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Revisiting Lower Bounds for the Kirchhoff Index of Graphs

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Abstract

The aims of this note are: (i) to identify clearly a family of graphs which attain the equality in several lower bounds for the Kirchhoff index $R(G)$ of a graph G; (ii) to enlarge the set of graphs which attain the equality in a classical lower bound for $R(G)$; (iii) to provide a new lower bound for $R(G)$ in terms of only four parameters (number of vertices, number of edges, number of pendent vertices and smallest non-pendant degree) which is better than or non-comparable to similar bounds obtained in the literature; (iv) to suggest how to obtain a cohort of lower bounds for $R(G)$ in terms of other descriptors, where the equalities are attained by large families of graphs, and to give two examples of such bounds.

1 Introduction

Let $G = (V, E)$ be a finite simple connected graph with vertex set $V = \{1, 2, \dots, n\}$, edge set E and degrees $\Delta = d_1 \geq d_2 = \delta_2 \geq \cdots \geq d_n = \delta$. A graph is d-regular if all its vertices have degree d. A graph is (a, b)-regular if its vertices have degree either a or b. For all graph theoretical terms the reader is referred to reference [22]. The Kirchhoff index is defined as

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

where R_{ij} is the effective resistance between $i, j \in v$ when the graph is considered as an electric network whose edges are unit resistors. It was introduced in [9] and arguably one of the most studied descriptors in Mathematical Chemistry. Of all aspects regarding this descriptor, we will focus here solely on the lower bounds.

The first general lower bound for $R(G)$ was given in [15] and it states that

$$R(G) \geq R(K_n), \tag{1}$$

where the equality is attained only for K_n.

The theme of lower bounds for $R(G)$ has attracted considerable attention through the years, and one particularly fruitful technique has been the use of majorization. Some relevant articles devoted to this theme, though not used in this note, are [2–4, 14].

In [23], Zhou and Trinajstić reported, among other lower bounds for $R(G)$, the following inequality:

$$R(G) \geq -1 + (n-1)I(G), \tag{2}$$

where $I(G)$ is the inverse degree index, defined as

$$I(G) = \sum_{i=1}^{n} \frac{1}{d_i}. \tag{3}$$

These authors stated that the equality is attained by the complete graph K_n and the complete bipartite graphs $K_{t,n-t}$, for $1 \leq t \leq \lceil \frac{n}{2} \rceil$.

In [17], we found that for d-regular graphs we have

$$R(G) \geq \frac{n^2 - n - d}{d}, \tag{4}$$

where the equality is attained by K_n and a family of graphs, later denoted Γ_d by E. Milovanović and I. Milovanović, that originally was described as the set of d-regular graphs with diameter 2 and such that the number of common neighbors between two vertices at distance 2 is d.

It is evident that (4) is a consequence of (2), and therefore our only real new contribution in [17] was to exhibit the family Γ_d, which attains the equality in (2), and that we showed to be nonempty by exhibiting specific examples. Later in [19] we reviewed these examples and noticed that they were all equal to the complete r-partite graph $K_{s,s,\ldots,s}$ for some r and s such that $rs = n$, and could not find any other examples.

E. Milovanović, I. Milovanović and their collaborators, found in a series of articles ([5, 6, 8]) a new generation of lower bounds for $R(G)$ where the equalities are attained by a large collection of graphs, which includes the family Γ_d, and that are given either in terms of a few parameters or in terms of other indices. Also in [7] they found some lower bounds expressed in terms of the number of spanning trees. Specifically, of interest for our purposes is this bound on two parameters found in [6]:

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

where the equality is attained by K_n, $K_{\frac{n}{2},\frac{n}{2}}$, or $G \in \Gamma_d$.

Also, in [6] there is a collection of lower bounds depending on at most four parameters from the set of parameters n, $|E|$, Δ, Δ_2 and δ, and where the equality is attained by a slightly larger set of graphs than that of (5). For example they have these two bounds:

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

and

$$R(G) \geq \frac{n-1-\Delta}{\Delta} + \frac{n-1}{\Delta_2} + \frac{(n-1)(n-2)^2}{2|E|-\Delta-\Delta_2}, \tag{7}$$

where the equalities are attained by K_n, $K_{1,n}$, $K_{\frac{n}{2},\frac{n}{2}}$, and $G \in \Gamma_d$.

When discussing a bound for a certain descriptor we can distinguish three aspects: (i) the universe of graphs for which the bound applies (for instance, in (2) the universe is the set of all graphs, in (4), only those which are regular); (ii) the set of parameters involved (for instance, in (2) the parameters are the degrees of all vertices, whereas in (4) the parameters are n and d); when the set of parameters for two bounds are the same, the authors in [6] say that bounds belong to the same *class*; (iii) the set of graphs for which the equality in the bound is attained, and that for lack of a better word we will call henceforth the *scope* of the bound.

In this note we identify the family Γ_d precisely as the set of all complete r-partite graphs $K_{s,s,\ldots,s}$ such that $rs = n$, thus clarifying what the scope is for many lower bounds of $R(G)$ in the literature. Also, we extend the scope of the lower bound (2) to include the complete r-partite graphs $K_{p_1,p_2,\ldots,p_r}$ such that $\sum_i p_i = n$ and the complete graph minus two non-adjacent edges, K_n^{--}. It should be noted that previously, in [5], they had extended this scope to include the graphs in Γ_d and K_n^{-}, the complete graph minus one edge. Also, we find a lower bound for $R(G)$ in terms of four parameters, different from the parameters used in the bounds in [6] (thus our bound is not in the same class of any of their bounds), but with the same scope. Finally, we take a quick look at some further lower bounds for $R(G)$ in terms of other descriptors, like the Hyper-Zagreb index and the first and second Zagreb indices.

2 The results

We prove now that for fixed n, the family Γ_d consists of all the complete r-partite graphs $K_{s,s,\ldots,s}$ such that $rs = n$ for some r and s. In [19] we noticed that all strongly regular graphs with parameters (n, d, ν, d) belong to Γ_d. Using proposition 3.1 in [12] we see that the parameters must satisfy $n - 2d + \nu = 0$ and this implies by proposition 3.5 in the same article that G must be complete multipartite. We can do better, without assuming the graph to be strongly regular. In fact, if we call $N(i)$ the set of neighbors of the vertex i, we can prove the following

Proposition 1 *Let G be an n-vertex d-regular diameter 2 graph such that $|N(i) \cap N(j)| = d$ whenever i and j are not neighbors. Then G is a complete r-partite graph $K_{s,s,\ldots,s}$ such that $n = rs$ and $d = (r-1)s$.*

Proof. Notice first that the condition $|N(i) \cap N(j)| = d$ actually implies $N(i) = N(j)$. Indeed, if k is a neighbor of i which is not in $N(j)$ then the degree of i is at least $d+1$, which is a contradiction to the fact that G is d-regular. A symmetric argument works if k is a neighbor of j which is not in $N(i)$.

Now let $\sim$ be the relation defined among the vertices of G by $i \sim j$ if and only if i and j are not neighbors. It is clear that $\sim$ is reflexive and symmetric. Now assume that $i \sim j$ and $j \sim k$. This implies that $N(i) = N(j)$ and $N(j) = N(k)$ and therefore $N(i) = N(k)$. Since the sets of neighbors of i and neighbors of k is the same and i is not a neighbor of i then k cannot be a neighbor of i. Therefore $i \sim k$ and the relation is transitive, and moreover it is an equivalence relation. Now G is a multipartite complete graph, the parts being the equivalence classes of $\sim$. Indeed, if $C_1, \ldots, C_r$ are the r classes, with $|C_j| = s_j$, and if $v \in C_j$, then v must be a neighbor of all vertices in $\bigcup_{i \neq j} C_i$, and the degree of v is

$$d(v) = d = \sum_{i \neq j} s_i = n - s_j.$$

Therefore all the cardinalities of the classes are equal: $s_j = n - d = s$, from where $n = rs$ and $d = n - s = rs - s = (r-1)s$ •

In light of this result, several of the inequalities in [5], [6], [8] and [19] need an update, replacing mentions of "Γ_d" with "complete r-partite $K_{s,s,\ldots,s}$ such that $rs = n$".

Our next result concerns the seminal inequality (2): we can extend its scope to include the complete r-partite graphs $K_{p_1,p_2,\ldots,p_r}$ as well as the complete graph minus two non-adjacent edges, denoted K_n^{--}.

Proposition 2 *The equality in (2) is attained by the complete r-partite graphs $K_{p_1,p_2,\ldots,p_r}$ and by K_n^{--}.*

Proof. It was shown in [1] that

$$R(K_{p_1,p_2,\ldots,p_r}) = r - 1 + n\sum_{i=1}^{r} \frac{p_i - 1}{n - p_i}.$$

Then we can write

$$R(K_{p_1,p_2,\ldots,p_r}) = r - 1 + n\sum_{i=1}^{r} \frac{p_i}{n - p_i} - n\sum_{i=1}^{r} \frac{1}{n - p_i}$$
$$= r - 1 + (n-1)\sum_{i=1}^{r} \frac{p_i}{n - p_i} + \sum_{i=1}^{r} \frac{-n + p_i}{n - p_i} = (n-1)I(R) - 1,$$

on account of the fact that there are p_i vertices with degree $n - p_i$, for $1 \leq i \leq r$.

Also, it is not difficult to compute that $R(K_n^{--}) = n - 1 + \frac{4}{n-2}$ (see for instance [16]), whereas $I(K_n^{--}) = \frac{4}{n-2} + \frac{n-4}{n-1}$. A little algebra shows $R(K_n^{--}) = -1 + (n-1)I(K_n^{--})$ •

The symmetric division deg index of G, defined by

$$SDD(G) = \sum_{(i,j)\in E} \left(\frac{d_i}{d_j} + \frac{d_j}{d_i} \right), \tag{8}$$

was introduced by Vukičević and Gašperov in [21] as one of the 148 so-called Adriatic indices, with a good predictive power for the total surface area of polychlorobiphenyls. The applicability of this index relative to other vertex-degree-based indices is studied in [11].

The following result gives a lower bound for $R(G)$ in terms of $SDD(G)$.

Proposition 3 *For any n vertex graph G we have*

$$R(G) \geq \frac{(SDD(G) + n^2)(n-1)}{2|E|} - n. \tag{9}$$

The equality is attained by K_n, K_n^-, K_n^{--} (for $n \geq 5$) and the complete r-partite graphs $K_{p_1,p_2,\ldots,p_r}$.

Proof. We showed in [18] that

$$SDD(G) \leq 2|E|(1 + I(G)) - n^2, \tag{10}$$

where the equality is attained by regular graphs, $(n-1, d)$-regular graphs for $1 \leq d < n-1$ and complete r-partite graphs $K_{p_1,p_2,\ldots,p_r}$. This fact, together with (2) and proposition 2, and considering the intersection of the scopes of (2) and (10) (notice that both K_n^- and K_n^{--}, for $n \geq 5$, are $(n-1, n-2)$-regular), yields the result •

As a corollary, we prove a lower bound for $R(G)$, in terms of only four parameters, with the same scope as the bounds (6) and (7) and several others in [6].

Proposition 4 *For any n vertex graph G with p pendent vertices and δ_1 the minimum non-pendent vertex degree we have*

$$R(G) \geq \frac{\left(n^2 + \frac{p(\delta_1-1)^2}{\delta_1}\right)(n-1)}{2|E|} - 1. \tag{11}$$

The equality is attained by K_n, the star $K_{1,n}$ and the complete r-partite graphs $K_{s,s,\ldots,s}$ with $rs = n$.

Proof. It was shown in [13] that

$$SDD(G) \geq p\left(\frac{\delta_1^2+1}{\delta_1}\right) + 2(|E| - p), \tag{12}$$

where the equality is attained by the star graph $K_{1,n}$ and all regular graphs.

Inserting (12) into (9) we get

$$\begin{aligned} R(G) &\geq \frac{\left(p\left(\frac{\delta_1^2+1}{\delta_1}\right) + 2(|E| - p) + n^2\right)(n-1)}{2|E|} - n \\ &= \frac{\left(n^2 + p\frac{(\delta_1-1)^2}{\delta_1} + 2|E|\right)(n-1)}{2|E|} - n \\ &= \frac{\left(n^2 + \frac{p(\delta_1-1)^2}{\delta_1}\right)(n-1)}{2|E|} - 1. \end{aligned}$$

Taking the intersection of the scopes of (12) and (9) ends the proof •

Remarks. Since $\frac{p(\delta_1-1)^2}{\delta_1} \geq 0$, (11) is always stronger than (5). Indeed, setting $\frac{p(\delta_1-1)^2}{\delta_1} = 0$ above we get

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

recovering (4) and (5).

By lemma 1 in [20] we can replace the term $\frac{p(\delta_1-1)^2}{\delta_1}$ with $\frac{2p}{3}$, but that improves the bound only when $\delta_1 = 2$.

The bound (11) is not in the same class as those in [6], and for completeness we can see that it is not comparable to (6) or (7). For the path graph P_n, (11) becomes $\frac{n^2}{2} - \frac{1}{2}$ whereas (6) and (7) become $\frac{n^2}{2} + \frac{n}{4} + \cdots$ On the other hand, if we take the tricyclic graph consisting of a cycle with two extra edges chosen so that $\Delta = 3$, $\Delta_2 = \delta = 2$, and $|E| = n + 2$, (11) becomes $\frac{n^2}{2} - n + \cdots$ whereas (6) and (7) become $n^2 - \frac{17}{12}n + \cdots$

The Hyper-Zagreb index, defined as

$$HM(G) = \sum_{uv\in E} (d_u + d_v)^2,$$

is used in [13] to give further lower bounds for $SDD(G)$, allowing us in turn to give more lower bounds for $R(G)$ in terms of $HM(G)$. We show one of these bounds and refer to [13] for further details:

Proposition 5 *For any n vertex graph G we have*

$$R(G) \geq \frac{\left(n^2 + \sqrt{\frac{n^2 HM(G)}{|E|} - 4|E|^2\left(\frac{\Delta}{\delta} - \frac{\delta}{\Delta}\right)^2}\right)(n-1)}{2|E|} - 2n + 1. \tag{13}$$

The equality is attained by K_n and the complete r-partite graphs $K_{s,s,\ldots,s}$ with $rs = n$.

Likewise, from lower bounds for $SDD(G)$ in terms of other indices obtained in [10], we can get lower bounds for $R(G)$ similar in form but with a scope slightly larger than the one in the previous proposition. For example, it is shown in [10] that if $M_1(G)$ and $M_2(G)$ are the first and second Zagreb indices of G then

$$SDD(G) \geq \frac{M_1(G)^2}{M_2(G)} - 2|E|, \tag{14}$$

where the equality is attained by regular graphs and semiregular bipartite graphs.

Then (14) together with (9), and intersecting the scopes of these two bounds proves the following

Proposition 6 *For any n vertex graph G we have*

$$R(G) \geq \frac{\left(n^2 + \frac{M_1(G)^2}{M_2(G)}\right)(n-1)}{2|E|} - 2n + 1. \tag{15}$$

The equality is attained by K_n, the complete bipartite graphs $K_{t,n-t}$, for $1 \leq t \leq \lceil \frac{n}{2} \rceil$, and the complete r-partite graphs $K_{s,s,\ldots,s}$ with $rs = n$.

We refer the reader to [10] for other lower bounds for $SDD(G)$ that yield more lower bounds for $R(G)$ in the manner described above.

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