

## THE SMALLEST HARMONIC INDEX OF TREES WITH GIVEN MAXIMUM DEGREE

REZA RASI

AND

SEYED MAHMOUD SHEIKHOESLAMI

*Department of Mathematics*  
*Azərbaycan Şahid Mədani University*  
*Tabriz, I.R. Iran*

**e-mail:** {r.rasi;s.m.sheikholeslami}@azaruniv.edu

### Abstract

The harmonic index of a graph  $G$ , denoted by  $H(G)$ , is defined as the sum of weights  $2/[d(u) + d(v)]$  over all edges  $uv$  of  $G$ , where  $d(u)$  denotes the degree of a vertex  $u$ . In this paper we establish a lower bound on the harmonic index of a tree  $T$ .

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### 1. INTRODUCTION

Let  $G$  be a simple connected graph with vertex set  $V = V(G)$  and edge set  $E = E(G)$ . The order  $|V|$  of  $G$  is denoted by  $n = n(G)$  and the size  $|E|$  of  $G$  is denoted by  $m = m(G)$ . For every vertex  $v \in V$ , the *open neighborhood*  $N(v)$  is the set  $\{u \in V(G) \mid uv \in E(G)\}$ . The *degree* of a vertex  $v \in V$  is  $d_v = d(v) = d_G(v) = |N(v)|$ . The *minimum degree* and the *maximum degree* of a graph  $G$  are denoted by  $\delta = \delta(G)$  and  $\Delta = \Delta(G)$ , respectively. An *leaf* of a tree  $T$  is a vertex of degree 1, a *stem* is a vertex adjacent to a leaf, whereas a *strong stem* is a stem adjacent to at least two leaves. An *end stem* is a stem whose all neighbors with exception at most one are leaves. For every two vertices  $x, y$  of a tree  $T$ , we denote the unique  $(x, y)$ -path by  $xTy$ . A path  $P = u_0u_1 \cdots u_k$  ( $k \geq 1$ ) in  $G$  is called a *pendant path* if  $d_{u_0} \geq 3$ ,  $d_{u_k} = 1$  and the degree of any other

vertex of the path is 2. To *contract* an edge  $e$  of a graph  $G$ , is to delete the edge and then identify its ends. The resulting graph is denoted by  $G/e$ . Let  $\mathcal{T}_{n,\Delta}$  be the family of trees  $T$  of order  $n$  and maximum degree  $\Delta$ .

A large variety of degree based topological indices has been defined in the mathematical and mathematico-chemical literature; for details we refer the reader to [4, 6]. Here, we focus on the harmonic index. For a simple graph  $G$ , the *harmonic index* of  $G$ , denoted  $H(G)$ , is defined in [3] as the sum of weights  $2/[d(u)+d(v)]$  of all edges  $uv$  of  $G$ . That is,  $H(G) = \sum_{uv \in E(G)} \frac{2}{d(u)+d(v)}$ . For some related works see [9, 17, 24–28, 30–33]. Wu *et al.* [20] established a lower bound on  $H(G)$  of a graph with minimum degree two. Favaron *et al.* [5] investigated the relation between graph eigenvalues of graphs and the harmonic index. Deng *et al.* [1] considered the relation between  $H(G)$  and the chromatic index  $\chi(G)$ , and proved that  $\chi(G) \leq 2H(G)$ . Liu [13] proposed a conjecture concerning the relation between the harmonic index and the diameter of a connected graph, and showed that the conjecture is true for trees. Relationships between the harmonic index and several other topological indices were established in [8, 22, 29]. For additional results on this index, see [11, 12, 14–17, 21].

In this paper we establish a lower bound for the harmonic index of a tree  $T$  in terms of its order and maximum degree. Our result is an extension of some well-known lower bound on the harmonic index of a tree  $T$ .

## 2. A LOWER BOUND ON THE HARMONIC INDEX OF TREES

In this section we prove the following lower bound for the harmonic index of a tree  $T$  of order  $n$  with maximum degree  $\Delta$ .

**Theorem 1.** *Let  $\Delta \geq 3$  and  $T \in \mathcal{T}_{n,\Delta}$ . If  $n \equiv r \pmod{\Delta-1}$ , then*

$$H(T) \geq \begin{cases} 2 \left( \frac{n(\Delta-2)}{\Delta^2-1} + \frac{\Delta-2}{2\Delta-2} + \frac{n-(\Delta-1)^2}{2\Delta(\Delta-1)} \right) & \text{if } r = 0 \text{ and } n > (\Delta-1)(\Delta-2), \\ 2 \left( \frac{(\Delta-1)^2-n}{(\Delta-1)^2} + \frac{n-\Delta+1}{\Delta+1} + \frac{n-\Delta+1}{2(\Delta-1)^2} \right) & \text{if } r = 0 \text{ and } n \leq (\Delta-1)(\Delta-2), \\ 2 \left( \frac{n(\Delta-2)+1}{\Delta^2-1} + \frac{\Delta-1}{2\Delta-1} + \frac{n-1-\Delta(\Delta-1)}{2\Delta(\Delta-1)} \right) & \text{if } r = 1 \text{ and } n > (\Delta-1)^2+1, \\ 2 \left( \frac{\Delta(\Delta-1)-n+1}{\Delta(\Delta-1)} + \frac{n-\Delta}{\Delta+1} + \frac{n-\Delta}{(2\Delta-1)(\Delta-1)} \right) & \text{if } r = 1 \text{ and } n \leq (\Delta-1)^2+1, \\ 2 \left( \frac{n(\Delta-2)+2}{\Delta^2-1} + \frac{n-\Delta-1}{2\Delta(\Delta-1)} \right) & \text{if } r = 2, \\ 2 \left( \frac{n(\Delta-2)+r-\Delta+1}{\Delta^2-1} + \frac{r-1}{\Delta+r-1} + \frac{n-(r-1)\Delta-1}{2\Delta(\Delta-1)} \right) & \text{if } r \geq 3 \text{ and } n \geq \Delta(r-1)+1, \\ 2 \left( \frac{(r-1)\Delta-n+1}{r(\Delta-1)} + \frac{n-r}{\Delta+1} + \frac{n-r}{(\Delta+r-1)(\Delta-1)} \right) & \text{if } r \geq 3 \text{ and } n < \Delta(r-1)+1. \end{cases}$$

For notational convenience, let  $h_\omega : E(T) \rightarrow \mathbb{R}$  denote a function defined by  $h_\omega(uv) = 1/[d(u) + d(v)]$ . Hence  $H(T) = 2 \sum_{e \in E(T)} h_\omega(e)$ . We begin with some lemmas.

**Lemma 2.** *Let  $T \in \mathcal{T}_{n,\Delta}$ . If  $u$  and  $v$  are two adjacent vertices each of degree at least two in  $T$  with  $d_T(u) + d_T(v) \leq \Delta + 1$ , then there exists a tree  $T'$  of order  $n$  with maximum degree  $\Delta(T)$  such that  $H(T') < H(T)$ .*

**Proof.** Let  $T' := (T/e) + up$  be the tree obtained from  $T$  by contracting the edge  $e = uv$  and adding a pendant edge  $up$ . Clearly,  $T'$  is a tree of order  $n$  with  $\Delta(T') \leq \Delta(T)$ . By the assumptions and the construction of  $T'$ , we have  $d_T(u) \leq \Delta - 1$ ,  $d_T(v) \leq \Delta - 1$ , and  $d_{T'}(u) \leq \Delta$ . If  $w \in V(T)$  is a vertex with maximum degree  $\Delta(T)$ , then we have  $w \notin \{u, v\}$  and  $d_T(w) = d_{T'}(w)$ . Hence  $\Delta(T') = \Delta(T)$ . Assume that  $d(u) = \alpha$ ,  $d(v) = \beta$ ,  $N(u) = \{x_1, \dots, x_{\alpha-1}, v\}$ ,  $N(v) = \{y_1, \dots, y_{\beta-1}, u\}$  and  $S = \{xu \mid x \in N(u)\} \cup \{yv \mid y \in N(v)\}$ . Then we have

$$\frac{1}{2}H(T) = \sum_{e \in E(T) - S} h_\omega(e) + \frac{1}{\alpha + \beta} + \sum_{i=1}^{\alpha-1} \frac{1}{d(x_i) + \alpha} + \sum_{i=1}^{\beta-1} \frac{1}{d(y_i) + \beta}$$

and

$$\frac{1}{2}H(T') = \sum_{e \in E(T) - S} h_\omega(e) + \frac{1}{\alpha + \beta} + \sum_{i=1}^{\alpha-1} \frac{1}{d(x_i) + \alpha + \beta - 1} + \sum_{i=1}^{\beta-1} \frac{1}{d(y_i) + \alpha + \beta - 1}.$$

Clearly  $H(T') < H(T)$  and the proof is complete.  $\blacksquare$

**Lemma 3.** *Let  $T \in \mathcal{T}_{n,\Delta}$ , let  $u$  and  $v$  be two vertices of  $T$  with  $d_T(u) = \alpha < \beta = d_T(v)$  and let  $x \in N(u)$  and  $y \in N(v)$  such that  $x, y \notin uTv$  or  $x, y \in uTv$ . If  $d_T(x) < d_T(y)$ , then there exists a tree  $T'$  of order  $n$  with maximum degree  $\Delta(T)$  such that  $H(T') < H(T)$ .*

**Proof.** Let  $T'$  be the tree obtained from  $T$  by removing the edges  $ux, vy$  and adding new edges  $vx, uy$  (see Figure 1). Clearly,  $T'$  is a connected graph of order  $n$  with  $n - 1$  edges and so  $T'$  is a tree. Also, we have  $d_T(z) = d_{T'}(z)$  for each  $z \in V(T)$  and hence  $\Delta(T') = \Delta(T)$ . Let  $S = \{ux, vy\}$ . Then we have

$$\frac{1}{2}H(T) = \sum_{e \in E(T) \setminus S} h_\omega(e) + \frac{1}{\alpha + d_T(x)} + \frac{1}{\beta + d_T(y)}$$

and

$$\frac{1}{2}H(T') = \sum_{e \in E(T) \setminus S} h_\omega(e) + \frac{1}{\beta + d_T(x)} + \frac{1}{\alpha + d_T(y)}.$$

It follows from  $\alpha < \beta$  and  $d_T(x) < d_T(y)$  that  $H(T') < H(T)$ .  $\blacksquare$

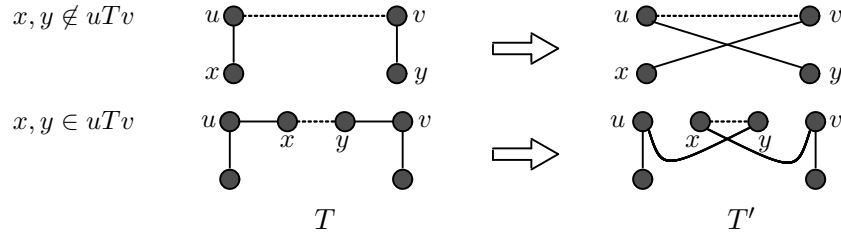


Figure 1. The switching process used in the proof of Lemma 3.

**Lemma 4.** Let  $T \in \mathcal{T}_{n,\Delta}$  be an extremal tree with the minimum harmonic index in  $\mathcal{T}_{n,\Delta}$ . If  $u$  and  $v$  are two vertices of  $T$  of degree  $\alpha$  with  $2 \leq \alpha \leq \Delta - 1$ , then there exists an extremal tree  $T^*$  with the minimum harmonic index in  $\mathcal{T}_{n,\Delta}$  such that  $V(T^*) = V(T)$ ,  $d_T(z) = d_{T^*}(z)$  for each  $z \in V(T)$ , and  $d_{T^*}(x) \geq d_{T^*}(y)$  for each  $x \in N_{T^*}(u) - V(uTv)$  and  $y \in N_{T^*}(v) - V(uTv)$ .

**Proof.** If  $d_T(x) \geq d_T(y)$  for each  $x \in N_T(u) - V(uTv)$  and  $y \in N_T(v) - V(uTv)$ , then we are done. Let  $d_T(x) < d_T(y)$  for some  $x \in N_T(u) - V(uTv)$  and some  $y \in N_T(v) - V(uTv)$ . Assume  $T_1$  to be the tree obtained from  $T$  by deleting the edges  $ux, vy$  and adding new edges  $uy, vx$ . Clearly,  $V(T_1) = V(T)$  and  $d_T(z) = d_{T_1}(z)$  for each  $z \in V(T)$  and hence  $T_1 \in \mathcal{T}_{n,\Delta}$ . Since  $d_{T_1}(u) = d_{T_1}(v) = \alpha$ , it is easy to verify that  $H(T) = H(T_1)$ . Thus  $T_1$  is a extremal tree with the minimum harmonic index in  $\mathcal{T}_{n,\Delta}$ . By repeating this process, we obtain a desired tree  $T^*$ . ■

**Lemma 5.** If  $T \in \mathcal{T}_{n,\Delta}$  is an extremal tree with the minimum harmonic index in  $\mathcal{T}_{n,\Delta}$ , then  $T$  has at most one vertex of degree  $1 < t < \Delta$ .

**Proof.** Assume, to the contrary, that  $T$  has two distinct vertices  $u$  and  $v$  such that  $1 < d(u) = \alpha \leq \beta = d(v) < \Delta$ . Also, suppose that among two vertices with this property we choose two distinct vertices  $u, v$  such that  $d(u, v)$  is as small as possible. Let  $N(u) = \{x_1, \dots, x_\alpha\}$ ,  $N(v) = \{y_1, \dots, y_\beta\}$ ,  $S = \{xu | x \in N(u)\} \cup \{yv | y \in N(v)\}$  and  $K = \sum_{e \in E(T) - S} h_\omega(e)$ . Assume that  $x_1, y_1 \in uTv$ ,  $d_{x_\alpha} \geq \dots \geq d_{x_2}$  and  $d_{y_\beta} \geq \dots \geq d_{y_2}$ . By Lemmas 3 and 4, we may suppose that  $d_{x_\alpha} \geq \dots \geq d_{x_2} \geq d_{y_\beta} \geq \dots \geq d_{y_2}$ . Let  $T' := T - ux_2 + vx_2$  be the tree obtained from  $T$  by removing the edge  $ux_2$  and adding a new edge  $vx_2$  (see Figure 2). We show that  $H(T') < H(T)$ . Consider four cases.

*Case 1.*  $uv \in E(T)$  and  $d_u = d_v = \alpha$ . Then  $x_1 = v$  and  $y_1 = u$ . By definition we have

$$\frac{1}{2}H(T) = K + \frac{1}{2\alpha} + \frac{1}{d_{x_2} + \alpha} + \sum_{i=3}^{\alpha} \frac{1}{d_{x_i} + \alpha} + \sum_{i=2}^{\alpha} \frac{1}{d_{y_i} + \alpha}$$

and

$$\frac{1}{2}H(T') = K + \frac{1}{2\alpha} + \frac{1}{d_{x_2} + \alpha + 1} + \sum_{i=3}^{\alpha} \frac{1}{d_{x_i} + \alpha - 1} + \sum_{i=2}^{\alpha} \frac{1}{d_{y_i} + \alpha + 1}.$$

Now, we have

$$\begin{aligned} & \frac{1}{2} (H(T') - H(T)) \\ &= \sum_{i=3}^{\alpha} \frac{1}{(d_{x_i} + \alpha)(d_{x_i} + \alpha - 1)} + \sum_{i=2}^{\alpha} \frac{-1}{(d_{y_i} + \alpha)(d_{y_i} + \alpha + 1)} \\ & \quad + \frac{-1}{(d_{x_2} + \alpha)(d_{x_2} + \alpha + 1)} \\ &= \sum_{i=3}^{\alpha} \left( \frac{1}{(d_{x_i} + \alpha)(d_{x_i} + \alpha - 1)} - \frac{1}{(d_{y_i} + \alpha)(d_{y_i} + \alpha + 1)} \right) \\ & \quad + \left( \frac{-1}{(d_{y_2} + \alpha)(d_{y_2} + \alpha + 1)} + \frac{-1}{(d_{x_2} + \alpha)(d_{x_2} + \alpha + 1)} \right) \\ &\leq \sum_{i=3}^{\alpha} \left( \frac{1}{(d_{x_2} + \alpha)(d_{x_2} + \alpha - 1)} - \frac{1}{(d_{x_2} + \alpha)(d_{x_2} + \alpha + 1)} \right) \\ & \quad + \left( \frac{-1}{(d_{x_2} + \alpha)(d_{x_2} + \alpha + 1)} + \frac{-1}{(d_{x_2} + \alpha)(d_{x_2} + \alpha + 1)} \right) \\ &\leq \sum_{i=3}^{\alpha} \left( \frac{2}{(d_{x_2} + \alpha)(d_{x_2} + \alpha - 1)(d_{x_2} + \alpha + 1)} \right) + \frac{-2}{(d_{x_2} + \alpha)(d_{x_2} + \alpha + 1)} \\ &\leq \frac{2(\alpha - 2)}{(d_{x_2} + \alpha)(d_{x_2} + \alpha - 1)(d_{x_2} + \alpha + 1)} + \frac{-2}{(d_{x_2} + \alpha)(d_{x_2} + \alpha + 1)} \\ &= \frac{-2d_{x_2} - 2}{(d_{x_2} + \alpha)(d_{x_2} + \alpha - 1)(d_{x_2} + \alpha + 1)} < 0. \end{aligned}$$

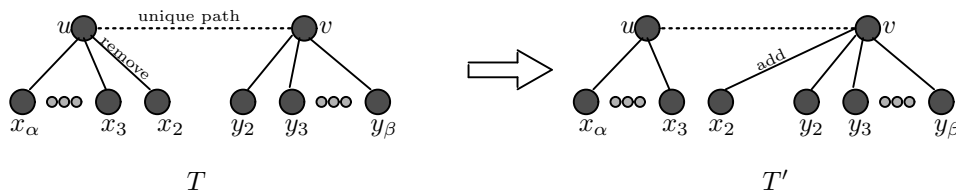


Figure 2. The switching process used in the proof of Lemma 5.

*Case 2.*  $uv \in E(T)$ ,  $d_u = \alpha < \beta = d_v$ . As above  $x_1 = v$  and  $y_1 = u$ . By definition we have

$$\frac{1}{2}H(T) = K + \frac{1}{\alpha + \beta} + \frac{1}{d_{x_2} + \alpha} + \frac{1}{d_{y_2} + \beta} + \sum_{i=3}^{\alpha} \frac{1}{d_{x_i} + \alpha} + \sum_{i=3}^{\beta} \frac{1}{d_{y_i} + \beta}$$

and

$$\begin{aligned} \frac{1}{2}H(T') &= K + \frac{1}{\alpha + \beta} + \frac{1}{d_{x_2} + \beta + 1} + \frac{1}{d_{y_2} + \beta + 1} \\ &\quad + \sum_{i=3}^{\alpha} \frac{1}{d_{x_i} + \alpha - 1} + \sum_{i=3}^{\beta} \frac{1}{d_{y_i} + \beta + 1}. \end{aligned}$$

Now, we have

$$\begin{aligned} &\frac{1}{2}(H(T') - H(T)) \\ &= \sum_{i=3}^{\alpha} \left( \frac{1}{(d_{x_i} + \alpha)(d_{x_i} + \alpha - 1)} - \frac{1}{(d_{y_i} + \beta)(d_{y_i} + \beta + 1)} \right) \\ &\quad + \sum_{i=\alpha+1}^{\beta} \frac{-1}{(d_{y_i} + \beta)(d_{y_i} + \beta + 1)} + \left( \frac{\alpha - \beta - 1}{(d_{x_2} + \alpha)(d_{x_2} + \beta + 1)} + \frac{-1}{(d_{y_2} + \beta)(d_{y_2} + \beta + 1)} \right) \\ &\leq \sum_{i=3}^{\alpha} \left( \frac{1}{(d_{x_2} + \alpha)(d_{x_2} + \alpha - 1)} - \frac{1}{(d_{x_2} + \beta)(d_{x_2} + \beta + 1)} \right) \\ &\quad + \sum_{i=\alpha+1}^{\beta} \frac{-1}{(d_{y_i} + \beta)(d_{y_i} + \beta + 1)} + \left( \frac{\alpha - \beta - 1}{(d_{x_2} + \alpha)(d_{x_2} + \beta + 1)} + \frac{-1}{(d_{x_2} + \beta)(d_{x_2} + \beta + 1)} \right) \\ &= \sum_{i=3}^{\alpha} \left( \frac{(\beta - \alpha + 1)(\alpha + \beta + 2d_{x_2})}{(d_{x_2} + \alpha)(d_{x_2} + \alpha - 1)(d_{x_2} + \beta)(d_{x_2} + \beta + 1)} \right) \\ &\quad + \sum_{i=\alpha+1}^{\beta} \frac{-1}{(d_{y_i} + \beta)(d_{y_i} + \beta + 1)} + \frac{(\alpha - \beta)(d_{x_2} + \beta) - (\alpha + \beta + 2d_{x_2})}{(d_{x_2} + \alpha)(d_{x_2} + \beta)(d_{x_2} + \beta + 1)} \\ &\leq \frac{(\alpha - 2)(\beta - \alpha + 1)(\alpha + \beta + 2d_{x_2})}{(d_{x_2} + \alpha)(d_{x_2} + \alpha - 1)(d_{x_2} + \beta)(d_{x_2} + \beta + 1)} \\ &\quad + \frac{\alpha - \beta}{(d_{x_2} + \beta)(d_{x_2} + \beta + 1)} + \frac{(\alpha - \beta)(d_{x_2} + \beta) - (\alpha + \beta + 2d_{x_2})}{(d_{x_2} + \alpha)(d_{x_2} + \beta)(d_{x_2} + \beta + 1)} \\ &= \frac{(\alpha - 2)(\beta - \alpha + 1)(\alpha + \beta + 2d_{x_2})}{(d_{x_2} + \alpha)(d_{x_2} + \alpha - 1)(d_{x_2} + \beta)(d_{x_2} + \beta + 1)} \\ &\quad + \frac{(\alpha - \beta)(d_{x_2} + \alpha) + (\alpha - \beta)(d_{x_2} + \beta) - (\alpha + \beta + 2d_{x_2})}{(d_{x_2} + \alpha)(d_{x_2} + \beta)(d_{x_2} + \beta + 1)} \\ &= \frac{(\alpha - 2)(\beta - \alpha + 1)(\alpha + \beta + 2d_{x_2})}{(d_{x_2} + \alpha)(d_{x_2} + \alpha - 1)(d_{x_2} + \beta)(d_{x_2} + \beta + 1)} + \frac{(\alpha - \beta - 1)(\alpha + \beta + 2d_{x_2})}{(d_{x_2} + \alpha)(d_{x_2} + \beta)(d_{x_2} + \beta + 1)} \end{aligned}$$

$$\begin{aligned}
&= \frac{(\alpha - 2)(\beta - \alpha + 1)(\alpha + \beta + 2d_{x_2}) + (\alpha - \beta - 1)(d_{x_2} + \alpha - 1)(\alpha + \beta + 2d_{x_2})}{(d_{x_2} + \alpha)(d_{x_2} + \beta)(d_{x_2} + \beta + 1)(d_{x_2} + \alpha - 1)} \\
&= \frac{(\beta - \alpha + 1)(\alpha + \beta + 2d_{x_2})(-d_{x_2} - 1)}{(d_{x_2} + \alpha)(d_{x_2} + \beta)(d_{x_2} + \beta + 1)(d_{x_2} + \alpha - 1)} < 0
\end{aligned}$$

*Case 3.*  $uv \notin E(T)$  and  $d_u = d_v = \alpha$ . By the choice of  $u, v$ , we may assume that  $d_{x_1} = d_{y_1} = \Delta$ . We have

$$\frac{1}{2}H(T) = K + \frac{1}{\alpha + \Delta} + \frac{1}{\alpha + \Delta} + \frac{1}{d_{x_2} + \alpha} + \frac{1}{d_{y_2} + \alpha} + \sum_{i=3}^{\alpha} \frac{1}{d_{x_i} + \alpha} + \sum_{i=3}^{\beta} \frac{1}{d_{y_i} + \alpha}$$

and

$$\begin{aligned}
\frac{1}{2}H(T') &= K + \frac{1}{\alpha + \Delta - 1} + \frac{1}{\alpha + \Delta + 1} + \frac{1}{d_{x_2} + \alpha + 1} + \frac{1}{d_{y_2} + \alpha + 1} \\
&\quad + \sum_{i=3}^{\alpha} \frac{1}{d_{x_i} + \alpha - 1} + \sum_{i=3}^{\beta} \frac{1}{d_{y_i} + \alpha + 1}.
\end{aligned}$$

Now, we have

$$\begin{aligned}
&\frac{1}{2}(H(T') - H(T)) \\
&= \sum_{i=3}^{\alpha} \frac{1}{(d_{x_i} + \alpha)(d_{x_i} + \alpha - 1)} + \sum_{i=3}^{\alpha} \frac{-1}{(d_{y_i} + \alpha)(d_{y_i} + \alpha + 1)} \\
&\quad + \frac{2}{(\alpha + \Delta)(\alpha + \Delta - 1)(\alpha + \Delta + 1)} + \frac{-1}{(d_{x_2} + \alpha)(d_{x_2} + \alpha + 1)} + \frac{-1}{(d_{y_2} + \alpha)(d_{y_2} + \alpha + 1)} \\
&\leq \sum_{i=3}^{\alpha} \left( \frac{1}{(d_{x_2} + \alpha)(d_{x_2} + \alpha - 1)} - \frac{1}{(d_{x_2} + \alpha)(d_{x_2} + \alpha + 1)} \right) \\
&\quad + \frac{2}{(\alpha + \Delta)(\alpha + \Delta - 1)(\alpha + \Delta + 1)} - \frac{2}{(d_{x_2} + \alpha)(d_{x_2} + \alpha + 1)} \\
&= \frac{2(\alpha - 2)}{(d_{x_2} + \alpha)(d_{x_2} + \alpha - 1)(d_{x_2} + \alpha + 1)} + \frac{2}{(\alpha + \Delta)(\alpha + \Delta - 1)(\alpha + \Delta + 1)} \\
&\quad - \frac{2}{(d_{x_2} + \alpha)(d_{x_2} + \alpha + 1)} \\
&= \frac{2(\alpha - 2) - 2(d_{x_2} + \alpha - 1)}{(d_{x_2} + \alpha)(d_{x_2} + \alpha - 1)(d_{x_2} + \alpha + 1)} + \frac{2}{(\alpha + \Delta)(\alpha + \Delta - 1)(\alpha + \Delta + 1)} \\
&= \frac{-2d_{x_2} - 2}{(d_{x_2} + \alpha)(d_{x_2} + \alpha - 1)(d_{x_2} + \alpha + 1)} + \frac{2}{(\alpha + \Delta)(\alpha + \Delta - 1)(\alpha + \Delta + 1)}
\end{aligned}$$

$$\begin{aligned}
&\leq \frac{-2d_{x_2} - 2}{(d_{x_2} + \alpha)(d_{x_2} + \alpha - 1)(d_{x_2} + \alpha + 1)} + \frac{2}{(\alpha + d_{x_2})(\alpha + d_{x_2} - 1)(\alpha + d_{x_2} + 1)} \\
&\leq \frac{-2d_{x_2}}{(d_{x_2} + \alpha)(d_{x_2} + \alpha - 1)(d_{x_2} + \alpha + 1)} < 0.
\end{aligned}$$

Case 4.  $uv \notin E(T)$  and  $d_u = \alpha < \beta = d_v$ . As in Case 3, we may assume that  $d_{x_1} = d_{y_1} = \Delta$ . By definition we have

$$\frac{1}{2}H(T) = K + \sum_{i=3}^{\alpha} \frac{1}{d_{x_i} + \alpha} + \sum_{i=3}^{\beta} \frac{1}{d_{y_i} + \beta} + \frac{1}{\alpha + \Delta} + \frac{1}{\beta + \Delta} + \frac{1}{d_{x_2} + \alpha} + \frac{1}{d_{y_2} + \beta}$$

and

$$\begin{aligned}
\frac{1}{2}H(T') &= K + \sum_{i=3}^{\alpha} \frac{1}{d_{x_i} + \alpha - 1} + \sum_{i=3}^{\beta} \frac{1}{d_{y_i} + \beta + 1} + \frac{1}{\alpha + \Delta - 1} + \frac{1}{\beta + \Delta + 1} \\
&\quad + \frac{1}{d_{x_2} + \beta + 1} + \frac{1}{d_{y_2} + \beta + 1}.
\end{aligned}$$

Then we have

$$\begin{aligned}
&\frac{1}{2}(H(T') - H(T)) \\
&= \sum_{i=3}^{\alpha} \frac{1}{(d_{x_i} + \alpha)(d_{x_i} + \alpha - 1)} + \sum_{i=3}^{\beta} \frac{-1}{(d_{y_i} + \beta)(d_{y_i} + \beta + 1)} + \frac{1}{(\alpha + \Delta)(\alpha + \Delta - 1)} \\
&\quad + \frac{-1}{(\beta + \Delta)(\beta + \Delta + 1)} + \frac{\alpha - \beta - 1}{(d_{x_2} + \alpha)(d_{x_2} + \beta + 1)} + \frac{-1}{(d_{y_2} + \beta)(d_{y_2} + \beta + 1)} \\
&\leq \sum_{i=3}^{\alpha} \left( \frac{1}{(d_{x_2} + \alpha)(d_{x_2} + \alpha - 1)} - \frac{1}{(d_{x_2} + \beta)(d_{x_2} + \beta + 1)} \right) \\
&\quad + \sum_{i=\alpha+1}^{\beta} \frac{-1}{(d_{x_2} + \beta)(d_{x_2} + \beta + 1)} + \frac{1}{(\alpha + \Delta)(\alpha + \Delta - 1)} \\
&\quad + \frac{-1}{(\beta + \Delta)(\beta + \Delta + 1)} + \frac{\alpha - \beta - 1}{(d_{x_2} + \alpha)(d_{x_2} + \beta + 1)} + \frac{-1}{(d_{x_2} + \beta)(d_{x_2} + \beta + 1)} \\
&= \frac{(\alpha - 2)((d_{x_2} + \beta)(d_{x_2} + \beta + 1) - (d_{x_2} + \alpha)(d_{x_2} + \alpha - 1))}{(d_{x_2} + \alpha)(d_{x_2} + \alpha - 1)(d_{x_2} + \beta)(d_{x_2} + \beta + 1)} + \frac{\alpha - \beta}{(d_{x_2} + \beta)(d_{x_2} + \beta + 1)} \\
&\quad + \frac{1}{(\alpha + \Delta)(\alpha + \Delta - 1)} + \frac{-1}{(\beta + \Delta)(\beta + \Delta + 1)} + \frac{(\alpha - \beta - 1)(d_{x_2} + \beta) - (d_{x_2} + \alpha)}{(d_{x_2} + \alpha)(d_{x_2} + \beta)(d_{x_2} + \beta + 1)}
\end{aligned}$$



$$\begin{aligned}
&= \frac{(\alpha - 2)(\beta - \alpha + 1)(\alpha + \beta + 2d_{x_2})}{(d_{x_2} + \alpha)(d_{x_2} + \alpha - 1)(d_{x_2} + \beta)(d_{x_2} + \beta + 1)} + \frac{1}{(\alpha + \Delta)(\alpha + \Delta - 1)} \\
&+ \frac{-1}{(\beta + \Delta)(\beta + \Delta + 1)} + \frac{(\alpha - \beta)(d_{x_2} + \beta) - (\alpha + \beta + 2d_{x_2}) + (\alpha - \beta)(d_{x_2} + \alpha)}{(d_{x_2} + \alpha)(d_{x_2} + \beta)(d_{x_2} + \beta + 1)} \\
&= \frac{(\alpha - 2)(\beta - \alpha + 1)(\alpha + \beta + 2d_{x_2})}{(d_{x_2} + \alpha)(d_{x_2} + \alpha - 1)(d_{x_2} + \beta)(d_{x_2} + \beta + 1)} + \frac{1}{(\alpha + \Delta)(\alpha + \Delta - 1)} \\
&+ \frac{-1}{(\beta + \Delta)(\beta + \Delta + 1)} + \frac{(\alpha - \beta - 1)(\alpha + \beta + 2d_{x_2})}{(d_{x_2} + \alpha)(d_{x_2} + \beta)(d_{x_2} + \beta + 1)} \\
&= \frac{(\alpha - 2)(\beta - \alpha + 1)(\alpha + \beta + 2d_{x_2}) + (d_{x_2} + \alpha - 1)(\alpha - \beta - 1)(\alpha + \beta + 2d_{x_2})}{(d_{x_2} + \alpha)(d_{x_2} + \alpha - 1)(d_{x_2} + \beta)(d_{x_2} + \beta + 1)} \\
&+ \frac{1}{(\alpha + \Delta)(\alpha + \Delta - 1)} + \frac{-1}{(\beta + \Delta)(\beta + \Delta + 1)} \\
&= \frac{(\alpha + \beta + 2d_{x_2})(\beta - \alpha + 1)(-d_{x_2} - 1)}{(d_{x_2} + \alpha)(d_{x_2} + \alpha - 1)(d_{x_2} + \beta)(d_{x_2} + \beta + 1)} + \frac{1}{(\alpha + \Delta)(\alpha + \Delta - 1)} \\
&+ \frac{-1}{(\beta + \Delta)(\beta + \Delta + 1)} \\
&\leq \frac{(\alpha + \beta + 2d_{x_2})(\beta - \alpha + 1)(-d_{x_2} - 1)}{(\Delta + \alpha)(\Delta + \alpha - 1)(\Delta + \beta)(\Delta + \beta + 1)} + \frac{1}{(\alpha + \Delta)(\alpha + \Delta - 1)} + \frac{-1}{(\beta + \Delta)(\beta + \Delta + 1)} \\
&= \frac{(\alpha + \beta + 2d_{x_2})(\beta - \alpha + 1)(-d_{x_2} - 1) + (\alpha + \beta + 2\Delta)(\beta - \alpha + 1)}{(\Delta + \alpha)(\Delta + \alpha - 1)(\Delta + \beta)(\Delta + \beta + 1)} \\
&= \frac{(\beta - \alpha + 1)((\alpha + \beta + 2d_{x_2})(-d_{x_2} - 1) + (\alpha + \beta + 2\Delta))}{(\Delta + \alpha)(\Delta + \alpha - 1)(\Delta + \beta)(\Delta + \beta + 1)}.
\end{aligned}$$

Since  $\alpha + \beta + 2d_{x_2} < 2\Delta + 2d_{x_2}$  and  $-d_{x_2} - 1 \leq -2$ , we deduce that

$$(\alpha + \beta + 2d_{x_2})(-d_{x_2} - 1) + (\alpha + \beta + 2\Delta) < -4\Delta - 4d_{x_2} + (\alpha + \beta + 2\Delta) < -4d_{x_2} < 0$$

and hence  $\frac{1}{2}(H(T') - H(T)) < 0$ .

Thus all cases lead to a contradiction since  $T$  has the minimum harmonic index. This completes the proof.  $\blacksquare$

**Lemma 6.** Let  $T \in \mathcal{T}_{n,\Delta}$  be an extremal tree with the minimum harmonic index in  $\mathcal{T}_{n,\Delta}$  where  $\Delta \geq 3$ ,  $n = (\Delta - 1)k + r$  and  $0 \leq r \leq \Delta - 2$ . If  $n_i$  is the number of vertices of  $T$  of degree  $i$  for each  $i = 1, 2, \dots, \Delta$ , then the following hold:

1. if  $r = 0, 1$ , then  $n_\Delta = k - 1$ ,  $n_{\Delta-2+r} = 1$  and  $n_1 = n - k$ ,
2. if  $r = 2$ , then  $n_\Delta = k$  and  $n_1 = n - k$ ,
3. if  $r \geq 3$ , then  $n_\Delta = k$ ,  $n_{r-1} = 1$  and  $n_1 = n - k - 1$ .

**Proof.** Let  $n_i$  be the number of vertices of  $T$  of degree  $i$  for each  $i = 1, 2, \dots, \Delta$ . Then  $n_1 + n_2 + \dots + n_\Delta = n$  and  $n_1 + 2n_2 + \dots + \Delta n_\Delta = 2n - 2$  and hence

$$(1) \quad n_2 + 2n_3 + \dots + (\Delta - 1)n_\Delta = n - 2.$$

By Lemma 5 we have  $n_2 + n_3 + \dots + n_{\Delta-1} \leq 1$  that yields

$$(2) \quad n_2 + 2n_3 + \dots + (\Delta - 2)n_{\Delta-1} \leq \Delta - 2.$$

Assume  $n_t = 1$  if  $n_2 + n_3 + \dots + n_{\Delta-1} = 1$ .

(1) If  $r = 0, 1$ , then we deduce from (1) that  $n_2 + n_3 + \dots + n_{\Delta-1} = 1$  and so

$$(t - 1) + (\Delta - 1)n_\Delta = (\Delta - 1)k + r - 2 = (\Delta - 1)(k - 1) + (\Delta - 3 + r).$$

This implies that  $n_\Delta = k - 1$ ,  $n_t = n_{\Delta-2+r} = 1$  and  $n_1 = n - k$ .

(2) If  $r = 2$ , then we conclude from (1) and (2) that  $n_2 + n_3 + \dots + n_{\Delta-1} = 0$  and so  $n_\Delta = k$  and  $n_1 = n - k$ .

(3) Let  $r \geq 3$ . Then we have

$$(t - 1) + (\Delta - 1)n_\Delta = (\Delta - 1)k + r - 2,$$

and this implies that  $n_\Delta = k$ ,  $n_t = n_{r-1} = 1$  and  $n_1 = n - k - 1$ . ■

Let  $E_{i,j}$  denote the set of all edges having a vertex of degree  $i$  at one end and a vertex of degree  $j$  at the other end and let  $\varepsilon_{i,j} = |E_{i,j}|$ .

**Lemma 7.** Let  $T \in \mathcal{T}_{n,\Delta}$  be an extremal tree with the minimum harmonic index in  $\mathcal{T}_{n,\Delta}$  and let  $T$  have a vertex  $v$  of degree  $t$  with  $1 < t < \Delta$ . Then  $\varepsilon_{1,t}$  is as small as possible.

**Proof.** It follows from Lemma 5 that  $\deg(u) = 1$  or  $\Delta$  for each  $u \in V(T) - \{v\}$  and hence  $E(T) = E_{1,t} \cup E_{1,\Delta} \cup E_{t,\Delta} \cup E_{\Delta,\Delta}$ . By definition we have

$$\begin{aligned} \frac{1}{2}H(T) &= \frac{\varepsilon_{1,t}}{1+t} + \frac{\varepsilon_{1,\Delta}}{1+\Delta} + \frac{\varepsilon_{t,\Delta}}{t+\Delta} + \frac{\varepsilon_{\Delta,\Delta}}{2\Delta} \\ &= \frac{\varepsilon_{1,t}}{1+t} + \frac{n_1 - \varepsilon_{1,t}}{1+\Delta} + \frac{t - \varepsilon_{1,t}}{t+\Delta} + \frac{n - 1 - n_1 - \varepsilon_{t,\Delta}}{2\Delta} \\ &= \frac{\varepsilon_{1,t}}{1+t} + \frac{n_1 - \varepsilon_{1,t}}{1+\Delta} + \frac{t - \varepsilon_{1,t}}{t+\Delta} + \frac{n - 1 - n_1 - t + \varepsilon_{1,t}}{2\Delta} \\ &= \varepsilon_{1,t} \left( \frac{1}{1+t} + \frac{1}{2\Delta} \right) - \varepsilon_{1,t} \left( \frac{1}{1+\Delta} + \frac{1}{t+\Delta} \right) + \left( \frac{n_1}{1+\Delta} + \frac{t}{t+\Delta} + \frac{n - 1 - n_1 - t}{2\Delta} \right) \end{aligned}$$

$$\begin{aligned}
&= \varepsilon_{1,t} \left( \frac{2\Delta + t + 1}{2(1+t)\Delta} - \frac{2\Delta + t + 1}{(1+\Delta)(t+\Delta)} \right) + \left( \frac{n_1}{1+\Delta} + \frac{t}{t+\Delta} + \frac{n-1-n_1-t}{2\Delta} \right) \\
&= \varepsilon_{1,t}(2\Delta + t + 1) \left( \frac{1}{2\Delta(1+t)} - \frac{1}{(1+\Delta)(t+\Delta)} \right) + \left( \frac{n_1}{1+\Delta} + \frac{t}{t+\Delta} + \frac{n-1-n_1-t}{2\Delta} \right) \\
&= \varepsilon_{1,t}(2\Delta + t + 1) \left( \frac{t + \Delta + t\Delta + \Delta^2 - 2\Delta - 2t\Delta}{2\Delta(1+t)(1+\Delta)(t+\Delta)} \right) + \left( \frac{n_1}{1+\Delta} + \frac{t}{t+\Delta} + \frac{n-1-n_1-t}{2\Delta} \right) \\
&= \varepsilon_{1,t}(2\Delta + t + 1) \cdot \frac{(\Delta-1)(\Delta-t)}{2\Delta(1+t)(1+\Delta)(t+\Delta)} + \left( \frac{n_1}{1+\Delta} + \frac{t}{t+\Delta} + \frac{n-1-n_1-t}{2\Delta} \right).
\end{aligned}$$

Since  $\frac{(\Delta-1)(\Delta-t)}{2\Delta(1+t)(1+\Delta)(t+\Delta)} > 0$  and  $T$  is an extremal tree with the minimum harmonic index in  $\mathcal{T}_{n,\Delta}$ , we conclude that  $\varepsilon_{1,t}$  is as small as possible. ■

**Proof of Theorem 1.** Let  $T^* \in \mathcal{T}_{n,\Delta}$  be an extremal tree with the minimum harmonic index in  $\mathcal{T}_{n,\Delta}$ . We consider four cases.

*Case 1.*  $r = 0$ . Then  $n_\Delta = k - 1$ ,  $n_t = n_{\Delta-2} = 1$  and  $n_1 = n - k$  by Lemma 6. We have also  $\varepsilon_{1,\Delta} = n - k - \varepsilon_{1,t}$ ,  $\varepsilon_{t,\Delta} = \Delta - 2 - \varepsilon_{1,t}$  and  $\varepsilon_{\Delta,\Delta} = k - \Delta + \varepsilon_{1,t} + 1$ . Consider two subcases.

*Subcase 1.1.*  $k = \frac{n}{\Delta-1} > t = \Delta - 2$ , that is,  $n > (\Delta - 1)(\Delta - 2)$ . We conclude from Lemma 7 that  $\varepsilon_{1,t} = 0$  and hence  $\varepsilon_{1,\Delta} = n - k$ ,  $\varepsilon_{t,\Delta} = \Delta - 2$  and  $\varepsilon_{\Delta,\Delta} = k - \Delta + 1$ . Therefore,

$$\frac{1}{2}H(T^*) = \frac{n-k}{1+\Delta} + \frac{\Delta-2}{t+\Delta} + \frac{k-\Delta+1}{2\Delta} = \frac{n-k}{\Delta+1} + \frac{\Delta-2}{2\Delta-2} + \frac{k-\Delta+1}{2\Delta}.$$

*Subcase 1.2.*  $k = \frac{n}{\Delta-1} \leq t = \Delta - 2$ , that is,  $n \leq (\Delta - 1)(\Delta - 2)$ . Then we must have  $\varepsilon_{1,t} = t - n_\Delta = t - k + 1 = \Delta - k - 1$  which implies that  $\varepsilon_{1,\Delta} = n - \Delta + 1$ ,  $\varepsilon_{t,\Delta} = k - 1$  and  $\varepsilon_{\Delta,\Delta} = 0$ . Therefore,

$$\frac{1}{2}H(T^*) = \frac{\Delta-k-1}{1+t} + \frac{n-\Delta+1}{1+\Delta} + \frac{k-1}{t+\Delta} = \frac{\Delta-k-1}{\Delta-1} + \frac{k-1}{2\Delta-2} + \frac{n-\Delta+1}{\Delta+1}.$$

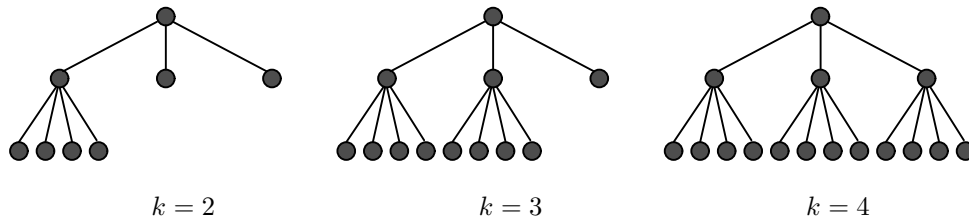


Figure 3.  $\Delta = 5$ ,  $r = 0$ ,  $t = \Delta - 2 = 3$ ,  $n = (\Delta - 1)k = 8, 12, 16$ .

*Case 2.*  $r = 1$ . As in Case 1, we have  $n_\Delta = k - 1$ ,  $n_t = n_{\Delta-1} = 1$ ,  $n_1 = n - k$ ,  $\varepsilon_{1,\Delta} = n - k - \varepsilon_{1,t}$ ,  $\varepsilon_{t,\Delta} = \Delta - 1 - \varepsilon_{1,t}$  and  $\varepsilon_{\Delta,\Delta} = k - \Delta + \varepsilon_{1,t}$ . If  $k = \frac{n-1}{\Delta-1} > t = \Delta - 1$  that is  $n > (\Delta - 1)^2 + 1$ , then as in Subcase 1.1. we have  $\varepsilon_{1,t} = 0$ ,  $\varepsilon_{1,\Delta} = n - k$ ,  $\varepsilon_{t,\Delta} = \Delta - 1$ ,  $\varepsilon_{\Delta,\Delta} = k - \Delta$  and by definition we have

$$\frac{1}{2}H(T^*) = \frac{n-k}{\Delta+1} + \frac{\Delta-1}{2\Delta-1} + \frac{k-\Delta}{2\Delta}.$$

If  $k \leq t = \Delta - 1$  that is  $n \leq (\Delta - 1)^2 + 1$ , then we have  $\varepsilon_{1,t} = \Delta - k$ ,  $\varepsilon_{1,\Delta} = n - \Delta$ ,  $\varepsilon_{t,\Delta} = k - 1$  and  $\varepsilon_{\Delta,\Delta} = 0$ . Hence

$$\frac{1}{2}H(T^*) = \frac{\Delta-k}{1+t} + \frac{n-\Delta}{1+\Delta} + \frac{k-1}{t+\Delta} = \frac{\Delta-k}{\Delta} + \frac{n-\Delta}{\Delta+1} + \frac{k-1}{2\Delta-1}.$$

*Case 3.*  $r = 2$ . In this case we have  $n_\Delta = k$ ,  $n_1 = n - k$ ,  $\varepsilon_{1,\Delta} = n_1 = n - k$  and  $\varepsilon_{\Delta,\Delta} = (n - 1) - (n - k) = k - 1$ . It follows from definition that

$$\frac{1}{2}H(T^*) = \frac{n-k}{\Delta+1} + \frac{k-1}{2\Delta}.$$

*Case 4.*  $r \geq 3$ . By Lemma 6 we have  $n_\Delta = k$ ,  $n_t = n_{r-1} = 1$  and  $n_1 = n - k - 1$ . Also we have  $\varepsilon_{1,\Delta} = n - k - 1 - \varepsilon_{1,t}$ ,  $\varepsilon_{t,\Delta} = r - 1 - \varepsilon_{1,t}$  and  $\varepsilon_{\Delta,\Delta} = k - r + \varepsilon_{1,t} + 1$ . An argument similar to that described in Case 1 shows that

$$\frac{1}{2}H(T^*) = \frac{n-k-1}{\Delta+1} + \frac{r-1}{\Delta+r-1} + \frac{k-r+1}{2\Delta}$$

if  $k = \frac{n-r}{\Delta-1} \geq t = r - 1$  that is  $n \geq \Delta(r - 1) + 1$ , and

$$\frac{1}{2}H(T^*) = \frac{r-k-1}{1+t} + \frac{n-r}{\Delta+1} + \frac{k}{\Delta+t} = \frac{r-k-1}{r} + \frac{n-r}{\Delta+1} + \frac{k}{\Delta+r-1}$$

when  $k < t = r - 1$  that is  $n < \Delta(r - 1) + 1$ .

Replacing  $k$  by  $\frac{n-r}{\Delta-1}$  in all cases, we arrive at the bounds of Theorem 1. This completes the proof.  $\blacksquare$

Applying Theorem 1, we can get two corollaries in the following.

**Corollary 8.** *Let  $T$  be a tree of order  $n$  and maximum degree  $\Delta$ . If  $\Delta \geq 3$  and  $n = (\Delta - 1)k + r$ ,  $0 \leq r \leq \Delta - 2$ , then*

$$H(T) \geq 2 \left( \frac{n(\Delta - 2) + r}{\Delta^2 - 1} + \frac{n - \Delta - r + 1}{2\Delta(\Delta - 1)} \right)$$

*with equality if and only if  $n - 2 = (\Delta - 1)k$  and  $n_\Delta = k$ .*

**Corollary 9** ([10]). *For any tree  $T$  of order  $n \geq 3$ ,*

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

*with equality if and only if  $T$  is a star.*

In Figure 4, we determine the harmonic index of all trees of order 6 and 7 with maximum degree at least 3.

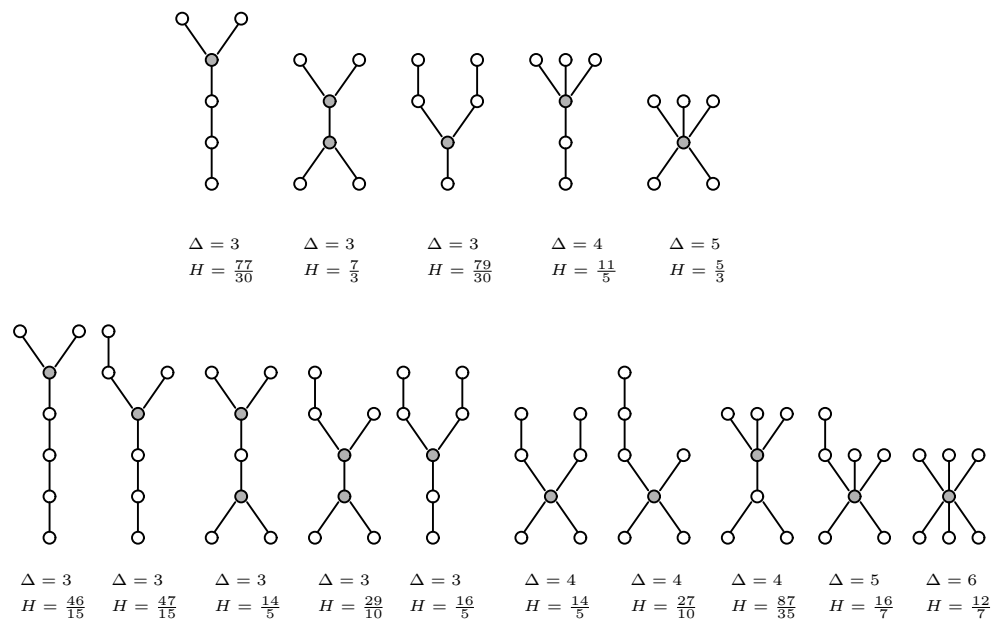


Figure 4. The harmonic index of all trees  $T$  of order 6 and 7 with  $\Delta(T) \geq 3$ .

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