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On Large Trees with Minimal Atom-Bond Connectivity Index

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Abstract

Finding trees with minimal atom-bond connectivity (ABC) index, in the general case, is still an open problem. I. Gutman and B. Furtula [*MATCH Commun. Math. Comput. Chem.* **86** (2012) 131-136] posed a conjecture on the structure of trees with a single high-degree vertex and smallest ABC index. Here we find a case when this conjecture fails for trees with more than 1185 vertices.

1. Introduction

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. [7].

In 1998, Estrada et al. defined a new topological index that displays an excellent correlation with the heats of formation of alkanes [8,9,15]. This index, named ABC (atom–bond connectivity) is defined as a modification of the Randić graph-theoretic invariant [17].

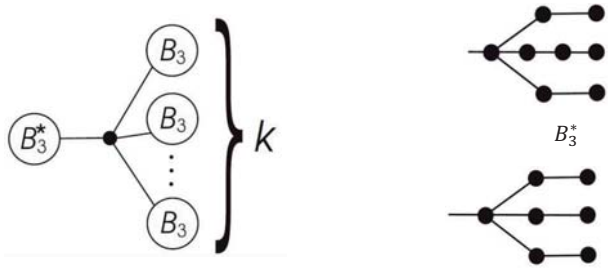
Let G be a simple graph with vertex set $V(G)$ and edge set $E(G)$. The degree of a vertex v is denoted by d_v. By the atom bond connectivity index of G we mean:

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

Recently a long series of mathematical investigations of the ABC index was communicated [1-6,10-14,16].

2. Main Results

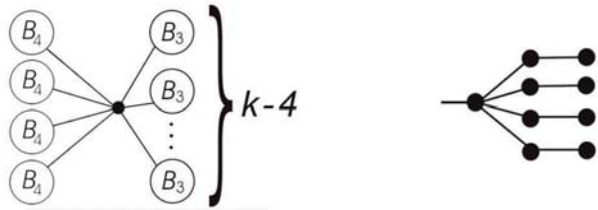
I. Gutman and B. Furtula conjectured that if $n \equiv 2 \pmod 7$, $k \geq 23$, and $n = 7k + 9$, then the minimum-ABC tree has the structure shown in Fig. 1 [13]. We denote such graphs in $7k$ +9 vertices by GF_k.



GF_k B_3

Fig. 1. Trees with $7k + 9$ vertices, for $k \geq 23$ introduced in Ref. [13].

In this case we found a family of graphs shown in Fig. 2, having smaller ABC index than the above structures. We denote such graphs on $7k + 9$ vertices by AHZ_k.



B_4

Fig. 2. Trees with $7k + 9$ vertices, for $k \geq 168$.

It is easy to see that:

$$ABC(GF_k) = (k+1)\sqrt{\frac{k+3}{4(k+1)}} + \frac{6k+7}{\sqrt{2}}$$

and

$$ABC(AHZ_k) = (k-4)\sqrt{\frac{k+2}{4k}} + 4\sqrt{\frac{k+3}{5k}} + \frac{6k+8}{\sqrt{2}}.$$

Here we are going to show that $ABC(GF_k) > ABC(AHZ_k)$ for k ≥ 168.

If the inequality $ABC(GF_k) > ABC(AHZ_k)$ holds, then by elementary calculation we obtain:

$$\frac{41}{400}k^{12} - \frac{3391}{200}k^{11} - \frac{138879}{4000}k^{10} + \frac{1179857}{4000}k^9 + \frac{167049681}{160000}k^8 - \frac{2179811}{40000}k^7$$
$$- \frac{427961721}{80000}k^6 - \frac{87810473}{8000}k^5 - \frac{1704407439}{160000}k^4 - \frac{1396511}{250}k^3$$
$$- \frac{937128}{625}k^2 - \frac{91648}{625}k + \frac{4098}{625} > 0$$

The largest root of the above polynomial is 167.33396, and its degree is even, therefore the value of the above polynomial is positive for $k > 167.33396$. Thus we have

$$ABC(GF_k) > ABC(AHZ_k) \text{ for } k \geq 168, \text{ i. e., for } n \geq 1185.$$

By this, the proof is complete.

Here we consider the behavior of $ABC(GF_k)$ and $ABC(AHZ_k)$ for sufficiently large *k*. Let $F(k) = ABC(GF_k) - ABC(AHZ_k)$. The function $F(k)$ is increasing and for $k \geq 1$, we have $F(k) < 0.00404$.

We show that $\lim_{k\to\infty} ABC(GF_k) - ABC(AHZ_k) = 0.0040388368$.

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

$$= \lim_{k\to\infty} \sqrt{\frac{k^2+4k+3}{4}} - \sqrt{\frac{k^3-6k^2+32}{4k}} - \frac{1}{\sqrt{2}} - \sqrt{\frac{16}{5}}$$

$$= \lim_{k\to\infty} \frac{\frac{k^2+4k+3}{4} - \frac{k^3-6k^2+32}{4k}}{\sqrt{\frac{k^2+4k+3}{4}} + \sqrt{\frac{k^3-6k^2+32}{4k}}} - \frac{1}{\sqrt{2}} - \sqrt{\frac{16}{5}}$$

$$= \lim_{k\to\infty} \frac{\frac{k^3+4k^2+3k-k^3+6k^2+32}{4k}}{\frac{k}{2}+\frac{k}{2}} - \frac{1}{\sqrt{2}} - \sqrt{\frac{16}{5}}$$

$$= \frac{5}{2} - \frac{1}{\sqrt{2}} - \sqrt{\frac{16}{5}} = 0.0040388368 \qquad (10D).$$

It should be noted that Gutman and Furtula calculated the ABC index of their purposed structure for trees with order less than 700 [13] and it seems that their results are valid for trees with order less than 1185.

Below we present numerical and graphical results to compare $ABC(GFk)$ and $ABC(AHZ_k)$ for some k. ($F(k) = ABC(GF_k) - ABC(AHZ_k)$)

k		k		k	$F(k)$	k		k	
25	-0.021435	100	-0.002670	170	0.000063	3000	0.003811	150000	0.004034
30	-0.017430	105	-0.002356	180	0.000281	4000	0.003868	200000	0.004035
35	-0.014514	110	-0.002071	190	0.000477	5000	0.003902	250000	0.004036
40	-0.012295	115	-0.001809	200	0.000654	6000	0.003925	300000	0.0040366
45	-0.010551	120	-0.001569	300	0.001775	7000	0.003941	400000	0.0040371
50	-0.009143	125	-0.001348	400	0.002338	8000	0.003953	500000	0.0040374
55	-0.007983	130	-0.001144	500	0.002677	9000	0.003963	600000	0.0040377
60	-0.007011	135	-0.000954	600	0.002904	10000	0.003971	700000	0.0040379
65	-0.006184	140	-0.000778	700	0.003065	15000	0.003993	800000	0.0040380
70	-0.005472	145	-0.000614	800	0.003187	20000	0.004005	900000	0.0040381
75	-0.004854	150	-0.000461	900	0.003281	30000	0.004016	1000000	0.0040382
80	-0.004310	155	-0.000318	1000	0.003357	40000	0.004022	2000000	0.0040385
85	-0.003829	160	-0.000183	1500	0.003584	50000	0.004025	3000000	0.0040386
90	-0.003401	167	-0.000008	2000	0.003698	60000	0.004027	5000000	0.0040387
95	-0.003017	168	0.000016	2500	0.003766	100000	0.004032	inf	0.0040388

Table 1. The difference between the ABC value of GF_k and AHZ_k for some k.

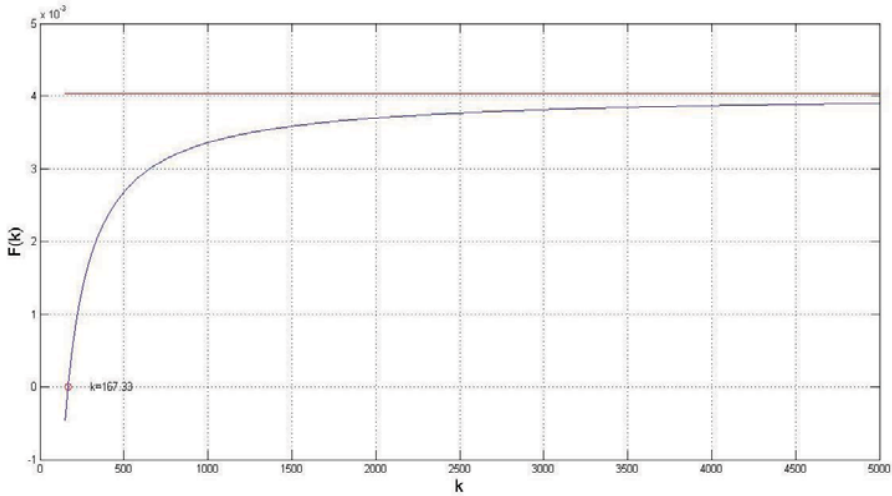


Fig. 3. The difference between $ABC(GF_k)$ and $ABC(AHZ_k)$.

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