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ORIGINAL PAPER

New Nordhaus-Gaddum-type results for the Kirchhoff index

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Abstract Let G be a connected graph. The resistance distance between any two vertices of G is defined as the net effective resistance between them if each edge of G is replaced by a unit resistor. The Kirchhoff index is the sum of resistance distances between all pairs of vertices in G. Zhou and Trinajstić (Chem Phys Lett 455 (1–3):120–123, 2008) obtained a Nordhaus-Gaddum-type result for the Kirchhoff index by obtaining lower and upper bounds for the sum of the Kirchhoff index of a graph and its complement. In this paper, by making use of the Cauchy-Schwarz inequality, spectral graph theory and Foster's formula, we give better lower and upper bounds. In particular, the lower bound turns out to be tight. Furthermore, we establish lower and upper bounds on the product of the Kirchhoff index of a graph and its complement.

Keywords Resistance distance · Kirchhoff index · Nordhaus-Gaddum-type result

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1 Introduction

Let G be a connected graph with vertices labeled as $1, 2, \ldots, n$. It is well known that the standard distance between two vertices i and j, denoted by $d_{ij}(G)$, is the length of a shortest path connecting them. The Wiener index [1], or Wiener-Bavelas index of G [2], denoted by $W(G)$, is a famous distance-based topological index and is defined as the sum of distances between all pairs of vertices in G:

$$W(G) = \sum_{i<j} d_{ij}(G).$$

In 1993, another novel distance function named resistance distance was identified [3]. They view G as an electrical network N by replacing each edge of G with a unit resistor. Then the resistance distance between i and j, denoted by $r_{ij}(G)$, is defined to be the net effective resistance between them in the network N. As an analogue to the Wiener index $W(G)$, they also defined the Kirchhoff index $Kf(G)$ of G as the sum of resistance distances between all pairs of vertices, that is

$$Kf(G) = \sum_{i<j} r_{ij}(G).$$

It is shown that the Kirchhoff index has very nice purely mathematical and physical interpretations. For example, Zhu et al. [4], and Gutman and Mohar [5] proved that the Kirchhoff index of a graph is the sum of reciprocal nonzero Laplacian eigenvalues of the graph multiplied by the number of vertices; Estrada and Hatano [6] showed that the Kirchhoff index of a (molecular) graph is simply the sum of the squared atomic displacements produced by small molecular vibrations multiplied by the number of atoms in the molecule. Besides, it also serves as an important molecular structure-descriptor in chemistry [7]. In view of the above, the Kirchhoff index is well studied in mathematical, physical and chemical literatures, the reader are referred to [8–23] and references therein.

A Nordhaus-Gaddum-type result is a (tight) lower or upper bound on the sum or product of a parameter of a graph and its complement. Problems of this type were first considered by Nordhaus and Gaddum [24] for the chromatic number. From then on various graph parameters including topological indices were taken into consideration, such as edge chromatic number [25], independence number [26], independent domination number [27], spectral radius [28], general Randić index [29], Wiener and Zagreb indices [30], energy and Laplacian energy [31]. In [21], Zhou and Trinajstić took the Kirchhoff index into account and obtained lower and upper bounds on the sum of the Kirchhoff index of a graph and its complement. In this paper, firstly we improve their bounds. By the Cauchy-Schwarz inequality and spectral graph theory, we obtain a sharp lower bound, fully characterizing the graphs achieving this lower bound, then by Foster's formula and the Nordhaus-Gaddum-type result for the Wiener index, we obtain a superior upper bound. Secondly, we give lower and upper bounds for the product of the Kirchhoff index of a graph and its complement.

2 Preliminaries

We recall some concepts, notations and results in graph theory.

The adjacency matrix $A(G)$ of G is an $n \times n$ matrix with the (i, j)-entry equal to 1 if vertices i and j are adjacent and 0 otherwise. Let $D(G) = \mathrm{diag}\,(d_1(G), d_2(G), \ldots, d_n(G))$ be the degree-diagonal matrix of G, where $d_i(G)$ is the degree of the vertex i, $i = 1, 2, \ldots, n$. Then $L(G) = D(G) - A(G)$ is called the Laplacian matrix of G. In addition, the eigenvalues of $A(G)$ and $L(G)$ are called eigenvalues and Laplacian eigenvalues of G, respectively.

Let $0 = \lambda_0 < \lambda_1 \leq \cdots \leq \lambda_{n-1}$ be the Laplacian eigenvalues of G. Then the Laplacian spectrum $S(G)$ of G is defined as

$$S(G) = (\lambda_0, \lambda_1, \ldots, \lambda_{n-1}).$$

Zhou [32] proved the following result

Theorem 2.1 *Let G be a connected graph with n vertices. Then $\lambda_1 = \lambda_2 = \cdots = \lambda_{n-1}$ if and only if $G \cong K_n$.*

As mentioned in the first section, the Kirchhoff index of G can be expressed via positive Laplacian eigenvalues as in the following theorem,

Theorem 2.2 [4,5] *For any connected n-vertex graph G, $n \geq 2$,*

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

In what follows, we introduce the concepts of strongly regular graphs including conference graphs, and review some properties of them.

Definition 2.3 A strongly regular graph with parameters (n, k, a, c), denoted by $\mathrm{srg}(n, k, a, c)$, is a k-regular graph on n vertices such that for every pair of adjacent vertices there are a vertices adjacent to both, and for every pair of non-adjacent vertices there are c vertices adjacent to both. We exclude $k = 0$ and $k = n - 1$ from being strongly regular.

There are three basic facts about strongly regular graphs.

Theorem 2.4 [33]

(a) *The complement of a strongly regular graph is strongly regular; precisely, the complement of a $\mathrm{srg}(n, k, a, c)$ is a $\mathrm{srg}(n, n-1-k, n-2-2k+c, n-2k+a)$.*

(b) *A strongly regular graph is disconnected if and only if it is isomorphic to mK_r (the disjoint union of m copies of K_r), for some positive integers m and r; this occurs if and only if $c = 0$.*

(c) *Every connected strongly regular graph has diameter 2.*

It is well known [34] that a srg(n, k, a, c) has eigenvalues

$$k, \text{ and } \theta_{\pm} = \frac{a - c \pm \sqrt{\Delta}}{2}$$

with corresponding multiplicities

$$1, \text{ and } m_{\mp} = \frac{1}{2}\left(n - 1 \mp \frac{(n-1)(c-a) - 2k}{\sqrt{\Delta}}\right),$$

where $\Delta = (a-c)^2 + 4(k-c) > 0$. Conversely, it is shown that

Theorem 2.5 [34] *A connected regular graph with exactly three distinct eigenvalues is strongly regular.*

Now we turn to an important class of strongly regular graphs-conference graphs.

Definition 2.6 A conference graph is a strongly regular graph with multiplicities $m_+ = m_-$.

A conference graph can also be defined in a another way as follows.

Lemma 2.7 [35] *A graph G is a conference graph if and only if G is a srg*$(n, \frac{n-1}{2}, \frac{n-5}{4}, \frac{n-1}{4})$.

It is easily verified that Theorem 2.4 (a) and (b) yield two simple properties of conference graphs.

Proposition 2.8 (a) *All conference graphs are connected.*

(b) *The complement of a conference graph is also a conference graph.*

At the end of this section, we prove a simple result which is used later.

Lemma 2.9 *Let G ba a connected* $srg(n, \frac{n-1}{2}, a, c)$. *Then*

$$a + c = \frac{n-3}{2}.$$

Proof As G has diameter two by Theorem 2.4 (c), we choose an arbitrary vertex v from $V(G)$ and denote by S_i the set of vertices at distance i to v, $i = 1, 2$. Clearly

$$|S_1| = |S_2| = \frac{n-1}{2}.$$

By the definition of strongly regular graphs, any vertex in S_1 has a neighbors in S_1, and thus has $(n-1)/2 - a - 1$ neighbors in S_2, while any vertex in S_2 has c neighbors in S_1. This indicates that $(n-1)/2 - a - 1 = c$ and the proof is completed. □

3 Bounds for $Kf(G) + Kf(\overline{G})$

In [21], Zhou and Trinajstić obtained a Nordhaus-Gaddum-type result for the Kirchhoff index.

Theorem 3.1 [21] *Let G be a connected (molecular) graph on $n \geq 5$ vertices with a connected $\overline{G}$. Then*

$$4n - 2 \leq Kf(G) + Kf(\overline{G}) < \frac{n^3 + 3n^2 + 2n - 6}{6}. \tag{2}$$

In this section, we improve their results by showing that

Theorem 3.2 *Let G be a connected (molecular) graph on $n \geq 5$ vertices with a connected $\overline{G}$. Then*

$$4n \leq Kf(G) + Kf(\overline{G}) < \frac{n^3 + 17n - 18}{6}, \tag{3}$$

and equality holds (at the lower bound) if and only if G is a conference graph.

Proof We first prove the lower bound. Let $d_1 \leq d_2 \leq \cdots \leq d_n$ and $0 = \lambda_0 < \lambda_1 \leq \cdots \leq \lambda_{n-1}$ be the vertex degrees and the Laplacian eigenvalues of G, respectively. Then it is well known that [36]

$$S(\overline{G}) = (0, n - \lambda_{n-1}, n - \lambda_{n-2}, \ldots, n - \lambda_1).$$

So by Theorem 2.2,

$$\begin{aligned} Kf(G) + Kf(\overline{G}) &= n \sum_{i=1}^{n-1} \frac{1}{\lambda_i} + n \sum_{i=1}^{n-1} \frac{1}{n - \lambda_i} \\ &= n \sum_{i=1}^{n-1} \left(\frac{1}{\lambda_i} + \frac{1}{n - \lambda_i} \right) \\ &= n^2 \sum_{i=1}^{n-1} \frac{1}{\lambda_i (n - \lambda_i)}, \end{aligned}$$

and by the Cauchy-Schwarz inequality, we have

$$\sum_{i=1}^{n-1} \frac{1}{\lambda_i (n - \lambda_i)} \geq \frac{(n-1)^2}{\sum_{i=1}^{n-1} \lambda_i (n - \lambda_i)}. \tag{4}$$

Since

$$\mathrm{tr}(L(G)) = \sum_{i=1}^{n} d_i = \sum_{i=0}^{n-1} \lambda_i$$

and

$$\mathrm{tr}(L(G)^2) = \sum_{i=1}^{n}(d_i^2 + d_i) = \sum_{i=0}^{n-1}\lambda_i^2,$$

so

$$\begin{aligned}\sum_{i=1}^{n-1}\lambda_i(n-\lambda_i) &= n\sum_{i=1}^{n-1}\lambda_i - \sum_{i=1}^{n-1}\lambda_i^2 = n\sum_{i=1}^{n}d_i - \sum_{i=1}^{n}(d_i^2+d_i)\\ &= \sum_{i=1}^{n}d_i(n-1-d_i) \le \sum_{i=1}^{n}\left(\frac{n-1}{2}\right)^2\\ &= \frac{n(n-1)^2}{4},\end{aligned} \tag{5}$$

and thus

$$Kf(G) + Kf(\overline{G}) = n^2\sum_{i=1}^{n-1}\frac{1}{\lambda_i(n-\lambda_i)} \ge n^2\frac{(n-1)^2}{\frac{n(n-1)^2}{4}} = 4n. \tag{6}$$

Now we discuss the sharpness of the lower bound. Equality holds in (6) if and only if equalities in both (4) and (5) hold. Equality can only hold in (4) if for all $1 \le i \ne j \le n-1$,

$$\lambda_i(n-\lambda_i) = \lambda_j(n-\lambda_j),$$

or equivalently

$$(\lambda_i - \lambda_j)(n - \lambda_i - \lambda_j) = 0,$$

which indicates that either $\lambda_i = \lambda_j$ or $\lambda_i + \lambda_j = n$; and equality can only hold in (5) if G is $(n-1)/2$−regular. From our hypothesis G is not complete, so by Theorem 2.1 we know $\lambda_1 = \lambda_2 = \cdots = \lambda_{n-1}$ is impossible, and equality can only hold in (4) if G has exactly two distinct non-zero Laplacian eigenvalues λ_1 and $n - \lambda_1$; in other words, G has exactly three distinct Laplacian eigenvalues 0, λ_1 and $n - \lambda_1$. Since G is $(n-1)/2$-regular, G also has exactly three distinct adjacency-matrix eigenvalues

$$\frac{n-1}{2},\ \frac{n-1}{2} - \lambda_1 \text{ and } \lambda_1 - \frac{n+1}{2}. \tag{7}$$

By Theorem 2.5, G is strongly regular and thus we may suppose that G is a srg$(n, \frac{n-1}{2}, a, c)$. Then by the spectral property of a strongly regular graph we get that the three distinct eigenvalues of G are

$$\frac{n-1}{2},\ \text{and } \theta_\pm = \frac{a-c\pm\sqrt{\Delta}}{2}, \tag{8}$$

where $\Delta = (a-c)^2 + 4((n-1)/2 - c)$. Comparing (7) with (8), we know

$$\theta_+ + \theta_- = \frac{a-c+\sqrt{\Delta}}{2} + \frac{a-c-\sqrt{\Delta}}{2} = a-c = \frac{n-1}{2} - \lambda_1 + \lambda_1 - \frac{n+1}{2} = -1,$$

that is

$$c - a = 1. \tag{9}$$

On the other hand, by Lemma 2.9,

$$a + c = \frac{n-3}{2}. \tag{10}$$

Combining (9) and (10), one finds $a = \frac{n-5}{4}$ and $c = \frac{n-1}{4}$. Hence G is a srg$(n, \frac{n-1}{2}, \frac{n-5}{4}, \frac{n-1}{4})$ and it follows that G is a conference graph by Lemma 2.7. Furthermore, by Proposition 2.8, $\overline{G}$ is also a conference graph. Hence

$$Kf(G) + Kf(\overline{G}) \geq 4n$$

with equality if and only if G is a conference graph.

To prove the upper bound, we use the famous Foster's formula [37], which states that the sum of resistance distances between all pairs of adjacent vertices in a connected n-vertex graph is $n-1$, whence $\sum_{i<j_{d_{ij}(G)=1}} r_{ij}(G) + \sum_{i<j_{d_{ij}(\overline{G})=1}} r_{ij}(\overline{G}) = 2(n-1)$. Clearly $\sum_{i<j_{d_{ij}(G)=1}} d_{ij}(G) + \sum_{i<j_{d_{ij}(\overline{G})=1}} d_{ij}(\overline{G}) = \frac{n(n-1)}{2}$ and recall that [30] $W(G) + W(\overline{G}) \leq \frac{n^3+3n^2+2n-6}{6}$ with equality if and only if $G = P_n$ or $G = \overline{P_n}$. Then it follows that

$$Kf(G) + Kf(\overline{G}) \leq W(G) + W(\overline{G}) - \left(\frac{n(n-1)}{2} - 2(n-1)\right) \leq \frac{n^3+17n-18}{6}. \tag{11}$$

For equality in (11) to hold requires not only $G = P_n$ or $G = \overline{P_n}$, but also the resistance distance between each pair of nonadjacent vertices in both G and $\overline{G}$ be equal to the distance between them. But this is impossible since the resistance distance between every pair of nonadjacent vertices in $\overline{P_n}$ is less than the shortest-path distance between them because they are connected by more than one path. So

$$Kf(G) + Kf(\overline{G}) < \frac{n^3+17n-18}{6}.$$

and the proof is completed. □

Though the upper bound is not sharp, we can show that it is nearly the best possible with an example. Take the n-vertex path P_n for an example. It is well known that

$$Kf(P_n) = W(P_n) = \frac{n^3 - n}{6},$$

so it suffices to compute $Kf(\overline{P_n})$. Since [38]

$$S(P_n) = \left(0, 4\sin^2\frac{\pi}{2n}, 4\sin^2\frac{2\pi}{2n}, \ldots, 4\sin^2\frac{(n-1)\pi}{2n}\right),$$

so

$$S(\overline{P_n}) = \left(0, n - 4\sin^2\frac{\pi}{2n}, n - 4\sin^2\frac{2\pi}{2n}, \ldots, n - 4\sin^2\frac{(n-1)\pi}{2n}\right).$$

Then by Theorem 2.2, we have

$$Kf(\overline{P_n}) = n\sum_{k=1}^{n-1}\frac{1}{n - 4\sin^2\frac{k\pi}{2n}}. \tag{12}$$

Thus

$$\begin{aligned} Kf(P_n) + Kf(\overline{P_n}) &= \frac{n^3 - n}{6} + n\sum_{k=1}^{n-1}\frac{1}{n - 4\sin^2\frac{k\pi}{2n}} \\ &> \frac{n^3 - n}{6} + n - 1 = \frac{n^3 + 5n - 6}{6}. \end{aligned}$$

Comparing $Kf(P_n) + Kf(\overline{P_n})$ with the upper bound in Theorem 3.2, we can conclude that the upper bound is nearly the best possible.

The above example not only illustrates that the upper bound is the best possible, but also motivates us to propose the following conjecture.

Conjecture 3.3 *Let G be a connected graph with a connected $\overline{G}$. Then*

$$Kf(G) + Kf(\overline{G}) \le \frac{n^3 - n}{6} + n\sum_{k=1}^{n-1}\frac{1}{n - 4\sin^2\frac{k\pi}{2n}}, \tag{13}$$

with equality holding if and only if $G = P_n$ or $G = \overline{P_n}$.

4 Bounds for $Kf(G) \times Kf(\overline{G})$

The diameter of a graph G, denoted by $d(G)$, is the maximum shortest-path distance between any two vertices in G. In this section, we give bounds for the product of

$Kf(G)$ and $Kf(\overline{G})$ in terms of the vertex number n and the maximum diameter of G and $\overline{G}$.

Theorem 4.1 *Suppose that* $d = \max\{d(G), d(\overline{G})\}$. *Then*

$$4(n-1)^2 < Kf(G) \times Kf(\overline{G}) < \begin{cases} \frac{1}{16}(9n^4 + 6n^3 - 23n^2 - 8n + 16), & \text{if } d=3, \\ \frac{d}{8}n^4 + \frac{1}{2}n^3 - \frac{d^2+2d-2}{4d}n^2 \\ \quad -\frac{d+2}{2d}n + \frac{d^2+4d+4}{8d}, & \text{otherwise.} \end{cases}$$

Proof Suppose that $E(G) = m$. By the Cauchy-Schwarz inequality,

$$\begin{aligned} Kf(G) \times Kf(\overline{G}) &= n^2 \sum_{i=1}^{n-1} \frac{1}{\lambda_i} \sum_{i=1}^{n-1} \frac{1}{n - \lambda_i} \\ &\geq n^2 \frac{(n-1)^2}{\sum_{i=1}^{n-1} \lambda_i} \times \frac{(n-1)^2}{\sum_{i=1}^{n-1}(n-\lambda_i)} \\ &= n^2 \frac{(n-1)^2}{2m} \times \frac{(n-1)^2}{n(n-1) - 2m} \\ &= \frac{n^2(n-1)^4}{2m(n(n-1)-2m)} \\ &\geq \frac{n^2(n-1)^4}{(\frac{n(n-1)}{2})^2} \\ &= 4(n-1)^2. \end{aligned} \tag{14}$$

Equality in (14) implies $\lambda_1 = \lambda_2 = \cdots = \lambda_{n-1}$, which is impossible by Theorem 2.1. Hence

$$Kf(G) \times Kf(\overline{G}) > 4(n-1)^2.$$

Now we prove the upper bound. Without loss of generality, suppose that $d = d(G)$. If $d = 3$, then $d(\overline{G}) \leq 3$ and

$$\begin{aligned} Kf(G) \times Kf(\overline{G}) &= \left[\sum_{i<j} r_{ij}(G)\right] \left[\sum_{i<j} r_{ij}(\overline{G})\right] \\ &= \left[\sum_{\substack{i<j \\ d_{ij}(G)=1}} r_{ij}(G) + \sum_{\substack{i<j \\ 2\leq d_{ij}(G)\leq 3}} r_{ij}(G)\right] \\ &\quad \times \left[\sum_{\substack{i<j \\ d_{ij}(\overline{G})=1}} r_{ij}(\overline{G}) + \sum_{\substack{i<j \\ 2\leq d_{ij}(\overline{G})\leq 3}} r_{ij}(\overline{G})\right]. \end{aligned}$$

But then noting that by Foster's theorem $\sum_{ij\in E} r_{ij} = n-1$, and further for $2 \le d_{ij} \le 3$ that the corresponding $r_{ij} \le d_{ij} \le 3$, we have

$$
\begin{aligned}
Kf(G) \times Kf(\overline{G}) &< \left[n-1+3\left(\frac{n(n-1)}{2}-m\right)\right][n-1+3m] \\
&= (n-1)^2 + 3(n-1)\frac{n(n-1)}{2} + 9\left(\frac{n(n-1)}{2}-m\right)m \\
&\le (n-1)^2 + 3(n-1)\frac{n(n-1)}{2} + 9\left(\frac{n(n-1)}{4}\right)^2 \\
&= \frac{1}{16}(9n^4+6n^3-23n^2-8n+16).
\end{aligned}
$$

Else, $d = 2$ or $d > 3$. Since if $d(G) > 3$, then $d(\overline{G}) < 3$ (cf. Exercise 1.6.12 in [39]), so it holds for both $d = 2$ and $d > 3$ that $d(\overline{G}) = 2$. Thus if $d = 2$ or $d > 3$, then

$$
\begin{aligned}
Kf(G) \times Kf(\overline{G}) &= \left[\sum_{i<j} r_{ij}(G)\right]\left[\sum_{i<j} r_{ij}(\overline{G})\right] \\
&= \left[\sum_{\substack{i<j \\ d_{ij}(G)=1}} r_{ij}(G) + \sum_{\substack{i<j \\ 2\le d_{ij}(G)\le d}} r_{ij}(G)\right] \\
&\quad \times \left[\sum_{\substack{i<j \\ d_{ij}(\overline{G})=1}} r_{ij}(\overline{G}) + \sum_{\substack{i<j \\ d_{ij}(\overline{G})=2}} r_{ij}(\overline{G})\right] \\
&< \left[n-1+d\left(\frac{n(n-1)}{2}-m\right)\right][n-1+2m] \\
&= -2dm^2 + (n-1)(dn-d+2)m + \frac{n(n-1)^2 d}{2} + (n-1)^2 \\
&= -2d\left[m - \frac{(n-1)(dn-d+2)}{4d}\right]^2 + \frac{d}{8}n^4 + \frac{1}{2}n^3 \\
&\quad - \frac{d^2+2d-2}{4d}n^2 - \frac{d+2}{2d}n + \frac{d^2+4d+4}{8d} \\
&\le \frac{d}{8}n^4 + \frac{1}{2}n^3 - \frac{d^2+2d-2}{4d}n^2 - \frac{d+2}{2d}n + \frac{d^2+4d+4}{8d}.
\end{aligned}
$$

□

If we choose G to be a conference graph on n vertices, then as indicated in the proof of Theorem 3.2,

$$Kf(G) = Kf(\overline{G}) = 2n.$$

Thus

$$Kf(G) \times Kf(\overline{G}) = 2n \times 2n = 4n^2,$$

which enables us to conclude that the lower bound obtained in Theorem 4.1 is nearly the best possible. However, as far as the upper bound is concerned, it can be seen from the proof process that it is somewhat rough, so we have every reason to believe that it will be improved in the future.

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