

## ECCENTRICITY OF NETWORKS WITH STRUCTURAL CONSTRAINTS <sup>1</sup>

MATJAŽ KRNC

*FAMNIT, University of Primorska, Koper*  
*Faculty of Information Studies*  
*Novo Mesto, Slovenia*

**e-mail:** matjaz.krnc@upr.si

JEAN-SÉBASTIEN SERENI

*Centre national de la recherche scientifique (C.N.R.S.)*  
*ICube, CSTB, Strasbourg, France*

**e-mail:** sereni@kam.mff.cuni.cz

RISTE ŠKREKOVSKI

*Faculty of Information Studies, Novo Mesto*  
*Faculty of Mathematics and Physics, University of Ljubljana*  
*FAMNIT, University of Primorska, Koper, Slovenia*

**e-mail:** skrekovski@gmail.com

AND

ZELEALEM B. YILMA

*Carnegie Mellon University Qatar*  
*Doha, Qatar*

**e-mail:** zyilma@qatar.cmu.edu

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### Abstract

The eccentricity of a node  $v$  in a network is the maximum distance from  $v$  to any other node. In social networks, the reciprocal of eccentricity is used as a measure of the importance of a node within a network. The associated centralization measure then calculates the degree to which a network is dominated by a particular node. In this work, we determine the maximum value of eccentricity centralization as well as the most centralized networks for various classes of networks including the families of bipartite networks (two-mode data) with given partition sizes and tree networks with fixed number of nodes and fixed maximum degree. To this end, we introduce and study a new way of enumerating the nodes of a tree which might be of independent interest.

**Keywords:** eccentricity, network, bipartite graph, complex network, maximum degree.

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## 1. INTRODUCTION

Over the last seven decades, graph theory has played an increasingly important role in social network analysis; social networks can be modeled using graphs and the properties of the networks as well as the actors within them can be studied and explored using graph theoretic means. One particular application of graph theory in social network analysis is that of identifying the most ‘important’ or ‘central’ actor or actors in a social network. As importance can be interpreted in different ways, various motivations lead to different measures of centrality and many of the terms used to measure centrality reflect their sociological origins [7, 16].

In 1979, Freeman [8] identified degree centrality, closeness centrality, and betweenness centrality as both relatively simple and widely applicable measures of centrality. However, when it comes to distance-based measures, eccentricity is arguably a much simpler notion than closeness [20]. The *eccentricity*  $e_G(v)$  of a node  $v$  in a connected network  $G$  is the maximum distance<sup>2</sup> (in the network) between  $v$  and  $u$ , over all nodes  $u$  of  $G$ . Figure 1 shows a simple network with the eccentricity of each node. For a disconnected network, all nodes are defined to have infinite eccentricity. To state this formally

$$e_G(v) := \max \{ \text{dist}_G(v, u) : u \in V(G) \} \in \mathbf{N} \cup \{ \infty \}.$$

*Eccentricity centrality* is defined as the reciprocal of the eccentricity of a node

$$\forall v \in V(G), \quad E_G(v) := \frac{1}{e_G(v)}.$$

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<sup>2</sup>The definition of all graph-theoretic terms can be found, for instance, in the monograph by McHugh [15].

The reciprocal of the eccentricity value is convenient, since it obeys the rule of monotonicity.

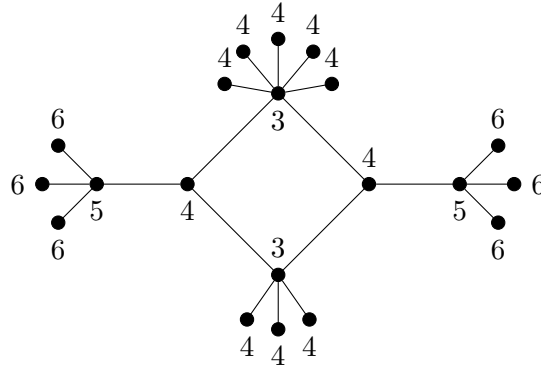


Figure 1. A network with the eccentricity of each node.

**Definition 1** (Rule of monotonicity). Let  $G$  be a network. A centrality measure  $X : V(G) \rightarrow \mathbf{R}$  on  $G$  obeys the rule of monotonicity if  $u$  is “more central” than  $v$  whenever  $X(u) > X(v)$ , for any two nodes  $u$  and  $v$  of  $G$ .

The *center* (or *Jordan center* [13]) of a network is the set of all nodes of minimum eccentricity, that is, the set of all those nodes  $v$  such that the greatest distance  $\text{dist}_G(v, u)$  to other nodes  $u$  is minimal. Equivalently, it is the set of nodes with eccentricity equal to the network’s radius. Thus nodes in the center (also called *central points*) minimize the maximal distance from other points in the network and we define  $c(G)$  to be the set of central nodes of the network  $G$ .

Hage and Harary [9], in proposing eccentricity as a measure of centrality, point out that, in the Marshall Islands, the islands belonging to the Jordan center (rather than those maximizing closeness) have historically been the politically and symbolically most important islands. The center of a network is also of paramount importance in *facility location problems*. As an example, in determining the optimal location for an emergency facility such as a hospital, the main objective is to find a site that minimizes the maximum response time between the facility and the site of a possible emergency. In a simple non-weighted version of this problem, the optimal locations are precisely the centers of the network.

The *centralization* of a network is a measure of how central its most central node is in relation to how central all the other nodes are. The general definition of centralization for non-weighted networks was proposed by Freeman [8] in 1979. Given a centrality measure, the centralization of a network is the sum of differences in centrality between the most central node in the network and all other nodes. Thus, every centrality measure can have its own centralization measure.

In order to calculate eccentricity centralization, we first define

$$\forall v \in V(G), \quad E_1(G, v) := \sum_{u \in V(G)} (E_G(v) - E_G(u)).$$

When there is no risk of confusion regarding the network  $G$ , we shall write  $E_1(v)$  instead of  $E_1(G, v)$ . The *eccentricity centralization* of the graph  $G$  is then defined to be

$$E_1(G) := \max \{E_1(v) : v \in V(G)\}.$$

Note that  $E_1(G) \geq 0$  for every network  $G$ . Moreover, if  $G$  is a disconnected network, then  $E_1(G) = 0$  since  $e_G(v) = \infty$  for every node  $v$  of  $G$ .

**Observation 2.** *If  $G$  is a network with  $n$  nodes, then  $E_1(G, v) = E_1(G)$  if and only if  $v \in c(G)$ .*

Indeed  $E_1(G, v) = n \cdot \frac{1}{e_G(v)} - \sum_{u \in V(G)} E_G(u)$  is maximized when  $e_G(v)$  is minimized, forcing  $v$  to be a member of the Jordan center.

Often, in order to allow comparison of networks of different orders, a centralization score is normalized by dividing it by the theoretically largest such score in any network of the same order [8]. Naturally, for networks on  $n$  vertices, the star graph  $S_n$  can be shown to be the most centralized graph with respect to many centralization scores (see [5] and [8], for example). However, comparisons with the star graph may not always be appropriate and it may be informative to define a class of “comparable” networks and determine the maximum centralization score and the extremal networks that attain the maximum within the pre-defined class. In Section 2 of this paper, we focus on bipartite networks with fixed part sizes. We also study the class of tree networks with fixed number of nodes and fixed maximum degree (Section 3). In the course of this study, we shall develop a new way of enumerating the nodes of a tree, coined  $S$ -enumerations, which might be useful in different contexts, too.

## 2. BIPARTITE NETWORKS WITH FIXED PARTITION SIZES

In 1991, Bonacich [1] introduced a method to calculate eigenvector centralities in two-mode data by, essentially, calculating the same on the underlying bipartite graph. He illustrated this method by applying it to the Davis, Gardner, Gardner data on the attendance of eighteen women at a series of fourteen events [3]. This approach can, in fact, be used to calculate centralities for any desired centrality measure. However, Borgatti and Everett [2] questioned the validity of using such scores as they fail to distinguish between the two modes. For example, if calculating degree centrality in the above data, the fact that there are more women than

events will, overall, give rise to higher centrality scores to events and lower centrality scores to women. Borgatti and Everett argue that, to appropriately compare the importance of nodes across modes, the raw centrality scores of each should be normalized by the maximum score attainable within their modes (Faust [6] also offers other interpretations and approaches to centrality in two-mode data).

These normalized centrality scores can then be used to calculate similarly normalized centralization scores. Borgatti and Everett [2] also suggested that in certain instances, it may even be instructive, when calculating the centralization of a network, to once again separate the two modes (that is, we should ask how centralized is the group of women and how centralized is the group of events). In either case, as a means to compare different networks, it is of interest to find the bipartite connected graphs with specified vertex sizes that maximize the centralization formula of choice.

Everett, Sinclair, and Dankelmann [5] studied betweenness centralization and provided a bipartite graph which they prove maximizes intra-mode betweenness centralization among all bipartite graphs on parts of sizes  $n_0$  and  $n_1$ . They conjectured that this same graph is also the extremal graph when centralization calculations are not restricted to be within one mode and proposed that it is similarly so for closeness centralization and eigenvector centralization. Sinclair [17, 18] settled the case for betweenness centralization and the authors of this paper [14] confirmed that it is extremal also for closeness centralization. Sinclair [19] showed that this same network is the most centralized with respect to the Gil Schmidt power centrality index.

In this section we examine eccentricity centralization on classes of bipartite networks with fixed partition sizes. Given two positive integers  $k$  and  $\ell$ , let  $\mathcal{B}_{k,\ell}$  be the set of all connected bipartite graphs with vertex sets  $K$  and  $L$  of respective sizes  $k$  and  $\ell$ . We will focus on the cases  $k, \ell \geq 2$  as, otherwise, the class contains only one network, namely, the star graph. Specifically, we shall prove the following result.

**Theorem 3.** *Let  $G \in \mathcal{B}_{k,\ell}$  with  $k, \ell \geq 2$  and let  $v$  be a node belonging to partition set  $K$ . If  $k = 2$ , then*

$$(1) \quad E_1(G, v) \leq \frac{\ell}{6},$$

*while if  $k \geq 3$ , then*

$$(2) \quad E_1(G, v) \leq \frac{\ell}{6} + \frac{k-1}{4}.$$

*Furthermore, both the bounds are tight.*

In the process of proving the theorem, we determine the extremal graphs that attain these bounds. Notably, and unlike in the cases of betweenness and

closeness, we find that for the case  $k \geq 3$ , there is not a unique extremal graph but rather a family of extremal graphs. It is also interesting to note that this same family remains extremal even when considering the normalized and one-mode versions of centralization.

### 2.1. The case $k = 2$ , $\ell \geq 2$

Let  $H \in \mathcal{B}_{2,\ell}$  with  $K = \{u, v\}$  and  $L = \{w_1, w_2, \dots, w_\ell\}$  be such that  $N(v) = L$  and  $N(u) = \{w_1\}$ .

**Proposition 4.**  $E_1(H, v) = \ell/6$ .

**Proof.** First of all, note that  $E_H(v) = \frac{1}{2}$ ,  $E_H(u) = \frac{1}{3}$ ,  $E_H(w_1) = \frac{1}{2}$ , and  $E_H(w_j) = \frac{1}{3}$  if  $2 \leq j \leq \ell$ . Therefore,  $E_1(H, v) = \left(\frac{1}{2} - \frac{1}{3}\right) + \left(\frac{1}{2} - \frac{1}{2}\right) + (\ell - 1)\left(\frac{1}{2} - \frac{1}{3}\right) = \frac{\ell}{6}$ . ■

Now let  $G$  be a connected bipartite graph on the same vertex set  $K \cup L$  and suppose, without loss of generality, that  $E_G(v) \geq E_G(u)$ . If  $N_G(v) \neq L$  then, as  $G$  is connected, it follows that  $E_G(v) = E_G(u) = 1/3$  and  $E_G(w_j) \geq \frac{1}{4}$  for every  $j \in \{1, \dots, \ell\}$ . Therefore,  $E_1(G, v) \leq \ell\left(\frac{1}{3} - \frac{1}{4}\right) = \frac{\ell}{12} \leq E_1(H, v)$ .

On the other hand, when  $N_G(v) = L$ , we obtain  $E_1(G, v) = 0$  if  $N_G(u) = L$  and, otherwise,  $E_1(G, v) = \frac{(\ell - |L'| + 1)}{6}$  where  $N_G(u) = L' \subset L$ . This is maximized when  $|L'| = 1$ , that is, when  $G$  is isomorphic to  $H$ , thereby proving the first part of Theorem 3. We also deduce that  $H$  is the unique extremal graph up to isomorphism.

### 2.2. The case $k \geq 3$ , $\ell \geq 2$

We now prove the remaining part of Theorem 3. Suppose that  $G \in \mathcal{B}_{k,\ell}$  and let  $v \in K$  be such that  $E_G(v) \geq E_G(u)$  for every  $u \in K$ . First, suppose that the eccentricity of  $v$  is some value  $r \geq 3$ . It follows from the triangle inequality that  $e_G(u) \leq 2r$  for every  $u \in K \cup L$ . Therefore,

$$E_1(G, v) \leq (k + \ell - 1) \left( \frac{1}{r} - \frac{1}{2r} \right) = \frac{k + \ell - 1}{2r} \leq \frac{k + \ell - 1}{6} < \frac{\ell}{6} + \frac{k - 1}{4}.$$

On the other hand if  $e_G(v) = 2$ , then it follows that  $N_G(v) = L$  and, once again, the triangle inequality implies that  $e_G(w) \leq 3$  for each  $w \in L$  and  $e_G(u) \leq 4$  for each  $u \in K$ . From here we deduce that  $E_1(G, v) \leq \frac{\ell}{6} + \frac{k-1}{4}$ .

What remains is to show that this bound is indeed achievable. To this end, consider the set  $\mathcal{T}_{k,\ell} \subset \mathcal{B}_{k,\ell}$  of trees of diameter 4 with the central node belonging to  $K$ . A schematic view of some of the elements in  $\mathcal{T}_{k,\ell}$  is given by Figure 2. Observe that the central node has eccentricity 2, all the other nodes in  $K$  have eccentricity 4 and all nodes in  $L$  have eccentricity 3. The eccentricity centralization score of the central node is therefore  $\frac{\ell}{6} + \frac{k-1}{4}$ . This set is not an exhaustive collection of all extremal graphs.

**Proposition 5.** *Let  $G \in \mathcal{B}_{k,\ell}$  and let  $v \in K$ . Then  $E_1(G, v) = \frac{\ell}{6} + \frac{k-1}{4}$  if and only if  $N_G(v) = L$  and for each  $u \in K \setminus \{v\}$ , there exists  $u' \in K$  such that  $N_G(u) \cap N_G(u') = \emptyset$ .*

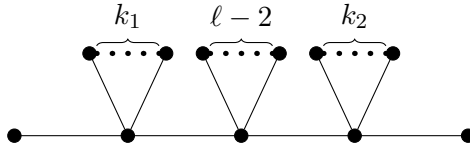


Figure 2. A schematic view of some members of  $\mathcal{T}$ , where  $k_1 + k_2 = k - 3$ .

**Proof.** These last conditions ensure that  $e_G(v) = 2$ ,  $e_G(w) = 3$  for every  $w \in L$ , and  $e_G(u) = 4$  for every  $u \in K - \{v\}$ . This shows the ‘if’ part, and we have already seen the ‘only if’ part above. ■

### 2.3. Normalized and one-mode centralization

Interestingly, the extremal graphs identified above remain extremal even if we consider normalized versions of eccentricity centralization. This is simply because, for  $k, \ell \geq 2$ , the maximum eccentricity centrality score any node can attain is  $1/2$  regardless of the actual values of  $k$  and  $\ell$ . Therefore, all centrality scores (and, by extension, centralization scores) are scaled by a factor of 2. Clearly, this linear scaling does not affect the extremal set.

It is notable, however, that if  $k = 1$  or  $\ell = 1$ , then the normalized eccentricity centrality scores of all nodes is exactly 1. Therefore, under this interpretation, the star graph has a centralization score of 0 and becomes among the least centralized networks.

When it comes to one-mode centralization, the centralization score for a node  $v \in K$  in the network  $G \in \mathcal{B}_{k,\ell}$  is calculated as  $E'_1(G, v) = \sum_{u \in K} (E_G(v) - E_G(u))$ . While the centralization score no longer depends directly on the centrality scores of nodes in  $L$ , these nodes still influence the centrality scores of nodes in  $K$ . Due to this indirect influence, we find that the extremal graphs for  $k \geq 3$  and  $\ell \geq 2$  are exactly the extremal graphs described in the previous section. However, in the case where  $k = 2$  and  $\ell \geq 2$ , every connected bipartite graph  $G$  with  $|N_G(v)| = \ell$  and  $|N_G(u)| < \ell$  receives the same centralization score of  $1/6$ , and hence is extremal.

## 3. TREE NETWORKS WITH PRESCRIBED ORDER AND MAXIMUM DEGREE

In this section we are interested in maximizing eccentricity centralization over the class of trees on a fixed number,  $n$ , of nodes and fixed maximum degree,  $\Delta$ .

The motivations for this are twofold. First of all, while a node in a network on  $n$  nodes can, in theory, have degree  $n - 1$ , often there are naturally occurring (such as Dunbar's number [4] for social capacity or the capacity of atoms to form chemical bonds) or artificially imposed (like Facebook's recently removed 5000-friend limit) bounds on the degree of a node. Secondly, the most centralized networks for many centralization measures, including eccentricity centralization, tend to be trees. In fact, given a network  $G$ , it is possible to remove edges from  $G$  to obtain a spanning tree  $T$  with  $E_1(G) \leq E_1(T)$ . In particular, a breadth-first search tree  $T$  rooted at a central node of  $G$  has this property. Therefore, tree networks with fixed number of nodes and maximum degree are a natural class of interest and many extremal results have been obtained on such classes for various centrality and topological measures (for example, see [10, 11] on the Merrifield-Simmons index and the Hosoya index and [12] on the eccentric connectivity index, see also [22]).

Given positive integers  $\Delta$  and  $n$  with  $\Delta < n$ , let  $\mathcal{T}_{n,\Delta}$  be the collection of all trees with  $n$  nodes and maximum degree  $\Delta$ . Our goal is to study

$$E_1^*(\mathcal{T}_{n,\Delta}) = \max \{E_1(T, v) : T \in \mathcal{T}_{n,\Delta} \text{ and } v \in V(T)\}.$$

We characterize all optimal trees from  $\mathcal{T}_{n,\Delta}$  and provide an efficient (algorithmic) way to build them all. We start with some preliminary remarks.

The situation is trivial for  $\Delta \leq 2$ , as the only trees with maximum degree at most two are paths. So we assume from now on that  $\Delta \geq 3$ . Moreover, there is only one tree with maximum degree  $\Delta$  and  $\Delta + 1$  nodes. Similarly, there is also only one tree with maximum degree  $\Delta$  and  $\Delta + 2$  nodes. So we assume from now on that  $n \geq \Delta + 3$ .

A tree is  $\Delta$ -regular if every node that has not degree  $\Delta$  is a leaf, that is, a vertex of degree 1. If  $T$  is a rooted tree with root  $r$ , then the *depth* of a node of  $T$  is its distance to  $r$ . The *depth of  $T$*  is the maximum of the depth over all nodes of  $T$ ; in other words, it is  $e_T(r)$ . A  $\Delta$ -regular rooted tree of depth  $k$  is *full* if every node of depth less than  $k$  has degree exactly  $\Delta$ . We let  $F_{\Delta,k}$  be the full  $\Delta$ -regular tree with depth  $k$ . In particular,  $F_{\Delta,k}$  contains  $\eta(\Delta, k) := 1 + \Delta \frac{(\Delta-1)^k - 1}{\Delta-2}$  nodes. As explained below, it is straightforward to obtain a (possibly tight) lower bound on the radius of a tree in terms of its maximum degree and its number of nodes.

**Lemma 6.** *Let  $k(n, \Delta)$  be the smallest integer  $k$  such that  $\mathcal{T}_{n,\Delta}$  contains a tree with radius  $k$ . Then*

$$k(n, \Delta) = \left\lceil \log_{\Delta-1} \left( (n-1) \cdot \frac{\Delta-2}{\Delta} + 1 \right) \right\rceil.$$

**Proof.** Fix  $T \in \mathcal{T}_{n,\Delta}$  and let  $k$  be the radius of  $T$ . Rooting  $T$  at a central vertex,



one sees that  $n$  is at most

$$1 + \Delta + \Delta(\Delta - 1) + \cdots + \Delta(\Delta - 1)^{k-1} = 1 + \Delta \frac{(\Delta - 1)^k - 1}{\Delta - 2}.$$

So,  $(\Delta - 1)^k \geq (n - 1) \cdot \frac{\Delta - 2}{\Delta} + 1$ , and hence

$$k \geq \log_{\Delta-1} \left[ (n - 1) \cdot \frac{\Delta - 2}{\Delta} + 1 \right].$$

This shows that  $k(n, \Delta) \geq \lceil \log_{\Delta-1} ((n - 1)(\Delta - 2)/\Delta + 1) \rceil$ . The equality is now straightforward.  $\blacksquare$

Let  $T$  be a tree of diameter  $d$  and assume that  $v_0 \cdots v_d$  is a longest path of  $T$ . It is well known (see, for example, [21]) that the radius of  $T$  is  $k := \lceil d/2 \rceil$  and every node is at distance at most  $k$  from each of  $v_{\lfloor d/2 \rfloor}$  and  $v_{\lceil d/2 \rceil}$ . Consider now  $T$  to be rooted at  $v_k$ . For each  $i \in \{1, \dots, k\}$ , the *layer*  $i$  of  $T$  is defined to be the set  $L_i(T)$  of all nodes  $v$  of  $T$  with depth  $i$ , that is, such that  $\text{dist}_T(v, v_k) = i$ . We set  $n_i(T) := |L_i(T)|$ . If  $uv$  is an edge such that  $u \in L_i(T)$  and  $v \in L_{i+1}(T)$ , then  $u$  is the *parent* of  $v$  and  $v$  is a *child* of  $u$ .

We shall demonstrate that, informally, every tree  $T$  in  $\mathcal{T}_{n, \Delta}^*$  has diameter  $2k(n, \Delta)$  and, subject to this, the following structure:  $n_k(T)$  is as large as possible, while  $n_i(T)$  contains, almost always, just as many vertices as needed so that every node in  $n_{i+1}(T)$  can have a parent (recall that the maximum degree cannot exceed  $\Delta$ ), for each  $i \in \{1, \dots, k - 1\}$ .

Before being precise, let us note a straightforward fact: in any tree  $T$  rooted at a node in its Jordan center and with even diameter, if one “re-arranges” the subtrees rooted at any fixed level so that neither the diameter nor the maximum degree changes, then the eccentricity centralization of the tree does not change either. Specifically, this follows from the fact that if a tree  $T$  with  $n$  nodes and diameter  $2k$  is rooted at a node in the Jordan center, then  $E_1(T) = \frac{n-1}{k} - \sum_{i=1}^k \frac{n_i(T)}{k+i}$ . Let  $v \in L_{i+1}(T)$  and define  $T'$  as the tree obtained from  $T$  by deleting the edge between  $v$  and its parent and adding an edge between  $v$  and any node in  $L_i(T)$  of degree less than  $\Delta$ . If  $T'$  has the same diameter as  $T$ , then it follows that  $E_1(T') = E_1(T)$ . In this case, the operation is said to be *valid*. Valid operations yield an equivalence relation between trees: two trees are *equivalent* if one is obtained from the other by a sequence of valid operations.

In the next subsection, we define  $\mathcal{F}_{\Delta, k}(n)$ , a class of trees all having fixed order  $n$ , maximum degree  $\Delta$  and (even) diameter  $2k$ . As we shall see, this class captures all trees with maximum eccentricity in the sense that every tree with  $n$  nodes, maximum degree  $\Delta$  and maximum eccentricity belongs to  $\mathcal{F}_{\Delta, k(n, \Delta)}(n)$ . To this end, we introduce  $S$ -enumerations of trees and prove a couple of useful properties of these enumerations.

### 3.1. $S$ -enumerations

In this section we provide an algorithmic procedure to label the vertices of a tree on  $n$  nodes all differently with labels  $0, \dots, n-1$ , which plays an important role in the characterisation of trees with maximum eccentricity (Theorem 7). Let  $T$  be a tree with  $n$  nodes and diameter  $d$ .

- We start from a longest path of  $T$  and label its nodes consecutively with  $0, \dots, d$ .
- We then consecutively label only those unlabeled nodes with a labeled parent. To this end, the following loop is performed. For  $i$  from 1 to  $\lfloor d/2 \rfloor$ , do the following two loops, in order:
  1. For each unlabeled child  $v$  of the node labeled  $i$ , label the nodes in the subtree rooted at  $v$  according to a depth-first search algorithm.
  2. For each unlabeled child  $v$  of the node labeled  $d-i$ , label the nodes in the subtree rooted at  $v$  according to a depth-first search algorithm.

Note that the running time of the procedure is  $O(|V(T)|)$ . Besides, the labeling is not uniquely defined, as it depends on the longest path chosen as well as the order in which the nodes are considered in each depth-first search procedure. Any labeling of the nodes of a tree  $T$  that can be obtained by the above procedure is called an  $S$ -enumeration of  $T$ . The longest path used in the  $S$ -enumeration is called the *root-path*. Figure 3 provides an example of an  $S$ -enumeration of a tree with maximum degree 4, diameter 8 and 16 nodes.

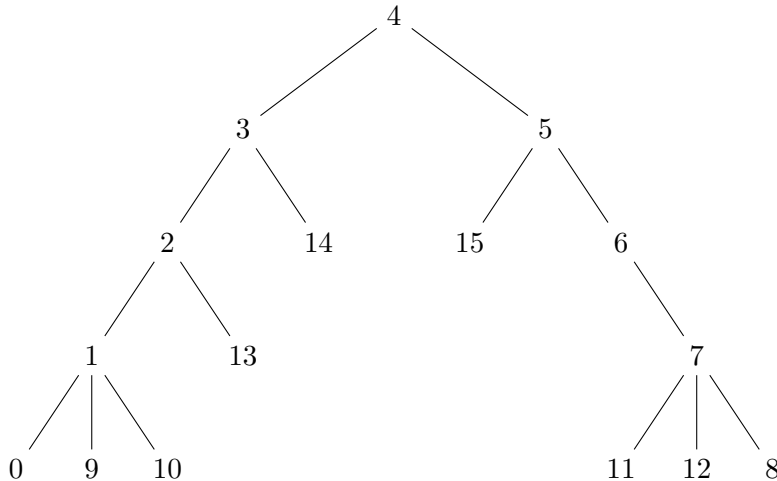


Figure 3. An  $S$ -enumeration of a tree with maximum degree 4, diameter 8 and 16 nodes.

For positive integers  $\Delta$ ,  $k$  and  $n$  with  $n \geq \max\{\Delta + 1, 2k\}$ , let  $F_{\Delta,k}(n)$  be the (unique) subtree of an  $S$ -enumeration of the full tree  $F_{\Delta,k}$  induced by the nodes

with labels in  $\{0, \dots, n - 1\}$ . Thus  $F_{\Delta,k}(n)$  has  $n$  nodes, maximum degree  $\Delta$ , radius  $k$  and diameter  $2k$ . The tree  $F_{4,4}(16)$  is depicted in Figure 4. Let  $\mathcal{F}_{\Delta,k}(n)$  be the collection of all trees that are equivalent to  $F_{\Delta,k}(n)$ .

The tree given in Figure 3 does not belong to  $\mathcal{F}_{4,4}(16)$ . Indeed, this tree contains two nodes on its root-path (namely 2 and 3) such that both have non-trivial subtrees, and the one further to the central node is not full. In particular, consider a tree  $T$  in  $\mathcal{F}_{\Delta,k}(n)$  with one of its  $S$ -enumerations: if  $u$  and  $v$  are two nodes on the root-path such that the level of  $u$  is smaller than that of  $v$ , then the degree of  $u$  cannot be greater than that of  $v$ .

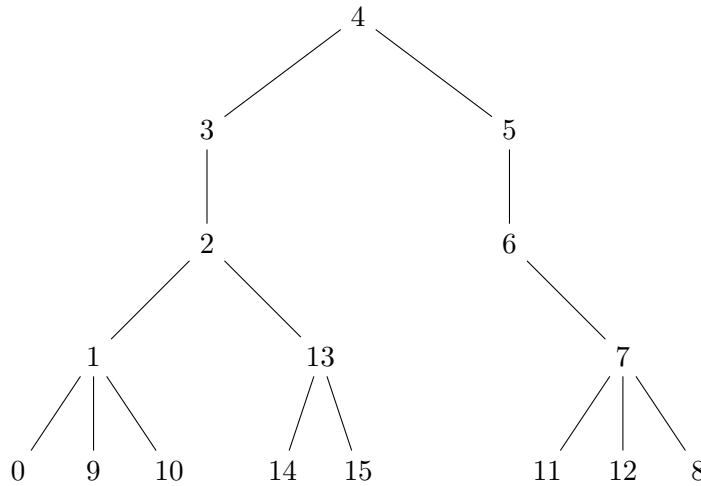


Figure 4. An  $S$ -enumeration of the tree  $F_{4,4}(16)$ .

We are now in a position to state the characterization of trees with maximum eccentricity.

**Theorem 7.** *Let  $\Delta$  and  $n$  be integers such that  $3 \leq \Delta \leq n - 3$ . It holds that  $\mathcal{T}_{n,\Delta}^* = \mathcal{F}_{\Delta,k(n,\Delta)}(n)$ .*

To prove Theorem 7, we first establish that  $F_{\Delta,k}(n)$  admits a particular partition of its nodes, which turns out to be useful to us. A path  $P$  of a tree  $T$  is *monotone* if  $P$  does not contain more than one node of each possible depth. In addition, let us define a  $D$ -tree of depth  $k$  to be a rooted tree in which every node of depth less than  $k$  has exactly  $D$  children. It will be useful to note that such a tree contains exactly  $D^i$  nodes of depth  $i$  for  $i \in \{0, \dots, k\}$ , and consequently precisely  $\nu(D, k) := \frac{D^{k+1}-1}{D-1}$  nodes in total. The partition defined in the next lemma is maybe better digested when read along with the example given after the proof of that lemma.

**Lemma 8.** *Define  $t$  to be the number of leaves of  $F := F_{\Delta,k}(n)$ . There exists a partition of the nodes of  $T$  into  $t$  sets  $V_1, \dots, V_t$  such that*

1. *for each  $i \in \{1, \dots, t\}$ , the nodes in  $V_i$  induce a monotone path in  $F$ ;*
2.  *$|V_1| = k$  and  $|V_i| \in \{1, \dots, k-1\}$  if  $2 \leq i \leq t$ ;*
3. *each set  $V_i$  contains exactly one leaf of  $F$  and, if  $i < t$ , then this leaf has depth  $k$ ; and*
4. *for every  $\ell \in \{1, \dots, k-1\}$ , if  $F$  contains  $(j+2)$  nodes of depth  $\ell$  for a positive integer  $j$ , then the number of  $(\Delta-1)$ -trees of depth  $k-\ell$  in  $F$  is at least  $j+1$ ; moreover,  $(j+1)(\Delta-1)^{k-\ell-1} \cdot (\Delta-2)$  sets among  $(V_i)_{0 \leq i \leq t+1}$  have order exactly 1 and are composed of a single leaf of depth  $k$ .*

**Proof.** The sought partition can be built as follows. We start from an  $S$ -enumeration of  $F_{\delta,k}$  such that  $F$  is the subtree induced by the nodes with labels in  $\{0, \dots, n-1\}$ . Let  $L$  be the set of nodes of  $F$  of depth  $k$ . Observe that  $|L| \in \{t-1, t\}$ . Let  $v_1, \dots, v_{|L|}$  be the elements of  $L$  increasingly ordered with respect to their label in the enumeration, so the label of  $v_1$  is 0 and that of  $v_2$  is  $2k$ . For convenience, set  $V_0 := \emptyset$ . For each index  $i$  from 1 up to  $|L|$ , let  $V_i$  be the set of nodes of the longest monotone path containing  $v_i$  in the network  $F - \bigcup_{0 \leq j < i} V_j$ . Observe that if  $|L| = t$ , that is, all leaves of  $F$  have depth  $k$ , then  $(V_i)_{1 \leq i \leq t}$  is a partition of  $V(F)$  into non-empty parts. If  $|L| = t-1$ , then we further define the set  $V_t$  to be  $V(F) \setminus \bigcup_{1 \leq j \leq t-1} V_j$ . Note that  $V_t$  contains a leaf (of depth less than  $k$ ) and induces a monotone path. Either way,  $(V_i)_{1 \leq i \leq t}$  is a partition of  $V(F)$  into  $t$  non-empty parts.

The partition  $(V_i)_{1 \leq i \leq t}$  of the nodes of  $F$  readily satisfies properties 1, 2 and 3. It remains to prove that property 4 is satisfied. To this end, let  $x_1, \dots, x_{j+2}$  be the nodes of  $F$  of depth  $\ell$  ordered increasingly with respect to their labels, so  $x_1$  is the node labeled  $k-\ell$  and  $x_2$  the node labeled  $k+\ell$ . Assume that  $j \geq 1$ . Then the definition of  $F$  implies that the subtree rooted at  $x_i$  is a  $(\Delta-1)$ -tree of depth  $k-\ell$  whenever  $1 \leq i \leq j+1$ , which implies the first statement. Moreover, our construction of the partition implies that for each node  $v$  of depth  $k-\ell-1$  in such a tree, exactly  $\Delta-2$  children of  $v$  are contained in a part of order 1. Therefore, in total, the partition  $(V_i)_{1 \leq i \leq t}$  contains at least  $(j+1)(\Delta-1)^{k-\ell-1} \cdot (\Delta-2)$  parts of order 1. ■

We use the following convention: when we build a partition of the nodes of  $F_{\Delta,k}(n)$ , we use the procedure given in the preceding proof and the leaves of  $F_{\Delta,k}(n)$  are considered in increasing order with respect to their labels in the  $S$ -enumeration.

**Example 9.** The partition obtained for the tree depicted in Figure 4 is  $V_0 := \{0, 1, 2, 3, 4\}$ ,  $V_1 := \{8, 7, 6, 5\}$ ,  $V_2 := \{9\}$ ,  $V_3 := \{10\}$ ,  $V_4 := \{11\}$ ,  $V_5 := \{12\}$ ,

$V_6 := \{14, 13\}$  and  $V_7 := \{15\}$ . As stated by Lemma 8 (because  $T$  has more than two nodes of depth 3), this partition contains at least  $2(\Delta - 1)^{k-3-1} \cdot (\Delta - 2) = 4$  singletons.

Eccentricity relates to  $S$ -enumerations of full regular trees as indicated in the next lemma.

**Lemma 10.** *If  $T$  is a tree in  $\mathcal{T}_{n,\Delta}$  with diameter  $2k$ , then  $E_1(T') \geq E_1(T)$  for every  $T' \in \mathcal{F}_{\Delta,k}(n)$ .*

To prove Lemma 10 we first recall that if  $T$  is a tree with  $n$  nodes and diameter  $2k$  rooted at a node in the Jordan center, then  $E_1(T) = \frac{n-1}{k} - \sum_{i=1}^k \frac{n_i(T)}{k+i}$ . Moreover, if  $T$  has maximum degree  $\Delta$ , then we know that  $n_1(T) \leq \Delta$  and  $n_{i+1}(T) \leq n_i(T)(\Delta - 1)$  if  $1 \leq i < k$ . This motivates the introduction of the following (more general) integer program.

**Definition 11.** Let  $k, \Delta$  and  $n$  be positive integers such that  $\max\{2k - 1, \Delta\} < n < \eta(\Delta, k)$  and  $\Delta \geq 2$ . Let  $\alpha_1, \dots, \alpha_k$  be a decreasing sequence of positive rational numbers. The integer program (P) with parameters  $k, \Delta, n$  and  $(\alpha_i)_{i=1}^k$  is

$$(3) \quad \min \quad \sum_{i=1}^k \alpha_i \cdot n_i$$

$$(4) \quad \text{s.t.} \quad \sum_{i=1}^k n_i = n$$

$$(5) \quad n_1 \leq \Delta$$

$$(6) \quad n_{i+1} \leq n_i(\Delta - 1) \quad \text{if } i \in \{1, \dots, k-1\}$$

$$(7) \quad n_i \in \mathbf{N} \setminus \{0, 1\} \quad \text{if } i \in \{1, \dots, k\}.$$

It turns out that the optimal solutions of (P) can be determined and they correspond to the sizes of the layers in specific trees with  $n$  nodes, diameter  $2k$  and maximum degree  $\Delta$ . Our strategy to prove Theorem 7 is to reduce the problem to the program (P) with some well-chosen parameters. In particular, in the proof of Theorem 7, the program (P) will be considered with parameter  $n - 1$  instead of  $n$ .

We solve the program (P) in the next proposition. Recall that  $\eta(\Delta, k)$  is  $1 + \Delta \frac{(\Delta-1)^k - 1}{\Delta-2}$ , the number of nodes in the full  $\Delta$ -regular tree of depth  $k$ , while  $\nu(D, k)$  is  $\frac{D^{k+1} - 1}{D-1}$ , the number of nodes in the  $D$ -tree of depth  $k$ . We shall often use that  $\eta(\Delta, k) = 1 + \Delta \cdot \nu(\Delta - 1, k - 1)$ .

**Proposition 12.** *Let  $k, \Delta$  and  $n$  be positive integers such that  $2k + \Delta - 1 \leq n < \eta(\Delta, k)$ , and  $\Delta \geq 3$ . Let  $\alpha_1, \dots, \alpha_k$  be a (strictly) decreasing sequence of*

positive rational numbers. The optimal value of the integer program (P) with parameters  $k$ ,  $\Delta$ ,  $n$  and  $(\alpha_i)_{i=1}^k$  is attained only by the feasible solution obtained in the following inductive way. Setting  $n_0 := 0$ , we define  $n_i$ , for each  $i \in \{1, \dots, k-1\}$ , to be the least integer  $s \geq 2$  such that  $s \cdot \nu(\Delta-1, k-i) \geq n - \sum_{j=0}^{i-1} n_j$ . Finally,  $n_k$  is defined to be  $n - \sum_{j=0}^{k-1} n_j$ .

**Proof.** For convenience, we set  $\sigma_i := \sum_{j=0}^i n_j$  for  $i \in \{0, \dots, k\}$ . First, we need to prove that the obtained solution  $(n_1, \dots, n_k)$  is feasible. As a preliminary remark, we note that  $n_k \geq 0$  since  $\nu(\Delta-1, k-i) \geq \frac{(\Delta-1)^2-1}{\Delta-2} \geq 3$  whenever  $1 \leq i \leq k-1$ , since  $\Delta \geq 3$ . Now, notice that (4) is satisfied since  $n_k$  is defined to be  $n - \sigma_{k-1}$ . Moreover,  $n_1 \leq \Delta$  since  $\Delta \cdot \nu(\Delta-1, k-1) = \eta(\Delta, k) - 1 \geq n$ .

We now prove that (6) is satisfied. Let  $i \in \{1, \dots, k-1\}$ . Since  $n_i \cdot \nu(\Delta-1, k-i) \geq n - \sigma_{i-1}$ , we deduce that

$$\begin{aligned} n - \sigma_i &= (n - \sigma_{i-1}) - n_i \leq n_i(\nu(\Delta-1, k-i) - 1) \\ &= n_i \left( \frac{(\Delta-1)^{k-i+1} - (\Delta-1)}{\Delta-2} \right) \\ &= n_i(\Delta-1) \cdot \nu(\Delta-1, k-(i+1)), \end{aligned}$$

and hence  $n_{i+1} \leq n_i(\Delta-1)$ .

It remains to prove that  $n_k \geq 2$ . If  $n_i = 2$  for every  $i \in \{1, \dots, k-1\}$ , then  $n_k \geq 2$  since  $n \geq 2k$ . Otherwise, let  $i$  be the largest integer such that  $n_i \geq 3$  and let us prove that  $n_k \geq 2$ . First, the definition of  $n_i$  implies that  $n \geq \sigma_{i-1} + (n_i - 1)\nu(\Delta-1, k-i) + 1$ . Moreover,  $\sigma_{k-1} = \sigma_{i-1} + n_i + 2(k-1-i)$ . Since  $n_k = n - \sigma_{k-1}$ , it follows that

$$(8) \quad n_k - 3 \geq n_i(\nu(\Delta-1, k-i) - 1) - \nu(\Delta-1, k-i) - 2k + 2i.$$

It therefore suffices to prove that

$$(9) \quad n_i(\nu(\Delta-1, k-i) - 1) - \nu(\Delta-1, k-i) - 2k + 2i \geq -1.$$

Since  $n_i \geq 3$  and  $\nu(\Delta-1, k-i) \geq 3$ , it thus suffices to prove that  $2\nu(\Delta-1, k-i) - 2(k+1-i) \geq 0$ . This holds because  $\nu(\Delta-1, k-i) \geq 2^{k-i+1} - 1 \geq k+1-i$  as  $i \in \{1, \dots, k-1\}$  and  $\Delta \geq 3$ . Since all constraints from Definition 11 are verified,  $(n_1, \dots, n_k)$  is feasible.

The optimality of  $(n_1, \dots, n_k)$  follows from the fact that  $(\alpha_i)_{i=0}^k$  is a (strictly) decreasing sequence of positive numbers. Let  $(n'_1, \dots, n'_k)$  be a feasible solution. Since  $\sum_{i=0}^k \alpha_i \cdot n_i \leq \sum_{i=0}^k \alpha_i \cdot n'_i$ , we may assume that  $n'_i < n_i$  for some index  $i \in \{1, \dots, k\}$ . Let  $i$  be the least positive integer such that  $n'_i < n_i$ . Observe that  $i > 1$ . Indeed, if  $n'_1 < n_1$ , then as  $n'_1 \geq 2$  the definition of  $n_1$  implies that

$n'_1 \nu(\Delta - 1, k - 1) < n$ . On the other hand, since  $n'_{j+1} \leq n'_j(\Delta - 1)$  for each  $j \in \{1, \dots, k - 1\}$  by (6), we deduce that

$$\sum_{j=1}^k n'_j \leq n'_1 \sum_{j=1}^k (\Delta - 1)^{j-1} = n'_1 \nu(\Delta - 1, k - 1) < n,$$

contrary to (5). This contradiction ensures that  $i > 1$ .

We assert that  $n'_j = n_j$  for each  $j \in \{1, \dots, i - 1\}$ . Otherwise, let  $\ell \in \{1, \dots, i - 1\}$  such that  $n'_\ell > n_\ell$  and  $n'_j = n_j$  if  $\ell < j < i$ . Let  $\mathbf{x} = (x_1, \dots, x_k)$  be defined by

$$x_j := \begin{cases} n'_\ell - 1 & \text{if } j = \ell, \\ n'_i + 1 & \text{if } j = i, \\ n'_j & \text{otherwise.} \end{cases}$$

Then  $\sum_{j=1}^k \alpha_j \cdot x_j = \sum_{j=1}^k \alpha_j \cdot n'_j + (\alpha_i - \alpha_\ell) < \sum_{j=1}^k \alpha_j \cdot n'_j$ , which shows that if  $\mathbf{x}$  is feasible, then  $(n'_1, \dots, n'_k)$  is not optimal. Thus it remains to prove that  $\mathbf{x}$  is feasible to conclude the proof of our assertion.

Note that  $\sum_{j=1}^k x_j = n$  by the definition. Moreover,  $x_\ell = n'_\ell - 1 \geq n_\ell \geq 2$  and  $x_i > n'_i \geq 2$ . Surely,  $x_{j+1} \leq x_j(\Delta - 1)$  if  $j \notin \{\ell, i - 1\}$ . It remains to prove that  $x_{\ell+1} \leq x_\ell(\Delta - 1)$  and  $x_i \leq x_{i-1}(\Delta - 1)$ . (These two inequalities are the same if  $\ell = i - 1$ .) For the sake of clarity, assume first that  $\ell \neq i - 1$ . Then, the former inequality holds because

$$x_{\ell+1} = n'_{\ell+1} = n_{\ell+1} \leq n_\ell(\Delta - 1) \leq (n'_\ell - 1)(\Delta - 1) = x_\ell(\Delta - 1),$$

while the latter inequality holds because

$$x_i = n'_i + 1 \leq n_i \leq n_{i-1}(\Delta - 1) = n'_{i-1}(\Delta - 1) = x_{i-1}(\Delta - 1).$$

If  $\ell = i - 1$ , then

$$x_i = n'_i + 1 \leq n_i \leq n_{i-1}(\Delta - 1) \leq (n'_{i-1} - 1)(\Delta - 1) = x_{i-1}(\Delta - 1).$$

Therefore,  $\mathbf{x}$  is feasible if  $n'_j > n_j$  for some  $j \in \{1, \dots, i - 1\}$ . We conclude that  $n'_j = n_j$  if  $j < i$ .

However, this leads to a contradiction. Indeed, since  $2 \leq n'_i < n_i$ , the definition of  $n_i$  implies that  $n'_i \cdot \nu(\Delta - 1, k - i) < n - \sigma_{i-1}$ . Moreover,  $\sigma_{i-1} = \sum_{j=1}^{i-1} n'_j$  by what precedes. But

$$\sum_{j=i}^k n'_j \leq n'_i \cdot \sum_{j=i}^k (\Delta - 1)^{j-i} = n'_i \cdot \nu(\Delta - 1, k - i),$$

which implies that  $\sum_{j=1}^k n'_j \leq \sigma_{i-1} + n'_i \cdot \nu(\Delta - 1, k - 1) < n$ , a contradiction. ■

A key consequence of Proposition 12 is that if a tree  $T$  belongs to  $\mathcal{F}_{\Delta,k}(n)$ , then the vector  $(n_1(T), \dots, n_k(T))$  is the optimal solution of the program (P) with parameters  $k, n-1, \Delta$  and  $\alpha_i := \frac{1}{k+i}$  for  $i \in \{1, \dots, k\}$ . Lemma 10 follows from this observation.

**Proof of Lemma 10.** Let  $T$  be a tree in  $\mathcal{T}_{n,\Delta}$  with diameter  $2k$ . Set  $n := |V(T)|$  and let  $T' \in \mathcal{F}_{\Delta,k}(n)$ . The vector  $(n_1(T), \dots, n_k(T))$  is a feasible solution of the program (P) with parameters  $k, n-1, \Delta$  and  $\alpha_i := \frac{1}{k+i}$  for  $i \in \{1, \dots, k\}$ . Therefore  $\sum_{i=1}^k \frac{n_i(T)}{k+i} \geq \sum_{i=1}^k \frac{n_i(T')}{k+i}$  by the remark above. Consequently  $\frac{n-1}{k} - \sum_{i=1}^k \frac{n_i(T)}{k+i}$  is at most  $\frac{n-1}{k} - \sum_{i=1}^k \frac{n_i(T')}{k+i}$ , which is to say that  $E_1(T)$  is at most  $E_1(T')$ . ■

We are now ready to establish Theorem 7.

### 3.2. The Proof of Theorem 7

Let  $T$  be a tree in  $\mathcal{T}_{n,\Delta}^*$  and let  $d$  be the diameter of  $T$ . So  $n \geq d + \Delta - 1 \geq d + 2$ , as  $\Delta \geq 3$ . Clearly, the conclusion holds for networks with diameter less than 3, so we assume that  $d$  is at least 3. Our first aim is to show that the diameter  $d$  of  $T$  is  $2k(n, \Delta)$ . (Recall that  $k(n, \Delta)$  is defined in Lemma 6.) We set  $k_0 := k(n, \Delta)$  for convenience and proceed in two steps: we establish that  $d$  is even and, next, we prove that if  $d \geq 2k_0 + 2$ , then there exists a network  $T'$  of diameter  $d - 2$  with  $n$  nodes and maximum degree  $\Delta$  such that  $E_1(T') > E_1(T)$ .

Suppose, for a contradiction, that  $d = 2s + 1$  for some positive integer  $s$ . Then the number  $n$  of nodes of  $T$  is at least  $2s + 3$ . In addition,  $T$  must contain a longest path  $P = v_0 \cdots v_d$  and a leaf that does not belong to  $P$ . Suppose first that there exists a leaf  $u$  not on  $P$  such that  $T - u$  still has maximum degree  $\Delta$ . Then let  $T'$  be the network obtained from  $T$  by deleting the edge incident to  $u$  and adding the edge  $\{u, v_d\}$ . The network  $T'$  is a tree of diameter  $d + 1 = 2s + 2$  with  $n$  nodes and maximum degree  $\Delta$ . Moreover, as  $e_{T'}(v) \geq e_T(v)$  for every node  $v$  with strict inequality for (exactly) one of  $v_s$  and  $v_{s+1}$ , it follows that  $E_1(T') > E_1(T)$ , which is a contradiction. Thus we may in particular assume that  $T$  has a unique node  $v$  of degree  $\Delta$ , all leaves of  $T$  not on  $P$  are adjacent to  $v$  and there are at least  $\Delta - 2$  of them. In addition, note that exactly one node  $v_i$  of  $P$  has degree greater than 2. Without loss of generality, we may assume that  $i \leq s + 1$ .

If  $v_i = v$ , that is,  $v_i$  is the unique node of  $T$  with degree  $\Delta$ , then  $n = d + \Delta - 1$  and  $T$  is composed of the path  $P$  and  $\Delta - 2$  leaves attached to  $v_i$ . In this case, a straightforward check ensures that  $E_1(T)$  is maximized only if  $i = 1$  (recalling that  $i \leq s + 1$ ). Let  $T'$  be the tree obtained by deleting the edge incident to  $v_d$  and next adding an edge between  $v_d$  and  $v_{d-2}$ . The tree  $T'$  has  $n$  nodes and



maximum degree  $\Delta$ . Moreover, one sees that

$$E_1(T') = E_1(T', v_s) = \frac{n-1}{s} - 2 \sum_{i=1}^{s-1} (s+i)^{-1} - \frac{\Delta+1}{2s}.$$

As

$$E_1(T) = E_1(T, v_{s+1}) = \frac{n}{s+1} - 2 \sum_{i=1}^s (s+i)^{-1} - \frac{\Delta}{2s+1},$$

we deduce that

$$\begin{aligned} E_1(T') - E_1(T) &= \frac{n-s-1}{s(s+1)} + \frac{2s+1-\Delta}{2s(2s+1)} \\ &= \frac{s(4n-2s-3-\Delta) + 2n-1-\Delta}{2s(s+1)(2s+1)} \\ &= \frac{s(3n-3) + n+2s-1}{2s(s+1)(2s+1)} > 0, \end{aligned}$$

where the last line uses that  $n = d + \Delta - 1 = 2s + \Delta > 1$ .

We conclude that  $v$  is not on  $P$ . In this case,  $v$  is adjacent to exactly  $\Delta - 1$  leaves  $u_1, \dots, u_{\Delta-1}$ . For each  $i \in \{1, \dots, \Delta - 1\}$ , we delete the edge  $\{v, u_i\}$  and add the edge  $\{v_d, u_i\}$ . It follows that  $T'$  has maximum degree  $\Delta$ , order  $n$ , diameter  $d + 1$  and  $E_1(T') > E_1(T)$ , a contradiction. This contradiction shows that  $d$  must be even.

Suppose now that  $d = 2k + 2$  with  $k \geq k(n, \Delta)$ . In particular,  $k \geq 2$  since  $d \geq 4$ . Our goal is to obtain a contradiction by showing the existence of a tree  $T'$  with  $n$  nodes, maximum degree  $\Delta$  and diameter  $2k$  such that  $E_1(T') > E_1(T)$ . Since  $d$  is even, Lemma 10 allows us to assume that  $T$  belongs to  $\mathcal{F}_{\Delta, k+1}(n)$ . Recall that  $n \leq \eta(\Delta, k(n, \Delta)) \leq \eta(\Delta, k)$ .

Notice that the central node of  $T$ , which is the node labeled  $k+1$ , has degree 2 in  $T$ . Indeed, if it had degree more than 2, then as  $T$  belongs to  $\mathcal{F}_{\Delta, k+1}(n)$ , we infer that the subtrees of  $T$  rooted at the nodes labeled  $k$  and  $k+2$  are both  $(\Delta - 1)$ -trees of depth  $k$  by Lemma 8(4). Consequently, each of these trees contains  $\nu(\Delta - 1, k)$  nodes. Therefore, the total number of nodes of  $T$  would be greater than  $2 \cdot \nu(\Delta - 1, k)$ , which is at least  $\eta(\Delta, k)$  as  $\Delta \geq 3$  and  $k \geq 2$ , a contradiction.

In other words,  $T$  contains exactly two nodes of depth 1. A similar counting argument allows us to establish that  $T$  contains at most  $\Delta$  nodes of depth 2. Indeed, let  $x$  be the number of nodes of  $T$  of depth 2, hence  $2 \leq x \leq 2\Delta - 2$ . Since  $T \in \mathcal{F}_{\Delta, k+1}(n)$ , if  $x > 2$  then all but at most one of the  $x$  subtrees of  $T$  rooted at the nodes of depth 2 are  $(\Delta - 1)$ -trees of depth  $k - 1$ . Consequently,  $T$  contains more than  $1 + (x - 1) \cdot \nu(\Delta - 1, k - 1)$  nodes. Therefore,

$$1 + (x - 1) \cdot \nu(\Delta - 1, k - 1) < n \leq \eta(\Delta, k) = 1 + \Delta \cdot \nu(\Delta - 1, k - 1),$$

which implies that  $x - 1 < \Delta$ , that is,  $x \leq \Delta$  as asserted.

We now define a new tree  $T'$ . (An example of the construction is given in Figure 5.) Let  $P = v_0 \cdots v_d$  be the root-path of  $T$ , that is, the path induced by nodes with labels in  $\{0, \dots, d\}$ . For each node  $v$  in  $P$ , let  $S(v)$  be the collection of all neighbors of  $v$  in  $T$  that do not belong to  $P$ . To obtain  $T'$ , we start from a path  $v'_1 \cdots v'_{d-1}$ , so, in particular,  $T'$  will have diameter at least (and, actually, exactly)  $d-2$ . For each  $i$  from 1 to  $d-1$  and for each node  $v$  in  $S(v_i)$ , we define  $T_v$  to be the subtree of  $T$  rooted at  $v$ . We add to  $T'$  a copy of  $T_v$  and join its root to the node  $v'_j$  of  $T'$  with

$$j := \begin{cases} i + 1 & \text{if } i \in \{1, \dots, k\}, \text{ and} \\ i - 1 & \text{if } i \in \{k + 2, \dots, d - 1\}. \end{cases}$$

Note that, as we proved earlier, the node labeled  $k + 1$  in  $T$  has exactly two children, which both belong to  $P$ . Hence the tree  $T'$  is well defined and so far it contains exactly  $n - 2$  nodes. Moreover, as proved earlier,  $T$  contains at most  $\Delta$  nodes of depth 2. Consequently, the degree of  $v_{d/2}$  in  $T'$  is at most  $\Delta$ . In total, the maximum degree of  $T'$  is hence exactly  $\Delta$ . Last, the radius of  $T'$  is  $k$  since each node is at distance at most  $k$  from  $v_{d/2}$  by the construction.

We finish the construction of  $T'$  by doing twice the following: among all nodes of degree less than  $\Delta$  and depth less than  $k$ , we choose a node  $v$  with the largest possible depth and we add a new neighbor to  $v$ . These last two steps are always possible, since  $n \leq 1 + \Delta \frac{(\Delta-1)^{k-1}}{\Delta-2}$ . In case there are more than one such node, we choose the one corresponding to the node of  $T$  with the smallest label. Let  $v'_0$  and  $v'_d$  be these two added nodes.

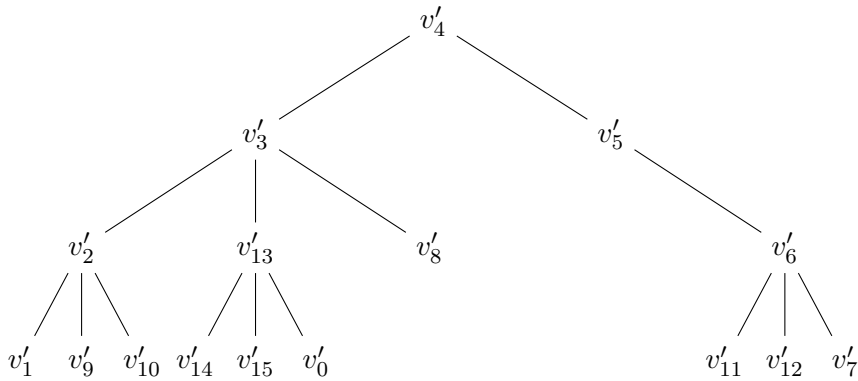


Figure 5. The tree  $T'$  obtained if  $T$  is  $F_{4,4}(16)$ , the tree of Figure 4.

Observe that  $T' \in \mathcal{F}_{\Delta,k}(n)$ , with root-path  $v'_1 \cdots v'_{d-1}$ . Notice also that there is a natural one-to-one correspondence between the nodes of  $T$  and  $T'$ , with  $v'_0$

and  $v'_d$  corresponding to  $v_0$  and  $v_d$ . Consequently, we shall make no distinction between nodes of  $T$  and  $T'$  in what follows, and we call  $V$  the common set of nodes of  $T$  and  $T'$ .

It remains to show that  $E_1(T') > E_1(T)$ . To this end, we set for convenience  $\mu'(v) := E_{T'}(v_{k+1}) - E_{T'}(v)$  and  $\mu(v) := E_T(v_{k+1}) - E_T(v)$  for every node  $v \in V$ . We consider partitions  $(V_i)_{1 \leq i \leq t}$  and  $(V'_i)_{1 \leq i \leq t'}$  of the nodes of  $T$  and  $T'$  given by Lemma 8, respectively. Notice that  $t' \in \{t, t+1, t+2\}$ , depending on whether  $v'_0$  was joined to a node of degree  $\Delta - 1$  or not and of depth  $k - 1$  or less (recall that  $v'_0$  is the last but one node added to  $T'$  in the construction process). Hence

$$E_1(T') - E_1(T) \geq \sum_{i=1}^t \left( \sum_{v \in V'_i} \mu'(v) - \sum_{v \in V_i} \mu(v) \right).$$

We shall now establish that  $E_1(T') - E_1(T) > 0$  by proving that  $\sum_{v \in V'_i} \mu'(v) - \sum_{v \in V_i} \mu(v) \geq 0$  for each  $i \in \{1, \dots, t\}$ , with strict inequality for at least one index.

The set  $V_1$  is composed of  $v_0, \dots, v_{k+1}$  and the set  $V_2$  of  $v_{k+2}, \dots, v_{2k+2}$ . The set  $V'_1$  is composed of  $v_1, \dots, v_{k+1}$  and the set  $V'_2$  of  $v_{k+2}, \dots, v_{2k+1}$ . Since  $\mu'(v_{k+1}) = 0 = \mu(v_{k+1})$ , we deduce that  $\sum_{v \in V_1} \mu(v) = \sum_{v \in V_2} \mu(v)$  and also that  $\sum_{v \in V'_1} \mu'(v) = \sum_{v \in V'_2} \mu'(v)$ . Hence, it follows that for each  $i \in \{1, 2\}$ ,

$$\begin{aligned} \sum_{v \in V'_i} \mu'(v) - \sum_{v \in V_i} \mu(v) &= \sum_{j=0}^{k-1} \left( \frac{1}{k} - \frac{1}{2k-j} \right) - \sum_{j=0}^k \left( \frac{1}{k+1} - \frac{1}{2k+2-j} \right) \\ &= \frac{1}{2k+2} + \frac{1}{2k+1} - \frac{1}{k+1} = \frac{1}{2k+1} - \frac{1}{2k+2} > 0. \end{aligned}$$

Now, fix  $i \in \{3, \dots, t-1\}$ . Since  $T \in \mathcal{F}_{\Delta, k+1}(n)$ , there is at most one leaf of  $T$  with depth less than  $k+1$ , which necessarily belongs to  $V_i$ . Thus the monotone path  $P_i$  induced by  $V_i$  in  $T$  starts from a leaf of depth  $k+1$ . Similarly, the monotone path  $P'_i$  induced by  $V'_i$  in  $T'$  starts from a leaf of depth  $k$ . Observe that  $|V_i| = |V'_i| \in \{1, \dots, k\}$ . Consequently, setting  $\ell := |V_i|$ , we deduce that

$$\begin{aligned} &\sum_{v \in V'_i} \mu'(v) - \sum_{v \in V_i} \mu(v) \\ &= \left( \frac{\ell}{k} - \sum_{j=0}^{\ell-1} \frac{1}{2k-j} \right) - \left( \frac{\ell}{k+1} - \sum_{j=0}^{\ell-1} \frac{1}{2k+2-j} \right) \\ &= \frac{\ell}{k(k+1)} - \sum_{j=0}^{\ell-1} \frac{1}{2k-j} + \sum_{j=-2}^{\ell-3} \frac{1}{2k-j} \end{aligned}$$

$$\begin{aligned}
&= \frac{\ell}{k(k+1)} - \frac{1}{2k+1-\ell} - \frac{1}{2k+2-\ell} + \frac{1}{2k+2} + \frac{1}{2k+1} \\
&= \frac{\ell \cdot f(k, \ell)}{2k(k+1)(2k+1)(2k+1-\ell)(2k+2-\ell)},
\end{aligned}$$

where  $f(k, \ell) := 8k^3 - k^2(12\ell - 20) + k(4\ell^2 - 17\ell + 15) + 2\ell^2 - 6\ell + 4$ . As a function of  $\ell \in [1, k]$ , we see that  $f(k, \ell)$  is decreasing so  $f(k, \ell) \geq f(k, k) = 5k^2 + 9k + 4$ , which is positive.

It remains to consider the sets  $V_t$  and  $V'_t$ . Note that  $V_t \subseteq V'_t$ . Therefore, the exact same reasoning as above applies, using  $|V_t|$  for  $\ell$  and ignoring the nodes in  $V'_t \setminus V_t$ , which is possible as  $\mu'(v) \geq 0$  for every node  $v$ . Consequently,  $E_1(T') > E_1(T)$ , which is a contradiction. We conclude that  $T$  is a tree of diameter  $2k_0$ .

Now if  $n = \nu(\Delta, k_0)$ , then  $T$  is the full  $\Delta$ -regular tree  $F_{\Delta, k_0}$ , which is the unique element of  $\mathcal{T}_{\Delta, k_0}(n)$ . Otherwise,  $n < \nu(\Delta, k_0)$  and, in particular,  $(n_1(T), \dots, n_{k_0}(T))$  must be an optimal solution to the problem (P) with parameters  $k_0, n-1, \Delta$  and  $\alpha_i := \frac{1}{k_0+i}$  for  $i \in \{1, \dots, k_0\}$ . Proposition 12 thus implies that  $(n_1(T), \dots, n_{k_0}(T))$  is uniquely defined and corresponds to the sizes of the layers of a tree in  $\mathcal{F}_{\Delta, k_0}(n)$ . We infer that  $T$  belongs to  $\mathcal{F}_{\Delta, k_0}(n)$ , which finishes the proof of Theorem 7.

We conclude by pointing out that valid operations provide an efficient algorithmic way of building all possible networks in  $\mathcal{T}_{n, \Delta}^*$ . We also notice that central nodes in tree networks with fixed maximum degree  $\Delta$  need not have degree  $\Delta$ .

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