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Some Additional Bounds for the Kirchhoff Index

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Abstract

We find new upper and lower bounds for the Kirchhoff index $R(G)$ of a graph $G = (V, E)$ using standard tools of electric networks. We compare our lower bounds with those found in the literature and we report a sharp threshold for $R(G)$: when the minimum degree exceeds $\lfloor \frac{|V|}{2} \rfloor$ then $R(G)$ is linear in $|V|$; if the minimum degree is strictly less than $\lfloor \frac{|V|}{2} \rfloor$, there are graphs for which $R(G)$ is quadratic in $|V|$.

1 Introduction

Let $G = (V, E)$ be a finite simple connected graph with vertex set $V = \{1, 2, \ldots, n\}$ and degrees d_i for $1 \leq i \leq n$, with δ and Δ the smallest and largest such degrees, respectively. The most popular resistive descriptor in Mathematical Chemistry is the Kirchhoff index $R(G)$, introduced in [12], and defined by

$$R(G) = \sum_{i<J} R_{ij}$$

where R_{ij} is the effective resistance between the vertices i and j. There exists an abundant literature about this index, of which the bibliography at the end of this article is but a sampler of the variety of approaches used through the years, and referred mostly to upper and lower bounds for $R(G)$.

Possibly the first general bound for $R(G)$ was the proof in [14] that the minimum of $R(G)$ is attained by the complete graph K_n, that is

$$R(G) \geq n - 1 = R(K_n) \tag{1}$$

for all G. Another simple proof of (1) using Foster's first formula is found in [15]. It should be mentioned that the inequality in (1) is strict if G is not K_n because the Kirchhoff index is strictly increasing in the number of edges (see [14, 19, 24] for three different and increasingly briefer proofs of this fact).

After the discovery (see [10] and [27], and also [11] and [17] for alternative proofs) that $K(G)$ can be expressed in terms on the non-zero eigenvalues λ_i of the Laplacian as

$$R(G) = n \sum_{i=2}^{n} \frac{1}{\lambda_i} \tag{2}$$

a cornucopia of *general* bounds (in the sense that they are applicable to all graphs) and also some more *particular* bounds (for graphs which are regular, bipartite, planar, edge-transitive, c-cyclic, with diameter 2, etc.) were found by applying a variety of approaches to maximize and minimize the expression (2) with real analysis, and the use of standard inequalities, majorization and Schur-convex functions. Other approaches with slightly different flavors are those that include the ideas of random walks on graphs and Wiener capacities. A relevant list of works, focused chiefly on bounds and hardly exhaustive, would include [1–3, 5, 7, 10–27].

Perhaps not so frequent in the literature, with some exceptions like direct calculations in [14] and sporadic mentions to Foster's formulas ([15, 16, 19, 22, 23]), is the use of well known facts from electric networks in order to produce upper and lower bounds for $R(G)$. In this article we return to the electrical ideas in order to find new bounds in terms of the number of vertices n, the number of edges $|E|$ and the largest and smallest degrees, Δ and δ, respectively. We compare our lower bounds to those found in the literature that depend on the same parameters. Lower bounds involving other parameters, such as the number of spanning trees, connectivity, chromatic number, independence number, clique number, etc., will not be discussed here. We also give some upper bounds, particularly when $\delta \geq \lfloor n/2 \rfloor$, in which case $R(G)$ is linear in n, and finally show that there is a sharp threshold at $\delta = \lfloor n/2 \rfloor$, in the sense that if $\delta < \lfloor n/2 \rfloor$ then $R(G)$ can be quadratic in n.

2 Lower bounds

We present in this section what we believe are new and simple upper and lower bounds for the Kirchhoff index which are derived from well known electric principles.

Proposition 1 *For any n-vertex graph G we have*

$$R(G) \geq n - 1 + \frac{2}{\Delta}\left(\binom{n}{2} - |E|\right). \tag{3}$$

This lower bound is attained by K_n.

Proof. Using Foster's first formula (see [9]) which states that $\sum_{i<j:d(i,j)=1} R_{ij} = n-1$, and the fact (see [6]) that

$$R_{ij} \geq \frac{1}{d_i} + \frac{1}{d_j} \geq \frac{2}{\Delta},$$

whenever i and j are not neighbors, we can write

$$R(G) = \sum_{i<j:d(i,j)=1} R_{ij} + \sum_{i<j:d(i,j)>1} R_{ij} = n-1+\sum_{i<j:d(i,j)>1} R_{ij}$$

$$\geq n-1+\sum_{i<j:d(i,j)>1} \frac{2}{\Delta} = n-1+\frac{2}{\Delta}\left(\binom{n}{2} - |E|\right).$$

It is clear that this lower bound is greater than or equal to $n-1$ and becomes this value if and only if the graph is K_n •

We obtain immediately the following

Corollary 1 *For any d-regular graph we have*

$$R(G) \geq n-1+\frac{n}{d}(n-1-d). \tag{4}$$

We are going to show now that the equality in the lower bound (4) (and therefore in (3)) is attained not only by K_n but by a large family of regular graphs. Let $N(i)$ be the neighborhood of the vertex i, i.e., the set of its neighbors, and let the diameter D be defined as $D = \max_{i,j}\{d(i,j) : i,j \in V\}$. Then we have

Proposition 2 *The bound (4) is attained by any n-vertex d-regular graph G for which $D = 2$ and $|N(i) \cap N(j)| = d$ for all i, j such that $d(i,j) = 2$.*

Proof. First we get an upper bound for R_{ij} when $d(i,j) = 2$. By the monotonicity principle (see [8]) and by deleting enough edges, R_{ij} is bounded above by the effective resistance of a graph which consists of d linear graphs of length 2 set in parallel between i and j, and the effective resistance of such a graph, using the rules of resistors in series and in parallel is $\frac{2}{d}$. Now using Foster's first formula we get

$$R(G) = n-1+\sum_{i<j:d(i,j)=2} R_{ij} \leq n-1+\sum_{i<j:d(i,j)=2} \frac{2}{d}$$

$$= n-1+\frac{2}{d}\sum_{i<j:d(i,j)=2} 1 = n-1+\frac{2}{d}\left(\binom{n}{2} - \frac{nd}{2}\right),$$

which coincides with (4) •

To show that the set of graphs satisfying the previous proposition is nonempty consider, for $j \geq 1, p \geq 1$, the graph $G(j,p)$ on $n = (p+1)(j+1)$ vertices which is d-regular, with $d = j(p+1)$, defined by the neighbors of its vertices thus: the neighbors of vertex v come in $p+1$ bunches of j consecutive vertices (the first bunch would be $v+1, v+2, \ldots, v+j-1$) separated by a non-neighbor (the first non-neighbor would be $v+j$). Here the addition is mod n. The densest of these examples occurs when $p = 1$; in that case $d = n-2$ and $G(j,1)$ can be described thus: from the complete graph K_{2j} we delete the j edges $(i, i+j)$, for $1 \leq i \leq j$, i.e., any vertex is connected to all others but its "opposite vertex". The least dense example occurs when $j = 1$; in that case $d = \frac{n}{2}$ and $G(1,p)$ can be described thus: every odd vertex is connected to all even vertices and every even vertex is connected to all odd vertices.

We now give a brief summary of the lower bounds for $R(G)$ found in the literature that resemble ours, in the sense that they are given in terms of n, $|E|$ and some of the degrees of the vertices.

Zhou and Trinajstić in [25] found that

$$R(G) \geq \frac{n}{1+\Delta} + \frac{n(n-2)^2}{2|E|-1-\Delta} \tag{5}$$

with equality if and only if $G = K_n$ or $G = K_{1,n-1}$.

In [7], Das et al. obtained the following bounds

$$R(G) \geq \frac{n}{\Delta+1} + \frac{n}{2|E|-\Delta-1}\left((n-2)^2 + \frac{(\Delta_2-\delta)^2}{\Delta_2\delta}\right), \tag{6}$$

where Δ_2 is the second largest degree, and the equality holds if and only if G is either $K_{1,n-1}$ or K_n. Also

$$R(G) \geq 1 + \frac{n}{\delta} + \frac{n(n-3)^2}{2|E|-\Delta-\delta-1}, \tag{7}$$

where the equality holds if and only if G is either $K_{1,n-1}$, $K_n - e$ (the complete graph K_n minus an edge e) or $Ki_{n,n-1}$ (a complete graph K_{n-1} with an extra edge between one of the vertices of the K_{n-1} and a pendent vertex).

In [13], refining the ideas used in [25] and [7] Li found two bounds for which we need some additional notation. Let Δ_3 be the third largest degree, let $N(v)$ be the set of neighbors of v and

$$c_{u,v} = |N(u) \cup N(v)|,$$

$$d_i^* = |\{v : d_v \geq i\}|.$$

If $d_u = \Delta$ and $d_v = \Delta_2$, define

$$a_{u,v} = \frac{1}{2}\left(d_v + 2 + \sqrt{(d_v+2)^2 - 8d_v + 4c_{u,v}}\right),$$

in case u and v are neighbors and

$$a_{u,v} = \frac{1}{2}\left(d_v + 1 + \sqrt{(d_v+1)^2 - 4c_{u,v}}\right),$$

otherwise. Finally, define

$$a = \max\{a_{u,v} : d_u = \Delta, d_v = \Delta_2, u \neq v\}.$$

Then if G is neither K_n nor $K_{1,n-1}$ and $n \geq 4$ we have

$$R(G) \geq n\left(\frac{1}{n} + \frac{1}{n + d_2^* - \Delta - 1} + \frac{1}{\delta} + \frac{(n-4)^2}{2|E| - \Delta - 1 - a - \delta}\right), \tag{8}$$

with equality if and only if G is $K_n - e, K_2 \vee K_{n-2}^c, K_2 \vee K_{1,n-2}^c, K_1 \vee K_{1,n-1}^c, K_{1,n} + e$ or $K_1 \vee (K_1 \cup K_{1,n-2})$.

Also, for a non-complete G with $n \geq 5$ Li showed that

$$R(G) \geq 1 + \frac{n}{\delta} + \frac{n}{n + d_2^* + d_3^* - \Delta - \Delta_2 - 1}$$
$$+ \frac{n}{n + d_2^* - \Delta - 1} + \frac{n(n-5)^2}{2|E| - \Delta - \Delta_2 - \Delta_3 - \delta}\,. \tag{9}$$

Now we will show that our bound (3) is not comparable to (5), (6), (7), (8) and (9). Indeed, (3) does not attain the equality for $K_{1,n-1}$, as (5), (6) and (7) do, in fact its value is $2n-3$ for that graph. Likewise, (3) does not attain the equality for $K_n - e$ as (8) does, but the value $n - 1 + \frac{2}{n-1} < R(K_n - e) = n - 1 + \frac{2}{n-2}$. Finally, even though (9) is not optimal for $K_{1,n-1}$, its value is $3n + 1 + \frac{n(n-5)^2}{n-4}$, which beats our value $2n-3$. This shows that our bound is outperformed by all others in the specific examples mentioned.

On the other hand, the graph $G(j,1)$, which has $n = 2j + 2$ vertices and degree $d = 2j = n - 2$, attains the equality in our bound (3), with a value equal to $n + \frac{2}{n-2}$, while (5), (6), (7) and (8) do not, because $G(j,1)$ is not among the maximal graphs of these bounds. Lastly, for this same n-vertex $(n-2)$-regular graph, the bound (9) becomes

$$n + \frac{2}{n-2} - \frac{3}{n+3} - \frac{1}{n+1} - \frac{7n-32}{n^2-6n+8},$$

which is strictly smaller than the actual value $n + \frac{2}{n-2}$ attained by our bound when $n \geq 5$.

3 Upper bounds

We first get a simple and general upper bound in the next

Proposition 3 *For any G we have*

$$R(G) \leq n-1+\left(\binom{n}{2}-|E|\right)R, \tag{10}$$

where $R=\max_{i,j} R_{ij}$.

Proof. Write, using Foster's first formula

$$R(G)=n-1+\sum_{i<j:d(i,j)\geq 2} R_{ij} \leq n-1+R\sum_{i<j:d(i,j)\geq 2} 1$$

$$=n-1+\left(\binom{n}{2}-|E|\right)R \qquad \bullet$$

Of course, the bound (10) is not very useful unless we have a good grip on the value of R. In general R can be very large, indeed its largest value for an n-vertex graph occurs when i and j are the endpoints of a linear path, in which case $R_{ij}=n-1$; using this and the fact that $|E|\geq n-1$ in (10) we obtain the following

Corollary 2 *For any n-vertex graph we have*

$$R(G) \leq \frac{(n-1)(n^2-3n+4)}{2} \ . \tag{11}$$

This corollary establishes correctly the order of the maximum value of $R(G)$, but little else, not even the right constant, because this maximum is attained by the linear graph on n vertices, whose value is $\dfrac{n^3-n}{6}$.

We can do much better than the above corollary for those graphs whose smallest degree is larger than $\lfloor\frac{n}{2}\rfloor$, for which $R(G)$ is *linear* in n. Specifically we obtain the following

Proposition 4 *For any G for which $\delta \geq \lfloor\frac{n}{2}\rfloor$ we have*

$$R(G) \leq 3n-1 \ . \tag{12}$$

Proof. Using the monotonicity principle, it is shown in [4] that if $\delta \geq \lfloor\frac{n}{2}\rfloor$ then $R\leq\frac{4}{\delta}$. Also $|E|\geq\dfrac{n\delta}{2}\geq\dfrac{1}{2}\dbinom{n}{2}$. Inserting these bounds for R and $|E|$ into (10) we get $R(G)\leq(n-1)\left(1+\frac{n}{\delta}\right)$. It is easy to see that this latter bound becomes $3n-3$ is n is even and $3n-1$ if n is odd $\bullet$

It would be interesting to determine whether (12) is a tight bound.

Adapting the discussion in [4] to our context, it should be pointed out that there is a sharp threshold at $\delta=\lfloor\frac{n}{2}\rfloor$. Indeed, when going from $\delta=\lfloor\frac{n}{2}\rfloor-1$ to $\delta=\lfloor\frac{n}{2}\rfloor$ the

Kirchhoff index drops from an n^2 order to an n order, as the previous proposition and the following example show.

Example. To simplify the discussion, let us take n to be even. Consider $G_1 = G_2 = K_{\lfloor \frac{n}{2} \rfloor}$. Delete edges (a_i, b_i) from G_i for $i = 1, 2$, and join the resulting graphs with the edges (a_1, a_2) and (b_1, b_2). The n-vertex graph thus built is $(\lfloor \frac{n}{2} \rfloor - 1)$-regular, and if we choose $a \in G_1$, $b \in G_2$ then by shorting all vertices in each G_i, $i = 1, 2$ into single vertices, and applying the monotonicity principle we see that $R_{ab} \geq \frac{1}{2}$. Since there are roughly $\dfrac{n^2}{4}$ possibles choices for a and b, the Kirchhoff index of this graph is bounded below roughly by $\dfrac{n^2}{8}$ •

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