Appl. Math. J. Chinese Univ.
2020, 35(3): 308-320

On the ordering of the Kirchhoff indices of the complements of trees and unicyclic graphs

CHEN Xiao-dan* HAO Guo-liang JIN De-quan

Abstract. The Kirchhoff index $Kf(G)$ of a graph G is defined to be the sum of the resistance distances between all pairs of vertices of G. In this paper, we develop a novel method for ordering the Kirchhoff indices of the complements of trees and unicyclic graphs. With this method, we determine the first five maximum values of $Kf(\overline{T})$ and the first four maximum values of $Kf(\overline{U})$, where $\overline{T}$ and $\overline{U}$ are the complements of a tree T and unicyclic graph U, respectively.

§1 Introduction

The concept of the resistance distance of a graph was conceived by Klein and Randić [17] in 1993 based on the electrical network theory and graph theory. A (connected) graph G is regarded as an electrical network N by replacing each edge of G with a unit resistor and then, the resistance distance between a pair of vertices in G is defined to be the effective resistance between them in N, which is computed by the Ohm's and Kirchhoff's laws. As the common shortest-path distance, the resistance distance is a distance function on graphs, which not only has some nice purely mathematical and physical interpretations, but also has a substantial potential for chemical applications [17, 18].

All graphs considered throughout this paper are finite, undirected, and simple graphs. Let G be a graph with vertex set $V(G) = \{v_1, v_2, \ldots, v_n\}$. Denote by $r_G(v_i, v_j)$ the resistance distance between the vertices v_i and v_j in G. The Kirchhoff index of G [3, 17] is defined as

$$Kf(G) = \frac{1}{2}\sum_{i=1}^{n}\sum_{j=1}^{n} r_G(v_i, v_j).$$

Here G is allowed to be disconnected; in this case, we have $r_G(v_i, v_j) = +\infty$ for the vertices v_i and v_j in different components of G and $Kf(G) = +\infty$. Up to now, this resistance-distance-based graph invariant, as a molecular structure descriptor, has been found noteworthy

Received: 2018-03-15. Revised: 2019-09-11
MR Subject Classification: 05C35, 05C50, 05C12.
Keywords: Kirchhoff index, tree, unicyclic graph, complement, ordering.
Digital Object Identifier(DOI): https://doi.org/10.1007/s11766-020-3605-5.
Supported by the National Natural Science Foundation of China (11861011, 11501133, 11661010).
*Corresponding author.

applications in chemistry [2, 3, 9], and many of its mathematical properties have also been established [5–8, 10–12, 16, 19, 20, 24–32, 35, 36, 38, 39].

Recall that the Laplacian matrix of a graph G is defined to be $L(G) = D(G) - A(G)$, where $A(G)$ is the adjacency matrix of G and $D(G)$ is the diagonal matrix of vertex degrees of G. The eigenvalues of $L(G)$, usually known as the Laplacian eigenvalues of the graph G, are arranged (in non-increasing order) as $\mu_1(G) \geq \mu_2(G) \geq \cdots \geq \mu_n(G)$. It is well known that $\mu_n(G) = 0$ and, $\mu_{n-1}(G) > 0$ if and only if G is connected. For more details concerning the Laplacian eigenvalues of a graph one may refer to [23].

One of the most beautiful and important mathematical properties of the Kirchhoff index, due to Gutman and Mohar [12], and Zhu et al. [39], is the following relation between the Kirchhoff index and the Laplacian eigenvalues:

$$Kf(G) = n \sum_{i=1}^{n-1} \frac{1}{\mu_i(G)}, \tag{1}$$

for any connected graph G of order $n \geq 2$.

Another interesting mathematical property of the Kirchhoff index, given by Deng and Chen [7] recently, is to establish a relation between the Kirchhoff index of the complement $\overline{G}$ of a bipartite graph G and the numbers of closed walks in the subdivision graph $S(G)$ of G (that is, the graph obtained from G by inserting a new vertex in each edge of G):

$$Kf(\overline{G}) = \frac{n-m}{2} + \frac{1}{2} \sum_{k \geq 0} \frac{M_{2k}(S(G))}{n^k} - 1, \tag{2}$$

for any bipartite graph G with $n \geq 2$ vertices and m edges, where $M_k(G)$ is the number of closed walks of length k in G. The relation (2) provides alternative method for comparing the Kirchhoff indices of the complements of bipartite graphs, which is to compare directly the numbers of closed walks in the subdivision graphs of those bipartite graphs. Using this method, one successfully determined the first and second maximum values of $Kf(\overline{G})$ when G is a tree [7], bipartite unicyclic graph [8], and bipartite bicyclic graph [16].

However, for non-bipartite graphs, the method based on (2) will be no longer valid. In addition, even for trees T, it seems hard to apply the method based on (2) to extend the ordering of $Kf(\overline{T})$. Hence, it would be of interest to develop some efficient methods for ordering the Kirchhoff indices of the complements of (general) graphs. As a first step to this work, in the present paper we develop a novel method for ordering the Kirchhoff indices of the complements of trees and unicyclic graphs. With this method, we determine the first five maximum values of $Kf(\overline{T})$ and the first four maximum values of $Kf(\overline{U})$, where $\overline{T}$ and $\overline{U}$ are the complements of trees T and unicyclic graphs U, respectively.

§2 Preliminaries

In this section, we give some known results as necessary preliminaries.

Lemma 2.1 (see [23]). *If G is a graph with n vertices and $\overline{G}$ is its complement, then $\mu_n(\overline{G}) = 0$ and $\mu_i(\overline{G}) = n - \mu_{n-i}(G)$ $(i = 1, 2, \ldots, n-1)$.*

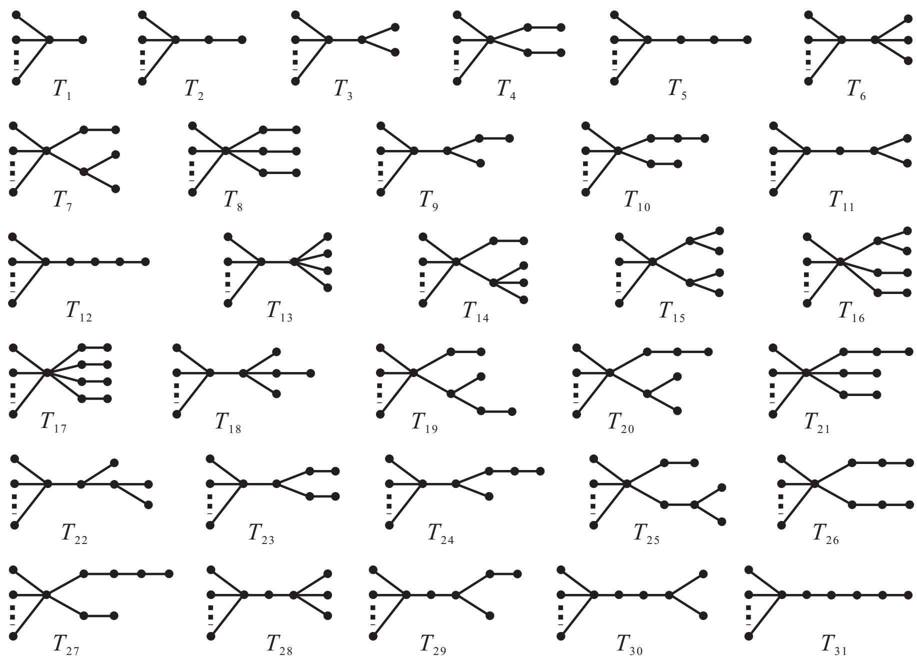

Figure 1: The trees $T_1, T_2, \ldots, T_{31}$.

Lemma 2.2 (see [1]). *For any graph G of order n, $\mu_1(G) \le n$ with equality if and only if $\overline{G}$ is disconnected.*

Let K_n and $K_{a,b}\,(a+b=n)$ denote the complete graph and the complete bipartite graph with n vertices, respectively.

Lemma 2.3 (see [4]). *If G is a connected graph with $n \ge 3$ vertices, then $\mu_2(G) = \mu_3(G) = \cdots = \mu_{n-1}(G)$ if and only if $G \cong K_n$, or $G \cong K_{n-1,1}$, or $G \cong K_{n/2,n/2}$ (n is even).*

Let $\mathcal{T}(n)$ and $\mathcal{U}(n)$ denote the sets of all trees and unicyclic graphs with n vertices, respectively.

Lemma 2.4 (see [13,33,34,37]). *For $n \ge 16$, if $T \in \mathcal{T}(n)\backslash\{T_1, T_2, \ldots, T_{31}\}$, then $\mu_1(T) \le n-4$, where $T_1, T_2, \ldots, T_{31}$ are depicted in Figure 1.*

Lemma 2.5 (see [15,21,22]). *For $n \ge 14$, if $U \in \mathcal{U}(n) \setminus \{U_1, U_2, \ldots, U_{16}\}$, then $\mu_1(U) \le n-2$, where $U_1, U_2, \ldots, U_{16}$ are depicted in Figure 2.*

For a square matrix M, denote by $\Phi(M;x)$ (or simply, $\Phi(M)$) the characteristic polynomial of M, i.e., $\Phi(M;x) = \det(xI - M)$. For a vertex $v \in V(G)$, let $L_v(G)$ be the principal submatrix of $L(G)$ obtained by deleting the row and column corresponding to the vertex v. The following result, due to Guo [14], is usually used to calculate the characteristic polynomial of $L(G)$.

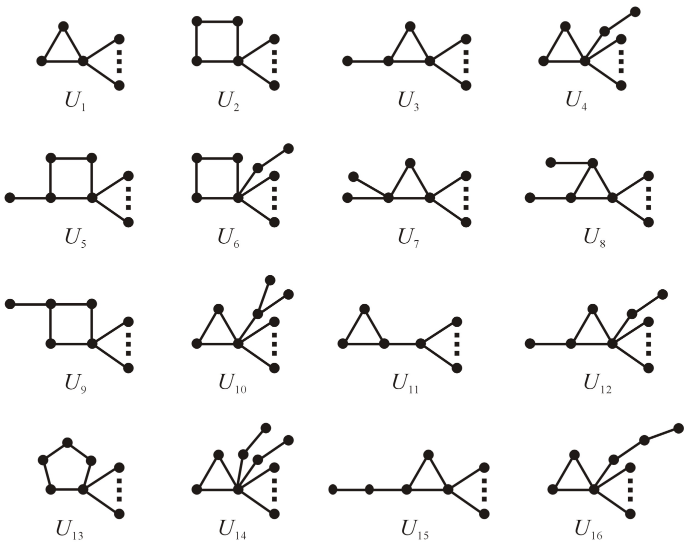

Figure 2: The unicyclic graphs $U_1, U_2, \ldots, U_{16}$.

Lemma 2.6 (see [14]). *If $G = G_1u : vG_2$ is the graph obtained by joining the vertex u of the graph G_1 to the vertex v of the graph G_2 by an edge, where G_1 and G_2 are vertex-disjoint, then*

$$\Phi(L(G)) = \Phi(L(G_1))\Phi(L(G_2)) - \Phi(L(G_1))\Phi(L_v(G_2)) - \Phi(L(G_2))\Phi(L_u(G_1)).$$

Clearly, for any graph G with n vertices, we have

$$\Phi(L(G); x) = x(x - \mu_1(G))(x - \mu_2(G)) \cdots (x - \mu_{n-1}(G)),$$

and then

$$\frac{\Phi'(L(G); x)}{\Phi(L(G); x)} = \sum_{i=1}^{n-1} \frac{1}{(x - \mu_i(G))} + \frac{1}{x},$$

which, together with (1) and Lemma 2.1, would yield the following result immediately (see also [7]).

Lemma 2.7 (see [7]). *If G is a graph with n vertices and $\overline{G}$ is its complement, then*

$$Kf(\overline{G}) = n\frac{\Phi'(L(G); n)}{\Phi(L(G); n)} - 1,$$

with a convention that $\frac{\alpha}{0} (\alpha \neq 0)$ means ∞.

§3 Main results

In this section, we provide a method for ordering the Kirchhoff indices of the complements of trees and unicyclic graphs.

The key to our method is the following result.

Theorem 3.1. *If G is a connected graph with n vertices and m edges, then*

$$Kf(G) \leq \frac{n(n-1)-2m}{\mu_{n-1}(G)} + n - 1, \tag{3}$$

with equality if and only if $G \cong K_n$, or $G \cong K_{n-1,1}$, or $G \cong K_{n/2,n/2}$ (n is even).

Proof. Recall first that $\sum_{i=1}^{n-1} \mu_i(G) = 2m$. From (1) it follows that

$$\begin{aligned} Kf(G) &= n\sum_{i=1}^{n-1}\frac{1}{\mu_i(G)} = n\left[\frac{n-1}{\mu_1(G)} + \sum_{i=2}^{n-1}\left(\frac{1}{\mu_i(G)} - \frac{1}{\mu_1(G)}\right)\right] \\ &= n\left[\frac{n-1}{\mu_1(G)} + \sum_{i=2}^{n-1}\frac{\mu_1(G)-\mu_i(G)}{\mu_1(G)\mu_i(G)}\right] \\ &\leq n\left[\frac{n-1}{\mu_1(G)} + \frac{\sum_{i=2}^{n-1}\big(\mu_1(G)-\mu_i(G)\big)}{\mu_1(G)\mu_{n-1}(G)}\right] \\ &= \frac{n\big[(n-1)\big(\mu_1(G)+\mu_{n-1}(G)\big)-2m\big]}{\mu_1(G)\mu_{n-1}(G)}. \end{aligned} \tag{4}$$

For $x > 0$, consider the following function

$$f(x) = \frac{(n-1)\big(x+\mu_{n-1}(G)\big)-2m}{x\mu_{n-1}(G)},$$

for which

$$f'(x) = \frac{2m-(n-1)\mu_{n-1}(G)}{x^2\mu_{n-1}(G)}.$$

Since $2m = \sum_{i=1}^{n-1}\mu_i(G) \geq (n-1)\mu_{n-1}(G)$, we have $f'(x) \geq 0$, implying that $f(x)$ is a increasing function for $x > 0$. Thus, noting that $\mu_1(G) \leq n$ (by Lemma 2.2), and by (4) we may obtain

$$Kf(G) \leq nf(\mu_1(G)) \leq nf(n) = \frac{n(n-1)-2m}{\mu_{n-1}(G)} + n - 1, \tag{5}$$

as desired, completing the first part of the proof.

We now suppose that the equality holds in (3). Then all inequalities in the above argument must be equalities. In fact, from the equality in (4), we have $\mu_2(G) = \mu_3(G) = \cdots = \mu_{n-1}(G)$, which implies that $G \cong K_n$, or $G \cong K_{n-1,1}$, or $G \cong K_{n/2,n/2}$ (by Lemma 2.3). Meanwhile, from the equality in (5), we get $\mu_1(G) = n$, implying that $\overline{G}$ is disconnected (by Lemma 2.2). Clearly, $\overline{K_n}$, $\overline{K_{n-1,1}}$, and $\overline{K_{n/2,n/2}}$ are disconnected. Therefore, the required result follows.

Conversely, if G is isomorphic to one of these graphs: K_n, $K_{n-1,1}$, and $K_{n/2,n/2}$, then one may easily check that the equality holds in (3), by noting that the Laplacian spectra of K_n, $K_{n-1,1}$, and $K_{n/2,n/2}$ are $\{n,\ldots,n,0\}$, $\{n,1,\ldots,1,0\}$, and $\{n,n/2,\ldots,n/2,0\}$, respectively.

This completes the proof. □

Remark 1. It should be mentioned that the idea of Theorem 3.1 comes from [25].

If $T \in \mathcal{T}(n) \setminus \{T_1, T_2, \ldots, T_{31}\}$, then by Lemma 2.4, we have $\mu_1(T) \leq n-4$, and hence, by Lemma 2.1, we get $\mu_{n-1}(\overline{T}) = n - \mu_1(T) \geq 4$. This, together with Theorem 3.1, would yield the next corollary.

Corollary 3.2. *For $n \geq 16$, if $T \in \mathcal{T}(n) \setminus \{T_1, T_2, \ldots, T_{31}\}$, then $Kf(\overline{T}) \leq \frac{3}{2}(n-1)$.*

Likewise, by Theorem 3.1 and Lemma 2.5, we may have the following.

Corollary 3.3. *For $n \geq 14$, if $U \in \mathcal{U}(n) \setminus \{U_1, U_2, \ldots, U_{16}\}$, then $Kf(\overline{U}) \leq 2n-1$.*

Now we are ready to present the main results of this paper.

Theorem 3.4. *For $n \geq 16$, if $T \in \mathcal{T}(n) \setminus \{T_1, T_2, T_3, T_4, T_5\}$, then $Kf(\overline{T_1}) > Kf(\overline{T_2}) > Kf(\overline{T_3}) > Kf(\overline{T_4}) > Kf(\overline{T_5}) > Kf(\overline{T})$.*

Proof. We first show that $Kf(\overline{T_1}) > Kf(\overline{T_2}) > Kf(\overline{T_3}) > Kf(\overline{T_4}) > Kf(\overline{T_5}) > \frac{3}{2}(n-1)$. Indeed, since $\overline{T_1}$ is disconnected, by convention we have $Kf(\overline{T_1}) = +\infty$. Furthermore, by Lemma 2.6 and some elementary calculation, we get

$$\begin{aligned}
\Phi(L(T_2);x) &= x(x-1)^{n-4}\big[x^3-(n+2)x^2+(3n-2)x-n\big],\\
\Phi(L(T_3);x) &= x(x-1)^{n-4}\big[x^3-(n+2)x^2+(4n-7)x-n\big],\\
\Phi(L(T_4);x) &= x(x-1)^{n-6}(x^2-3x+1)\big[x^3-(n+1)x^2+(3n-5)x-n\big],\\
\Phi(L(T_5);x) &= x(x-1)^{n-5}\big[x^4-(n+3)x^3+(5n-4)x^2-(6n-10)x+n\big],
\end{aligned}$$

and then, by Lemma 2.7, we obtain

$$\begin{aligned}
Kf(\overline{T_2}) &= \frac{2n^3-9n^2+11n+2}{(n-1)(n-3)},\\
Kf(\overline{T_3}) &= \frac{3n^3-17n^2+25n+7}{2(n-1)(n-4)},\\
Kf(\overline{T_4}) &= \frac{3n^5-23n^4+65n^3-67n^2-3n+5}{2(n-1)(n-3)(n^2-3n+1)},\\
Kf(\overline{T_5}) &= \frac{3n^4-20n^3+46n^2-31n-10}{(n-1)(2n^2-10n+11)}.
\end{aligned}$$

Thus, for $n \geq 16$, we may conclude that

$$\begin{aligned}
Kf(\overline{T_2})-Kf(\overline{T_3}) &= \frac{(n-1)^2(n-5)}{2(n-3)(n-4)} > 0,\\
Kf(\overline{T_3})-Kf(\overline{T_4}) &= \frac{5n^3-6n^2-22n-1}{2(n-1)(n-3)(n-4)(n^2-3n+1)} > 0,\\
Kf(\overline{T_4})-Kf(\overline{T_5}) &= \frac{(n-5)(n^4-13n^2+14n+1)}{2(n-1)(n-3)(n^2-3n+1)(2n^2-10n+11)} > 0,\\
Kf(\overline{T_5})-\frac{3}{2}(n-1) &= \frac{2n^3-7n^2+34n-53}{2(n-1)(2n^2-10n+11)} > 0.
\end{aligned}$$

Consequently, the desired result follows.

Next, by Corollary 3.2, we just need to verify that $Kf(\overline{T_i}) < \frac{3}{2}(n-1)$ for $i = 6, 7, \ldots, 31$. Indeed, based on the characteristic polynomials of $L(T_i)$ listed in Appendix, and bearing Lemma 2.7 in mind, one can conclude that, for $n \geq 16$,

$$\begin{aligned}
Kf(\overline{T_6})-\frac{3}{2}(n-1) &= -\frac{n^3-9n^2+9n-73}{6(n-1)(n-5)} < 0,\\
Kf(\overline{T_7})-\frac{3}{2}(n-1) &= -\frac{n^5-11n^4+30n^3-80n^2+213n-53}{2(n-1)(3n^3-21n^2+39n-11)} < 0,\\
Kf(\overline{T_8})-\frac{3}{2}(n-1) &= -\frac{n^5-10n^4+23n^3-65n^2+178n-43}{6(n-1)(n-3)(n^2-3n+1)} < 0,
\end{aligned}$$

$$Kf(\overline{T_9})-\frac{3}{2}(n-1) = -\frac{n^5-11n^4+31n^3-83n^2+190n-88}{2(n-1)(3n^3-21n^2+40n-18)}<0,$$

$$Kf(\overline{T_{10}})-\frac{3}{2}(n-1) = -\frac{n^6-12n^5+43n^4-106n^3+276n^2-330n+68}{2(n-1)(3n^4-24n^3+64n^2-62n+14)}<0,$$

$$Kf(\overline{T_{11}})-\frac{3}{2}(n-1) = -\frac{n^4-10n^3+22n^2-62n+113}{2(n-1)(3n^2-18n+23)}<0,$$

$$Kf(\overline{T_{12}})-\frac{3}{2}(n-1) = -\frac{n^4-10n^3+23n^2-54n+128}{2(n-1)(3n^2-18n+26)}<0,$$

$$Kf(\overline{T_{13}})-\frac{3}{2}(n-1) = -\frac{n^3-9n^2+7n-59}{4(n-1)(n-6)}<0,$$

$$Kf(\overline{T_{14}})-\frac{3}{2}(n-1) = -\frac{n^5-11n^4+29n^3-64n^2+179n-44}{2(n-1)(2n^3-16n^2+32n-9)}<0,$$

$$Kf(\overline{T_{15}})-\frac{3}{2}(n-1) = -\frac{n^5-11n^4+30n^3-58n^2+197n-39}{4(n-1)(n-4)(n^2-4n+1)}<0,$$

$$Kf(\overline{T_{16}})-\frac{3}{2}(n-1) = -\frac{n^7-13n^6+54n^5-127n^4+329n^3-570n^2+262n-34}{2(n-1)(n^2-3n+1)(2n^3-14n^2+26n-7)}<0,$$

$$Kf(\overline{T_{17}})-\frac{3}{2}(n-1) = -\frac{n^5-9n^4+17n^3-41n^2+133n-29}{4(n-1)(n-3)(n^2-3n+1)}<0,$$

$$Kf(\overline{T_{18}})-\frac{3}{2}(n-1) = -\frac{2n^5-22n^4+59n^3-133n^2+327n-133}{2(n-1)(4n^3-32n^2+65n-27)}<0,$$

$$Kf(\overline{T_{19}})-\frac{3}{2}(n-1) = -\frac{2n^7-26n^6+109n^5-261n^4+642n^3-1088n^2+641n-103}{2(n-1)(4n^5-40n^4+141n^3-209n^2+119n-21)}<0,$$

$$Kf(\overline{T_{20}})-\frac{3}{2}(n-1) = -\frac{2n^6-24n^5+85n^4-176n^3+468n^2-592n+93}{2(n-1)(4n^4-36n^3+105n^2-104n+19)}<0,$$

$$Kf(\overline{T_{21}})-\frac{3}{2}(n-1) = -\frac{2n^8-28n^7+137n^6-368n^5+876n^4-1800n^3+1938n^2-728n+83}{2(n-1)(n^2-3n+1)(4n^4-32n^3+85n^2-81n+17)}<0,$$

$$Kf(\overline{T_{22}})-\frac{3}{2}(n-1) = -\frac{n^5-11n^4+31n^3-62n^2+170n-79}{2(n-1)(2n^3-16n^2+35n-16)}<0,$$

$$Kf(\overline{T_{23}})-\frac{3}{2}(n-1) = -\frac{n^6-12n^5+43n^4-91n^3+222n^2-297n+74}{2(n-1)(n^2-3n+1)(2n^2-12n+15)}<0,$$

$$Kf(\overline{T_{24}})-\frac{3}{2}(n-1) = -\frac{2n^6-24n^5+86n^4-182n^3+447n^2-562n+173}{2(n-1)(4n^4-36n^3+106n^2-114n+35)}<0,$$

$$Kf(\overline{T_{25}})-\frac{3}{2}(n-1) = -\frac{n^6-12n^5+43n^4-90n^3+224n^2-302n+64}{2(n-1)(2n^4-18n^3+53n^2-56n+13)}<0,$$

$$Kf(\overline{T_{26}})-\frac{3}{2}(n-1) = -\frac{n^7-13n^6+56n^5-132n^4+303n^3-550n^2+431n-54}{2(n-1)(2n^2-10n+11)(n^3-5n^2+6n-1)}<0,$$

$$Kf(\overline{T_{27}})-\frac{3}{2}(n-1) = -\frac{2n^6-24n^5+88n^4-176n^3+431n^2-668n+143}{2(n-1)(4n^4-36n^3+110n^2-124n+29)}<0,$$

$$Kf(\overline{T_{28}})-\frac{3}{2}(n-1) = -\frac{2n^4-20n^3+41n^2-96n+193}{2(n-1)(4n^2-28n+39)}<0,$$

$$Kf(\overline{T_{29}})-\frac{3}{2}(n-1) = -\frac{2n^6-24n^5+87n^4-186n^3+427n^2-574n+208}{2(n-1)(4n^4-36n^3+107n^2-122n+42)}<0,$$

$$Kf(\overline{T_{30}})-\frac{3}{2}(n-1) = -\frac{2n^4-20n^3+45n^2-76n+233}{2(n-1)(4n^2-28n+47)}<0,$$

$$Kf(\overline{T_{31}})-\frac{3}{2}(n-1) = -\frac{2n^6-24n^5+89n^4-182n^3+413n^2-606n+248}{2(n-1)(4n^4-36n^3+111n^2-134n+50)}<0,$$

completing the proof. □

Remark 2. In fact, based on the above values of $Kf(\overline{T_i})$, one may further verify that $Kf(\overline{T_1}) > Kf(\overline{T_2}) > \cdots > Kf(\overline{T_{31}})$ holds for $n \geq 103$. On the other hand, based on the results in [13, 33, 34, 37], and using the method given in [34], one can also check that $\mu_1(T_1) > \mu_1(T_2) > \cdots > \mu_1(T_{31})$ holds for sufficiently large n. This would imply that the Kirchhoff indices of the complements of trees are likely to be relevant to the Laplacian spectral radii of those trees. Formally, we pose the following problem:

Problem. For any two trees T' and T'' of order n and sufficiently large n, is it true that $\mu_1(T') > \mu_1(T'')$ implies $Kf(\overline{T'}) > Kf(\overline{T''})$?

Theorem 3.5. *For $n \geq 14$, if $U \in \mathcal{U}(n)\backslash\{U_1, U_2, U_3, U_4\}$, then $Kf(\overline{U_1}) > Kf(\overline{U_2}) > Kf(\overline{U_3}) > Kf(\overline{U_4}) > Kf(\overline{U})$.*

Proof. This proof is analogous to the proof of Theorem 3.4. We first prove that $Kf(\overline{U_1}) > Kf(\overline{U_2}) > Kf(\overline{U_3}) > Kf(\overline{U_4}) > 2n-1$. Indeed, since $\overline{U_1}$ is disconnected, by convention we have $Kf(\overline{U_1}) = +\infty$. Furthermore, by Lemma 2.6 and some elementary calculation, we obtain

$$\begin{aligned}
\Phi(L(U_2);x) &= x(x-1)^{n-5}(x-2)\big[x^3-(n+3)x^2+(4n-2)x-2n\big],\\
\Phi(L(U_3);x) &= x(x-1)^{n-5}\big[x^4-(n+5)x^3+(6n+3)x^2-(9n-5)x+3n\big],\\
\Phi(L(U_4);x) &= x(x-1)^{n-5}(x-3)\big[x^3-(n+2)x^2+(3n-2)x-n\big],
\end{aligned}$$

and then, by Lemma 2.7, we have

$$\begin{aligned}
Kf(\overline{U_2}) &= \frac{2n^4-15n^3+39n^2-34n-4}{(n-1)(n-2)(n-4)},\\
Kf(\overline{U_3}) &= \frac{2n^4-15n^3+38n^2-32n-5}{(n-1)(n-2)(n-4)},\\
Kf(\overline{U_4}) &= \frac{2n^3-9n^2+13n+2}{(n-1)(n-3)}.
\end{aligned}$$

Thus, for $n \geq 14$, we may conclude that

$$\begin{aligned}
Kf(\overline{U_2})-Kf(\overline{U_3}) &= \frac{n-1}{(n-2)(n-4)} > 0,\\
Kf(\overline{U_3})-Kf(\overline{U_4}) &= \frac{2n+1}{(n-2)(n-3)(n-4)} > 0,\\
Kf(\overline{U_4})-(2n-1) &= \frac{3n+5}{(n-1)(n-3)} > 0,
\end{aligned}$$

as desired.

Next, by Corollary 3.3, we only need to check that $Kf(\overline{U_i}) < 2n-1$ for $i = 5, 6, \ldots, 16$. Actually, based on the characteristic polynomials of $L(U_i)$ listed in Appendix, and bearing in mind Lemma 2.7, one can conclude that, for $n \geq 14$,

$$\begin{aligned}
Kf(\overline{U_5})-(2n-1) &= -\frac{(n-3)(n^3-5n^2-4n-14)}{(n-1)(2n^2-14n+23)} < 0,\\
Kf(\overline{U_6})-(2n-1) &= -\frac{n^6-10n^5+29n^4-30n^3+50n^2-106n+36}{(n-1)(n-2)(2n^3-14n^2+27n-10)} < 0,\\
Kf(\overline{U_7})-(2n-1) &= -\frac{n^4-8n^3+10n^2-8n+37}{2(n-1)(n-2)(n-5)} < 0,
\end{aligned}$$

$$
\begin{aligned}
Kf(\overline{U_8})-(2n-1) &= -\frac{n^5-9n^4+19n^3-13n^2+55n-33}{2(n-1)(n-3)(n^2-5n+3)}<0,\\
Kf(\overline{U_9})-(2n-1) &= -\frac{n^5-9n^4+20n^3-16n^2+36n-52}{2(n-1)(n-2)(n^2-6n+7)}<0,\\
Kf(\overline{U_{10}})-(2n-1) &= Kf(\overline{U_{11}})-(2n-1)=-\frac{n^4-8n^3+12n^2-2n+45}{2(n-1)(n-3)(n-4)}<0,\\
Kf(\overline{U_{12}})-(2n-1) &= -\frac{n^6-10n^5+29n^4-32n^3+59n^2-108n+31}{(n-1)(2n^4-18n^3+54n^2-60n+17)}<0,\\
Kf(\overline{U_{13}})-(2n-1) &= -\frac{n^5-9n^4+21n^3-13n^2+35n-55}{2(n-1)(n-3)(n^2-5n+5)}<0,\\
Kf(\overline{U_{14}})-(2n-1) &= -\frac{n^5-7n^4+9n^3-5n^2+37n-11}{2(n-1)(n-3)(n^2-3n+1)}<0,\\
Kf(\overline{U_{15}})-(2n-1) &= -\frac{n^5-9n^4+21n^3-17n^2+39n-55}{(n-1)(2n^3-16n^2+39n-29)}<0,\\
Kf(\overline{U_{16}})-(2n-1) &= -\frac{n^5-9n^4+22n^3-16n^2+35n-63}{(n-1)(n-3)(2n^2-10n+11)}<0,
\end{aligned}
$$

completing the proof. □

Remark 3. Based on the above values of $Kf(\overline{U_i})$, one may further verify that $Kf(\overline{U_1}) > Kf(\overline{U_2}) > \cdots > Kf(\overline{U_{10}}) = Kf(\overline{U_{11}}) > \cdots > Kf(\overline{U_{16}})$ holds for $n \geq 28$, whereas it was shown in [15,21,22] that $\mu_1(U_1) > \mu_1(U_2) > \cdots > \mu_1(U_7) > \mu_1(U_9) > \mu_1(U_{10}) = \mu_1(U_{11}) > \mu_1(U_{12}) > \mu_1(U_8) = \mu_1(U_{13}) = \mu_1(U_{14}) > \mu_1(U_{15}) > \mu_1(U_{16})$. This means that the Kirchhoff indices of the complements of unicyclic graphs are likely to be irrelevant to the Laplacian spectral radii of those unicyclic graphs, which behaves in a way different from trees.

§4 Concluding remarks

We have provided a method for ordering the Kirchhoff indices of the complements of trees and unicyclic graphs, which is mainly based on Theorem 3.1. With this method, we have determined the first 5 maximum values of $Kf(\overline{T})$ for trees, which extends the ordering given by Deng and Chen [7]; we have also determined the first 4 maximum values of $Kf(\overline{U})$ for unicyclic graphs. Comparing with the method based on (2), our method seems to be more efficient to some extent. In fact, using our method, one can further extend the ordering given in Theorems 3.4 and 3.5 (for sufficient large n). For example, the first 12 maximum values of $Kf(\overline{T})$ would be determined as long as all the trees T with $\mu_1(T) > n-6$ could be drawn out from $\mathcal{T}(n)$, which are exactly those trees T with the maximum degree $\Delta(T) \geq n-7$ (see [34]). Likewise, the first 16 maximum values of $Kf(\overline{U})$ would be determined as long as all the unicyclic graphs U with $\mu_1(U) > n-4$ could be drawn out from $\mathcal{U}(n)$, which are exactly those unicyclic graphs U with $\Delta(U) \geq n-5$ (see [21]). The calculation in this extending work is, of course, considerably large and tedious.

Acknowledgements. The authors would like to thank the anonymous referees for their valuable comments and suggestions which have contributed to the final preparation of the paper.

Appendix

Here we list the Laplacian characteristic polynomials of the trees $T_1, T_2, \ldots, T_{31}$ (shown in Figure 1) and unicyclic graphs $U_1, U_2, \ldots, U_{16}$ (shown in Figure 2), which are computed by the software 'Mathematica 5.0' based on Lemma 2.6.

List 1. The characteristic polynomials of $L(T_1), L(T_2), \ldots, L(T_{31})$

$$
\begin{aligned}
\Phi(L(T_1);x) &= x(x-1)^{n-2}(x-n)\\
\Phi(L(T_2);x) &= x(x-1)^{n-4}[x^3-(n+2)x^2+(3n-2)x-n]\\
\Phi(L(T_3);x) &= x(x-1)^{n-4}[x^3-(n+2)x^2+(4n-7)x-n]\\
\Phi(L(T_4);x) &= x(x-1)^{n-6}(x^2-3x+1)[x^3-(n+1)x^2+(3n-5)x-n]\\
\Phi(L(T_5);x) &= x(x-1)^{n-5}[x^4-(n+3)x^3+(5n-4)x^2-(6n-10)x+n]\\
\Phi(L(T_6);x) &= x(x-1)^{n-4}[x^3-(n+2)x^2+(5n-14)x-n]\\
\Phi(L(T_7);x) &= x(x-1)^{n-6}[x^5-(n+4)x^4+(7n-7)x^3-(14n-32)x^2+(7n-10)x-n]\\
\Phi(L(T_8);x) &= x(x-1)^{n-8}(x^2-3x+1)^2[x^3-nx^2+(3n-8)x-n]\\
\Phi(L(T_9);x) &= x(x-1)^{n-6}[x^5-(n+4)x^4+(7n-7)x^3-(14n-32)x^2+(8n-17)x-n]\\
\Phi(L(T_{10});x) &= x(x-1)^{n-7}[x^6-(n+5)x^5+(8n-2)x^4-(22n-40)x^3\\
&\quad +(24n-53)x^2-(9n-13)x+n]\\
\Phi(L(T_{11});x) &= x(x-1)^{n-5}[x^4-(n+3)x^3+(6n-10)x^2-(8n-22)x+n]\\
\Phi(L(T_{12});x) &= x(x-1)^{n-5}[x^4-(n+3)x^3+(6n-9)x^2-(9n-25)x+n]\\
\Phi(L(T_{13});x) &= x(x-1)^{n-4}[x^3-(n+2)x^2+(6n-23)x-n]\\
\Phi(L(T_{14});x) &= x(x-1)^{n-6}[x^5-(n+4)x^4+(8n-15)x^3-(17n-56)x^2+(8n-17)x-n]\\
\Phi(L(T_{15});x) &= x(x-1)^{n-6}(x^2-4x+1)[x^3-nx^2+(4n-15)x-n]\\
\Phi(L(T_{16});x) &= x(x-1)^{n-8}(x^2-3x+1)[x^5-(n+3)x^4+(7n-14)x^3-(14n-45)x^2\\
&\quad +(7n-13)x-n]\\
\Phi(L(T_{17});x) &= x(x-1)^{n-10}(x^2-3x+1)^3[x^3-(n-1)x^2+(3n-11)x-n]\\
\Phi(L(T_{18});x) &= x(x-1)^{n-6}[x^5-(n+4)x^4+(8n-15)x^3-(17n-56)x^2+(9n-26)x-n]\\
\Phi(L(T_{19});x) &= x(x-1)^{n-8}[x^7-(n+6)x^6+(10n-4)x^5-(36n-84)x^4+(57n-170)x^3\\
&\quad -(39n-108)x^2+(11n-20)x-n]\\
\Phi(L(T_{20});x) &= x(x-1)^{n-7}[x^6-(n+5)x^5+(9n-9)x^4-(27n-75)x^3\\
&\quad +(30n-94)x^2-(10n-18)x+n]\\
\Phi(L(T_{21});x) &= x(x-1)^{n-9}(x^2-3x+1)[x^6-(n+4)x^5+(8n-10)x^4-(22n-61)x^3\\
&\quad +(24n-72)x^2-(9n-16)x+n]\\
\Phi(L(T_{22});x) &= x(x-1)^{n-6}[x^5-(n+4)x^4+(8n-14)x^3-(18n-60)x^2+(10n-31)x-n]\\
\Phi(L(T_{23});x) &= x(x-1)^{n-7}(x^2-3x+1)[x^4-(n+2)x^3+(6n-16)x^2-(8n-29)x+n]\\
\Phi(L(T_{24});x) &= x(x-1)^{n-7}[x^6-(n+5)x^5+(9n-9)x^4-(27n-75)x^3\\
&\quad +(31n-102)x^2-(12n-34)x+n]\\
\Phi(L(T_{25});x) &= x(x-1)^{n-7}[x^6-(n+5)x^5+(9n-9)x^4-(27n-75)x^3\\
&\quad +(31n-101)x^2-(11n-25)x+n]\\
\Phi(L(T_{26});x) &= x(x-1)^{n-8}(x^3-5x^2+6x-1)[x^4-(n+1)x^3+(5n-14)x^2-(6n-21)x+n]\\
\Phi(L(T_{27});x) &= x(x-1)^{n-7}[x^6-(n+5)x^5+(9n-8)x^4-(28n-76)x^3\\
&\quad +(34n-112)x^2-(12n-28)x+n]
\end{aligned}
$$

$$\begin{aligned}
\Phi(L(T_{28});x) &= x(x-1)^{n-5}\big[x^4-(n+3)x^3+(7n-18)x^2-(10n-38)x+n\big]\\
\Phi(L(T_{29});x) &= x(x-1)^{n-7}\big[x^6-(n+5)x^5+(9n-9)x^4-(27n-75)x^3\\
&\qquad +(32n-109)x^2-(13n-41)x+n\big]\\
\Phi(L(T_{30});x) &= x(x-1)^{n-5}\big[x^4-(n+3)x^3+(7n-16)x^2-(12n-46)x+n\big]\\
\Phi(L(T_{31});x) &= x(x-1)^{n-7}\big[x^6-(n+5)x^5+(9n-8)x^4-(28n-76)x^3\\
&\qquad +(35n-119)x^2-(15n-49)x+n\big]
\end{aligned}$$

List 2. The characteristic polynomials of $L(U_1), L(U_2), \ldots, L(U_{16})$

$$\begin{aligned}
\Phi(L(U_1);x) &= x(x-1)^{n-3}(x-3)(x-n)\\
\Phi(L(U_2);x) &= x(x-1)^{n-5}(x-2)\big[x^3-(n+3)x^2+(4n-2)x-2n\big]\\
\Phi(L(U_3);x) &= x(x-1)^{n-5}\big[x^4-(n+5)x^3+(6n+3)x^2-(9n-5)x+3n\big]\\
\Phi(L(U_4);x) &= x(x-1)^{n-5}(x-3)\big[x^3-(n+2)x^2+(3n-2)x-n\big]\\
\Phi(L(U_5);x) &= x(x-1)^{n-5}\big[x^4-(n+5)x^3+(7n-1)x^2-(13n-19)x+4n\big]\\
\Phi(L(U_6);x) &= x(x-1)^{n-7}(x-2)\big[x^5-(n+5)x^4+(7n+1)x^3-(15n-17)x^2+(10n-8)x-2n\big]\\
\Phi(L(U_7);x) &= x(x-1)^{n-5}\big[x^4-(n+5)x^3+(7n-3)x^2-(11n-17)x+3n\big]\\
\Phi(L(U_8);x) &= x(x-1)^{n-6}(x^2-5x+3)\big[x^3-(n+1)x^2+(3n-5)x-n\big]\\
\Phi(L(U_9);x) &= x(x-1)^{n-6}(x-2)\big[x^4-(n+4)x^3+(6n-4)x^2-(8n-12)x+2n\big]\\
\Phi(L(U_{10});x) &= \Phi(L(U_{11});x)=x(x-1)^{n-5}(x-3)\big[x^3-(n+2)x^2+(4n-7)x-n\big]\\
\Phi(L(U_{12});x) &= x(x-1)^{n-7}\big[x^6-(n+7)x^5+(9n+10)x^4-(28n-18)x^3\\
&\qquad +(36n-42)x^2-(18n-14)x+3n\big]\\
\Phi(L(U_{13});x) &= x(x-1)^{n-6}(x^2-5x+5)\big[x^3-(n+1)x^2+(3n-5)x-n\big]\\
\Phi(L(U_{14});x) &= x(x-1)^{n-7}(x-3)(x^2-3x+1)\big[x^3-(n+1)x^2+(3n-5)x-n\big]\\
\Phi(L(U_{15});x) &= x(x-1)^{n-6}\big[x^5-(n+6)x^4+(8n+4)x^3-(20n-22)x^2+(17n-26)x-3n\big]\\
\Phi(L(U_{16});x) &= x(x-1)^{n-6}(x-3)\big[x^4-(n+3)x^3+(5n-4)x^2-(6n-10)x+n\big]
\end{aligned}$$

References

[1] W N Anderson, T D Morley. *Eigenvalues of Laplacian of a graph*, Linear Multilinear Algebra, 1985, 18: 141-145.

[2] D Babić, D J Klein, I Lukovits, S Nikolić, N Trinajstić. *Resistance distance matrix: a computational algorithm and its application*, Int J Quantum Chem, 2002, 90: 166-176.

[3] D Bonchev, A T Balaban, X Liu, D J Klein. *Molecular cyclicity and centricity of polycyclic graphs: I. Cyclicity based on resistance distances or reciprocal distances*, Int J Quantum Chem, 1994, 50: 1-20.

[4] K C Das. *A sharp upper bound for the number of spanning trees of a graph*, Graphs Combin, 2007, 23: 625-632.

[5] K C Das. *On Kirchhoff index of graphs*, Z Naturforsch, 2013, 68a: 531-538.

[6] H Deng. *On the minimum Kirchhoff index of graphs with a given number of cut edges*, MATCH Commun Math Comput Chem, 2010, 63: 171-180.

[7] Q Deng, H Chen. *On the Kirchhoff index of the complement of a bipartite graph*, Linear Algebra Appl, 2013, 439: 167-173.

[8] Q Deng, H Chen. *On extremal bipartite unicyclic graphs*, Linear Algebra Appl, 2014, 444: 89-99.

[9] E Estrada, N Hatano. *Topological atomic displacements, Kirchhoff and Wiener indices of molecules*, Chem Phys Lett, 2010, 486: 166-170.

[10] L Feng, G Yu, K Xu, Z Jiang. *A note on the Kirchhoff index of bicyclic graphs*, Ars Combin, 2014, 114: 33-40.

[11] X Gao, Y Luo, W Liu. *Resistance distances and the Kirchhoff index in Cayley graphs*, Discrete Appl Math, 2011, 159: 2050-2057.

[12] I Gutman, B Mohar. *The quasi-Wiener and the Kirchhoff indices coincide*, J Chem Inf Comput Sci, 1996, 36: 982-985.

[13] J Guo. *On the Laplacian spectral radius of a tree*, Linear Algebra Appl, 2003, 368: 379-385.

[14] J Guo. *On the second largest Laplacian eigenvalue of trees*, Linear Algebra Appl, 2005, 404: 251-261.

[15] S Guo. *The largest eigenvalues of Laplacian matrices of unicyclic graphs (in Chinese)*, Appl Math J Chinese Univ Ser A, 2001, 16(2): 131-135.

[16] J Huang, S Li, Q Zhao. *On extremal bipartite bicyclic graphs*, J Math Anal Appl, 2016, 436: 1242-1255.

[17] D J Klein, M Randić. *Resistance distance*, J Math Chem, 1993, 12: 81-95.

[18] D J Klein. *Graph geometry, graph metrics, and Wiener*, MATCH Commun Math Comput Chem, 1997, 35: 7-27.

[19] R Li. *Lower bounds for the Kirchhoff index*, MATCH Commun Math Comput Chem, 2013, 70: 163-174.

[20] J Liu, X Pan, L Yu, D Li. *Complete characterization of bicyclic graphs with minimal Kirchhoff index*, Discrete Appl Math, 2016, 200: 95-107.

[21] M Liu, F Wei, Y Zhu. *A new method to order the unicyclic graphs by their Laplace spectral radii (in Chinese)*, J Huizhou Univ, 2008, 28(6): 10-14.

[22] Y Liu, J Shao, X Yuan. *Some results on the ordering of the Laplacian spectral radii of unicyclic graphs*, Discrete Appl Math, 2008, 156: 2679-2697.

[23] B Mohar. *The Laplacian spectrum of graphs*, in: Y Alavi, G Chartrand, O R Oellermann, A J Schwenk (Eds), Graph Theory, Combinatorics, and Applications, Wiley, New York, 1991, 2: 871-898.

[24] J L Palacios. *On the Kirchhoff index of graphs with diameter 2*, Discrete Appl Math, 2015, 184: 196-201.

[25] S Pirzada, H A Ganie, I Gutman. *Comparison between the Laplacian-energy-like invariant and the Kirchhoff index*, Electron J Linear Algebra, 2016, 31: 27-41.

[26] H Wang, H Hua, D Wang. *Cacti with minimum, second-minimum, and third-minimum Kirchhoff indices*, Math Commun, 2010, 15: 347-358.

[27] W Wang, D Yang, Y Luo. *The Laplacian polynomial and Kirchhoff index of graphs derived from regular graphs*, Discrete Appl Math, 2013, 161: 3063-3071.

[28] W Xiao, I Gutman. *Resistance distance and Laplacian spectrum*, Theor Chem Acc, 2003, 110: 284-289.

[29] K Xu, H Liu, K C Das. *The Kirchhoff index of quasi-tree graphs*, Z Naturforsch, 2015, 70a: 135-139.

[30] K Xu, K C Das, X Zhang. *Ordering connected graphs by their Kirchhoff indices*, Int J Comput Math, 2016, 93: 1741-1755.

[31] Y Yang, X Jiang. *Unicyclic graphs with extremal Kirchhoff index*, MATCH Commun Math Comput Chem, 2008, 60: 107-120.

[32] Y Yang, D J Klein. *Comparison theorems on resistance distances and Kirchhoff indices of S, T-isomers*, Discrete Appl Math, 2014, 175: 87-93.

[33] A Yu, M Lu, F Tian. *Ordering trees by their Laplacian spectral radii*, Linear Algebra Appl, 2005, 405: 45-59.

[34] X Yuan, H Shan, Y Liu. *On the Laplacian spectral radii of trees*, Discrete Math, 2009, 309: 4241-4246.

[35] H Zhang, X Jiang, Y Yang. *Bicyclic graphs with extremal Kirchhoff index*, MATCH Commun Math Comput Chem, 2009, 61: 697-712.

[36] W Zhang, H Deng. *The second maximal and minimal Kirchhoff indices of unicyclic graphs*, MATCH Commun Math Comput Chem, 2009, 61: 683-695.

[37] X Zhang, J Li. *The two largest eigenvalues of Laplacian matrices of trees (in Chinese)*, J China Univ Sci Technol, 1998, 28(5): 513-518.

[38] B Zhou, N Trinajstić. *A note on Kirchhoff index*, Chem Phys Lett, 2008, 455: 120-123.

[39] H Zhu, D J Klein, I Lukovits. *Extensions of the Wiener number*, J Chem Inf Comput Sci, 1996, 36: 420-428.

*College of Mathematics and Information Science, Guangxi University, Nanning 530004, China.
Email: x.d.chen@live.cn

Guangxi Center for Mathematical Research, Guangxi University, Nanning 530004, China.

College of Science, East China University of Technology, Nanchang 330013, China.