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A Resistive Upper Bound for the ABC Index

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Abstract

Let G be a connected undirected graph with vertex set $\{1, 2, \ldots, n\}$ and degrees d_i, for $1 \le i \le n$. Then we show that

$$ABC(G) = \sum_{i \sim j} \sqrt{\frac{d_i + d_j - 2}{d_i d_j}} \le \sum_{i \sim j} \sqrt{R_{ij}},$$

where R_{ij} is the effective resistance between i and j.

This general bound allows us to obtain many other particular bounds and asymptotic maximal results for the ABC index with elementary proofs.

1 Introduction

Among the various descriptors in Mathematical Chemistry, the Kirchhoff index $R(G)$ and the ABC index, have received considerable attention in recent times. For a connected undirected graph $G = (V, E)$ with vertex set $\{1, 2, \ldots, n\}$ and edge set E, the Kirchhoff index was defined by Klein and Randić in [1] as

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

where R_{ij} is the effective resistance between vertices i and j. We refer the reader to references [2] through [5], among others, for a variety of approaches expressing this index in terms of eigenvalues of the Laplacian matrix, hitting times of random walks and the average of the Wiener capacities of its vertices. The ABC index, proposed by Estrada et al. in [6], and reintroduced in [7] was defined as

$$ABC(G) = \sum_{i \sim j} \sqrt{\frac{d_i + d_j - 2}{d_i d_j}}, \tag{1}$$

where $i \sim j$ means that the vertices i and j are neighbors and d_i is the index of the vertex i. (For all graph theoretical terms the reader is referred to reference [8])

The index $ABC(G)$ has been studied in a large number of references of which we mention [9], [10] and [11] for their own interest and for many other related references found in them.

In this article we want to give a new upper bound for $ABC(G)$ that uses some ideas pertinent to the Kirchhoff and other resistive descriptors. This upper bound yields a number of particular bounds and asymptotic maximal results with proofs that we believe are easier than those found in the literature, and introduces new electrical insights in the study of the ABC index.

With the exception of proposition 3, in what follows we will assume that the graphs satisfy $n \geq 3$ in order to avoid cases where $i \sim j$ and $d_i = d_j = 1$.

2 The bounds

The following proposition was shown first in [12] and we include a refined version of its proof here for completeness

Proposition 1 *For any G with $n \geq 3$, if $i \sim j$ then*

$$R_{ij} \geq \frac{d_i + d_j - 2}{d_i d_j - 1}. \tag{2}$$

Proof. There is an edge between i and j. If $d_i = 1$ or $d_j = 1$ then $R_{ij} = 1$ and (2) holds. So we take $d_i \geq 2$ and $d_j \geq 2$. Consider now all the endpoints of all the other $d_i - 1$ edges stemming out of i and all the $d_j - 1$ edges stemming out of j. Short all these. Then we get two edges in parallel: one with resistance 1 and the other with resistance $\frac{1}{d_i - 1} + \frac{1}{d_j - 1}$. Solving this into a single resistor, and applying the monotonicity principle (see [13]), finishes the proof •

Now we obtain as a corollary

Proposition 2 *For any G with $n \geq 3$ we have*

$$ABC(G) \leq \sum_{i \sim j} \sqrt{\frac{d_i + d_j - 2}{d_i d_j - 1}} \leq \sum_{i \sim j} \sqrt{R_{ij}}. \tag{3}$$

Proof. Obvious •

The middle term in (3) could be thought of as an alternative definition of the ABC index that we will call $ABC^*(G)$. The rightmost term is the bound, that we will call P, from which we will be extracting all the information. As we mentioned above, effective resistances can be studied from a variety of viewpoints, and given in terms of eigenvalues of the Laplacian matrix (see also [14]), or of Wiener capacities, or of hitting times of random walks, and these approaches might lead to new results for the ABC index. In this note, however, we will concentrate on purely electrical ideas. The first question of interest is: how small can P be? We answer that question in the next

Proposition 3 *For any G we have*

$$P \geq n - 1. \tag{4}$$

Proof. It is well known that in a simple connected graph, if $i \sim j$ then $\frac{2}{n} \leq R_{ij} \leq 1$ and therefore

$$P = \sum_{i \sim j} \sqrt{R_{ij}} \geq \sum_{i \sim j} R_{ij} = n - 1,$$

where the last equality is Foster's first formula (see [15]) •

It is evident that this lower value for P is attained by all trees. The next question is: how large can P be and how good can it be to bound $ABC(G)$? This is answered in the next

Proposition 4 *For any graph G with $n \geq 3$ we have*

$$ABC(G) \leq ABC^*(G) \leq \sqrt{|E|(n-1)} \leq \frac{\sqrt{n}(n-1)}{\sqrt{2}}. \tag{5}$$

Proof. The Cauchy Schwarz inequality tells us that

$$P^2 = \left(\sum_{i \sim j} \sqrt{R_{ij}} \right)^2 \leq \sum_{i \sim j} 1 \sum_{i \sim j} R_{ij} = |E|(n-1),$$

where the last equality uses Foster's first formula •

Notice that the inequality $P \leq \sqrt{|E|(n-1)}$ becomes an equality whenever the graph is edge transitive, in which case all the edges have the same resistance $\frac{n-1}{|E|}$. Now for the star graph S_n it is easy to compute $ABC^*(S_n) = n-1$ and $ABC(S_n) = \sqrt{(n-1)(n-2)}$, so the middle inequality in (5) shows that S_n is maximal among trees for ABC^* and asymptotically maximal for ABC, because for trees $\sqrt{|E|(n-1)} = n-1$. For the complete graph K_n it is easily seen that $ABC^*(K_n) = \frac{n\sqrt{n-1}}{\sqrt{2}}$ and $ABC(K_n) = \frac{n\sqrt{n-2}}{\sqrt{2}}$, so the rightmost inequality in (5) shows that K_n is asymptotically maximal for both ABC and ABC^*.

Even though the bounds in (5) are easy to prove and give the right order of magnitude of the maximal tree and maximal general graph for the descriptor ABC, up to the constant coefficient, they are weaker than the exact known results of maximality for this descriptor given in [9] for trees and in [10] for general graphs. The more useful inequality in (5) is the middle one that enables us to prove better results, when the graph is not a tree, than the naive bound $ABC(G) \leq |E|$ valid for all graphs. Thus for example the following two propositions provide bounds with little effort, that do not seem to be obtainable easily from the direct application of the definition (1).

Proposition 5 *If G is c-cyclic, $c \geq 0$, and $n \geq 3$, then*

$$ABC(G) \leq ABC^*(G) \leq \sqrt{(n-1+c)(n-1)}. \tag{6}$$

Proof. Use in (5) that $|E| = n-1+c$ •

Proposition 6 *If G is planar and $n \geq 3$ then*

$$ABC(G) \leq ABC^*(G) \leq \sqrt{3(n-1)(n-2)}. \tag{7}$$

Proof. It is well known that for a planar graph $|E| \leq 3(n-2)$. Use this in (5) •

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