

On the extremal values of the ratios of number of paths

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Received 12 July 2008, accepted 1 January 2010, published online 26 December 2010

Abstract

In this paper, we analyze the ratios of the numbers of paths $p_i(G)$ and $p_j(G)$ of different length in graph G . Namely, we are interested in the extremal values of these ratios for acyclic and cyclic graphs with given maximal degree. The values of infimum and supremum for graphs with given maximal degree are obtained. Also, the infimum of these ratios for trees with given maximal degree are obtained. Suprema for trees of given maximal degree are given when ratios of paths of length 1 and 2 are observed, and when ratios of paths of lengths 1 and 3 are observed. As the main result, a linear algorithm (in terms of maximal degree) for finding suprema of the ratios of the numbers of paths of length 2 and 3 for trees with given maximal degree is presented.

Keywords: Extremal graph, path, push to leaves.

Math. Subj. Class.: 05C35, 05C38

1 Introduction

In this paper, we analyze the possible values of the ratio of the numbers of the paths of lengths i and j , $i > j$. Namely we are interested in the extremal values [2] of the ratio $\frac{p_i(G)}{p_j(G)}$ where $p_i(G)$ and $p_j(G)$ are the numbers of (unoriented) paths of length i and j , respectively. We restrict ourselves to the simple graphs and henceforth the term graph shall imply simple graph.

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Denote by $\mathcal{T}(\Delta, j)$ the family of all trees with maximum degree Δ that contain at least one path of length j and by $\mathcal{G}(\Delta, j)$ family of connected graphs of maximum degree Δ that contain at least one path of length j . We define functions: $\phi_{ij}^G, \Phi_{ij}^G, \phi_{ij}^T, \Phi_{ij}^T : N \setminus \{1\} \rightarrow R$ by

$$\begin{aligned} \phi_{ij}^G(\Delta) &= \inf_{G \in \mathcal{G}(\Delta, j)} \frac{p_i(G)}{p_j(G)}; \\ \phi_{ij}^T(\Delta) &= \inf_{T \in \mathcal{T}(\Delta, j)} \frac{p_i(T)}{p_j(T)}; \\ \Phi_{ij}^G(\Delta) &= \sup_{G \in \mathcal{G}(\Delta, j)} \frac{p_i(G)}{p_j(G)}; \\ \Phi_{ij}^T(\Delta) &= \sup_{T \in \mathcal{T}(\Delta, j)} \frac{p_i(T)}{p_j(T)}. \end{aligned}$$

for all $i, j \in N, i > j$.

Remark 1.1. Removing the requirement of connectivity in the definition of $\mathcal{G}(\Delta, j)$, then $\phi_{ij}^G(\Delta) = 0$, since

$$\lim_{x \rightarrow \infty} \frac{p_i(G + x \cdot P_{j+1})}{p_j(G + x \cdot P_{j+1})} = \lim_{x \rightarrow \infty} \frac{p_i(G)}{p_j(G) + x} = 0.$$

for all $G \in \mathcal{G}(\Delta, j)$ where $G + x \cdot P_{j+1}$ is the disjoint union of G and x paths of length j . On the other hand if G is a graph with connected components G_1, \dots, G_k we have

$$\begin{aligned} \frac{p_i(G)}{p_j(G)} &\leq \max \left\{ \frac{p_i(G_1)}{p_j(G_1)}, \dots, \frac{p_i(G_k)}{p_j(G_k)} \right\} \leq \max \{ \Phi_{ij}^G(1), \Phi_{ij}^G(2), \dots, \Phi_{ij}^G(\Delta) \} \\ &= \{ \text{see remark 2.14} \} \leq \Phi_{ij}^G(\Delta) \end{aligned}$$

hence Φ_{ij}^G does not change whether we require connectivity or not. Therefore, we can restrict ourselves to connected graphs. From now on, we use the term graph to imply simple connected graph.

Finding an extremal value of, not a single invariant, but an arithmetic operation on two invariants is not a new concept. It is the concept at the core of AutoGraphX software [1]. Here, we choose paths. They are well known mathematical objects. But, they are also important descriptors in chemistry, especially paths of length two and three. Their numbers are closely related to the Zagreb indices M_1 and M_2 which are very well known in chemistry (see [3, 6, 8] and references within), defined by:

$$\begin{aligned} M_1(G) &= \sum_{v \in V(G)} d_G(v)^2; \\ M_2(G) &= \sum_{uv \in E(G)} d_G(u) \cdot d_G(v); \end{aligned}$$

where $d_G(u)$ is the degree of a vertex u in the graph G , $V(G)$ is the set of vertices of G , and $E(G)$ is the set of edges of G . It can be shown that:

$$p_2(G) = \frac{1}{2}M_1(G) - e(G),$$

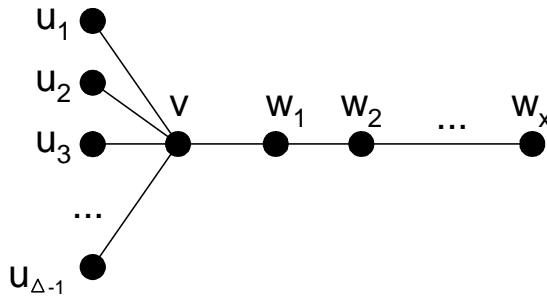
where $e(G)$ is the number of edges of graph G and that

$$p_3(G) = M_2(G) - M_1(G) + e(G)$$

for all triangle-free graphs. Comparisons of the Zagreb indices have been extensively studied [4, 9, 10, 11]. Besides this, path numbers are themselves interesting molecular descriptors. References about the use of path numbers in defining molecular descriptors and their applications in chemistry can be found in [7].

2 Results for the infimum

Denote by $G(\Delta, x)$ the graph presented in the following figure:



Let us prove:

Proposition 2.1. *It holds that $\phi_{ij}^G(\Delta) = 0$ and $\phi_{ij}^T(\Delta) = 0$ for all $j < i, i \geq 3$ and $\Delta \in N \setminus \{1\}$.*

Proof. Just note that $p_i(G(\Delta, j - 1)) = 0$ and that $p_j(G(\Delta, j - 1)) > 0$. □

Proposition 2.2. *It holds that*

$$\phi_{21}^G(2) = \phi_{21}^T(2) = \frac{1}{2} \text{ and } \phi_{21}^G(\Delta) = \phi_{21}^T(\Delta) = 1$$

for all $\Delta \in N \setminus \{1, 2\}$.

Proof. The only graphs with $\Delta = 2$ are the path P_n on n vertices and the cycle C_n on n vertices, where $n \geq 3$. It holds that:

$$\frac{p_2(C_n)}{p_1(C_n)} = \frac{n}{n} = 1,$$

and

$$\frac{p_2(P_n)}{p_1(P_n)} = \frac{n - 2}{n - 1},$$

hence

$$\phi_{21}^G(2) = \phi_{21}^T(2) = \inf_{n \geq 3} \frac{n - 2}{n - 1} = \frac{1}{2}.$$

Note that

$$\frac{p_2(G(\Delta, x))}{p_1(G(\Delta, x))} = \frac{\binom{\Delta}{2} + (x-1) \cdot \binom{2}{2}}{\Delta - 1 + x},$$

hence

$$\phi_{21}^G(\Delta) \leq \phi_{21}^T(\Delta) \leq \lim_{x \rightarrow \infty} \frac{\binom{\Delta}{2} + (x-1) \cdot \binom{2}{2}}{\Delta - 1 + x} = 1.$$

In order to prove that

$$\phi_{21}^T(\Delta) \geq \phi_{21}^G(\Delta) \geq 1,$$

for every $\Delta \geq 3$, it is sufficient to show that

$$p_2(G) - p_1(G) \geq 0 \text{ for each } G \text{ with } \Delta \geq 3$$

Denote by n_i the number of vertices of degree i in graph G with maximum degree at least 3, and by $v(G)$ the (total) number of its vertices. We have

$$\begin{aligned} e(G) &\geq v(G) - 1 \\ \frac{\sum_{i=1}^{\Delta} i \cdot n_i}{2} &\geq \sum_{i=1}^{\Delta} n_i - 1 \\ n_1 &\leq \sum_{i=3}^{\Delta} (i-2) n_i + 2 \\ n_1 &\leq \sum_{i=3}^{\Delta} i \cdot n_i \end{aligned}$$

hence

$$\begin{aligned} p_2(G) - p_1(G) &= \sum_{i=1}^{\Delta} \binom{i}{2} n_i - \frac{\sum_{i=1}^{\Delta} i \cdot n_i}{2} = \frac{1}{2} \sum_{i=1}^{\Delta} (i^2 - 2i) n_i = \\ &= \frac{1}{2} \left[\sum_{i=3}^{\Delta} (i^2 - 2i) n_i - n_1 \right] \geq \frac{1}{2} \left[\sum_{i=3}^{\Delta} (i^2 - 2i) n_i - \sum_{i=3}^{\Delta} i \cdot n_i \right] = \\ &= \frac{1}{2} \sum_{i=1}^{\Delta} (i^2 - 3i) n_i \geq 0. \end{aligned}$$

□

Let P be any path. We say that P' is an end-subpath of P if it is a subpath of P and if it contains an end-vertex of P .

Proposition 2.3. *Let $\Delta \geq 2$ and $i > j$. Then,*

$$\Phi_{ij}^G(\Delta) = (\Delta - 1)^{i-j}.$$

Proof. Let G be any graph. Note that each path of length i contains two paths of length j as end-subpaths. On the other hand any path of length j can be end-subpath of at most

$2 \cdot (\Delta - 1)^{i-j}$ paths of length i , because we have 2 choices for the direction of the extension and at most $\Delta - 1$ choices for adding each subsequent vertex. Therefore,

$$p_j(G) \leq \frac{2 \cdot (\Delta - 1)^{i-j}}{2} \leq (\Delta - 1)^{i-j},$$

hence

$$\Phi_{ij}^G(\Delta) \leq (\Delta - 1)^{i-j}.$$

Now, let G be a Δ -uniform graph (i.e. a graph in which all vertices have degree Δ) without a cycle of length less than $\Delta + 1$. The existence of such graph follows from the results of paper [5]. Then

$$\frac{p_i(G)}{p_j(G)} = \frac{\frac{1}{2} \cdot v(G) \cdot \Delta \cdot (\Delta - 1)^{i-1}}{\frac{1}{2} \cdot v(G) \cdot \Delta \cdot (\Delta - 1)^{j-1}} = (\Delta - 1)^{i-j}.$$

This proves the Theorem. □

Determining the functions Φ_{ij}^T is a much harder problem. Here, we restrict ourselves to the cases $i, j \leq 3$, i.e. to analyses of the functions Φ_{21}^T, Φ_{31}^T and Φ_{32}^T . First, let us determine Φ_{21}^T :

Proposition 2.4. *Let $\Delta \geq 2$. Then*

$$\Phi_{21}^T(\Delta) = \frac{\Delta}{2}.$$

Proof. Let T be any tree and n_i number of the vertices of degree $i, i = 1, \dots, \Delta$. It holds that:

$$\frac{p_2(T)}{p_1(T)} = \frac{\sum_{i=1}^{\Delta} \binom{i}{2} n_i}{\frac{1}{2} \sum_{i=1}^{\Delta} i \cdot n_i} = \frac{\sum_{i=1}^{\Delta} (i^2 - i) n_i}{\sum_{i=1}^{\Delta} i \cdot n_i} = (*).$$

From $e(T) = v(T) - 1$, it follows that

$$\begin{aligned} \frac{\sum_{i=1}^{\Delta} i \cdot n_i}{2} &= \sum_{i=1}^{\Delta} n_i - 1 \\ n_1 - 2 &= \sum_{i=3}^{\Delta} (i - 2) n_i. \end{aligned}$$

Hence

$$\begin{aligned} (*) &= \frac{n_1 \cdot (1^2 - 1) + n_2 \cdot (2^2 - 2) + \sum_{i=3}^{\Delta} (i^2 - i) n_i}{2 \cdot 1 + (n_1 - 2) \cdot 1 + n_2 \cdot 2 + \sum_{i=3}^{\Delta} i \cdot n_i} \\ &= \frac{0 + 2n_2 + \sum_{i=3}^{\Delta} (i^2 - i) n_i}{2 + 2n_2 + \sum_{i=3}^{\Delta} (2i - 2) \cdot n_i} \\ &\leq \max \left\{ \left\{ \frac{0}{2}, \frac{2}{2} \right\} \cup \left\{ \frac{i^2 - i}{2i - 2} : i = 3, \dots, \Delta \right\} \right\} = \frac{\Delta}{2}. \end{aligned}$$

Therefore $\Phi_{21}^T(\Delta) \leq \frac{\Delta}{2}$. Let $T(\Delta, k)$ be a tree with the distinguished vertex v such that all vertices have degree either Δ or 1, and all leaves are at distance k from the root. Then

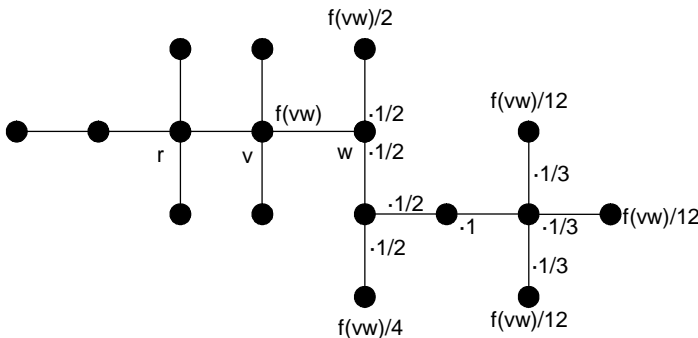
$$\begin{aligned} \lim_{k \rightarrow \infty} \frac{p_2(T(\Delta, k))}{p_1(T(\Delta, k))} &= \lim_{k \rightarrow \infty} \frac{\left(1 + \Delta \cdot \sum_{i=0}^{k-2} (\Delta - 1)^i\right) \cdot \left(\frac{\Delta}{2}\right)}{\left[\left(1 + \Delta \cdot \sum_{i=0}^{k-2} (\Delta - 1)^i\right) \cdot \Delta + \Delta \cdot (\Delta - 1)^{k-1}\right] / 2} \\ &= \lim_{k \rightarrow \infty} \frac{\Delta \cdot \frac{(\Delta - 1)^{k-1} - 1}{\Delta - 2} \cdot \Delta \cdot (\Delta - 1)}{\Delta \cdot \frac{(\Delta - 1)^{k-1} - 1}{\Delta - 2} \cdot \Delta + \Delta \cdot (\Delta - 1)^{k-1}} = \\ &= \lim_{k \rightarrow \infty} \frac{\Delta \cdot (\Delta - 1)^{k-1} \cdot \Delta \cdot (\Delta - 1)}{\Delta \cdot (\Delta - 1)^{k-1} \cdot \Delta + \Delta \cdot (\Delta - 1)^{k-1} \cdot (\Delta - 2)} = \\ &= \frac{\Delta \cdot (\Delta - 1)}{\Delta + (\Delta - 2)} = \frac{\Delta^2 - \Delta}{2\Delta - 2} = \frac{\Delta}{2}. \end{aligned}$$

Hence, $\Phi_{21}^T(\Delta) \geq \frac{\Delta}{2}$. □

Now, we shall need the concept of "pushed to leaves" function. Let T be a rooted tree with root r and let $\rho : E(T) \rightarrow R$ be any function. The "pushed to leaves" function $\rho^r : L(T) \rightarrow R$ ($L(T)$ from the set of leaves to the set of real numbers) is defined by pushing the weight of the edges to the leaves in the following way: Let l be any leaf and $rv_1 \dots v_k l$ a path from r to l . Then

$$\begin{aligned} \rho^r(l) &= \frac{\rho(rv_1)}{(d(v_1) - 1)(d(v_2) - 1) \dots (d(v_k) - 1)} + \frac{\rho(v_1 v_2)}{(d(v_2) - 1) \dots (d(v_k) - 1)} + \\ &\quad + \dots + \frac{\rho(v_{k-1} v_k)}{d(v_k) - 1} + \rho(v_k l). \end{aligned}$$

An example of how the weight of a single edge is pushed to the leaves is presented in the following figure:



It can easily be seen that $\sum_{uv \in E(T)} \rho(uv) = \sum_{v \in L(T)} \rho^r(v)$. Now, let us prove:

Proposition 2.5. *Let $\Delta \geq 2$. Then*

$$\Phi_{31}^T(\Delta) = \Delta - 1.$$

Proof. First, let us prove that $\Phi_{31}^T(\Delta) = \Delta - 1$. Let T be any tree. Note that the number of paths of length 3 having a middle edge uv is $(d(u) - 1) \cdot (d(v) - 1)$. Hence

$$p_3(T) = \sum_{uv \in E(T)} (d(u) - 1) \cdot (d(v) - 1);$$

$$p_1(T) = \sum_{uv \in E(T)} 1$$

Choose any vertex $r \in V(T) \setminus L(T)$. Since p_3 and p_2 are expressed as the sum of the contributions of edge-weights, the functions p_1^r and p_2^r can be defined and we have:

$$\frac{p_3(T)}{p_1(T)} = \frac{p_3^r(T)}{p_1^r(T)} = \frac{\sum_{v \in L(T)} p_3^r(v)}{\sum_{v \in L(T)} p_1^r(v)} \leq \max_{v \in L(T)} \frac{p_3^r(v)}{p_1^r(v)}$$

Let $vv_1v_2 \dots v_{k-1}v_k$ ($v_k = r$) be a path from v to r and denote $d_i = d(v_i)$. We have:

$$\begin{aligned} \max_{v \in L(T)} \frac{p_3^r(v)}{p_2^r(v)} &= \\ &= \frac{\left[(1-1) \cdot (d_1-1) + \frac{(d_1-1) \cdot (d_2-1)}{d_1-1} + \frac{(d_2-1) \cdot (d_3-1)}{(d_1-1) \cdot (d_2-1)} + \right. \\ &\quad \left. + \dots + \frac{(d_{k-1}-1) \cdot (d_k-1)}{(d_1-1) \cdot (d_2-1) \cdot \dots \cdot (d_{k-2}-1) \cdot (d_{k-1}-1)} \right]}{\left[1 + \frac{1}{d_1-1} + \frac{1}{(d_1-1) \cdot (d_2-1)} + \right. \\ &\quad \left. + \dots + \frac{1}{(d_1-1) \cdot (d_2-1) \cdot \dots \cdot (d_{k-2}-1)} + \frac{1}{(d_1-1) \cdot (d_2-1) \cdot \dots \cdot (d_{k-2}-1) \cdot (d_{k-1}-1)} \right]} \\ &\leq \frac{(d_2-1) + \frac{d_3-1}{(d_1-1)} + \dots + \frac{d_k-1}{(d_1-1) \cdot (d_2-1) \cdot \dots \cdot (d_{k-2}-1)}}{\left[1 + \frac{1}{d_1-1} + \frac{1}{(d_1-1) \cdot (d_2-1)} + \right. \\ &\quad \left. + \dots + \frac{1}{(d_1-1) \cdot (d_2-1) \cdot \dots \cdot (d_{k-2}-1)} + \frac{1}{(d_1-1) \cdot (d_2-1) \cdot \dots \cdot (d_{k-2}-1) \cdot (d_{k-1}-1)} \right]} \\ &\leq \frac{\Delta - 1 + \frac{\Delta-1}{(d_1-1)} + \dots + \frac{\Delta-1}{(d_1-1) \cdot (d_2-1) \cdot \dots \cdot (d_{k-2}-1)}}{\left[1 + \frac{1}{d_1-1} + \frac{1}{(d_1-1) \cdot (d_2-1)} + \right. \\ &\quad \left. + \dots + \frac{1}{(d_1-1) \cdot (d_2-1) \cdot \dots \cdot (d_{k-2}-1)} + \frac{1}{(d_1-1) \cdot (d_2-1) \cdot \dots \cdot (d_{k-2}-1) \cdot (d_{k-1}-1)} \right]} \\ &\leq \Delta - 1. \end{aligned}$$

Hence, $\Phi_{31}^T(\Delta) \leq \Delta - 1$. Let $T(\Delta, k)$ be defined as above. We have:

$$\begin{aligned} \lim_{k \rightarrow \infty} \frac{p_3(T(\Delta, k))}{p_1(T(\Delta, k))} &= \\ &= \lim_{k \rightarrow \infty} \frac{\left(\Delta \cdot \sum_{i=0}^{k-2} (\Delta - 1)^i \right) \cdot (\Delta - 1)^2 + \left(\Delta \cdot (\Delta - 1)^{k-1} \right) \cdot (\Delta - 1) \cdot (1 - 1)}{\left(\Delta \cdot \sum_{i=0}^{k-1} (\Delta - 1)^i \right)} \\ &= \lim_{k \rightarrow \infty} \frac{\Delta \cdot \frac{(\Delta-1)^{k-1}-1}{\Delta-1-1} \cdot (\Delta - 1)^2}{\Delta \cdot \frac{(\Delta-1)^k-1}{\Delta-1-1}} = \lim_{k \rightarrow \infty} \frac{(\Delta - 1)^{k-1} \cdot (\Delta - 1)^2}{(\Delta - 1)^k} = \Delta - 1 \end{aligned}$$

Hence, $\Phi_{31}^T(\Delta) \geq \Delta - 1$. □

Determining of Φ_{32}^T is much more complex problem. Let us start with the simplest case:

Proposition 2.6. $\Phi_{32}^T(2) = 1$.

Proof. The tree with maximum degree 2 is a path. Denote by P_n the path on n vertices. It holds that $\frac{p_3(P_n)}{p_2(P_n)} = \frac{n-3}{n-2}$ and therefore

$$\sup_{T \in \mathcal{T}(2,2)} \frac{p_3(T)}{p_2(T)} = \sup_{n \geq 3} \frac{n-3}{n-2} = 1.$$

□

Denote

$$f(x_1, x_2, \dots, x_k) = \frac{\frac{x_1 x_2}{x_1} + \frac{x_2 x_3}{x_1 x_2} + \dots + \frac{x_{k-1} x_k}{x_1 \dots x_{k-1}}}{x_1 + \frac{x_1 + x_2}{x_1} + \frac{x_2 + x_3}{x_1 x_2} + \dots + \frac{x_{k-1} + x_k}{x_1 \dots x_{k-1}}}.$$

Note that $f(x_1, x_2, \dots, x_k) \leq m/2$ for all x_1, x_2, \dots, x_m . Hence, it can be defined:

$$\Gamma(m) = \sup_{k \in \mathbb{N}, x_1, \dots, x_{k-1} \in \{1, \dots, m\}} f(x_1, x_2, \dots, x_{k-1}, m).$$

Note that $k = 1$ on the right hand-side implies that we observe $f(m)$. Now, we shall prove several auxiliary lemmas:

Lemma 2.7. $\Phi_{32}(\Delta) = 2 \cdot \Gamma(\Delta - 1)$ for all $\Delta > 2$.

Proof. Recall that the number of paths of length 3 with a middle edge uv is $(d(u) - 1) \cdot (d(v) - 1)$ and that the number of paths of length 2 with middle vertex v is $\binom{d(v)}{2}$. Hence

$$\begin{aligned} p_3(T) &= \sum_{uv \in E(T)} (d(u) - 1) \cdot (d(v) - 1); \\ p_2(T) &= \sum_{v \in V(T)} \binom{d(v)}{2} = \frac{1}{2} \sum_{v \in V(T)} d(v) \cdot (d(v) - 1) = \\ &= \frac{1}{2} \sum_{v \in V(T)} \sum_{u \in V(T): uv \in E(T)} (d(v) - 1) = \frac{1}{2} \sum_{uv \in E(T)} [(d(u) - 1) + (d(v) - 1)]. \end{aligned}$$

Choose any vertex $r \in V(T)$ of degree Δ . Since p_3 and p_2 are expressed as the sum of the contributions of edge-weights, functions p_3^r and p_2^r can be defined and we have:

$$\frac{p_3(T)}{p_2(T)} = \frac{p_3^r(T)}{p_2^r(T)} = \frac{\sum_{v \in L(T)} p_3^r(v)}{\sum_{v \in L(T)} p_2^r(v)}.$$

First, let us prove that

$$\Phi_{32}(\Delta) \leq 2 \cdot \Gamma(\Delta - 1).$$

It is sufficient to prove that for each $T \in \mathcal{T}(\Delta, 2)$ it holds that:

$$\frac{p_3(T)}{p_2(T)} = \frac{\sum_{v \in L(T)} p_3^r(v)}{\sum_{v \in L(T)} p_2^r(v)} \leq 2 \cdot \sup_{k \in \mathbb{N}, x_1, \dots, x_{k-1} \in \{1, \dots, \Delta-1\}} f(x_1, x_2, \dots, x_{k-1}, \Delta - 1).$$

Note that

$$\frac{\sum_{v \in L(T)} p_3^r(v)}{\sum_{v \in L(T)} p_2^r(v)} \leq \max_{l \in L(T)} \frac{p_3^r(l)}{p_2^r(l)}.$$

Denote by l the leaf for which the observed ratio obtains its maximum and let $lv_1v_2 \dots v_q$ ($v_q = r$) be a path from l to r . Denote $d_i = d(v_i)$. We have:

$$\begin{aligned} \max_{v \in L(T)} \frac{p_3^p(v)}{p_2^p(v)} &= \\ &= \frac{\left[\begin{aligned} &(1-1) \cdot (d_1-1) + \frac{(d_2-1)(d_1-1)}{(d_1-1)} + \\ &+ \frac{(d_3-1)(d_2-1)}{(d_1-1)(d_2-1)} + \dots + \frac{(d_{q-1}-1)(d_q-1)}{(d_1-1)(d_2-1) \cdot (d_{q-1}-1)} \end{aligned} \right]}{\frac{1}{2} \left[\begin{aligned} &(1-1) + (d_1-1) + \frac{(d_2-1)+(d_1-1)}{(d_1-1)} + \\ &+ \frac{(d_3-1)+(d_2-1)}{(d_1-1)(d_2-1)} + \dots + \frac{(d_{q-1}-1)+(d_q-1)}{(d_1-1)(d_2-1) \cdot (d_{q-1}-1)} \end{aligned} \right]} \\ &= 2 \cdot f(d_1-1, d_2-1, \dots, d_q-1) \\ &\leq 2 \cdot \sup_{k \in \mathbb{N}, x_1, \dots, x_{k-1} \in \{1, \dots, \Delta-1\}} f(x_1, x_2, \dots, x_{k-1}, \Delta-1) = 2 \cdot \Gamma(\Delta-1). \end{aligned}$$

Now, let us prove that

$$\Phi(\Delta) \geq 2 \cdot \Gamma(\Delta-1).$$

It is sufficient to prove that

$$\Phi(\Delta) \geq 2 \cdot f(x_1, x_2, \dots, x_{k-1}, \Delta-1)$$

for each (x_1, \dots, x_{k-1}) where $x_i \in \{1, \dots, \Delta-1\}, i = 1, \dots, k$. Set $x_k = \Delta-1$. Denote by $T(x_1, \dots, x_k)$ a tree such that the following hold:

1) There is a distinguished vertex $r \in V(T(x_1, \dots, x_k))$ of degree $x_k + 1$ such that all leaves are at distance k from r

2) Let $lv_1 \dots v_{k-1}r$ be a path from any leaf l to v . Then, $d(v_i) = x_i + 1$ for every vertex v_i .

We have:

$$\Phi(\Delta) \geq \frac{p_3(T(x_1, \dots, x_k))}{p_2(T(x_1, \dots, x_k))} = \frac{\sum_{v \in L(T(x_1, \dots, x_k))} p_3^r(v)}{\sum_{v \in L(T(x_1, \dots, x_k))} p_2^r(v)} = 2 \cdot f(x_1, \dots, x_k).$$

□

Lemma 2.8. Let $m \geq 2$, then

$$\Gamma(m) \leq \frac{m^{3/2}}{m+1}$$

Proof. For each $k \in N$, each $x_1, \dots, x_{k-1} \in \{1, \dots, m\}$, $x_k = m$, and each $\lambda \in [0, 1]$, we have

$$\begin{aligned} & \frac{\frac{x_1 x_2}{x_1} + \frac{x_2 x_3}{x_1 x_2} + \dots + \frac{x_{k-1} x_k}{x_1 \dots x_{k-1}}}{x_1 + \frac{x_1 + x_2}{x_1} + \frac{x_2 + x_3}{x_1 x_2} + \dots + \frac{x_{k-1} + x_k}{x_1 \dots x_{k-1}}} = \\ & = \frac{\frac{x_1 x_2}{x_1} + \frac{x_2 x_3}{x_1 x_2} + \dots + \frac{x_{k-1} x_k}{x_1 \dots x_{k-1}}}{(1 - \lambda) x_1 + \frac{\lambda x_1^2 + x_1 + (1 - \lambda) x_2}{x_1} + \frac{\lambda x_2^2 + x_2 + (1 - \lambda) x_3}{x_1 x_2} + \dots + \frac{\lambda x_{k-1}^2 + x_{k-1} + x_k}{x_1 \dots x_{k-1}}} \\ & = \frac{\left[\frac{\lambda x_1^2 + x_1 + (1 - \lambda) x_2}{x_1} \cdot \frac{x_1 x_2}{\lambda x_1^2 + x_1 + (1 - \lambda) x_2} + \right. \\ & \quad \left. + \frac{\lambda x_2^2 + x_2 + (1 - \lambda) x_3}{x_1 x_2} \cdot \frac{x_2 x_3}{\lambda x_2^2 + x_2 + (1 - \lambda) x_3} + \dots + \right. \\ & \quad \left. \frac{\lambda x_{k-1}^2 + x_{k-1} + x_k}{x_1 \dots x_{k-1}} \cdot \frac{x_{k-1} x_k}{\lambda x_{k-1}^2 + x_{k-1} + x_k} \right]}{(1 - \lambda) x_1 + \frac{\lambda x_1^2 + x_1 + (1 - \lambda) x_2}{x_1} + \frac{\lambda x_2^2 + x_2 + (1 - \lambda) x_3}{x_1 x_2} + \dots + \frac{\lambda x_{k-1}^2 + x_{k-1} + x_k}{x_1 \dots x_{k-1}}} = (*) \end{aligned}$$

Let

$$S = \inf_{\lambda \in [0, 1]} \max_{a, b \in \{1, \dots, m\}} \frac{ab}{a + \lambda a^2 + (1 - \lambda) b}$$

We have

$$(*) \leq \frac{\left[\frac{x_1 + x_2 + \lambda x_2^2}{x_2 x_3 \dots x_k} \cdot S + \frac{(1 - \lambda) x_2 + x_3 + \lambda x_3^2}{x_3 \dots x_k} \cdot S + \dots + \frac{(1 - \lambda) x_{k-1} + x_k + \lambda x_k^2}{x_k} \cdot S \right]}{\left[\frac{x_1 + x_2 + \lambda x_2^2}{x_2 x_3 \dots x_k} + \frac{(1 - \lambda) x_2 + x_3 + \lambda x_3^2}{x_3 \dots x_k} + \dots + \frac{(1 - \lambda) x_{k-1} + x_k + \lambda x_k^2}{x_k} \right]} \leq S$$

Let us calculate the upper bound of $\max_{a, b \in \{1, \dots, m\}} \frac{ab}{a + \lambda a^2 + (1 - \lambda) b}$. We have

$$\begin{aligned} & \max_{a, b \in \{1, \dots, m\}} \frac{ab}{a + \lambda a^2 + (1 - \lambda) b} = \\ & = \max_{a, b \in \{1, \dots, m\}} \frac{ab}{a^2 \cdot \left(\lambda + \frac{1}{a} \right) + (1 - \lambda) b} \\ & \leq \max_{a, b \in \{1, \dots, m\}} \frac{ab}{2 \cdot \sqrt{\left(\lambda + \frac{1}{a} \right) a^2 \cdot b (1 - \lambda)}} \\ & = \max_{a, b \in \{1, \dots, m\}} \frac{\sqrt{b}}{2 \cdot \sqrt{(1 - \lambda) \left(\lambda + \frac{1}{a} \right)}} \\ & \leq \{ \text{increasing in } a \text{ and } b \} \leq \frac{\sqrt{m}}{2 \cdot \sqrt{(1 - \lambda) \left(\lambda + \frac{1}{m} \right)}} \end{aligned}$$

Using simple analytical calculation to maximize $(1 - \lambda) \left(\lambda + \frac{1}{m} \right)$ for $\lambda \in [0, 1]$, we obtain

$$S = \inf_{\lambda \in [0, 1]} \frac{\sqrt{m}}{2 \cdot \sqrt{(1 - \lambda) \left(\lambda + \frac{1}{m} \right)}} = \frac{m^{3/2}}{1 + m}.$$

which proves the claim. □

Denote

$$\begin{aligned}
 X(m) &= \{(x_1, m, m) : x_1 \in \{1, \dots, m\}\} \cup \\
 &\cup \left\{ (x_1, x_2, m) : x_1 \in \left\{ 1, \dots, \left\lfloor \frac{m^{3/2}}{m+1} \right\rfloor \right\}, x_2 \in \{1, \dots, m\} \right\} \cup \\
 &\cup \left\{ (x_1, x_2, x_3) : x_1, x_2 \in \left\{ 1, \dots, \left\lfloor \frac{m^{3/2}}{m+1} \right\rfloor \right\}, x_3 \in \{1, \dots, m\} \right\} \\
 g_m(x_1, x_2, x_3) &= \frac{\frac{x_1 x_2}{x_1} + \frac{x_2 x_3}{x_1 x_2} + \frac{x_3 m}{x_1 x_2 x_3} + \frac{1}{x_1 x_2 x_3} \cdot \frac{m^2}{m-1}}{x_1 + \frac{x_1+x_2}{x_1} + \frac{x_2+x_3}{x_1 x_2} + \frac{x_3+m}{x_1 x_2 x_3} + \frac{1}{x_1 x_2 x_3} \cdot \frac{2m}{m-1}}
 \end{aligned}$$

and

$$\Psi(m) = \max_{(x_1, x_2, x_3) \in X(m)} g_m(x_1, x_2, x_3)$$

Let us prove:

Lemma 2.9. *Let $m \geq 2$, then*

$$\frac{m}{m+1} \leq \Psi(m) \leq \frac{m^{3/2}}{m+1} \leq \frac{m}{2}.$$

Proof. First, let us prove that $\Gamma(m) \geq \frac{m}{m+1}$. It is sufficient to prove that

$$g(1, m, m) \geq \frac{m}{m+1},$$

i.e. that

$$\begin{aligned}
 \frac{2m+1 + \frac{1}{m-1}}{4+m + \frac{2}{m} + \frac{2}{m(m-1)}} &\geq \frac{m}{m+1} \\
 2m^2 + 3m + 1 + \frac{m+1}{m-1} &\geq m^2 + 4m + 2 + \frac{2}{m-1} \\
 m^2 &\geq m
 \end{aligned}$$

which is obviously true.

Simple calculation shows that

$$\frac{m^{3/2}}{m+1} \leq \frac{m}{2}.$$

Now, let us prove that $\Gamma(m) \leq \frac{m^{3/2}}{m+1}$. It is sufficient to prove that for each

$$(x_1, x_2, x_3) \in X,$$

it holds that:

$$g_m(x_1, x_2, x_3) \leq \frac{m^{3/2}}{m+1}.$$

Note that

$$\lim_{n \rightarrow \infty} f \left(x_1, x_2, x_3, \underbrace{m, \dots, m}_{n\text{-times}} \right) = g_m(x_1, x_2, x_3).$$

Hence,

$$g_m(x_1, x_2, x_3) \leq \Gamma(m) \leq \frac{m^{3/2}}{m+1}.$$

This proves the Lemma. □

Let us prove:

Lemma 2.10. *Let k and $m \geq 2$ be positive integers and r real number such that $\frac{m}{m+1} \leq r \leq \frac{m}{2}$, and $k \geq 2$. Then*

$$\begin{aligned} \max_{t_1, t_2, \dots, t_k \in \{1, \dots, m\}} & \frac{t_1 t_2 - r t_1 - r t_2}{t_1} + \frac{t_2 t_3 - r t_2 - r t_3}{t_1 t_2} + \dots + \frac{t_{k-1} t_k - r t_{k-1} - r t_k}{t_1 t_2 t_3 \dots t_{k-1}} \\ & \leq (m - 2r) \cdot \frac{1 - \frac{1}{m^k}}{1 - \frac{1}{m}}. \end{aligned}$$

Proof. We prove the claim by induction on k . First suppose that $k = 2$. It is sufficient to prove that

$$\frac{t_1 t_2 - r t_1 - r t_2}{t_1} \leq m - 2r$$

Note that $m - 2r \geq 0$. If $t_1 \leq r$ then $t_1 t_2 - r t_1 - r t_2$ is negative and the claim holds. If $t_1 > r$, the left hand-side is increasing in t_2 , hence

$$\frac{t_1 t_2 - r t_1 - r t_2}{t_1} \leq \frac{t_1 m - r t_1 - r m}{t_1} = m - r - \frac{r m}{t_1} \leq \{\text{increasing in } t_1\} \leq m - 2r.$$

Now, suppose that $k > 2$ and that claim holds for smaller values of k . We have:

$$\begin{aligned} & \frac{t_1 t_2 - r t_1 - r t_2}{t_1} + \frac{t_1 t_2 - r t_1 - r t_2}{t_1 t_2} + \frac{t_2 t_3 - r t_2 - r t_3}{t_1 t_2 t_3} + \dots + \frac{t_{k-1} t_k - r t_{k-1} - r t_k}{t_1 t_2 t_3 \dots t_{k-1}} \\ &= \frac{t_1 t_2 - r t_1 - r t_2}{t_1} + \\ & \quad \frac{1}{t_1} \cdot \left(\frac{t_2 t_3 - r t_2 - r t_3}{t_2} + \frac{t_3 t_4 - r t_3 - r t_4}{t_2 t_3} + \dots + \frac{t_{k-1} t_k - r t_{k-1} - r t_k}{t_2 t_3 \dots t_{k-1}} \right) \\ & \leq \{\text{by the inductive hypothesis}\} \\ &= \frac{t_1 t_2 - r t_1 - r t_2}{t_1} + \frac{1}{t_1} (m - 2r) \cdot \frac{1 - \frac{1}{m^{k-1}}}{1 - \frac{1}{m}} \end{aligned}$$

If $t_1 \leq r$ then

$$\begin{aligned} \frac{t_1 t_2 - r t_1 - r t_2}{t_1} + \frac{1}{t_1} (m - 2r) \cdot \frac{1 - \frac{1}{m^{k-1}}}{1 - \frac{1}{m}} & \leq \frac{1}{t_1} (m - 2r) \cdot \frac{1 - \frac{1}{m^{k-1}}}{1 - \frac{1}{m}} \\ & \leq (m - 2r) \cdot \frac{1 - \frac{1}{m^{k-1}}}{1 - \frac{1}{m}} \\ & \leq (m - 2r) \cdot \frac{1 - \frac{1}{m^k}}{1 - \frac{1}{m}}. \end{aligned}$$

Otherwise,

$$\begin{aligned} \frac{t_1 t_2 - r t_1 - r t_2}{t_1} + \frac{1}{t_1} (m - 2r) \cdot \frac{1 - \frac{1}{m^{k-1}}}{1 - \frac{1}{m}} &\leq \{\text{increasing in } t_2\} \\ &\leq \frac{m t_1 - r t_1 - r m}{t_1} + \frac{1}{t_1} (m - 2r) \cdot \frac{1 - \frac{1}{m^{k-1}}}{1 - \frac{1}{m}} \\ &= m - r + \frac{1}{t_1} \cdot \left[(m - 2r) \cdot \frac{1 - \frac{1}{m^{k-1}}}{1 - \frac{1}{m}} - r m \right] = (*) \end{aligned}$$

In order to prove that (*) is increasing in t_1 , we need to prove that

$$(m - 2r) \cdot \frac{1 - \frac{1}{m^{k-1}}}{1 - \frac{1}{m}} - r m \leq 0.$$

It is sufficient to prove that

$$\frac{m - 2r}{1 - \frac{1}{m}} \leq r m,$$

but this is equivalent to

$$\begin{aligned} m &\leq r m - r + 2r \\ r &\geq \frac{m}{m + 1} \end{aligned}$$

Therefore, (*) is increasing in t_1 , and

$$\begin{aligned} (*) &\leq m - r + \frac{1}{m} \cdot \left[(m - 2r) \cdot \frac{1 - \frac{1}{m^{k-1}}}{1 - \frac{1}{m}} - r m \right] \\ &= (m - 2r) \cdot \left(1 + \frac{1}{m} \cdot \frac{1 - \frac{1}{m^{k-1}}}{1 - \frac{1}{m}} \right) = (m - 2r) \cdot \frac{1 - \frac{1}{m^k}}{1 - \frac{1}{m}}, \end{aligned}$$

which proves the Lemma. □

Now, let us prove the key Lemma.

Lemma 2.11. *Let $m \geq 2$, then*

$$\Gamma(m) = \Psi(m).$$

Proof. Denote $r = \Psi(m)$ and denote $(y_1, y_2, y_3) \in X(m)$ such that $g_m(y_1, y_2, y_3) = r$. We have:

$$\begin{aligned} \Gamma(m) &= \sup_{k \in \mathbb{N}, x_1, \dots, x_k \in \{1, 2, \dots, m\}} f(x_1, \dots, x_k) \geq \lim_{k \rightarrow \infty} f \left(y_1, y_2, y_3, \underbrace{m, \dots, m}_{(k-3)\text{-times}} \right) \\ &= \lim_{k \rightarrow \infty} \frac{\frac{y_1 y_2}{y_1} + \frac{y_2 y_3}{y_1 y_2} + \frac{y_3 m}{y_1 y_2 y_3} + \frac{m^2}{y_1 y_2 y_3} \cdot \left(\frac{1}{m} + \frac{1}{m^2} + \dots + \frac{1}{m^{k-4}} \right)}{y_1 + \frac{y_1 + y_2}{y_1} + \frac{y_2 + y_3}{y_1 y_2} + \frac{y_3 + m}{y_1 y_2 y_3} + \frac{2m}{y_1 y_2 y_3} \cdot \left(\frac{1}{m} + \frac{1}{m^2} + \dots + \frac{1}{m^{k-4}} \right)} \\ &= g_m(y_1, y_2, y_3) = r \end{aligned}$$

Suppose to the contrary that

$$\sup_{k \in N, x_1, \dots, x_{k-1} \in \{1, 2, \dots, m\}} f(x_1, \dots, x_{k-1}, m) > r. \tag{2.1}$$

Denote by S_1 set of finite ordered sequences $(x_1, \dots, x_{k-1}, x_k)$ such that $x_k = m$ and

$$f(x_1, \dots, x_k) > r.$$

Note that this last relation can be rewritten as

$$h(x_1, \dots, x_k) = -rx_1 + \frac{x_1x_2 - rx_1 - rx_2}{x_1} + \frac{x_2x_3 - rx_2 - rx_3}{x_1x_2} + \dots + \frac{x_{k-1}x_k - rx_{k-1} - rx_k}{x_1 \dots x_{k-1}} > 0 \tag{2.2}$$

From (2.1), it follows that S_1 is a non-empty set. Let S_2 be the set of sequences in S_1 which have one of the following two properties:

- 1) There are no entries from $[r, m)$ and all m s are located at the end of the sequence;
- 2) There is a single entry from the set $[r, m)$; there is no m before this entry and all entries after this one are equal to m .

Let us prove that S_3 is non-empty. Let $(b_1, \dots, b_{k_2}) \in S_2$. Let i be the first entry greater or equal r (note that at least $b_{k_2} = m \geq r$). If $i = k_2$, then $(b_1, \dots, b_{k_2}) \in S_2$, hence

suppose that $i < k_2$. In order to prove that $\left(b_1, \dots, b_i, \underbrace{m, \dots, m}_{(k_2-i)\text{-times}} \right) \in S_2$, it is sufficient

to prove that

$$h\left(b_1, \dots, b_i, \underbrace{m, \dots, m}_{(k_2-i)\text{-times}} \right) \geq h(b_1, \dots, b_{k_2}) \geq 0,$$

i.e. that

$$h\left(b_1, \dots, b_i, \underbrace{m, \dots, m}_{(k_2-i)\text{-times}} \right) - h(b_1, \dots, b_{k_2}) \geq 0.$$

We have:

$$\begin{aligned} & \left(h\left(b_1, \dots, b_i, \underbrace{m, \dots, m}_{(k_2-i)\text{-times}} \right) - h(b_1, \dots, b_{k_2}) \right) \cdot b_1 b_2 \dots b_i = \\ & = (b_i m - r m - r b_i) + \frac{m \cdot m - 2rm}{m} + \frac{m \cdot m - 2rm}{m^2} + \dots + \frac{m \cdot m - 2rm}{m^{k_2-i-1}} \\ & \quad - (b_i b_{i+1} - r b_i - r b_{i+1}) - \frac{b_{i+1} b_{i+2} - r b_{i+1} - r b_{i+2}}{b_{i+1}} - \dots \\ & \quad - \frac{b_{k_2-1} b_{k_2} - r b_{k_2-1} - r b_{k_2}}{b_{i+1} \dots b_{k_2}} = \\ & = [(b_i - r) \cdot (m - b_{i+1})] \\ & \quad + \left[\left(\frac{m \cdot m - 2rm}{m} + \frac{m \cdot m - 2rm}{m^2} + \dots + \frac{m \cdot m - 2rm}{m^{k_2-i-1}} \right) - \right. \\ & \quad \left. \left(\frac{b_{i+1} b_{i+2} - r b_{i+1} - r b_{i+2}}{b_{i+1}} + \dots + \frac{b_{k_2-1} b_{k_2} - r b_{k_2-1} - r b_{k_2}}{b_{i+1} \dots b_{k_2}} \right) \right]. \end{aligned}$$

The first square bracket is non-negative because it is the product of two non-negative numbers. From Lemma 2.9 it follows that $\frac{m}{m+2} \leq r \leq \frac{m}{2}$ and then from Lemma 2.10, it follows that the second square bracket is non-negative, so S_2 is non-empty. Let $c = (c_1, \dots, c_{k_2})$ be an element of S_2 with the following properties:

- 1) c has the least number of entries smaller than r ;
- 2) Among all the elements of S_2 with the same number of entries smaller than r , c is the shortest sequence.

Note that all these entries are at the beginning of the sequence. Hence, assume that c_1, \dots, c_j are smaller than r and c_{j+1}, \dots, c_{k_3} are larger than r . Distinguish two cases:

CASE 1: $h(c_1, \dots, c_{k_3}) \geq h(c_1, c_2)$

SUBCASE 1.1: $j \geq 3$.

Because of the minimality of (c_1, \dots, c_{k_3}) , it follows that $(c_1, c_3, c_4, c_{k_3}) \notin S_3$, hence

$$\begin{aligned} h(c_1, \dots, c_{k_3}) &> 0 \\ h(c_1, c_3, c_4, \dots, c_{k_3}) &< 0 \end{aligned}$$

Therefore

$$h(c_1, \dots, c_{k_3}) > h(c_1, c_3, c_4, \dots, c_{k_3}).$$

We have:

$$\begin{aligned} h(c_1, \dots, c_{k_3}) &\leq h(c_1, \dots, c_{k_3}) + (c_2 - 1) \cdot (h(c_1, \dots, c_{k_3}) - h(c_1, c_2)) \\ &\leq -rc_1 + \frac{c_1c_2 - rc_1 - rc_2}{c_1} + \frac{c_2c_3 - rc_2 - rc_3}{c_1} + \frac{c_3c_4 - rc_3 - rc_4}{c_1c_3} + \dots \\ &\quad + \frac{c_{k_3-1}c_{k_3} - rc_{k_3-1} - rc_{k_3}}{c_1c_3 \dots c_{k_3-1}} \leq \\ &\leq h(c_1, c_3, c_4, \dots, c_{k_3}) + \frac{c_1c_2 - rc_1 - rc_2}{c_1} + \frac{c_2c_3 - rc_2 - rc_3}{c_1} - \frac{c_1c_3 - rc_1 - rc_3}{c_1} \\ &\leq h(c_1, c_3, c_4, \dots, c_{k_3}) + \frac{\overset{\leq 0}{(c_1 - r)c_2}}{c_1} + \frac{c_2 \cdot \overset{\leq 0}{(c_3 - r)}}{c_1} - \frac{c_1c_3}{c_1} \\ &\leq h(c_1, c_3, c_4, \dots, c_{k_3}), \end{aligned}$$

which is a contradiction.

SUBCASE 1.2: $j \leq 2$.

If $k_3 = 2$, then $c_2 = m$ and

$$\begin{aligned} 0 &< -rc_1 + \frac{c_1m - rc_1 - rm}{c_1} < \\ &< -rc_1 + \frac{c_1m - rc_1 - rm}{c_1} + \frac{m^2 - 2rm}{c_1m} + \frac{m^2 - 2rm}{c_1m^2}, \end{aligned}$$

hence $(c_1, m, m, m) \in S_1$. If $k_3 = 3$, then $c_3 = m$ and

$$\begin{aligned} 0 &< -rc_1 + \frac{c_1c_2 - rc_1 - rc_2}{c_1} + \frac{c_2m - rc_2 - rm}{c_1c_2} < \\ &< -rc_1 + \frac{c_1c_2 - rc_1 - rc_2}{c_1} + \frac{c_2m - rc_2 - rm}{c_1c_2} + \frac{m^2 - 2rm}{c_1c_2m}, \end{aligned}$$

hence $(c_1, c_2, m, m) \in S_1$. If $k_3 > 3$, then $c_3 \geq r$ and all entries after c_3 are equal to m .

Hence, in any case there is an element of S_1 of the form $c' = \left(z_1, z_2, z_3, \underbrace{m, \dots, m}_{t\text{-times}} \right)$,

where $t \geq 1$ and $(z_1, z_2, z_3) \in X$. Since, $c' \in S_1$, it follows that $f(c') > g(z_1, z_2, z_3)$, i.e.

$$\frac{\frac{x_1x_2}{x_1} + \frac{x_2x_3}{x_1x_2} + \frac{x_3m}{x_1x_2x_3} + \frac{1}{x_1x_2x_3} \cdot m^2 \cdot \frac{1-\frac{1}{m^t}}{m-1}}{x_1 + \frac{x_1+x_2}{x_1} + \frac{x_2+x_3}{x_1x_2} + \frac{x_3+m}{x_1x_2x_3} + \frac{1}{x_1x_2x_3} \cdot 2m \cdot \frac{1-\frac{1}{m^t}}{m-1}} > \frac{\frac{x_1x_2}{x_1} + \frac{x_2x_3}{x_1x_2} + \frac{x_3m}{x_1x_2x_3} + \frac{1}{x_1x_2x_3} \cdot m^2 \cdot \frac{1}{m-1}}{x_1 + \frac{x_1+x_2}{x_1} + \frac{x_2+x_3}{x_1x_2} + \frac{x_3+m}{x_1x_2x_3} + \frac{1}{x_1x_2x_3} \cdot 2m \cdot \frac{1}{m-1}} \quad (2.3)$$

Denote

$$\begin{aligned} \alpha_1 &= \frac{x_1x_2}{x_1} + \frac{x_2x_3}{x_1x_2} + \frac{x_3m}{x_1x_2x_3} \\ \beta_1 &= x_1 + \frac{x_1+x_2}{x_1} + \frac{x_2+x_3}{x_1x_2} + \frac{x_3+m}{x_1x_2x_3} \\ \gamma_1 &= \frac{1}{x_1x_2x_3} \cdot 2m \cdot \frac{1-\frac{1}{m^t}}{m-1} \\ \delta_1 &= \frac{1}{x_1x_2x_3} \cdot 2m \cdot \frac{1}{m-1} \end{aligned}$$

Inequality (2.3) can be rewritten as

$$\begin{aligned} \frac{\alpha_1 + \frac{m}{2}\gamma_1}{\beta_1 + \gamma_1} &> \frac{\alpha_1 + \frac{m}{2}\delta_1}{\beta_1 + \delta_1} \\ \alpha_1\delta_1 - \alpha_1\gamma_1 + \frac{m}{2}\gamma_1\beta_1 - \frac{m}{2}\beta_1\delta_1 &> 0 \\ \left(\alpha_1 - \frac{m}{2}\beta_1\right) (\delta_1 - \gamma_1) &> 0 \end{aligned}$$

Since $\delta_1 > \gamma_1$, it follows that $\alpha_1 - \frac{m}{2}\beta_1 > 0$, but

$$\begin{aligned} \alpha_1 - \frac{m}{2}\beta_1 &= \\ &= \frac{x_1x_2 - \frac{m}{2}x_1 - \frac{m}{2}x_2}{x_1} + \frac{x_2x_3 - \frac{m}{2}x_2 - \frac{m}{2}x_3}{x_1x_2} + \frac{x_3m - \frac{m}{2}x_3 - \frac{m}{2}m}{x_1x_2x_3} - \frac{m}{2}x_1 \\ &\leq \{\text{inequality between arithmetic and geometric mean}\} \leq \\ &\leq \frac{x_1x_2 - m\sqrt{x_1x_2}}{x_1} + \frac{x_2x_3 - m\sqrt{x_2x_3}}{x_1x_2} + \frac{x_3m - m\sqrt{x_3m}}{x_1x_2x_3} - \frac{m}{2}x_1 \leq \\ &\leq \{m \geq \sqrt{x_1x_2}, \sqrt{x_2x_3}, \sqrt{x_3m}\} \leq -\frac{m}{2}x_1 \leq 0, \end{aligned}$$

which is a contradiction.

CASE 2: $h(c_1, \dots, c_{k_3}) < h(c_1, c_2)$

In this case $h(c_1, c_2) > 0$, hence $f(c_1, c_2) > \Psi(m) \geq g_m(c_1, c_2, m)$, i. e.

$$\frac{\frac{c_1 c_2}{c_1}}{c_1 + \frac{c_1 + c_2}{c_1}} > \frac{\frac{c_1 c_2}{c_1} + \frac{c_2 m}{c_1 c_2} + \frac{m^2}{c_1 c_2 m} + \frac{1}{c_1 c_2 m} \cdot \frac{m^2}{m-1}}{c_1 + \frac{c_1 + c_2}{c_1} + \frac{c_2 + m}{c_1 c_2} + \frac{2m}{c_1 c_2 m} + \frac{1}{c_1 c_2 m} \cdot \frac{2m}{m-1}}$$

$$\frac{c_2}{c_1 + \frac{c_1 + c_2}{c_1}} > \frac{c_2 + \left(\frac{c_2 m}{c_1 c_2} + \frac{1}{c_1 c_2} \cdot \frac{m^2}{m-1}\right)}{\left(c_1 + \frac{c_1 + c_2}{c_1}\right) + \left(\frac{c_2 + m}{c_1 c_2} + \frac{1}{c_1 c_2} \cdot \frac{2m}{m-1}\right)}.$$

In order to obtain a contradiction, it is sufficient to prove that

$$\frac{\frac{c_2 m}{c_1 c_2} + \frac{1}{c_1 c_2} \cdot \frac{m^2}{m-1}}{\frac{c_2 + m}{c_1 c_2} + \frac{1}{c_1 c_2} \cdot \frac{2m}{m-1}} \geq \frac{c_2}{c_1 + \frac{c_1 + c_2}{c_1}}$$

$$\frac{c_2 m + \frac{m^2}{m-1}}{c_2 + m + \frac{2m}{m-1}} \geq \frac{c_1 c_2}{c_1^2 + c_1 + c_2}$$

Note that

$$\frac{c_1 c_2}{c_1^2 + c_1 + c_2} \leq \frac{c_1 \cdot \frac{m}{2} + c_2 \cdot \frac{m}{2}}{c_1^2 + c_1 + c_2} \leq \frac{m}{2} = \frac{\frac{m^2}{m-1}}{\frac{2m}{m-1}},$$

hence it is sufficient to prove that

$$\frac{c_2 m}{c_2 + m} \geq \frac{c_1 c_2}{c_1^2 + c_1 + c_2}.$$

This is equivalent to $c_1^2 c_2 m + c_2^2 m \geq c_1 c_2^2$, which obviously holds. Hence, a contradiction is obtained. □

From Lemmas 2.7 and 2.11, our main result follows:

Theorem 2.12. *Let $\Delta \geq 3$, then*

$$\Phi_{32}(\Delta) = 2 \cdot \Psi(\Delta - 1)$$

This Theorem is very useful, because the number $\Psi(\Delta - 1)$ can be determined in $\sim \Delta^2$ operations. The program for calculating the function Ψ is produced and Table 1 of values for $\Phi_{32}(\Delta)$ is obtained.

Remark 2.13. Note that X has $\sim \Delta^2$ elements. However, we can restrict our search for the maximum to only linear number of elements. Let $G_m : [1, m]^3 \rightarrow R$ be the function defined by

$$G_m(x_1, x_2, x_3) = \frac{\frac{x_1 x_2}{x_1} + \frac{x_2 x_3}{x_1 x_2} + \frac{x_3 m}{x_1 x_2 x_3} + \frac{1}{x_1 x_2 x_3} \cdot \frac{m^2}{m-1}}{x_1 + \frac{x_1 + x_2}{x_1} + \frac{x_2 + x_3}{x_1 x_2} + \frac{x_3 + m}{x_1 x_2 x_3} + \frac{1}{x_1 x_2 x_3} \cdot \frac{2m}{m-1}}$$

Let

$$h : [1, m] \rightarrow R$$

Δ	$\Phi_{32}(\Delta)$	Δ	$\Phi_{32}(\Delta)$	Δ	$\Phi_{32}(\Delta)$	Δ	$\Phi_{32}(\Delta)$	Δ	$\Phi_{32}(\Delta)$
1	Not def.	41	6.6904	81	9.3623	121	11.3872	161	13.0876
2	1.0000	42	6.7731	82	9.4180	122	11.4327	162	13.1281
3	1.5000	43	6.8571	83	9.4730	123	11.4779	163	13.1683
4	1.8750	44	6.9393	84	9.5273	124	11.5227	164	13.2083
5	2.1538	45	7.0195	85	9.5810	125	11.5671	165	13.2480
6	2.4074	46	7.0980	86	9.6339	126	11.6111	166	13.2875
7	2.6667	47	7.1747	87	9.6862	127	11.6547	167	13.3267
8	2.8913	48	7.2498	88	9.7379	128	11.6980	168	13.3657
9	3.0877	49	7.3232	89	9.7889	129	11.7410	169	13.4045
10	3.2609	50	7.3950	90	9.8442	130	11.7835	170	13.4430
11	3.4146	51	7.4653	91	9.9000	131	11.8258	171	13.4813
12	3.5794	52	7.5341	92	9.9552	132	11.8711	172	13.5193
13	3.7500	53	7.6015	93	10.0098	133	11.9167	173	13.5571
14	3.9080	54	7.6675	94	10.0638	134	11.9619	174	13.5947
15	4.0546	55	7.7321	95	10.1172	135	12.0068	175	13.6321
16	4.1912	56	7.8031	96	10.1701	136	12.0514	176	13.6692
17	4.3186	57	7.8750	97	10.2224	137	12.0957	177	13.7062
18	4.4378	58	7.9457	98	10.2741	138	12.1396	178	13.7429
19	4.5495	59	8.0151	99	10.3253	139	12.1832	179	13.7793
20	4.6730	60	8.0834	100	10.3760	140	12.2265	180	13.8156
21	4.8000	61	8.1505	101	10.4261	141	12.2695	181	13.8516
22	4.9211	62	8.2165	102	10.4757	142	12.3121	182	13.8900
23	5.0367	63	8.2813	103	10.5248	143	12.3545	183	13.9286
24	5.1472	64	8.3451	104	10.5734	144	12.3965	184	13.9669
25	5.2528	65	8.4079	105	10.6215	145	12.4383	185	14.0050
26	5.3540	66	8.4696	106	10.6691	146	12.4797	186	14.0430
27	5.4509	67	8.5304	107	10.7162	147	12.5209	187	14.0807
28	5.5439	68	8.5902	108	10.7629	148	12.5617	188	14.1182
29	5.6331	69	8.6490	109	10.8091	149	12.6023	189	14.1555
30	5.7322	70	8.7069	110	10.8589	150	12.6426	190	14.1927
31	5.8333	71	8.7639	111	10.9091	151	12.6825	191	14.2296
32	5.9313	72	8.8260	112	10.9588	152	12.7223	192	14.2663
33	6.0262	73	8.8889	113	11.0081	153	12.7617	193	14.3028
34	6.1182	74	8.9509	114	11.0570	154	12.8009	194	14.3392
35	6.2073	75	9.0120	115	11.1054	155	12.8397	195	14.3753
36	6.2939	76	9.0724	116	11.1534	156	12.8813	196	14.4112
37	6.3778	77	9.1319	117	11.2010	157	12.9231	197	14.4470
38	6.4594	78	9.1906	118	11.2481	158	12.9646	198	14.4826
39	6.5386	79	9.2486	119	11.2949	159	13.0058	199	14.5180
40	6.6156	80	9.3058	120	11.3412	160	13.0468	200	14.5532

Figure 1: Table of values for for $\Phi_{32}(\Delta)$.

be any function. Denote by $\text{MaxInt}(h)$ its maximum on the set $\{1, \dots, m\}$. Let us observe the following functions

$$\begin{aligned}
 &h_m : [1, m] \rightarrow R \text{ defined by } h_m(x_1) = G_m(x_1, m, m) \\
 &\quad \text{where } m \in N \setminus \{1\}; \\
 &h_{x_1, m} : [1, m] \rightarrow R \text{ defined by } h_{x_1, m}(x_2) = G_m(x_1, x_2, m) \\
 &\quad \text{where } m \in N \setminus \{1\}, x_1 \in N \text{ and } x_1 \leq m; \\
 &h_{x_1, x_2, m} : [1, m] \rightarrow R \text{ defined by } h_{x_1, x_2, m}(x_3) = G_m(x_1, x_2, x_2) \\
 &\quad \text{where } m \in N \setminus \{1\}, x_1, x_2 \in N \text{ and } x_1, x_2 \leq m.
 \end{aligned}$$

It can be easily seen that all of these functions are infinitely differentiable. Also, using Mathematica, it can be verified that they have at most two stationary points (null-points of the first derivation). Let $h : [1, m] \rightarrow R$ be an infinitely derivable function:

- 1) with no stationary points - then $\text{MaxInt}(h) = \max\{h(1), h(m)\}$;
 - 2) with one stationary point x - then $\text{MaxInt}(h) = \max\{h(1), h(m), h(\lfloor x \rfloor), h(\lceil x \rceil)\}$;
 - 3) with two stationary points x and y - then $\text{MaxInt}(h) = \max\{h(1), h(m), h(\lfloor x \rfloor), h(\lceil x \rceil), h(\lfloor y \rfloor), h(\lceil y \rceil)\}$.
- Hence, in order to determine the $\Psi(m)$ it is sufficient to check at most

$$6 \cdot \left(1 + \left\lfloor \frac{m^{3/2}}{m+1} \right\rfloor + \left\lfloor \frac{m^{3/2}}{m+1} \right\rfloor^2 \right)$$

values, which can be done in linear time.

Remark 2.14. In order to prove that the function Φ_{32} is increasing, it is sufficient to show that

$$\begin{aligned}
 &\frac{\frac{x_1 x_2}{x_1} + \frac{x_2 x_3}{x_1 x_2} + \frac{x_3 m}{x_1 x_2 x_3} + \frac{1}{x_1 x_2 x_3} \cdot \frac{m^2}{m-1}}{x_1 + \frac{x_1+x_2}{x_1} + \frac{x_2+x_3}{x_1 x_2} + \frac{x_3+m}{x_1 x_2 x_3} + \frac{1}{x_1 x_2 x_3} \cdot \frac{2m}{m-1}} \\
 &\leq \frac{\frac{x_1 x_2}{x_1} + \frac{x_2 x_3}{x_1 x_2} + \frac{x_3(m+1)}{x_1 x_2 x_3} + \frac{1}{x_1 x_2 x_3} \cdot \frac{(m+1)^2}{m}}{x_1 + \frac{x_1+x_2}{x_1} + \frac{x_2+x_3}{x_1 x_2} + \frac{x_3+m+1}{x_1 x_2 x_3} + \frac{1}{x_1 x_2 x_3} \cdot \frac{2(m+1)}{m}}
 \end{aligned}$$

for every $m \geq 3$ and x_1, x_2, x_3 which maximizes g_m . We need to prove that

$$\begin{aligned}
 &\frac{\frac{x_1 x_2}{x_1} + \frac{x_2 x_3}{x_1 x_2} + \frac{x_3 m}{x_1 x_2 x_3} + \frac{1}{x_1 x_2 x_3} \cdot \frac{m^2}{m-1}}{x_1 + \frac{x_1+x_2}{x_1} + \frac{x_2+x_3}{x_1 x_2} + \frac{x_3+m}{x_1 x_2 x_3} + \frac{1}{x_1 x_2 x_3} \cdot \frac{2m}{m-1}} \\
 &\leq \frac{\left(\frac{x_1 x_2}{x_1} + \frac{x_2 x_3}{x_1 x_2} + \frac{x_3 m}{x_1 x_2 x_3} + \frac{1}{x_1 x_2 x_3} \cdot \frac{m^2}{m-1} \right) +}{\left(x_1 + \frac{x_1+x_2}{x_1} + \frac{x_2+x_3}{x_1 x_2} + \frac{x_3+m}{x_1 x_2 x_3} + \frac{1}{x_1 x_2 x_3} \cdot \frac{2m}{m-1} \right) +} \\
 &\quad + \left(\frac{x_3}{x_1 x_2 x_3} + \frac{1}{x_1 x_2 x_3} \cdot \left(\frac{(m+1)^2}{m} - \frac{m^2}{m-1} \right) \right) \\
 &\quad + \left(\frac{1}{x_1 x_2 x_3} + \frac{1}{x_1 x_2 x_3} \cdot \left(\frac{2(m+1)}{m} - \frac{2m}{m-1} \right) \right)
 \end{aligned}$$

It is sufficient to show that

$$\frac{\frac{x_1 x_2}{x_1} + \frac{x_2 x_3}{x_1 x_2} + \frac{x_3 m}{x_1 x_2 x_3} + \frac{1}{x_1 x_2 x_3} \cdot \frac{m^2}{m-1}}{x_1 + \frac{x_1+x_2}{x_1} + \frac{x_2+x_3}{x_1 x_2} + \frac{x_3+m}{x_1 x_2 x_3} + \frac{1}{x_1 x_2 x_3} \cdot \frac{2m}{m-1}} \leq \frac{\frac{x_3}{x_1 x_2 x_3} + \frac{1}{x_1 x_2 x_3} \cdot \left(\frac{(m+1)^2}{m} - \frac{m^2}{m-1}\right)}{\frac{1}{x_1 x_2 x_3} + \frac{1}{x_1 x_2 x_3} \cdot \left(\frac{2(m+1)}{m} - \frac{2m}{m-1}\right)}$$

$$\frac{\frac{x_1 x_2}{x_1} + \frac{x_2 x_3}{x_1 x_2} + \frac{x_3 m}{x_1 x_2 x_3} + \frac{1}{x_1 x_2 x_3} \cdot \frac{m^2}{m-1}}{x_1 + \frac{x_1+x_2}{x_1} + \frac{x_2+x_3}{x_1 x_2} + \frac{x_3+m}{x_1 x_2 x_3} + \frac{1}{x_1 x_2 x_3} \cdot \frac{2m}{m-1}} \leq \frac{(m^2 - m) x_3 + m^2 - m - 1}{(m^2 - m) - 2}.$$

From the proof of the Lemma 2.11, it follows that

$$\frac{\frac{x_1 x_2}{x_1} + \frac{x_2 x_3}{x_1 x_2} + \frac{x_3 m}{x_1 x_2 x_3} + \frac{1}{x_1 x_2 x_3} \cdot \frac{m^2}{m-1}}{x_1 + \frac{x_1+x_2}{x_1} + \frac{x_2+x_3}{x_1 x_2} + \frac{x_3+m}{x_1 x_2 x_3} + \frac{1}{x_1 x_2 x_3} \cdot \frac{2m}{m-1}} \leq x_3$$

and the claim follows.

The behavior of this function on its boundary is described by the following theorem:

Theorem 2.15. *It holds that*

$$\lim_{\Delta \rightarrow \infty} \frac{\log \Phi_{32}(\Delta)}{\log \Delta} = \frac{1}{2}.$$

Proof. First, let us prove that $\lim_{\Delta \rightarrow \infty} \frac{\log \Phi_{32}(\Delta)}{\log \Delta} \leq \frac{1}{2}$. We have:

$$\begin{aligned} \lim_{\Delta \rightarrow \infty} \frac{\log \Phi_{32}(\Delta)}{\log \Delta} &= \lim_{\Delta \rightarrow \infty} \frac{\log(2 \cdot \Gamma(\Delta - 1))}{\log \Delta} \leq \{\text{from Lemma 2.8}\} \leq \\ &\leq \lim_{\Delta \rightarrow \infty} \frac{\log\left(2 \cdot \frac{(\Delta-1)^{3/2}}{\Delta}\right)}{\log \Delta} \leq \lim_{\Delta \rightarrow \infty} \left(\frac{\log 2 + \frac{1}{2} \log \Delta}{\log \Delta}\right) = \frac{1}{2}. \end{aligned}$$

Now, let us prove that $\lim_{\Delta \rightarrow \infty} \frac{\log \Phi_{32}(\Delta)}{\log \Delta} \geq \frac{1}{2}$. We have:

$$\begin{aligned} \lim_{\Delta \rightarrow \infty} \frac{\log \Phi_{32}(\Delta)}{\log \Delta} &= \lim_{\Delta \rightarrow \infty} \frac{\log(2 \cdot \Gamma(\Delta - 1))}{\log \Delta} \geq \lim_{\Delta \rightarrow \infty} \frac{\log(2 \cdot \Psi(\Delta - 1))}{\log \Delta} \\ &\geq \lim_{\Delta \rightarrow \infty} \frac{\log(2 \cdot g_{\Delta-1}(\lceil \sqrt{\Delta-1} \rceil, \Delta, \Delta))}{\log \Delta} \\ &= \lim_{\Delta \rightarrow \infty} \frac{\log\left(2 \cdot \frac{\frac{[\sqrt{\Delta-1}]^{\Delta-1}}{[\sqrt{\Delta-1}]^{\Delta-1}} + \frac{\Delta-1}{[\sqrt{\Delta-1}]^{\Delta-1}} + \frac{1}{[\sqrt{\Delta-1}]^{\Delta-1}} + \frac{1}{[\sqrt{\Delta-1}]^{\Delta-1} \cdot (\Delta-2)}}{[\sqrt{\Delta-1}] + \frac{[\sqrt{\Delta-1}]^{\Delta-1}}{[\sqrt{\Delta-1}]^{\Delta-1}} + \frac{2}{[\sqrt{\Delta-1}]^{\Delta-1}} + \frac{2}{[\sqrt{\Delta-1}]^{\Delta-1} \cdot (\Delta-1)} + \frac{2}{[\sqrt{\Delta-1}]^{\Delta-1} \cdot (\Delta-1) \cdot (\Delta-1)}}}\right)}{\log \Delta} \\ &\geq \lim_{\Delta \rightarrow \infty} \frac{\log\left(2 \cdot \frac{\Delta-1}{9^{\lceil \sqrt{\Delta-1} \rceil}}\right)}{\log \Delta} \geq \lim_{\Delta \rightarrow \infty} \frac{\log\left(\frac{2}{9} \cdot \sqrt{\Delta-1}\right)}{\log \Delta} = \frac{1}{2}. \end{aligned}$$

□

3 Acknowledgement

Partial support of Croatian Ministry of Science, Education and Sports is gratefully acknowledged (grant no. 177-0000000-0884 and grant no. 037-0000000-2779). Help with English language of Sarah Michelle Rajtmajer is also gratefully acknowledged.

References

- [1] M. Aouchiche, J. M. Bonnefoy, A. Fidahoussen, G. Caporossi, P. Hansen, P. L. Hiesse, J. Lacheré and A. Monhait, Variable neighborhood search for extremal graphs 14, The Auto-GraphiX 2 system, in: L. Liberti and N. Maculan (eds.), *Global Optimization: From Theory to Implementation*, Springer, 2005.
- [2] B. Bollobás, *Extremal Graph Theory*, Academic Press, London, 1978.
- [3] I. Gutman and K. C. Das, The First Zagreb Index 30 Years After, *MATCH – Commun. Math. Comput. Chem.* **50** (2004), 83–92.
- [4] P. Hansen and D. Vukičević, Comparing the Zagreb Indices, *Croatica Chemica Acta* **80** (2007), 165–168.
- [5] W. Imrich, Explicit Construction of Regular Graphs Without Small Cycles, *Combinatorica* **4** (1984), 53–39.
- [6] S. Nikolić, G. Kovačević, A. Miličević and N. Trinajstić, The Zagreb Indices 30 Years After, *Croat. Chem. Acta* **76** (2003), 113–124.
- [7] R. Todeschini and V. Consonni, *Handbook of Molecular Descriptors*, Wiley-VCH, Weinheim, 2000.
- [8] N. Trinajstić, *Chemical Graph Theory*, CRC Press, Boca Raton, 1992.
- [9] D. Vukičević, Comparing variable Zagreb indices, *MATCH – Commun. Math. Comput. Chem.* **57** (2007), 633–641.
- [10] D. Vukičević and A. Graovac, Comparing Zagreb M1 and M2 indices for acyclic molecules, *MATCH – Commun. Math. Comput. Chem.* **57** (2007), 587–590.
- [11] D. Vukičević and A. Graovac, Comparing variable Zagreb M1 and M2 indices for acyclic molecules, *MATCH – Commun. Math. Comput. Chem.* **60** (2008), 37–44.