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ABC Index of Trees with Fixed Number of Leaves

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Abstract

Given a graph G, the atom-bond connectivity (ABC) index is defined to be $ABC(G) = \sum_{uv\in E(G)} \sqrt{\frac{d_G(u)+d_G(v)-2}{d_G(u)\,d_G(v)}}$, where $E(G)$ is the edge set of graph G and $d_G(v)$ is the degree of vertex v in graph G. The paper [10] claims to classify tho trees with a fixed number of leaves which minimize the ABC index. Unfortunately, there is a gap in the proof, leading to other examples that contradict the main result of that work. These examples and the problem are discussed in this note.

1 Introduction

Given a graph G with vertex set $V(G)$ and edge set $E(G)$, the atom–bond connectivity (ABC) index is defined to be [4]

$$ABC(G) := \sum_{uv\in E(G)} \sqrt{\frac{d_G(u)+d_G(v)-2}{d_G(u)\,d_G(v)}}$$

where $d_G(v)$ is the degree (the number of incident vertices) of a vertex $v \in V(G)$ in graph G.

An early (and easy) mathematical result on the ABC index is that of all trees on n vertices, the star has the highest ABC index [5]. An analogous problem, namely the characterization of trees on n vertices with smallest ABC index, turned out to be prohibitively difficult. In spite of numerous attempts, its solution is still unknown. Details of the search for trees with minimal ABC index are outlined in [9]; for more recent works along the same lines see [1–3]. Also of interest is to maximize and minimize chemical indices on trees with a fixed number of leaves. In [6, 8], a tight inequality is suggested for the first and the second Zagreb indices over trees with a fixed number of leaves. In [7] a dynamic programming approach is used to characterize the minimizers of the generalized first Zagreb index and the second Zagreb index. For the ABC index, there is no maximum value on a fixed number of leaves, since a broom (a path with one end joined to the center of a star) has a fixed number of leaves but arbitrarily large ABC index as the length of the path grows.

2 Observations

Regarding the minimum ABC index over trees with a fixed number of leaves, the following result was claimed in [10].

Theorem 1. [10] *Among all trees with $k \geq 19$ leaves, the balanced double–star has the smallest ABC index. Among all trees with $2 \leq k < 19$ leaves, the star has the smallest ABC index.*

Unfortunately, a gap was soon noticed in the proof,* leading to counterexamples to Theorem 1. In particular, a tree with 40 pendent vertices, which has smaller value of ABC index than the respective balanced double star, can be found in [7] (see Figure 1).

In [7] a routine based on a dynamic programming technique was suggested to calculate numerically the minimizers for the second–Zagreb–like indices of the form

$$C_2(G) = \sum_{uv \in E(G)} c_2(d_G(u), d_G(v))$$

*In the proof of Claim 1 in [10], in the expression for $ABC(w)$, instead of the term $(d'-1)\sqrt{\frac{d'}{d'+1}}$, it was erroneously written $d'\sqrt{\frac{d'}{d'+1}}$. This seemingly benign mistake caused a major error in the final result.

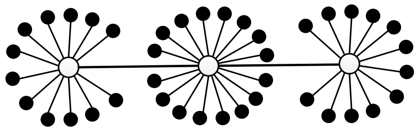

Figure 1: A counterexample to Theorem 1: The ABC index of this tree with 40 pendent vertices is smaller than that of a double–star.

over all trees with given number of pendent vertices. Here $c_2(d,d')$ is a symmetric non-negative function of two natural arguments, d and d'.

This routine is based on the notion of the *attached pendent–rooted tree*, where the root is a pendent vertex, which is considered as a vertex of degree d when calculating C_2 for this tree. The idea of the routine is that if a tree T delivers the minimum to $C_2(\cdot)$ over all trees with n pendent vertices, and one selects any internal vertex $v \in V(T)$ of degree d, then T is a union of d attached rooted trees $T_1,\ldots,T_d$ having their roots in vertex v, and T_i minimizes the ABC index over all rooted trees with n_i pendent vertices and the root of degree d.

Moreover, if we denote by $C_2^*(n,d)$ the minimum value of the ABC index for an attached rooted tree with n pendent vertices and the root of degree d, then we can write the *Bellman equation* as

$$C_2(T) = \min_{d=2,\ldots,n} \min_{n_1,\ldots,n_d} \left\{ \sum_{i=1}^{d} C_2^*(n_i,d) : n_1+\cdots+n_d = n \right\}$$

which can be used to calculate by induction the minimizers of C_2 over trees with n pendent vertices.

If we know that the vertex degree in any extremal tree does not exceed Δ, then C_2-minimizers can be efficiently calculated in $O(n^\Delta)$ operations.

It is clear that the second Zagreb index M_2 is a special case of C_2 for $c_2(d,d') = dd'$, and the ABC index is a special case for $c_2(d,d') = \sqrt{\frac{d+d'-2}{d\,d'}}$. Therefore, the trees with n vertices delivering the minimum to M_2 are characterized in [7]. For the ABC index, the maximal degree in an extremal tree was not estimated, so only extremal chemical trees (those having maximum vertex degree 4) were characterized in [7].

Although evaluation of ABC index minimizers becomes too expensive for large n, we calculated numerically all trees with the smallest ABC index among the trees with $n \le 53$ pendent vertices.

A star S_n minimizes the ABC index for $n = 1, \dots, 18$. A balanced double–star minimizes the ABC index for $n = 19, \dots, 35$ (Figure 2 shows the example for $n = 28$). A caterpillar with the central path of length 3 minimizes the ABC index for $n = 36, \dots, 49$ if and only if the vertices of the central path have n_1, n_2, and n_3 pendants, respectively, as indicated in Table 2. An example of such a caterpillar for $n = 40$ is shown in Figure 1.

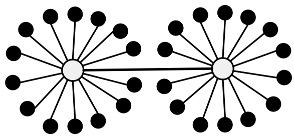

Figure 2: The balanced double–star with 28 pendent vertices.

Table 1: Number of pendent vertices incident to vertices of the central path of a caterpillar, required that the ABC index of a tree with n pendent vertices be minimal.

n	n_1	n_2	n_3	n	n_1	n_2	n_3
36	11	14	11	43	13	17	13
37	11	15	11	44	13	18	13
38	11	16	11	45	13	18	14
39	11	16	12	46	13	19	14
40	12	16	12	47	14	19	14
41	12	17	12	48	14	20	14
42	12	17	13	49	15	20	14

A star S_3 with n_1, n_2, and n_3 additional pendent vertices attached to its leaves and n_c additional pendent vertices attached to its center, minimizes the ABC index for $n = 50, \dots, 53$ if an only if n_1, n_2, n_3, and n_c assume the values indicated in Table 2. An example for $n = 50$ is shown in Figure 3.

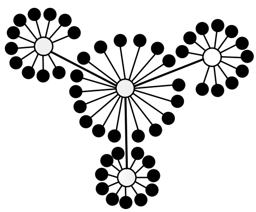

Figure 3: A foliated star S_3 with 50 pendent vertices.

Table 2: Number of additional pendent vertices attached to the vertices of the star S_3, required that the ABC index of a tree with n pendent vertices be minimal.

n	n_1	n_2	n_3	n_c
50	11	11	11	17
51	11	11	11	18
52	11	11	12	18
53	11	11	12	19

3 Conclusion

The results outlined in this note show that Theorem 1 from the recent paper [10], holds only for trees up to $n = 35$ leaves. For $n \geq 36$, trees significantly different from double–stars have minimal ABC index among all trees with n leaves. Much like the problem of finding the minimum ABC index over all trees on n vertices, the problem of finding the minimum ABC index over trees with a fixed number of leaves appears to be elusive. The solution of both problems remains a task and challenge for the future.

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