2$ we have that

$$-n(\Delta - 2) + (\Delta^2 - 4) \leq -n + \Delta,$$

and, thus, (5) becomes $W(G) \leq W(T_{n,\Delta}) - (n - \Delta)$, which is in contradiction with (1).

On the other hand, if u is adjacent to the spine vertices only, let d be the distance in G from the atlas to the nearest spine neighbor of u. Note that $0 \leq d \leq n - \Delta - 2$, since u may not be a distant leaf. Thus, its distance to the atlas is $d+1$, the distance to the atlas neighbors (not the one on the spine) is $d+2$, while the distance to the spine vertices goes from 1 to $d+1$ towards the atlas, and from 1 to $n - \Delta - d$ towards the distant leaf of $G - u$. Therefore,

$$\begin{aligned} d_G(u) &\leq (\Delta-1)(d+2) + [1+2+\ldots+(d+1)] + [2+3+\ldots+(n-\Delta-d)] \\ &= (\Delta-1)(d+2) + \frac{(d+1)(d+2)}{2} + \frac{(n-\Delta-d+2)(n-\Delta-d-1)}{2} \\ &= d^2 - d(n-2\Delta) + \left(\frac{n^2}{2} + \frac{\Delta^2}{2} - n\Delta + \frac{n}{2} + \frac{3\Delta}{2} - 2\right) \\ &= f_{n,\Delta}(d). \end{aligned}$$

The bound $f_{n,\Delta}(d)$ is a quadratic function in d, which, having in mind that the range of d is $[0, n-\Delta-2]$, reaches its maximum at $d = n - \Delta - 2$. Thus,

$$W(G) \leq W(G-u) + d_G(u)$$

$$\begin{aligned}
&\leq W(T_{n-1,\Delta}) + \frac{n^2-\Delta^2-3n+3\Delta}{2} + 2 \\
&= W(T_{n,\Delta}) - \frac{(n-\Delta+1)(n+\Delta-2)}{2} + \frac{n^2-\Delta^2-3n+3\Delta}{2} + 2 \\
&= W(T_{n,\Delta}) - (n-3) \\
&\leq W(T_{n,\Delta}) - (n-\Delta),
\end{aligned}$$

which is also in contradiction with (1). ■

3 Further observations

Let $T^{\dagger}_{n,\Delta}$ be the graph obtained from $T_{n,\Delta}$ by joining two atlas neighbors with an edge: one that is a leaf and the other one that belongs to the spine. It holds that

$$W(T^{\dagger}_{n,\Delta}) = W(T_{n,\Delta}) - (n-\Delta).$$

Further, let $T^{\diamond}_{n,\Delta}$ be the graph obtained from $T_{n-1,\Delta}$ by duplicating its distant leaf. We have that

$$W(T^{\diamond}_{n,\Delta}) = W(T_{n,\Delta}) - (n-3).$$

The graphs $T^{\dagger}_{10,4}$ and $T^{\diamond}_{10,4}$ are shown in Fig. 2.

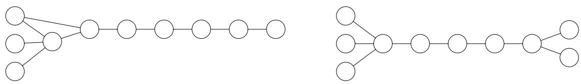

Figure 2: The trees $T^{\dagger}_{10,4}$ and $T^{\diamond}_{10,4}$.

In the list of graphs from $\mathcal{G}_{n,\Delta}$ ordered by the non-increasing value of the Wiener index, the graphs from $\mathcal{T}_{n,\Delta,m}$, $m < n-\Delta$, will always appear first. However, from the proof of Theorem 2 it is also evident that the graphs $T^{\dagger}_{n,\Delta}$, $T^{\diamond}_{n,\Delta}$ and $T^{*}_{n,\Delta}$ will appear high in the list. Such a list for $(n,\Delta) = (10,4)$, containing the first thirty graphs, is shown in Table 1.

The first thing we may notice from Table 1 is a more-or-less general conclusion that, whatever the set of graphs is given, maximizing the Wiener index means finding the structure with the largest diameter, while minimizing the Wiener index means finding the structure with the least diameter. This is in accordance not only with the results proved here, but also with the results of [5, 7, 8] both on minimizing the Wiener index of trees with maximum degree at most Δ and on maximizing the Wiener index in the restricted set of trees with two distinct vertex degrees only. These principles also emerge from the old results stating that the paths have the maximum Wiener index among the connected graphs, while the complete graphs and the stars minimize the Wiener index among the connected graphs and among the trees, respectively.

Further, the graphs in Table 1 share some prominent similarities to $T_{n,\Delta}$:

- their diameter is very close to the upper bound from Lemma 3, equal to either 6 or 7 in all thirty graphs,
- a vertex of degree Δ is found near the end of the longest path, at the distance 1 or 2 from its end.

The number of graphs in $\mathcal{G}_{n,\Delta}$ is much larger than the maximum Wiener index, and so there will be many graphs having the same Wiener index. In order to follow the change in the Wiener index, we may consider a lattice of graphs, where the graphs are positioned in levels according to their Wiener index, with two graphs being related if one can be obtained from another by a small perturbation. Theorems 1 and 2 thus describe the top of this lattice. At least close to the lattice top, the Wiener index will in most cases decrease by one by adding an edge between the leaves having a common neighbor. However, it will also make bigger changes, especially at the lower levels when the graphs become denser.

In the case of trees with maximum degree at most Δ, the bottom of corresponding lattice is very well described in the papers [5, 7, 8]. However, we have to leave as an open problem the characterization of the graphs from $\mathcal{G}_{n,\Delta}$ having the minimum Wiener index.

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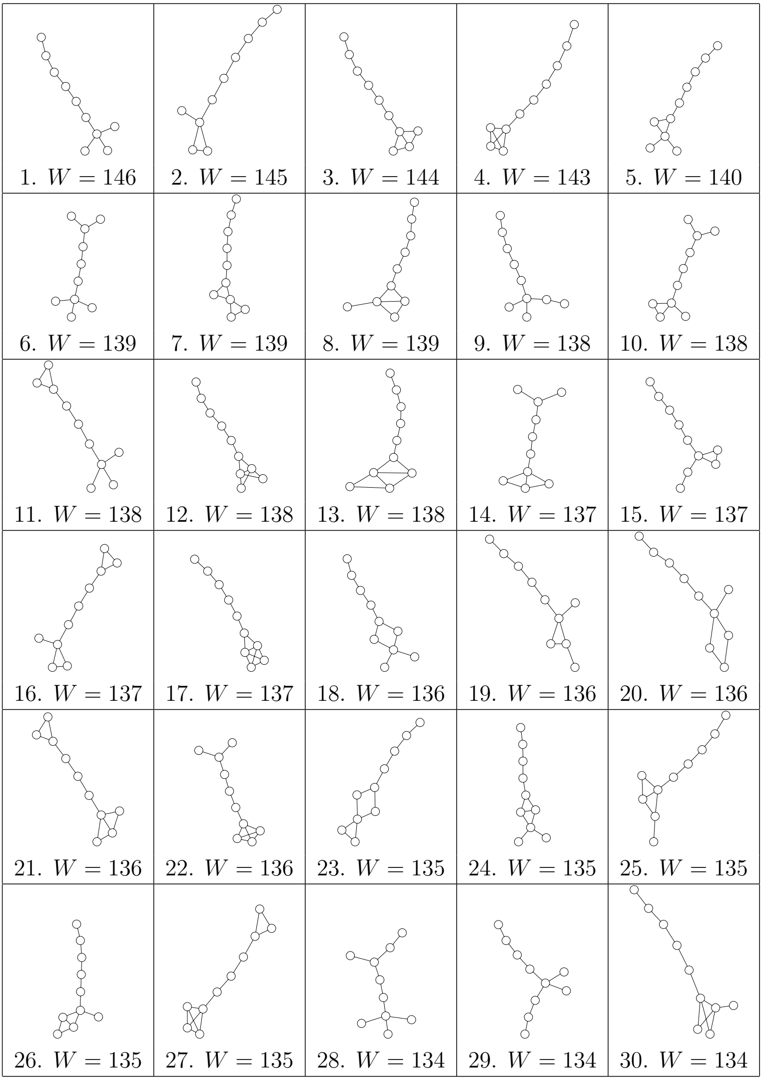

Table 1: The first thirty graphs with 10 vertices and the maximum degree 4, ordered by the non-increasing value of the Wiener index