Wiener Index, Kirchhoff Index in Graphs with Given Girth and Maximum Degree

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Abstract

The Wiener index is defined as the sum of all distances between all pairs of unordered vertices in a connected graph. Replacing the ordinary distance by resistance distance in Wiener index, one gets the Kirchhoff index which is defined as the sum of all resistance distances between all pairs of unordered vertices in a connected graph. This two distance-based invariants are viewed as important measures associated with a (molecular) network which correlate nicely to chemical and physical properties, and have been studied extensively in the past decades. In this paper, we determine respectively the graphs which have the maximum Wiener index and Kirchhoff index among all connected graphs of order n with girth g and maximum degree Δ . The corresponding extremal graphs are characterized completely.

1 Introduction

Let G = (V(G), E(G)) be a graph consisting of a finite set V(G) of vertices and a finite set E(G) of edges. The degree $d_G(v)$ of a vertex $v \in V(G)$ is the

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number of vertices adjacent to v. The neighborhood $N_G(v)$ of v is the set of vertices adjacent to v in graph G. The maximum vertex degree of graph G, denoted by $\Delta(G)$ or Δ for short, is the maximum degree of its vertices. The girth g = g(G) of a graph G is equal to the length of a shortest cycle in G. The distance $d_G(u, v)$ between a pair of vertices u and v in a connected graph G is the numbers of edges of a shortest path connecting u and v. As usual, we denote the path, cycle and star on n vertices by P_n , C_n and $K_{1,n-1}$, respectively. If $P = uu_1u_2 \dots u_\ell$ is an induced path of length ℓ in G such that $d_G(u_\ell) = 1$, $d_G(u_1) = d_G(u_2) = \dots = d_G(u_{\ell-1}) = 2$ and $d_G(u) \geq 2$, then we call P a pendant path with u as its origin and u_ℓ as its terminus. If $\ell = 1$, the the pendant path P is called the pendant edge.

A topological index is a number to a (molecular) graph which remains unchanged under graph isomorphisms. Distance-based topological indices were investigated intensively in the past decades. Among the category of distance-based topological indices, the Wiener index is regarded as the oldest and most thoroughly studied invariant related to molecular branching. It was introduced in 1947 by the chemist H. Wiener [24] who observed it correlation with the chemical, physical and biological properties of certain molecules and molecular compounds. The Wiener index W(G) of a graph G is defined as the distances between all unordered pairs of vertices of a connected graph G. That is

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

where D(u|G) denotes the sum of distances between u and all other vertices of G, namely,

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

The resistance distance was first introduced by Klein and Randić [13] as a new distance function in 1993. For two vertices u and v in G, the resistance distance $r_G(u, v)$ between u and v is defined as the effective resistance between u and v in the electrical network for which nodes correspond to the vertices of G and each edge of G is replaced by a resistor of unit resistance.

Analogy to the Wiener index, the Kirchhoff index of a graph G is defined as [13]

$$Kf(G) = \sum_{\{u,v\} \subseteq V(G)} r_G(u,v) = \frac{1}{2} \sum_{u \in V(G)} R(u|G),$$

where R(u|G) denotes the sum of resistance distances between u and all other vertices of G, namely,

$$R(u|G) = \sum_{v \in V(G)} r_G(u, v)$$

Nowadays, due to their extensive applications there are still much interesting work related to Wiener index and Kirchhoff index being reported constantly. Some recent developments on Wiener index and Kirchhoff index can be referred to [1-10, 12, 14-18, 21-23]. The present paper was motivated by a recent article of Horoldagva *et al.* [11] on average eccentricity, where they obtained the maximum average eccentricity of graphs of order *n* in terms of girth and maximum degree. We take further the line of this extremal problem by investigating the Wiener index and Kirchhoff index for graphs with given order, girth and maximum degree.

The rest of the paper is organised as follows. In Section 2, we first recall some necessary known results for Wiener index and Kirchhoff index and then give some lemmas and definitions which will be used in the proof of the main results in the subsequent sections. In Section 3, we determine the maximum Wiener index among all n order connected graphs with given girth and maximum degree. In Section 4, we study the maximum Kirchhoff index in graphs of given order, grith and maximum degree. In the concluding Section 5 we pose some open problems arising from our investigations.

2 Preliminaries

In what follows we recall some basic known results on Wiener index and Kirchhoff index, and then give several lemmas and definitions which will be needed in the subsequent considerations.

It is well-known that $d_G(u, v) \ge r_G(u, v)$ with equality if and only if there is a unique path connecting vertices u and v in graph G. So, it is clear that Kf(G) = W(G) when G is a tree.

Let P_n be the path of n vertices from the vertex u to the vertex v. The most basic upper bound of W(G) states that, if G is a connected graph of order n, then $W(G) \leq W(P_n)$ with the equality if and only if $G \cong P_n$. It is known that

$$W(P_n) = Kf(P_n) = \frac{n(n^2 - 1)}{6}$$

and

$$D(v|P_n) = R(v|P_n) = D(u|P_n) = R(u|P_n) = \frac{n(n-1)}{2}.$$

Let $K_{1,n-1}$ be the star with *n* vertices. Then we have

$$W(K_{1,n-1}) = Kf(K_{1,n-1}) = (n-1)^2$$

Let $C_n = v_1 v_2 \dots v_n$ be the *n*-vertex cycle with vertices labeled consecutively by v_1, v_2, \dots, v_n . Then it is known that

$$d_{C_n}(v_i, v_j) = \min\{j - i, n - j + i\}$$

and

$$r_{C_n}(v_i, v_j) = \frac{(j-i)[n-(j-i)]}{n},$$

where $1 \leq i < j \leq n$. It is easy to verify that $\max\{d_{C_n}(v_i, v_j) : v_i, v_j \in V(C_n)\} = \lfloor \frac{n}{2} \rfloor$ and $\max\{r_{C_n}(v_i, v_j) : v_i, v_j \in V(C_n)\} = \frac{1}{n} \lfloor \frac{n}{2} \rfloor \lceil \frac{n}{2} \rceil$ with equality if and only $j - i = \lfloor \frac{n}{2} \rfloor$. Moreover, for any $v \in V(C_n)$ we have

$$D(v|C_n) = \begin{cases} \frac{n^2 - 1}{4}, & n \text{ is odd,} \\ \frac{n^2}{4}, & n \text{ is even} \end{cases} \text{ and } R(v|C_n) = \frac{n^2 - 1}{6}.$$

The Wiener index and Kirchhoff index of cycle C_n can be given respectively by

$$W(C_n) = \begin{cases} \frac{n(n^2 - 1)}{8}, & n \text{ is odd,} \\ \frac{n^3}{8}, & n \text{ is even} \end{cases} \text{ and } Kf(C_n) = \frac{n^3 - n}{12}.$$

The following result is well-known in the literature.

Lemma 2.1. Let v be a cut vertex of a graph G, u and w the vertices coming from different components which arise upon deletion of v. Then we have $d_G(u, w) = d_G(u, v) + d_G(v, w)$ and $r_G(u, w) = r_G(u, v) + r_G(v, w)$.

Let v be a cut vertex of a graph G such that G-v consists two disjoint subgraphs $G_1 - v$ and $G_2 - v$, then we denote the graph G by G_1vG_2 . From Lemma 2.1, one can derive Lemma 2.2 immediately.

Lemma 2.2. [19, 20, 25] Let G_1vG_2 be the graph defined as above. Then

- (i) $W(G_1vG_2) = W(G_1) + W(G_2) + (|V(G_2)| 1)D(v|G_1) + (|V(G_1)| 1)D(v|G_2).$
- (ii) $Kf(G_1vG_2) = Kf(G_1) + Kf(G_2) + (|V(G_2)| 1)R(v|G_1) + (|V(G_1)| 1)R(v|G_2).$

By the definitions of Wiener index and Kirchhoff index, we can see that this two indices are monotonically increasing when we delete an edge such that the resulting graph remains connected.

Lemma 2.3. Let G be a connected graph of order n. If G - e is still connected, then we have W(G - e) > W(G) and Kf(G - e) > Kf(G).

Lemma 2.4. Let G be the graph obtained from a graph H and a tree $T_k \not\cong P_k$ on k vertices by identifying one vertex of H and one vertex of T_k such that $V(H) \cap V(T_k) = \{v\}$, namely $G = HvT_k$. We modify G to obtain G' by replacing T_k with P_k , i.e., G' is obtained from H and a path P_k by identifying one pendant vertex of P_k with the vertex v of H. Then we have W(G') > W(G) and Kf(G') > Kf(G).

Proof. For a tree $T_k \not\cong P_k$ with k vertices, it is known that $W(P_k) > W(T_k)$ and $D(v|P_k) > D(w|T_k)$, where v is a pendant vertex of P_k and w is an arbitrary vertex of T_k . Then, according to Lemma 2.2, it follows that

$$W(G) = W(H) + W(T_k) + (|V(H)| - 1)D(v|T_k) + (k - 1)D(v|H),$$

$$W(G') = W(H) + W(P_k) + (|V(H)| - 1)D(v|P_k) + (k - 1)D(v|H).$$

Thus, we have

$$W(G') - W(G) = W(P_k) - W(T_k) + (|V(H)| - 1)(D(v|P_k) - D(v|T_k)) > 0,$$

which leads to W(G') > W(G).

Analogously, by Lemma 2.2 one can get Kf(G') > Kf(G).

Lemma 2.5. Let G be the graph obtained from a graph H by attaching two pendant paths $P = uu_1u_2...u_s$ and $Q = vv_1v_2...v_t$ to u and v in H, respectively. Let $G' = G - vv_1 + v_1u_s$ and $G'' = G - uu_1 + u_1v_t$.

- (i) If $D(v|H) \le D(u|H)$, then W(G') > W(G). If $D(v|H) \ge D(u|H)$, then W(G'') > W(G).
- (ii) If $R(v|H) \le R(u|H)$, then Kf(G') > Kf(G). If $R(v|H) \ge R(u|H)$, then Kf(G'') > Kf(G).

Proof. According to Lemma 2.2, one can get that

$$W(G) = W(PuH) + W(Q) + (|V(Q)| - 1)D(v|PuH) + (|V(PuH)| - 1)D(v|Q)$$
(1)

$$=W(QvH) + W(P) + (|V(P)| - 1)D(u|QvH) + (|V(QvH)| - 1)D(u|P),$$
(2)

$$W(G') = W(PuH) + W(Q) + (|V(Q)| - 1)D(u_s|PuH) + (|V(PuH)| - 1)D(v|Q),$$
(3)

$$W(G'') = W(QvH) + W(P) + (|V(Q)| - 1)D(v_t|QuH) + (|V(PvH)| - 1)D(u|P).$$
(4)

If $D(v|H) \leq D(u|H)$, then it is easy to see that $D(v|PuH) < D(u_s|PuH)$. Thus, from (1) and (3) we have

$$W(G') - W(G) = (|V(Q)| - 1)(D(u_s|PuH) - D(v|PuH)) > 0,$$

which means that W(G') > W(G).

On the other hand, if $D(v|H) \geq D(u|H)$, then it is obvious that

 $D(u|QvH) < D(v_t|QuH)$. Thus, from (2) and (4) we have

$$W(G'') - W(G) = (|V(Q)| - 1)(D(v_t|QuH) - D(u|QvH)) > 0,$$

which implies that W(G'') > W(G). We have thus proved the statement (i).

Using Lemma 2.2, the proof of the second part of this lemma follows in a similar manner.



Figure 1. The graphs $H^1_{n,g,\Delta}$, $H^2_{n,g,\Delta}$ and $H^3_{n,g,\Delta}$.

Let $\mathscr{G}_n(g, \Delta)$ be the set of all simple connected graphs of order n with the girth g and maximum degree Δ . Then it must have $g + \Delta \leq n + 2$. Denote by $H^1_{n,g,\Delta}$ the graph obtained from C_g by attaching $\Delta - 2$ pendant edges and one pendant path of length $n - g - \Delta + 2$ to two opposite vertices of C_g , respectively. Denote by $H^2_{n,g,\Delta}$ the graph obtained from C_g by attaching $\Delta - 3$ pendant edges and one pendant path of length $n - g - \Delta + 3$ to one vertex of C_g . Let $H^3_{n,g,\Delta}$ be the graph obtained by identifying two pendant vertices of the path $P_{n-g-\Delta+2}$ with the center of star $K_{1,\Delta-1}$ and one vertex of cycle C_g , respectively. See Figure 1 for the graphs $H^1_{n,g,\Delta}$, $H^2_{n,g,\Delta}$ and $H^3_{n,g,\Delta}$. There is just one graph obtained by attaching $\Delta - 2$ pendant vertices to a vertex of C_g in $\mathscr{G}_n(g, \Delta)$ when $\Delta = n - g + 2$. Thus, we consider in this paper that $g \geq 3$ and $3 \leq \Delta \leq n-g+1$. It is easy to see that $H^1_{n,g,\Delta}, H^2_{n,g,\Delta} \in \mathscr{G}_n(g,\Delta)$ for $3 \leq \Delta \leq n-g+1$ and $H^3_{n,g,\Delta} \in \mathscr{G}_n(g,\Delta)$ for $3 \leq \Delta \leq n-g$.

3 Maximum Wiener index of graphs with given girth and maximum degree

In this section, we determine the maximum Wiener index among all graphs in $\mathscr{G}_n(g, \Delta)$.

Theorem 3.1. Let G be a graph in $\mathscr{G}_n(g, \Delta)$.

- (i) If g = 3 and $\Delta \ge 3$, then $W(G) \le W(H^2_{n,3,\Delta})$ with equality iff $G \cong H^2_{n,3,\Delta}$.
- (ii) If $\Delta = 3$ and g > 3, then $W(G) \leq W(H_{n,g,3}^2)$ with equality iff $G \cong H_{n,g,3}^2$.

- (vi) Let $\Delta > 5$ and $g \ge 5$ is odd. If $\Delta < n g \frac{2}{g-3}$, then $W(G) \le W(H_{n,g,\Delta}^3)$ with equality iff $G \cong H_{n,g,\Delta}^3$. If $\Delta > n g \frac{2}{g-3}$, then $W(G) \le W(H_{n,g,\Delta}^1)$ with equality iff $G \cong H_{n,g,\Delta}^1$. If g = 5 and $\Delta = n 6$, then $W(G) \le W(H_{n,5,n-6}^1) = W(H_{n,5,n-6}^3)$ with equality iff $G \in \{H_{n,5,n-6}^1, H_{n,5,n-6}^3\}$.
- (vii) Let $\Delta > 5$ and $g \ge 6$ is even. If $\Delta < n g \frac{4}{g-4}$, then we have $W(G) \le W(H_{n,g,\Delta}^3)$ with equality iff $G \cong H_{n,g,\Delta}^3$. If $\Delta > n g \frac{4}{g-4}$, then $W(G) \le W(H_{n,g,\Delta}^1)$ with equality iff $G \cong H_{n,g,\Delta}^1$. If g = 6 and $\Delta = n 8$, then $W(G) \le W(H_{n,g,\Delta}^1) = W(H_{n,g,\Delta}^3)$ with equality iff $G \in \{H_{n,6,n-8}^1, H_{n,6,n-8}^3\}$.

Proof. Let G^* be a graph in $\mathscr{G}_n(g, \Delta)$ with maximum Wiener index. In the following, we always assume that w is a maximum degree vertex in G^* .

Claim 1. G^* is unicyclic.

Let E_w be the set of edges incident to the maximum degree vertex w and C a cycle of length g in G^* . If C is the unique cycle in G, then we are done. Otherwise, there is another cycle C' in G. It is clear that there is an edge e in C' satisfying $e \notin E_w \cup E(C)$. Then, one can consider the graph G' = G - e. It is easily seen that $G' \in \mathscr{G}_n(g, \Delta)$ and W(G') > W(G) by Lemma 2.3. If G' is still not a uncyclic graph, then by the same argument as above, one can finally arrive at a unicyclic graph G'' such that $W(G^*) < W(G') < W(G'')$. Thus, the claim follows.

Claim 2. Let u be a cut vertex in G^* other than the maximum degree vertex w and T an induced subtree of G^* . If $G^* = HuT$ and $w \notin V(T)$, then T is isomorphic to a path.

Suppose to the contrary that G^* can be viewed as the composition graph HuT, where T is the induced subtree of G^* and not isomorphic to a path. Then we let G' be the graph obtained from H by identifying a pendant vertex of a path which has the same orders as T to u. Clearly, $G' \in \mathscr{G}_n(g, \Delta)$. By Lemma 2.4 we have $W(G^*) < W(G')$, a contradiction.

Claim 3. G^* has at most one pendant path such that its origin is different from the maximum degree vertex, and G^* has at most one pendant path of length greater than one.

If G^* has two pendant paths $P = uz_1z_2...z_s$ and $P' = vv_1v_2...v_t$, where $u \neq w, v \neq w, t \geq 1$ and $s \geq 1$. Let $G' = G - uz_1 + z_1v_t$ and $G'' = G - vv_1 + v_1z_s$. Clearly, $G' \in \mathscr{G}_n(g, \Delta)$ and $G'' \in \mathscr{G}_n(g, \Delta)$. Then by Lemma 2.5, we have $W(G') > W(G^*)$ or $W(G'') > W(G^*)$, which is a contradiction.

If G^* has two pendant paths $P = wz_1z_2...z_s$ and $P' = ww_1w_2...w_t$ where $t \ge s \ge 2$, then let $G' = G - z_1z_2 + z_2w_t$ and it is clear that $G' \in \mathscr{G}_n(g, \Delta)$. By Lemma 2.4, we have $W(G') > W(G^*)$, which is a contradiction.

If G^* has two pendant paths $P = uz_1z_2...z_s$ and $P' = ww_1w_2...w_t$ where $u \neq w, t \geq 2$ and $s \geq 1$. Let $G' = G - uz_1 + z_1w_t$ and $G'' = G - w_1w_2 + w_2z_s$. It is easy to see that $G' \in \mathscr{G}_n(g, \Delta)$ and $G'' \in \mathscr{G}_n(g, \Delta)$. By Lemma 2.4 we have $W(G') > W(G^*)$ or $W(G'') > W(G^*)$, which is a contradiction.

Thus, the claim follows.

Claim 4. Let $C = x_1 x_2 \dots x_g$ be the unique cyclic in G^* . If G^* has a pendant path P with length greater than one and the maximum degree $w \notin V(P)$, then $G^* \cong (Tx_1C)x_{\lfloor \frac{g}{2} \rfloor+1}P$, where T is an induced subtree in G^* .

Clearly, from above we have $G^* \cong (Tx_1C)x_iP$ for some $i \in \{1, 2, \ldots, g\}$ and T is an induced subtree which contains the maximum degree vertex w. It can be easily verified that $W((Tx_1C)x_iP) < W((Tx_1C)x_{\lfloor \frac{g}{2} \rfloor + 1}P)$ for any $i \neq 1$ and $i \neq \lfloor \frac{g}{2} \rfloor + 1$. Thus, the claim follows. Claim 5. If the maximum degree vertex w is not on the unique cycle C, then G^* does not contain a pendant path of length greater than one.

Otherwise, let $P := uu_1u_2...u_s$ be a pendant path in G^* and $P' := z_1(=w)z_2...z_t$ a path connecting the maximum degree vertex w to the cycle C, where u_s is a pendant vertex, $z_t \in V(C)$, $s \ge 2$ and $t \ge 2$. If $u \in V(C)$, let $G' = G^* - z_{t-1}z_t + z_{t-1}u_s$. Then, by Lemma 2.2 and direct computation one can get that $W(G') > W(G^*)$, a contradiction. If u = w, let $G'' = G^* - \{wv : v \in N_{G^*}(w) \setminus \{z_2, u_1\}\} + \{u_{s-1}v : v \in N_{G^*}(w) \setminus \{z_2, u_1\}\}$. Then, by the use of Lemma 2.2 one can easily get that $W(G'') > W(G^*)$, a contradiction. The required claim follows.

From the discussion above, we can get $G^* \in \{H^1_{n,g,\Delta}, H^2_{n,g,\Delta}, H^3_{n,g,\Delta}\}$, see Figure 1. According to Lemma 2.2, one can get the Wiener indices of $H^1_{n,g,\Delta}, H^2_{n,g,\Delta}$ and $H^3_{n,g,\Delta}$, respectively, by direct calculations.

If g is odd, then we have

$$\begin{split} W(H_{n,g,\Delta}^{1}) &= \frac{5g^{3}-6g^{2}(n-2\Delta+6)-g[12n(\Delta-3)-12\Delta^{2}+60\Delta-79]}{24} \\ &+ \frac{2n^{3}-n(6\Delta^{2}-36\Delta+53)+4\Delta^{3}-24\Delta^{2}+38\Delta-12}{12}, \\ W(H_{n,g,\Delta}^{2}) &= \frac{(g^{2}-1)(2n-g)}{8} + \frac{(g-n+\Delta-4)(g-n+\Delta-3)(2g+n+2\Delta-7)}{6} \\ &+ (n-1)(\Delta-3), \\ W(H_{n,g,\Delta}^{3}) &= \frac{5g^{3}-6g^{2}(n+2)+g(12n+7)+4n^{3}-2n(6\Delta^{2}-18\Delta+17)}{24} \\ &+ \frac{2\Delta^{3}-3\Delta^{2}-5\Delta+6}{6}. \end{split}$$

If g is even, then we have

$$\begin{split} W(H_{n,g,\Delta}^1) = & \frac{5g^3 - 6g^2(n - 2\Delta + 6) - 4g[3n(\Delta - 3) - 3\Delta^2 + 18\Delta - 25]}{24} \\ &+ \frac{n^3 - n(3\Delta^2 - 21\Delta + 31) + 2\Delta^3 - 15\Delta^2 + 31\Delta - 18}{6}, \\ W(H_{n,g,\Delta}^2) = & \frac{g^2(2n - g)}{8} + \frac{(g - n + \Delta - 4)(g - n + \Delta - 3)(2g + n + 2\Delta - 7)}{6} \\ &+ (n - 1)(\Delta - 3), \\ W(H_{n,g,\Delta}^3) = & \frac{5g^3}{24} - \frac{g^2(n + 2)}{4} + \frac{g(3n + 1)}{6} + \frac{n^3 - n(3\Delta^2 - 9\Delta + 7)}{6} \\ &+ \frac{2\Delta^3 - 3\Delta^2 - 5\Delta + 6}{6}. \end{split}$$

Furthermore, we have

$$W(H_{n,g,\Delta}^{1}) - W(H_{n,g,\Delta}^{2}) = \begin{cases} \frac{[(g-3)(\Delta-4)-2](n-g-\Delta+2)}{2}, & g \text{ is odd,} \\ \frac{(g-2)(\Delta-4)(n-g-\Delta+2)}{2}, & g \text{ is even,} \end{cases}$$
(5)

$$W(H_{n,g,\Delta}^{1}) - W(H_{n,g,\Delta}^{3}) = \begin{cases} \frac{(\Delta-2)[g^{2}+g(-n+\Delta-3)+3n-3\Delta+2]}{2}, & g \text{ is odd,} \\ \frac{(\Delta-2)[g^{2}+g(-n+\Delta-4)+4(n-\Delta+1)]}{2}, & g \text{ is even} \end{cases}$$
(6)

and

$$W(H_{n,g,\Delta}^2) - W(H_{n,g,\Delta}^3) = g^2(\Delta - 3) - g(\Delta - 3)(n - \Delta + 4) + n(3\Delta - 8) - 3(\Delta - 2)^2.$$
(7)

Next, we consider the following cases respectively.

If g = 3, then from (5) and (7) we have $W(H_{n,3,\Delta}^1) - W(H_{n,3,\Delta}^2) = \Delta - n + 1 < 0$ and $W(H_{n,3,\Delta}^2) - W(H_{n,3,\Delta}^3) = n - 3 > 0$. Thus, we get the desired result (i).

If $\Delta = 3$ and g > 3, then from (5) and (7) we have

$$W(H_{n,g,3}^1) - W(H_{n,g,3}^2) = \begin{cases} \frac{(g-1)(g+1-n)}{2} < 0, & g \text{ is odd,} \\ \frac{(g-2)(g+1-n)}{2} < 0, & g \text{ is even,} \end{cases}$$

and

$$W(H_{n,g,3}^2) - W(H_{n,g,3}^3) = n - 3 > 0.$$

Thus, we get the result of (ii).

If $\Delta = 4$ and $g \geq 4$ is even, then from (5) we have $W(H_{n,g,4}^1) = W(H_{n,g,4}^2)$. It is easy to check that $W(H_{n,g,4}^2) > W(H_{n,g,4}^3)$ for $7 \leq n < 12$ by (6). For $n \geq 12$, from (6) we have

$$W(H_{n,g,4}^1) - W(H_{n,g,4}^3) = \left(g - \frac{n - \sqrt{n^2 - 16n + 48}}{2}\right) \left(g - \frac{n + \sqrt{n^2 - 16n + 48}}{2}\right).$$

It is easy to verify that $4 < \frac{n - \sqrt{n^2 - 16n + 48}}{2} \le 6$ for $n \ge 12$, $\frac{n - \sqrt{n^2 - 16n + 48}}{2} = \frac{n + \sqrt{n^2 - 16n + 48}}{2} = 6$ when n = 12, $\frac{n - \sqrt{n^2 - 16n + 48}}{2} = 5$ and $\frac{n + \sqrt{n^2 - 16n + 48}}{2} = 8$ when n = 13, and $\frac{n - \sqrt{n^2 - 16n + 48}}{2}$ and $\frac{n + \sqrt{n^2 - 16n + 48}}{2}$ can not be positive

integers when n > 13. Thus, we can get that $W(H_{n,g,4}^1) < W(H_{n,g,4}^3)$ for $\frac{n-\sqrt{n^2-16n+48}}{2} < g < \frac{n+\sqrt{n^2-16n+48}}{2}$, $W(H_{n,g,4}^1) > W(H_{n,g,4}^3)$ for $g < \frac{n-\sqrt{n^2-16n+48}}{2}$ or $g > \frac{n+\sqrt{n^2-16n+48}}{2}$, $W(H_{12,6,4}^1) = W(H_{12,6,4}^2) = W(H_{12,6,4}^3)$ and $W(H_{13,8,4}^1) = W(H_{13,8,4}^2) = W(H_{13,8,4}^3)$. The desired result (iii) follows.

If $\Delta = 4$ and $g \geq 5$ is odd, then from (5) we have $W(H_{n,g,4}^1) - W(H_{n,g,4}^2) = g - n + 2 < 0$. It is east to check that $W(H_{n,g,4}^2) - W(H_{n,g,4}^3) > 0$ for $8 \leq n < 12$. Now, we consider the case of $n \geq 12$. When $\Delta = 4$, Equation (7) can be phrased as

$$W(H_{n,g,4}^2) - W(H_{n,g,4}^3) = \left(g - \frac{n - \sqrt{n^2 - 16n + 48}}{2}\right) \left(g - \frac{n + \sqrt{n^2 - 16n + 48}}{2}\right).$$

Thus, we have that $W(H_{n,g,4}^1) < W(H_{n,g,4}^2) < W(H_{n,g,4}^3)$ for $n \ge 12$ and $\frac{n-\sqrt{n^2-16n+48}}{2} < g < \frac{n+\sqrt{n^2-16n+48}}{2}$, $W(H_{n,g,4}^2) > W(H_{n,g,4}^3)$ and $W(H_{n,g,4}^2) > W(H_{n,g,4}^1)$ for $n \ge 12$ and $g < \frac{n-\sqrt{n^2-16n+48}}{2}$ or $g > \frac{n+\sqrt{n^2-16n+48}}{2}$, and $W(H_{13,5,4}^2) = W(H_{13,5,4}^3) > W(H_{13,5,4}^1)$. Therefore, the desired result (iv) holds.

Let $g = \Delta = 5$. From (5) and (6) we have $W(H_{n,5,5}^1) = W(H_{n,5,5}^2)$ and $W(H_{n,5,5}^1) - W(H_{n,5,5}^3) = 3(11 - n)$. So, we have $W(H_{11,5,5}^1) = W(H_{11,5,5}^2) = W(H_{11,5,5}^3) = 151$ for n = 11, $W(H_{n,5,5}^1) < W(H_{n,5,5}^3)$ for n > 11 and $W(H_{n,5,5}^1) = W(H_{n,5,5}^2) > W(H_{n,5,5}^3)$ for $9 \le n < 11$. Thus, we get the desired result (v).

Let $g \ge 5$ and $\Delta > 5$. From (5) we have

$$W(H_{n,g,\Delta}^1) - W(H_{n,g,\Delta}^2) = \begin{cases} \frac{[(g-3)(\Delta-4)-2](n-g-\Delta+2)}{2} > 0, & g \text{ is odd,} \\ \frac{(g-2)(\Delta-4)(n-g-\Delta+2)}{2} > 0, & g \text{ is even.} \end{cases}$$

Thus, we get that $W(H^1_{n,g,\Delta}) > W(H^2_{n,g,\Delta})$ for g > 5 and $\Delta > 5$.

From (6) we have

$$W(H_{n,g,\Delta}^1) - W(H_{n,g,\Delta}^3) = \frac{1}{2}(g-3)(\Delta-2)\left(\Delta - n + g + \frac{2}{g-3}\right)$$

for odd $g \geq 5$. Thus, we have $W(H_{n,g,\Delta}^1) > W(H_{n,g,\Delta}^3)$ for $n - g - \frac{2}{g-3} < \Delta < n - g + 1$, $W(H_{n,g,\Delta}^1) < W(H_{n,g,\Delta}^3)$ for $\Delta < n - g - \frac{2}{g-3}$ and $W(H_{n,g,\Delta}^1) = W(H_{n,g,\Delta}^3)$ for g = 5 and $\Delta = n - 6$.

Similarly, we have

$$W(H_{n,g,\Delta}^1) - W(H_{n,g,\Delta}^3) = \frac{1}{2}(g-4)(\Delta-2)\left(\Delta - n + g + \frac{4}{g-4}\right)$$

for even $g \geq 6$. Thus, we have $W(H_{n,g,\Delta}^1) > W(H_{n,g,\Delta}^3)$ for $n - g - \frac{4}{g-4} < \Delta < n - g + 1$, $W(H_{n,g,\Delta}^1) < W(H_{n,g,\Delta}^3)$ for $\Delta < n - g - \frac{4}{g-4}$ and $W(H_{n,g,\Delta}^1) = W(H_{n,g,\Delta}^3)$ for g = 6 and $\Delta = n - 8$.

Hence, the statements in (vi) and (vii) are proved.

4 Maximum Kirchhoff index of graphs with given girth and maximum degree

In this section we proceed to determine the maximum Kirchhoff index among all graphs with given grith and maximum degree.

Theorem 4.1. Let G be a graph in $\mathscr{G}_n(g, \Delta)$, where $g \ge 3$ and $3 \le \Delta \le n - g + 1$.

- (i) If g = 3 and $\Delta \ge 3$, then we have $Kf(G) \le Kf(H_{n,3,\Delta}^2)$ with equality iff $G \cong H_{n,3,\Delta}^2$.
- (ii) Let g = 4. If $\frac{n-\sqrt{n^2-16n+48}}{2} < \Delta < \frac{n+\sqrt{n^2-16n+48}}{2}$, then $Kf(G) \leq Kf(H_{n,4,\Delta}^3)$ with equality iff $G \cong H_{n,4,\Delta}^3$. If $\Delta < \frac{n-\sqrt{n^2-16n+48}}{2}$ or $\Delta > \frac{n+\sqrt{n^2-16n+48}}{2}$, then $Kf(G) \leq Kf(H_{n,g,\Delta}^2)$ with equality iff $G \cong H_{n,3,\Delta}^2$. If $\Delta = \frac{n\pm\sqrt{n^2-16n+48}}{2}$, then $Kf(G) \leq Kf(H_{n,4,\Delta}^3) = Kf(H_{n,4,\Delta}^2)$ with equality iff $G \in \{H_{n,4,\Delta}^2, H_{n,4,\Delta}^3\}$.

(iii) Let $g \geq 5$. We set $\theta_1(n,g) = \frac{n+4-g}{2} - \sqrt{\frac{(g-n)(g^2-gn+g+3n-8)}{4(g-3)}}$ and $\theta_2(n,g) = \frac{n+4-g}{2} + \sqrt{\frac{(g-n)(g^2-gn+g+3n-8)}{4(g-3)}}$. If $\theta_1(n,g) < \Delta < \theta_2(n,g)$ then $Kf(G) \leq Kf(H_{n,g,\Delta}^3)$ with equality iff $G \cong H_{n,g,\Delta}^3$. If $3 \leq \Delta < \theta_1(n,g)$ or $\theta_2(n,g) < \Delta < n-g+1$, then $Kf(G) \leq Kf(H_{n,g,\Delta}^2)$ with equality iff $G \cong H_{n,g,\Delta}^2$. If $\Delta = \theta_1(n,g)$ or $\Delta = \theta_2(n,g)$, then $Kf(G) \leq Kf(H_{n,g,\Delta}^2) = Kf(H_{n,g,\Delta}^3)$ with equality iff $G \in \{H_{n,g,\Delta}^2, H_{n,g,\Delta}^3\}$.
$$\begin{array}{ll} ({\rm v}) \ \ Let \ \Delta &= n-g+1 \ \ and \ g \ \geq \ 6 \ \ is \ \ even. \ \ If \ n \ < \ \frac{g^2+g-12}{g-4}, \ then \\ Kf(G) \le Kf(H_{n,g,n-g+1}^2) \ \ with \ \ equality \ \ iff \ G \cong H_{n,g,n-g+1}^2. \ \ If \ n \ > \\ \frac{g^2+g-12}{g-4}, \ \ then \ \ we \ have \ \ Kf(G) \le Kf(H_{n,g,n-g+1}^1) \ \ with \ \ equality \ \ iff \\ G \cong H_{n,g,n-g+1}^1. \ \ If \ n \ = \ \frac{g^2+g-12}{g-4}, \ \ then \ \ Kf(G) \le Kf(H_{n,g,n-g+1}^1) = \\ Kf(H_{n,g,n-g+1}^2) \ \ with \ \ \ equality \ \ iff \ \ G \in \{H_{n,g,n-g+1}^1, H_{n,g,n-g+1}^2\}. \end{array}$$

Proof. Let G^* be a graph in $\mathscr{G}_n(g, \Delta)$ with maximum Kirchhoff index. Then, proceeding as in the proof of Theorem 3.1, one can get that $G^* \in \{H^1_{n,g,\Delta}, H^2_{n,g,\Delta}, H^3_{n,g,\Delta}\}$, and the graphs $H^1_{n,g,\Delta}, H^2_{n,g,\Delta}$ and $H^3_{n,g,\Delta}$ are illustrated in Figure 1. By Lemma 2.2 and a series of straightforward calculations we can get the explicit expressions for $Kf(H^1_{n,g,\Delta}), Kf(H^2_{n,g,\Delta})$ and $Kf(H^3_{n,g,\Delta})$, respectively. If g is odd, then the Kirchhoff index of $H^1_{n,g,\Delta}$ can be given by

$$\begin{split} Kf(H^1_{n,g,\Delta}) = & \frac{3g^3 - g^2(4n - 9\Delta + 24) + g[n(24 - 9\Delta) + 9\Delta^2 - 48\Delta + 63] + 2n^3}{12} \\ & - \frac{n(6\Delta^2 - 42\Delta + 64) - 4\Delta^3 + 30\Delta^2 - 65\Delta + 42}{12} - \frac{(\Delta - 2)(n - \Delta + 2)}{4g}. \end{split}$$

If g is even, then the Kirchhoff index of $H^1_{n,q,\Delta}$ can be given by

$$Kf(H_{n,g,\Delta}^{1}) = \frac{3g^{3} + g^{2}(-4n + 9\Delta - 24) + g[n(24 - 9\Delta) + 9\Delta^{2} - 48\Delta + 63]}{12} + \frac{n^{3} + n(-3\Delta^{2} + 21\Delta - 32) + 2\Delta^{3} - 15\Delta^{2} + 31\Delta - 18}{6}.$$

The Kirchhoff indices $Kf(H^2_{n,g,\Delta})$ and $Kf(H^3_{n,g,\Delta})$ can be given respectively by

$$Kf(H_{n,g,\Delta}^2) = \frac{3g^3 - 2g^2(2n - 6\Delta + 21) - 3g(2\Delta - 7)(2n - 2\Delta + 7)}{12} + \frac{n^3 + n(-3\Delta^2 + 27\Delta - 56) + 2\Delta^3 - 21\Delta^2 + 67\Delta - 66}{6}$$

 $\frac{698}{and}$

$$Kf(H_{n,g,\Delta}^3) = \frac{3g^3 - 2g^2(2n+3) + g(6n+3) + 2[n^3 - n(3\Delta^2 - 9\Delta + 8) + 2\Delta^3 - 3\Delta^2 - 5\Delta + 6]}{12}$$

Furthermore, we have

$$Kf(H_{n,g,\Delta}^{1}) - Kf(H_{n,g,\Delta}^{2}) = \begin{cases} \frac{[g^{2}(\Delta-6) - 4g(\Delta-4) - \Delta+2](n+2-g-\Delta)}{4g}, & g \text{ is odd,} \\ \frac{[g(\Delta-6) - 4(\Delta-4)](n+2-g-\Delta)}{4}, & g \text{ is even,} \end{cases}$$
(8)

$$Kf(H_{n,g,\Delta}^{1}) - Kf(H_{n,g,\Delta}^{3}) = \begin{cases} \frac{(\Delta-2)[3g^{3}+g^{2}(-3n+3\Delta-10)+g(8n-8\Delta+9)-n+\Delta-2]}{4g}, & g \text{ is odd,} \\ \frac{(\Delta-2)[3g^{2}+g(-3n+3\Delta-10)+8(n-\Delta+1)]}{4}, & g \text{ is even} \end{cases}$$
(9)

and

$$Kf(H_{n,g,\Delta}^2) - Kf(H_{n,g,\Delta}^3) = g^2(\Delta - 3) - g(n + 4 - \Delta)(\Delta - 3) - 3(\Delta - 2)^2 + n(3\Delta - 8).$$
(10)

Next, we consider the following cases respectively. If g = 3 and $\Delta \ge 3$, then from (8) and (10) we have

$$Kf(H_{n,3,\Delta}^1) - Kf(H_{n,3,\Delta}^2) = \frac{(\Delta+1)(\Delta+1-n)}{3} < 0$$

and

$$Kf(H_{n,3,\Delta}^2) - Kf(H_{n,3,\Delta}^3) = n - 3 > 0.$$

Thus, we have $Kf(H^2_{n,3,\Delta}) > Kf(H^1_{n,3,\Delta})$ and $Kf(H^2_{n,3,\Delta}) > Kf(H^3_{n,3,\Delta})$ for $\Delta \geq 3$. The required result (i) follows.

If g = 4 and $\Delta \ge 3$, then from (8) and (10) we have

$$Kf(H_{n,4,\Delta}^1) - Kf(H_{n,4,\Delta}^2) = 2(\Delta + 2 - n) < 0$$

and

$$Kf(H_{n,4,\Delta}^2) - Kf(H_{n,4,\Delta}^3) = \left(\Delta - \frac{n - \sqrt{n^2 - 16n + 48}}{2}\right) \left(\Delta - \frac{n + \sqrt{n^2 - 16n + 48}}{2}\right).$$

Thus, we can get that $Kf(H_{n,4,\Delta}^3) > Kf(H_{n,4,\Delta}^2) > Kf(H_{n,4,\Delta}^1)$ for $\frac{n-\sqrt{n^2-16n+48}}{2} < \Delta < \frac{n+\sqrt{n^2-16n+48}}{2}, Kf(H_{n,g,\Delta}^2) > Kf(H_{n,g,\Delta}^1)$ and $Kf(H_{n,g,\Delta}^2) > Kf(H_{n,g,\Delta}^3)$ for $\Delta < \frac{n-\sqrt{n^2-16n+48}}{2}$ or $\Delta > \frac{n+\sqrt{n^2-16n+48}}{2}$ and $Kf(H_{n,4,\Delta}^3) = Kf(H_{n,4,\Delta}^2) > Kf(H_{n,4,\Delta}^1)$ for $\Delta = \frac{n\pm\sqrt{n^2-16n+48}}{2}$. The required result (ii) follows.

If $g \ge 5$ and $3 \le \Delta \le n - g$, then from (9) we have

$$\begin{split} &Kf(H^1_{n,g,\Delta}) - Kf(H^3_{n,g,\Delta}) \\ &= \begin{cases} \frac{(\Delta - 2)(1 - 8g + 3g^2)}{4g} \left(\Delta - \frac{-3g^3 + 3g^2n + 10g^2 - 8gn - 9g + n + 2}{3g^2 - 8g + 1}\right), & g \text{ is odd}, \\ \frac{(\Delta - 2)(3g - 8)}{4} \left(\Delta - \frac{-3g^2 + 3gn + 10g - 8n - 8}{3g - 8}\right), & g \text{ is even}, \end{cases} \end{split}$$

Note that

$$n-g+1 > \frac{-3g^3+3g^2n+10g^2-8gn-9g+n+2}{3g^2-8g+1} = n-g + \frac{2g^2-8g+2}{3g^2-8g+1} > n-g$$

and

$$n-g+1 > \frac{-3g^2+3gn+10g-8n-8}{3g-8} = n-g + \frac{2g-8}{3g-8} > n-g.$$

Thus we have $Kf(H^3_{n,g,\Delta}) > Kf(H^1_{n,g,\Delta})$ for all $\Delta \le n - g$.

We can rewrite Equation (10) as

$$Kf(H_{n,g,\Delta}^2) - Kf(H_{n,g,\Delta}^3) = \left(\Delta - \frac{n+4-g}{2} + \sqrt{\frac{(g-n)(g^2 - gn + g + 3n - 8)}{4(g-3)}}\right)$$
$$\times \left(\Delta - \frac{n+4-g}{2} - \sqrt{\frac{(g-n)(g^2 - gn + g + 3n - 8)}{4(g-3)}}\right)$$
$$= (\Delta - \theta_1(n,g))(\Delta - \theta_2(n,g)),$$

where
$$\theta_1(n,g) = \frac{n+4-g}{2} - \sqrt{\frac{(g-n)(g^2 - gn + g + 3n - 8)}{4(g-3)}}$$
 and $\theta_2(n,g) = \frac{n+4-g}{2} + \sqrt{\frac{(g-n)(g^2 - gn + g + 3n - 8)}{4(g-3)}}$.
It is easy to get that $\frac{g^3 - 2g^2 n + g^2 + gn^2 + 2gn - 8g - 3n^2 + 8n}{4(g-3)} - \left(\frac{n-g-2}{2}\right)^2 =$

 $\frac{3-n}{g-3} < 0$, then we have

$$\theta_2(n,g) - (n-g+1) = \sqrt{\frac{g^3 - 2g^2n + g^2 + gn^2 + 2gn - 8g - 3n^2 + 8n}{4(g-3)}} + \frac{g+2-n}{2} < \frac{n-g-2}{2} + \frac{g+2-n}{2} = 0,$$

which means $\theta_2(n,g) < n-g+1$.

Thus, we have $Kf(H^3_{n,g,\Delta}) > Kf(H^1_{n,g,\Delta})$ and $Kf(H^3_{n,g,\Delta}) > Kf(H^2_{n,g,\Delta})$ for $\theta_1(n,g) < \Delta < \theta_2(n,g)$, $Kf(H^2_{n,g,\Delta}) > Kf(H^3_{n,g,\Delta}) > Kf(H^1_{n,g,\Delta})$ for $3 \leq \Delta < \theta_1(n,g)$ or $\theta_2(n,g) < \Delta \leq n-g$ and $Kf(H^2_{n,g,\Delta}) = Kf(H^3_{n,g,\Delta}) > Kf(H^1_{n,g,\Delta})$ for $\Delta = \theta_1(n,g)$ or $\Delta = \theta_2(n,g)$. The required result (iii) follows.

If $g \ge 5$ and $\Delta = n - g + 1$, then we have $G^* \in \{H^1_{n,g,\Delta}, H^2_{n,g,\Delta}\}$. One can get by (8) that

$$\begin{split} Kf(H^1_{n,g,n-g+1}) - Kf(H^2_{n,g,n-g+1}) \\ &= \begin{cases} \frac{g^2 - 4g - 1}{4g} \big(n - \frac{g^3 + g^2 - 13g - 1}{g^2 - 4g - 1}\big), & g \text{ is odd}, \\ \frac{g - 4}{4} \big(n - \frac{g^2 + g - 12}{g - 4}\big), & g \text{ is even.} \end{cases} \end{split}$$

Thus, if $g \ge 5$ is odd, then we have $Kf(H_{n,g,n-g+1}^1) < Kf(H_{n,g,n-g+1}^2)$ for $n < \frac{g^3 + g^2 - 13g - 1}{g^2 - 4g - 1}$, $Kf(H_{n,g,n-g+1}^1) > Kf(H_{n,g,n-g+1}^2)$ for $n > \frac{g^3 + g^2 - 13g - 1}{g^2 - 4g - 1}$ and $Kf(H_{n,g,n-g+1}^1) = Kf(H_{n,g,n-g+1}^2)$ for $n = \frac{g^3 + g^2 - 13g - 1}{g^2 - 4g - 1}$. If $g \ge 6$ is even, then we have $Kf(H_{n,g,n-g+1}^1) < Kf(H_{n,g,n-g+1}^2)$ for $n < \frac{g^2 + g - 12}{g - 4}$, $Kf(H_{n,g,n-g+1}^1) > Kf(H_{n,g,n-g+1}^2)$ for $n > \frac{g^2 + g - 12}{g - 4}$ and $Kf(H_{n,g,n-g+1}^1) = Kf(H_{n,g,n-g+1}^2)$ for $n < \frac{g^2 + g - 12}{g - 4}$. Hence, the statements (iv) and (v) follows.

5 Open problems

In this paper we have obtained the maximum Wiener index and Kirchhoff index for graphs of order n in terms of girth and maximum degree, respectively. On the other side, what about the minimum value of Wiener index (resp. Kirchhoff index) for graphs of given order, girth and maximum degree? It is still an open problem. **Problem 5.1.** Determine the minimum Wiener index (resp. Kirchhoff index) among all graphs of order n with given girth and maximum degree.

It is also interesting to consider the problem restricted in 2-connected graphs.

Problem 5.2. Determine the maximum or minimum Wiener index (resp. Kirchhoff index) among all 2-connected graphs of order n with given girth and maximum degree.

Similar questions can be asked for other important graph invariants, such as the number of subtrees, matching energy, Hosoya index, Merrifield-Simmons index, spectral radius, (signless) Laplacian spectral radius, distance spectral radius, Estrada index and so forth. We look forward to see these problems solved in the near future.

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