## MINIMUM HARMONIC INDEX OF TREES

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## Brief History

In the 1980s S.Fajtlowicz created a computer program for automatic generation of conjectures in graph theory. Thus the harmonic index first appeared in On conjectures on Graffiti-II,Congr. Numer.60(1987) 187-197.

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- Zhong et al. studied the harmonic index of bicyclic graphs and characterized the corresponding extremal graphs in their paper The harmonic index on bicyclic graphs, Utilitas Mathematica, 90 (2013), in press.

Deng et al. determined the trees with the second to the sixth maximum harmonic indices, and bicyclic graphs with the first four maximum harmonic indices and they gave a lower bound for harmonic index of trees and chemical trees with given number of pendant vertices in their papers On harmonic indices of trees, unicyclic graphs and bicyclic graphs, preprint and Harmonic indices of trees and chemical trees with a given number of pendant vertices, preprint.

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- Deng et al. considered the relation between the harmonic index H(G) and the chromatic number χ(G) and proved that χ(G) ≤ 2H(G) by using the effect of removal of a minimum degree vertex on the harmonic index in their paper On the harmonic index and the chromatic number of a graph, Discrete Appl. Math. 161(2013) 2740-2744.

 Gutman gave a survey of selected degree-based topological indices and summarized their properties in his paper Degree-based topological indices, Croat. Chem. Acta 86 (4)(2013)351-361.

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## HARMONIC INDEX

The Harmonic index H(G) of a graph G is defined as the sum of the weights  $\frac{2}{d(u) + d(v)}$  of all edges uv of G, where d(u) denotes the degree of the vertex u in G.

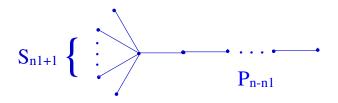
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## COMET

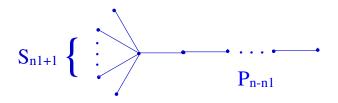
A comet is a tree composed of a star and an appended path. We denote by  $T(n, n_1)$  the comet of order n with  $n_1$  pendant vertices, that is, a tree formed by a path  $P_{n-n_1}$  of which one end vertex coincides with a pendant vertex of a star  $S_{n_1+1}$ , where  $2 \le n_1 \le n-1$ .



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If  $n_1 \leq n-2$ , the harmonic index of  $T(n, n_1)$  is

$$H(T(n, n_1)) = \frac{2(n_1 - 1)}{n_1 + 1} + \frac{2}{n_1 + 2} + \frac{2(n - n_1 - 2)}{4} + \frac{2}{3}$$

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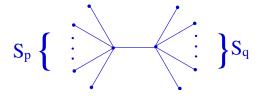
## DOUBLE STAR

A tree is called a double star  $S_{p,q}$  if it is obtained from connecting the centres of  $S_p$  and  $S_q$  by an edge, where  $1 , as shown in the figure below. Then for a double star <math>S_{p,q}$  with *n* vertices, we have p + q = n and  $p \le \lfloor \frac{n}{2} \rfloor$ .

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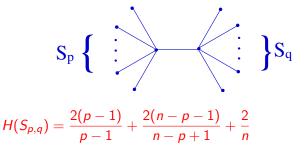
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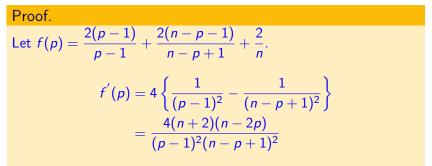
The harmonic index of  $S_{p,q}^{c}$  is given by  $H(S_{p,q}^{c}) = \frac{n-3}{2} + \frac{2(p-1)}{n+p-3} + \frac{2(n-p-1)}{2n-p-3}$ 

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## The harmonic index of the double star $S_{p,q}$ is monotonically increasing for $n \ge 4$ in p.

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Since  $n \ge 4$  and p > 1, we have n - 2p > 0. This implies f'(p) > 0 and then  $S_{p,q}$  is increasing for  $n \ge 4$  in p.

# The harmonic index of $S_{p,q}^c$ is monotonically increasing for $n \ge 4$ in p.

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The harmonic index of  $S_{p,q}^c$  is monotonically increasing for  $n \ge 4$  in p.

Proof.

Let 
$$f(p) = \frac{n-3}{2} + \frac{2(p-1)}{n+p-3} + \frac{2(n-p-1)}{2n-p-3}$$
.

$$f'(p) = \frac{2n-4}{(n+p-3)^2} - \frac{2n-4}{(2n-p-3)^2}$$
$$= 2(n-2) \left\{ \frac{1}{(n+p-3)^2} - \frac{1}{(2n-p-3)^2} \right\}$$
$$= \frac{6(n-2)^2(n-2p)}{(n+p-3)^2(2n-p-3)^2}$$

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Since  $n \ge 4$  and p > 1, we have n - 2p > 0. This implies f'(p) > 0 and then  $S_{p,q}^c$  is increasing for  $n \ge 4$  in p.

The harmonic index of the Nordhaus-Gaddum type for a double star  $S_{p,q}$  is monotonically increasing for  $n \ge 4$  in p.

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Jerline *et al.*<sup>1</sup> gave the formula for calculating the harmonic index of a graph with more than one cut-vertex as follows.

#### Lemma

Let  $\mathscr{C} = \{v_1, v_2, \dots, v_l\}$  be the set of all cut-vertices and  $\mathscr{B} = \{B_1, B_2, \dots, B_k\}$  be the set of all blocks of a simple connected graph *G*. Then

$$H(G) = \sum_{i=1}^{k} H(B_i) - 2 \sum_{i=1}^{l} \sum_{B \in B'_i} \sum_{\substack{x \in N_B(v_i) \\ x \notin \mathscr{C}}} \left\{ \frac{1}{d_B(v_i) + d_B(x)} - \frac{1}{d_G(v_i) + d_G} - \sum_{i=1}^{l} \sum_{B \in B'_i} \sum_{\substack{x \in \mathscr{C} \\ x \in \mathscr{C}}} \left\{ \frac{1}{d_B(v_i) + d_B(x)} - \frac{1}{d_G(v_i) + d_G(x)} \right\}$$
  
where  $B'_i = \{B \in \mathscr{B} | v_i \in B\}, \quad 1 \le i \le l.$ 

## Observation

Suppose that e = uv be an edge such that u is a cut-vertex and  $u \in B_i$ . Then the contribution of e to the calculation H(G) is denoted by  $\frac{1}{d_{B_i}(u) + d_{B_i}(v)} - \frac{1}{d_G(u) + d_G(v)} \ge 0.$ 

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## Observation

From the above equation, it is clear that

H(G) = sum of the harmonic indices of blocks-

2(sum of the contribution of each edge one of whose end vertex is a cut-vertex)-

2(sum of the contribution of each edge both of whose end vertices are cut-vertices)

=sum of the harmonic indices of blocks-2x-2y

where

x = sum of the contribution of each edge one of whose end vertex is a cut-vertex and <math>y = sum of the contribution of each edge both of whose end vertices are cut-vertices.

Let T be a tree with n vertices and  $n_0$  pendent vertices. Then

$$H(T) \geq n-1-n_0\left\{\frac{n-2}{n}\right\}$$

with equality if and only if  $T \cong S_n$  and

$$H(T) \leq \frac{n-1}{2} + n_0 \left\{ \frac{1}{6} \right\}$$

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Proof. The least value of H(T) will exist for trees with all the edges having one end is a cut-vertex and the other end is not a cut-vertex. That is,  $n_0 = n - 1$  and in all the blocks the degree of one end is n - 1 and the other is 1. Therefore  $\begin{pmatrix} 1 & 1 \end{pmatrix}$ 

 $x \ge (n-1)\left(\frac{1}{2}-\frac{1}{n}\right)$  and y = 0.

$$H(T) \ge n - 1 - 2(n - 1)\left(\frac{1}{2} - \frac{1}{n}\right)$$
  
=  $n - 1 - n_0\left\{\frac{n - 2}{n}\right\}$ 

There is a tree structure of this type, namely star. Therefore equality holds for star.

The greatest value of H(T) will exist for trees with all the edges having both the ends as cut-vertex. Since a tree has at least two pendant vertices  $n_0 \ge 2$ . Therefore  $x \le n_0 \frac{1}{6}$  and

$$y \le (n-1-n_0)rac{1}{4}.$$
  
 $H(T) \le n-1-2n_0rac{1}{6}-2(n-1-n_0)rac{1}{4}$   
 $\le rac{n-1}{2}+n_0\left\{rac{1}{6}
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There is a tree structure of this type, namely path. Therefore equality holds for path.

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The function 
$$f(n,x) = \frac{2(x-1)}{x+1} + \frac{2}{x+2} + \frac{(n-x-2)}{2} + \frac{2}{3}$$
 is a decreasing function for  $3 \le x \le n-2$  in x.

<sup>&</sup>lt;sup>2</sup>Deng H, Balachandran S, Ayyaswamy S K, Venkatakrishnan Y B, Harmonic indices of trees and chemical trees with a given number of pendant vertices, preprint.

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#### Lemma

For any n,  $H(T(n,2)) > H(T(n,3)) > H(T(n,4)) > \cdots > H(T(n,n-3)) > H(T(n,n-2)).$ 

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#### Lemma

<sup>2</sup> Let T be a tree of order  $n \ge 4$  with  $n_1$  pendant vertices. If  $n_1 \le n-2$ , that is, T is not a star then,  $H(T) \ge H(T(n, n_1))$ .

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Among all n-vertex trees, for  $n \ge 4$ , the comet T(n,n-2) are the trees with the second minimum harmonic index, which is equal to  $\frac{2(n-3)}{n-1} + \frac{2}{n} + \frac{2}{3}.$ 

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- Let T be a tree of order  $n \ge 4$  with  $n_1$  pendant vertices.
- If  $n_1 \le n-2$ ,  $H(T) \ge H(T(n, n_1))$ .
- ►  $H(T(n, n_1)) > H(T(n, n-2))$  for all  $n_1 \ge n-3$  with equality if and only if  $n_1 = n-2$ .

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- If  $n_1 \leq n-2$ ,  $H(T) \geq H(T(n, n_1))$ .
- ►  $H(T(n, n_1)) > H(T(n, n-2))$  for all  $n_1 \ge n-3$  with equality if and only if  $n_1 = n-2$ .
- Since T(n, n − 2) is the unique tree, this T(n, n − 2) is the unique tree of order n with second minimum harmonic Index.

**Note:** There can exist trees with n - 2 pendant vertices that is not a *comet* but has H(T) > H(T(n, n-2)) and H(T) < H(T(n, n-3)).

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$$H(T(10,8)) = \frac{109}{45}, \quad H(S_{7,3}) = \frac{27}{10} \text{ and } H(T(10,7)) = \frac{26}{9}$$

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So, for the third minimum harmonic Index, we have to search in double star with n - 2 pendant vertices.

Among all n-vertex trees, for  $n \ge 6$ , the double star  $S_{3,n-3}$  are the trees with the third minimum harmonic index, which is equal to  $3n^2 - 8n - 4$ 

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#### Proof.

► The harmonic index of the double star S<sub>p,q</sub> is monotonically increasing.

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• So the third minimum harmonic index is for  $S_{3,n-3}$ .

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## **THANK YOU**