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On Trees with Minimal Atom Bond Connectivity Index

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Abstract

In a recent work, I. Gutman and B. Furtula posed the structure of trees with a single high-degree vertex and smallest ABC index [1]. Here we provide a family of trees with smaller ABC index in one case of their conjectures. The smallest tree violating the Gutman-Furtula conjecture has 312 vertices.

1. Introduction

Graph-based molecular structure descriptors (often referred to as "topological indices") are useful tools for modeling physical and chemical properties of molecules, for design of pharmacologically active compounds, for recognizing environmentally hazardous materials, etc. [2–4]. The atom-bond connectivity index (ABC) is a molecular structure descriptor that recently found a remarkable application in rationalizing the stability of linear and branched alkanes as well as the strain energy of cycloalkanes [5,6]. Let G be a simple graph with vertex set $V(G)$ and edge set $E(G)$. The degree of a vertex v is denoted by d_v. The atom bond connectivity index of G is defined as

$$\mathrm{ABC}(\mathrm{G}) = \sum_{\mathrm{uv}\,\in\,\mathrm{E(G)}} \sqrt{\frac{d_u + d_v - 2}{d_u d_v}}.$$

The mathematical properties of this index were reported in [2,3,7-13].

I. Gutman and B. Furtula conjectured [1] that if n ≡ 4 (mod 7), k ≥ 6, and n = 7k + 11, then the minimum-ABC tree has the structure shown in Fig. 1. We denote such graphs with 7k+11 vertices by GF_k.

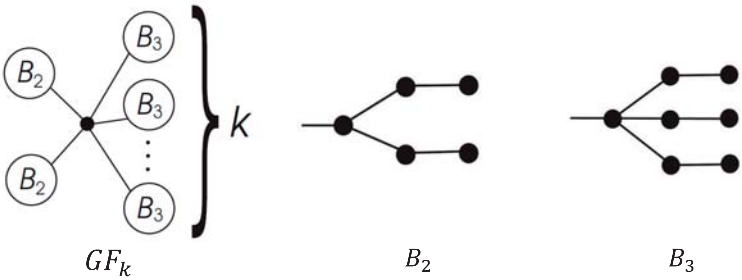
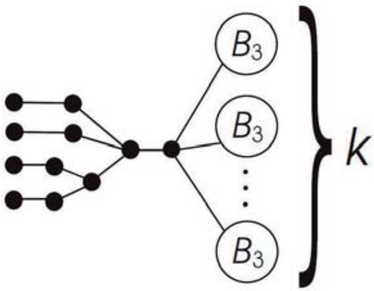


Fig. 1. Trees with $7k + 11$ vertices, for $k \geq 6$ introduced by I. Gutman and B. Furtula.

In this case we found a family of graphs shown in Fig. 2, that have smaller ABC index than the above structures. We denote such graphs with $7k + 11$ vertices by AHS_k.



It is easy to see that:

$$ABC(GF_k) = k\sqrt{\frac{k+4}{4(k+2)}} + 2\sqrt{\frac{k+3}{3(k+2)}} + \frac{6k+8}{\sqrt{2}}$$

and

$$ABC(AHS_k) = (k+1)\sqrt{\frac{k+3}{4(k+1)}} + \sqrt{\frac{5}{12}} + \frac{6k+8}{\sqrt{2}}$$

Here we are going to show that $ABC(GF_k) > ABC(AHS_k)$ for $k \geq 43$.

If the inequality $ABC(GF_k) > ABC(AHS_k)$ holds, it implies that:

$$\frac{1}{2}\sqrt{k^3+4k^2} + \frac{1}{2\sqrt{3}}\sqrt{16k+48} > \frac{1}{2}\sqrt{k^3+6k^2+11k+6} + \frac{1}{2\sqrt{3}}\sqrt{5k+10}$$

By elementary calculation and squaring the above relation and rearranging for three times, we get

$$4k^8 - 120k^7 - 1900k^6 - \frac{26960}{4}k^5 - \frac{146480}{9}k^4 - \frac{46400}{9}k^3 + 14720k^2 + \frac{102400}{9}k + \frac{6400}{9} > 0$$

The largest root of the above polynomial is 42.480136, and its degree is even, therefore the value of the above polynomial is positive for $k > 42.480136$. Thus we have

$$ABC(GF_k) > ABC(AHS_k) \quad \text{for } k \geq 43,$$

and the proof is complete.

One can ask about the behavior of ABC(GF_k) and ABC(AHS_k) for sufficiently large k. To answer this question we show that $\lim_{k\to\infty} ABC(GF_k) - ABC(AHS_k) = 0.0092$.

$$\lim_{k\to\infty} k\sqrt{\frac{k+4}{4(k+2)}} + 2\sqrt{\frac{k+3}{3(k+2)}} - (k+1)\sqrt{\frac{k+3}{4(k+1)}} - \sqrt{\frac{5}{12}}$$

$$= \lim_{k\to\infty} \sqrt{\frac{k^3+4k^2}{4(k+2)}} - \sqrt{\frac{k^2+4k+3}{4}} + \frac{2}{\sqrt{3}}\sqrt{\frac{k+3}{(k+2)}} - \sqrt{\frac{5}{12}}$$

$$= \lim_{k\to\infty} \frac{\frac{k^3+4k^2}{4(k+2)} - \frac{k^2+4k+3}{4}}{\sqrt{\frac{k^3+4k^2}{4(k+2)}} + \sqrt{\frac{k^2+4k+3}{4}}} + \frac{2}{\sqrt{3}} - \sqrt{\frac{5}{12}}$$

$$= \lim_{k\to\infty} \frac{\frac{k^3+4k^2-k^3-6k^2-11k-6}{4(k+2)}}{\sqrt{\frac{k^3+4k^2}{4(k+2)}} + \sqrt{\frac{k^2+4k+3}{4}}} + \frac{2}{\sqrt{3}} - \sqrt{\frac{5}{12}}$$

$$= \lim_{k\to\infty} \frac{\frac{-2k^2 - 11k - 6}{4(k+2)}}{\frac{k}{2} + \frac{k}{2}} + \frac{2}{\sqrt{3}} - \sqrt{\frac{5}{12}}$$

$$= \lim_{k\to\infty} \frac{-2k^2 - 11k - 6}{4k^2 + 8k} + \frac{2}{\sqrt{3}} - \sqrt{\frac{5}{12}} = -\frac{1}{2} + \frac{2}{\sqrt{3}} - \sqrt{\frac{5}{12}} = 0.0092 \quad (4D)$$

Below we present numerical result showing that $ABC(GFk)$ is greater than $ABC(AHS_k)$ for $k \geq 43$. Let $A = ABC(GF_k) - ABC(AHS_k)$.

k	A	k	A	k	A	k	A	k	A
6	-0.035277	21	-0.008080	36	-0.001511	51	0.001440	66	0.003117
7	-0.031076	22	-0.007402	37	-0.001247	52	0.001580	67	0.003203
8	-0.027594	23	-0.006775	38	-0.000995	53	0.001715	68	0.003287
9	-0.024662	24	-0.006193	39	-0.000754	54	0.001845	69	0.003369
10	-0.022160	25	-0.005652	40	-0.000525	55	0.001971	70	0.003448
11	-0.020001	26	-0.005148	41	-0.000306	56	0.002093	71	0.003526
12	-0.018119	27	-0.004677	42	-0.000097	57	0.002211	72	0.003601
13	-0.016464	28	-0.004236	43	0.000103	58	0.002324	73	0.003674
14	-0.014998	29	-0.003822	44	0.000295	59	0.002434	74	0.003745
15	-0.013689	30	-0.003433	45	0.000479	60	0.002541	75	0.003815
16	-0.012515	31	-0.003066	46	0.000655	61	0.002645	76	0.003883
17	-0.011455	32	-0.002720	47	0.000824	62	0.002745	77	0.003949
18	-0.010494	33	-0.002393	48	0.000987	63	0.002842	78	0.004014
19	-0.009618	34	-0.002084	49	0.001144	64	0.002936	79	0.004076
20	-0.008816	35	-0.001790	50	0.001295	65	0.003028	80	0.004138

Table 1. ABC index for trees GF_k and AHS_k , $k = 6, \dots, 80$.

We conclude this section with a related conjecture about this problem. Let *T* be a tree with *n* vertices with a single high-degree vertex denoted by *GF*, which is introduced in [1]. Then $ABC(T)$ and $ABC(GF)$ have the same behavior for sufficiently large *n*, i. e.,

$$\lim_{n\to\infty} ABC(GF) - ABC(T) \leq c$$

where c is a sufficiently small constant.

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