Publ. Math. Debrecen
77/3-4 (2010), 347–367

Asymptotics of the extremal values of certain graph parameters in trees with bounded degree

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Abstract. In a recent paper, the authors of this note determined the trees of given maximum degree which maximize the number of independent vertex subsets and minimize the number of independent edge subsets respectively. It turned out that some kind of digit representation plays a major role in the characterization of the optimal trees. In the current paper, we study the asymptotic behavior of the optimal parameter values. It turns out that they increase exponentially, but with fluctuations which can be described by means of the aforementioned digit system.

1. Introduction

Characterizing the graphs or trees which maximize or minimize a certain graph parameter is a problem that has already been the topic of a vast amount of papers, see for instance [5], [11], [14], [18]. Most typically, the extremal values of a graph parameter among all trees of a prescribed size are given for the star and the path respectively. Among others, this is the case for the number of *independent vertex subsets* and the number of *independent edge subsets*, which will be discussed in the current work. An exception to this rule is the number of *maximal independent sets* (cf. Wilf [18]). If the maximum degree is bounded above, the path stays extremal, of course, but the star does not for obvious reasons. However, this is a pretty natural restriction not only for theoretical considerations,

2000 *Mathematics Subject Classification:* 05A16, 05C69, 05C05, 11A63.
Key words and phrases: independent sets, d-ary trees, digit expansion, asymptotics.
C. Heuberger is supported by the Austrian Science Foundation FWF, project S9606, that is part of the Austrian National Research Network "Analytic Combinatorics and Probabilistic Number Theory".

but also for applications: several graph parameters are known to be of interest in theoretical chemistry, where they are used for predicting the behavior of molecules [2], [3], [4], [8]. Trees with given maximum degree are frequently studied in mathematical chemistry, see for instance [12], [15], [19], where the graph energy, largest eigenvalue and Laplacian spectral radius are investigated.

In recent articles of SZÉKELY and WANG [16], [17], binary trees maximizing the number of *subtrees* are determined and formulæ for the resulting maximal numbers are given; the more general case of trees with bounded maximum degree was treated by KIRK and WANG [9]. Similarly, the authors of this paper investigated the number of independent vertex subsets and edge subsets for trees with bounded maximum degree, thereby also improving upon work of LV and YU [13]. The results are quite surprising–in particular, the following theorem [7] was proved:

Theorem 1. *Let n be a positive integer and $d \geq 2$. Then there is a unique (up to isomorphism) tree X_n with n vertices and maximum degree $\leq d+1$ that maximizes the number of independent vertex subsets; the same tree also minimizes the number of independent edge subsets. It can be decomposed as,*

with $M_{k,1}, \ldots, M_{k,d-1} \in \{C_k, C_{k+2}\}$ for $0 \leq k < \ell$ and either $M_{\ell,1} = \cdots = M_{\ell,d} = C_{\ell-1}$ or $M_{\ell,1} = \cdots = M_{\ell,d} = C_\ell$ or $M_{\ell,1}, \ldots, M_{\ell,d} \in \{C_\ell, C_{\ell+1}, C_{\ell+2}\}$, where at least two of $M_{\ell,1}, \ldots, M_{\ell,d}$ equal $C_{\ell+1}$. Here, C_h denotes the complete d-ary tree of height $h-1$ (and C_0 is the empty graph).

It was also shown that there is a natural connection to *digital systems*: if a_k denotes the number of $M_{k,j}$s which are isomorphic to C_{k+2}, and if $\tilde{a}_\ell$ is the number of $M_{\ell,j}$s which are isomorphic to $C_{\ell+1}$, we have

$$n = \sum_{k=0}^{\ell-1} (1 + (d+1)a_k)d^k + (1 + \tilde{a}_\ell + (d+1)a_\ell)d^\ell + \frac{d^\ell - 1}{d-1}. \tag{1}$$

In the case that $M_{\ell,1} = \cdots = M_{\ell,d} = C_{\ell-1}$, we set $a_\ell = 0$ and $\tilde{a}_\ell = -1$. It follows immediately that a_k is uniquely determined by the remainder of $(d-1)n$ modulo

d^{k+1}. The numbers a_k (or $1+(d+1)a_k$) can thus be interpreted as *digits*. Indeed, any positive integer n can be written uniquely in the form (1).

However, nice explicit formulæ (as in the aforementioned papers of Székely and Wang) for the corresponding extremal values of the two graph parameters cannot be expected in view of the rather complicated structure. It is possible to determine the values recursively (as exhibited in Section 3), and these recursions could theoretically be turned into explicit formulæ involving multiple sums, but without being very enlightening. In this paper, the asymptotic behavior of the number of independent vertex subsets and independent edge subsets of X_n is exhibited. The main result is the following:

Theorem. *Let $\sigma(X_n)$ and $Z(X_n)$ denote the number of independent vertex subsets and independent edge subsets of X_n respectively. There exist constants $\beta = \beta(d)$ and $\delta = \delta(d)$, such that*

$$\sigma(X_n) = \rho_n \beta^{(d-1)n} \quad \text{and} \quad Z(X_n) = \tau_n \delta^{(d-1)n},$$

where ρ_n and τ_n are bounded above and below by positive constants depending only on d.

The values ρ_n and τ_n depend on the digits a_k in representation (1) in a rather complicated way. It is shown, though, that ρ_n is Cesàro-convergent for $d \leq 4$ and that τ_n is Cesàro-convergent for arbitrary d. This surprisingly complicated asymptotic behavior is an indication that simple explicit formulæ are most probably not available.

2. Notations and preliminaries

Definition 2.1.

(1) Let G be a graph. Then $\sigma(G)$ is defined to be the number of independent vertex subsets of G, and $Z(G)$ is the number of independent edge subsets (matchings) of G.

(2) For a rooted tree T with root v, we also define $\sigma_0(T)$ to be the number of independent vertex subsets of T not containing the root v and $\sigma_1(T)$ to be the number of independent vertex subsets of T containing the root v. Analogously, $Z_0(T)$ denotes the number of independent edge subsets of T not containing an edge incident with the root v, and $Z_1(T)$ the number of independent edge subsets of T containing an edge incident with the root v.

Note that we do not mention the root v in the notations $\sigma_0(T)$, $\sigma_1(T)$, $Z_0(T)$ and $Z_1(T)$ since the roots will usually be anonymous.

The empty set is always an independent (vertex or edge) subset of G, even if G is the empty graph. Therefore, $\sigma(G)$ and $Z(G)$ are always positive.

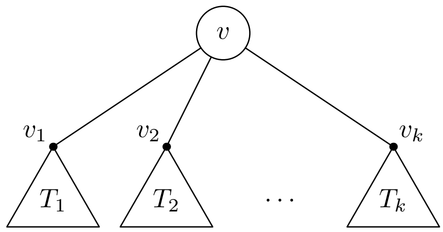

Figure 1. Rooted tree with branches

For a rooted tree T with root v, the connected components $T_1, \ldots, T_k$ of $T - v$ are called the branches of v, cf. Figure 1. Taking the neighbor v_j of v contained in T_j as root of T_j, T_j is again a rooted tree.

The following recursive formulæ are essential, but easy to prove (see for instance [4]), and will be used throughout the paper without specific reference.

Lemma 2.2. *Let T be a rooted tree with root v and branches $T_1, \ldots, T_k$. Then*

$$\sigma_0(T) = \prod_{j=1}^{k} \sigma(T_j), \qquad \sigma_1(T) = \prod_{j=1}^{k} \sigma_0(T_j),$$

$$Z_0(T) = \prod_{j=1}^{k} Z(T_j), \qquad Z_1(T) = Z_0(T) \sum_{j=1}^{k} \frac{Z_0(T_j)}{Z(T_j)}.$$

Since complete d-ary trees play a major role in the description of the optimal trees, we will need the asymptotics of $\sigma(C_h)$ and $Z(C_h)$. The former has been studied in a paper of Kirschenhofer, Prodinger and Tichy [10] – their result is the following:

Proposition 2.3. *The number of independent vertex subsets of a complete d-ary tree of height $h-1$ is*

$$s_h := \sigma(C_h) = \alpha_h \cdot \beta(d)^{d^h}$$

for a constant $\beta(d)$, and the limits

$$\lim_{k\to\infty} \alpha_{2k} = A_0(d) > 0 \quad \textit{and} \quad \lim_{k\to\infty} \alpha_{2k+1} = A_1(d) > 0$$

exist. For $d \leq 4$, $A_0(d) = A_1(d) =: A(d)$.

Remark 2.4. From Lemma 2.2, it is clear that

$$s_h = s_{h-1}^d + s_{h-2}^{d^2},$$

and so the constants $A_0 = A_0(d)$ and $A_1 = A_1(d)$ satisfy the equations

$$A_0 = A_1^d + A_0^{d^2} \quad \text{and} \quad A_1 = A_0^d + A_1^{d^2}. \tag{2}$$

From this, it also follows that $0 < A_0, A_1 < 1$. However, we need a refinement of this result for our purposes, which is given in the following proposition.

Proposition 2.5. *With α_h and A_0, A_1 as in Proposition 2.3, we have*

$$\alpha_{2k} = A_0 + O(B^k) \quad \textit{and} \quad \alpha_{2k+1} = A_1 + O(B^k)$$

for a constant $B = B(d) < 1$.

Proof. We first introduce the auxiliary quantity $\phi_h = \alpha_h \alpha_{h-1}^{-d} = s_h s_{h-1}^{-d}$. Then we have

$$\phi_h = 1 + \phi_{h-1}^{-d},$$

thus simplifying our recurrence to a first order recurrence. We will show that

$$\phi_{2k} = p_0 + O(B^k) \quad \text{and} \quad \phi_{2k+1} = p_1 + O(B^k) \tag{3}$$

for some constants p_0, p_1 and $0 < B < 1$ that depend only on d. This will be used to derive the original assertions.

It has already been shown in [10] that ϕ_{2k} is increasing, ϕ_{2k+1} is decreasing and $\phi_{2k} < \phi_{2k+1}$ for all k. Hence, the two sequences converge to limits p_0 and p_1 respectively, where $p_0 \leq p_1$, $p_0 = 1 + p_1^{-d}$ and $p_1 = 1 + p_0^{-d}$. If $\Phi(x) := 1 + (1 + x^{-d})^{-d}$, then $\phi_{2k+2} = \Phi(\phi_{2k})$ and $\phi_{2k+1} = \Phi(\phi_{2k-1})$, so p_0 and p_1 are fixed points of the map $x \mapsto \Phi(x)$. If we can show that $|\Phi'(p_0)|$ and $|\Phi'(p_1)|$ are both less than 1, then Φ is a contraction in a neighborhood of p_0 and p_1 respectively, and we have (3). To this end, consider the derivative of $\Phi(x)$, which is given by

$$\Phi'(x) = d^2 x^{-d-1}(1 + x^{-d})^{-d-1}.$$

We want to show that

$$d^2 p_0^{-d-1}(1+p_0^{-d})^{-d-1} < 1 \quad \text{and} \quad d^2 p_1^{-d-1}(1+p_1^{-d})^{-d-1} < 1.$$

Note that since $p_0 = 1 + p_1^{-d}$ and $p_1 = 1 + p_0^{-d}$, the two values are actually equal. Since we have monotone convergence to the points p_0, p_1, we know that the derivative cannot be > 1, so it remains to rule out the case that it is equal to 1, i.e., to prove that there is no solution to the system

$$p_0 = 1 + p_1^{-d},\ p_1 = 1 + p_0^{-d} \quad \text{and} \quad (p_0 p_1)^{d+1} = d^2. \tag{4}$$

This can be achieved as follows: from the first two equations, we deduce

$$(p_0 p_1)^d = \frac{1}{(p_0 - 1)(p_1 - 1)}$$

and thus

$$d^2 = (p_0 p_1)^{d+1} = \frac{p_0 p_1}{(p_0 - 1)(p_1 - 1)}.$$

It follows that $p_0 + p_1 = (1 - d^{-2})p_0 p_1 + 1 = (1 - d^{-2})d^{2/(d+1)} + 1$, so that p_0 and p_1 have to be the solutions of the quadratic equation

$$u^2 - \Big((1 - d^{-2})d^{2/(d+1)} + 1\Big)\, u + d^{2/(d+1)},$$

which are given by

$$\frac{1}{2}\left((1 - d^{-2})d^{2/(d+1)} + 1 \pm \sqrt{\Big((1 - d^{-2})d^{2/(d+1)} + 1\Big)^2 - 4d^{2/(d+1)}}\right).$$

This is only a necessary condition for the solutions to (4). We want to show that this is not sufficient, in fact, we will derive a contradiction to (4) by asympototic estimates. (For $2 \le d \le 4$, there are no real solutions, so these cases can be excluded immediately). Of the two solutions, p_0 is the smaller one (it is trivial to rule out the case $p_0 = p_1 = d^{1/(d+1)}$). Now we claim that

$$\sqrt{\Big((1 - d^{-2})d^{2/(d+1)} + 1\Big)^2 - 4d^{2/(d+1)}} \ge (1 - d^{-2})d^{2/(d+1)} - 1 - 2d^{-1} \tag{5}$$

for $d \ge 6$. To show this, note first that

$$\Big((1 - d^{-2})d^{2/(d+1)} + 1\Big)^2 - 4d^{2/(d+1)} = \Big((1 - d^{-2})d^{2/(d+1)} - 1\Big)^2 - 4d^{-2d/(d+1)}.$$

Of course, we only have to consider the case that the right hand side in (5) is positive. Thus, squaring the inequality (5) shows that it is equivalent to

$$4d^{-1}\Big((1-d^{-2})d^{2/(d+1)}-1\Big) \geq 4d^{-2d/(d+1)}+4d^{-2}.$$

We multiply by $d^{1-2/(d+1)}/4$ and rearrange the summands to get

$$1 \geq d^{-2/(d+1)}+d^{-1}+d^{-1-2/(d+1)}+d^{-2} = (1+d^{-1})(d^{-1}+d^{-2/(d+1)}).$$

This is equivalent to

$$d^{2/(d+1)} \geq 1+\frac{1+2d}{d^2-d-1},$$

which can be strengthened to

$$\frac{2\log d}{d+1} \geq \frac{1+2d}{d^2-d-1},$$

and this is true for $d \geq 6$. Now we get

$$p_0 \leq \frac{1}{2}\big((1-d^{-2})d^{2/(d+1)}+1-(1-d^{-2})d^{2/(d+1)}+1+2d^{-1}\big) = 1+d^{-1} \leq \exp(d^{-1}),$$

and it follows that

$$1+p_0^{-d} \geq 1+e^{-1}.$$

On the other hand,

$$p_1 = \frac{d^{2/(d+1)}}{p_0} \leq d^{2/(d+1)}$$

and since $d^{2/(d+1)} < 1+e^{-1}$ for $d \geq 18$, this yields a contradiction. For the remaining values $d \leq 17$, it can be checked directly that the equation $1+p_0^{-d} = p_1$ is not satisfied. Therefore, our estimate for ϕ_h is proved.

Now note that

$$\log s_h = d\log s_{h-1}+\log\phi_h$$

from which we deduce, by iteration,

$$\log s_h = d^h\log s_0+\sum_{k=1}^{h} d^{h-k}\log\phi_k = d^h\sum_{k=1}^{\infty} d^{-k}\log\phi_k - \sum_{k=h+1}^{\infty} d^{h-k}\log\phi_k,$$

and finally

$$\beta = \exp\left(\sum_{k=1}^{\infty} d^{-k}\log\phi_k\right)$$

and

$$\begin{aligned}
\alpha_h &= \exp\left(-\sum_{k=1}^{\infty} d^{-k}\log\phi_{h+k}\right)\\
&= \exp\left(-\sum_{k=1}^{\infty} d^{-2k+1}\big(\log p_1 + O(B^{h/2+k})\big) - \sum_{k=1}^{\infty} d^{-2k}\big(\log p_0 + O(B^{h/2+k})\big)\right)\\
&= \exp\left(-\frac{d}{d^2-1}\log p_1 - \frac{1}{d^2-1}\log p_0 + O(B^{h/2})\right)\\
&= (p_1^d p_0)^{-1/(d^2-1)} + O(B^{h/2}) = A_0 + O(B^{h/2})
\end{aligned}$$

for even h and analogously

$$\alpha_h = (p_0^d p_1)^{-1/(d^2-1)} + O(B^{h/2}) = A_1 + O(B^{h/2})$$

for odd h, which proves our claim. □

To the best of our knowledge, the asymptotic behavior of $Z(C_h)$ does not appear in the literature, so we give a short proof for it (the treatment is even easier than in the case of independent vertex subsets).

Proposition 2.6. *The number of independent edge subsets of a complete d-ary tree of height $h-1$ is*

$$z_h := Z(C_h) \sim \gamma(d)\cdot\delta(d)^{d^h}$$

for constants $\gamma(d), \delta(d)$, where

$$\gamma(d) = \left(\frac{1+\sqrt{4d+1}}{2}\right)^{-1/(d-1)}.$$

Proof. Lemma 2.2 readily yields the recursion

$$z_h = z_{h-1}^d + d z_{h-1}^{d-1} z_{h-2}^d$$

with initial values $z_0 = z_1 = 1$. Now, write $y_h = z_h z_{h-1}^{-d}$. Then the recurrence formula transforms to

$$y_h = 1 + \frac{d}{y_{h-1}},$$

and straightforward induction (note that $y_1 = 1$) yields

$$y_h = \frac{u^{h+1} - v^{h+1}}{u^h - v^h},$$

where $u := \frac{1+\sqrt{4d+1}}{2}$ and $v := \frac{1-\sqrt{4d+1}}{2}$, so y_h tends to $u = \frac{1+\sqrt{4d+1}}{2}$. Iterating $z_h = z_{h-1}^d y_h = z_{h-2}^{d^2} y_{h-1}^d y_h = \dots$ gives

$$z_h = \prod_{k=1}^{h} y_k^{d^{h-k}}.$$

Now we take logarithms again, the usual method in the analysis of polynomial recurrences (see [1]):

$$\begin{aligned}\log z_h &= d^h \sum_{k=1}^{h} d^{-k} \log y_k = d^h \sum_{k=1}^{\infty} d^{-k} \log y_k - d^h \sum_{k=h+1}^{\infty} d^{-k} \log y_k \\ &= d^h C(d) - d^h \sum_{k=h+1}^{\infty} d^{-k} \log y_k.\end{aligned}$$

$C(d)$ is a constant depending only on d – the sum converges since y_k tends to a limit and is thus bounded. Now

$$y_k = \frac{u^{k+1} - v^{k+1}}{u^k - v^k} = u + (u-v) \cdot \frac{v^k}{u^k - v^k} = u + O\left(\left|\frac{v}{u}\right|^k\right)$$

and thus

$$d^h \sum_{k=h+1}^{\infty} d^{-k} \log y_k = d^h \sum_{k=h+1}^{\infty} \left(d^{-k} \log u + O\left(\left|\frac{v}{ud}\right|^k\right)\right) = \frac{\log u}{d-1} + O\left(\left|\frac{v}{u}\right|^h\right).$$

Therefore,

$$z_h = \exp\left(C(d) \cdot d^h - \frac{\log u}{d-1} + O\left(\left|\frac{v}{u}\right|^h\right)\right),$$

and the proposition follows. □

3. Asymptotics for the optimal tree

Now, in order to obtain the asymptotic number of independent (vertex or edge) subsets of the tree described in Theorem 1, we first consider a slightly simpler tree defined as follows:

Definition 3.1. Let $T(a_0, a_1, \dots, a_\ell)$ $(0 \leq a_k < d)$ be the tree that can be decomposed as, with $M_{k,1},\dots,M_{k,a_k}=C_{k+2}$ and $M_{k,a_k+1},\dots,M_{k,d-1}=C_k$.

Then we have, by Lemma 2.2,

$$\begin{aligned}\sigma(T(a_0,\dots,a_\ell)) &= \sigma(C_\ell)^{d-1-a_\ell}\sigma(C_{\ell+2})^{a_\ell}\sigma(T(a_0,\dots,a_{\ell-1}))\\ &+\sigma(C_{\ell-1})^{d-1-a_{\ell-1}}\sigma(C_{\ell+1})^{a_{\ell-1}}\sigma_0(C_\ell)^{d-1-a_\ell}\sigma_0(C_{\ell+2})^{a_\ell}\sigma(T(a_0,\dots,a_{\ell-2}))\end{aligned} \tag{6}$$

and

$$\begin{aligned}Z(T(a_0,\dots,a_\ell)) &= Z(C_\ell)^{d-1-a_\ell}Z(C_{\ell+2})^{a_\ell}\\ &\times\left(1+\frac{(d-1-a_\ell)Z_0(C_\ell)}{Z(C_\ell)}+\frac{a_\ell Z_0(C_{\ell+2})}{Z(C_{\ell+2})}\right)Z(T(a_0,\dots,a_{\ell-1}))\\ &+Z(C_{\ell-1})^{d-1-a_{\ell-1}}Z(C_{\ell+1})^{a_{\ell-1}}Z(C_\ell)^{d-1-a_\ell}Z(C_{\ell+2})^{a_\ell}Z(T(a_0,\dots,a_{\ell-2})).\end{aligned}$$

Furthermore, denote the tree that maximizes σ and minimizes Z by X_n as in Theorem 1, and take a_k and $\tilde a_\ell$ as in (1). We have the following formula for the number of independent vertex subsets of X_n:

$$\begin{aligned}\sigma(X_n) &= \sigma(C_\ell)^{d-a_\ell-\tilde a_\ell}\sigma(C_{\ell+1})^{\tilde a_\ell}\sigma(C_{\ell+2})^{a_\ell}\sigma(T(a_0,\dots,a_{\ell-1}))\\ &+\sigma(C_{\ell-1})^{d-1-a_{\ell-1}}\sigma(C_{\ell+1})^{a_{\ell-1}}\sigma_0(C_\ell)^{d-a_\ell-\tilde a_\ell}\\ &\times\sigma_0(C_{\ell+1})^{\tilde a_\ell}\sigma_0(C_{\ell+2})^{a_\ell}\sigma(T(a_0,\dots,a_{\ell-2}))\end{aligned} \tag{7}$$

in the case that $\tilde a_\ell \neq -1$ and

$$\begin{aligned}\sigma(X_n) &= \sigma(C_{\ell-1})^{d}\sigma(T(a_0,\dots,a_{\ell-1}))\\ &+\sigma_0(C_{\ell-1})^{d}\sigma(C_{\ell-1})^{d-1-a_{\ell-1}}\sigma(C_{\ell+1})^{a_{\ell-1}}\sigma(T(a_0,\dots,a_{\ell-2}))\end{aligned}$$

otherwise. On the other hand, the number of independent edge subsets of X_n is given by

$$\begin{aligned}Z(X_n) &= \left(1+\frac{(d-a_\ell-\tilde a_\ell)Z_0(C_\ell)}{Z(C_\ell)}+\frac{\tilde a_\ell Z_0(C_{\ell+1})}{Z(C_{\ell+1})}+\frac{a_\ell Z_0(C_{\ell+2})}{Z(C_{\ell+2})}\right)\\ &\times Z(C_\ell)^{d-a_\ell-\tilde a_\ell}Z(C_{\ell+1})^{\tilde a_\ell}Z(C_{\ell+2})^{a_\ell}Z(T(a_0,\dots,a_{\ell-1}))\\ &+Z(C_{\ell-1})^{d-1-a_{\ell-1}}Z(C_{\ell+1})^{a_{\ell-1}}\\ &\times Z(C_\ell)^{d-a_\ell-\tilde a_\ell}Z(C_{\ell+1})^{\tilde a_\ell}Z(C_{\ell+2})^{a_\ell}Z(T(a_0,\dots,a_{\ell-2}))\end{aligned}$$

for $\tilde{a}_\ell \neq -1$ and

$$Z(X_n) = \left(Z(C_{\ell-1})^d + dZ_0(C_{\ell-1})Z(C_{\ell-1})^{d-1}\right) Z(T(a_0,\dots,a_{\ell-1})) \\ + Z(C_{\ell-1})^{d-1-a_{\ell-1}} Z(C_{\ell+1})^{a_{\ell-1}} Z(C_{\ell-1})^d Z(T(a_0,\dots,a_{\ell-2}))$$

otherwise. The first step in the derivation of the desired asymptotics is the following proposition:

Proposition 3.2. *Define $\lambda(a_0,\dots,a_\ell)$ by*

$$\sigma(T(a_0,a_1,\dots,a_\ell)) = \lambda(a_0,\dots,a_\ell)\cdot\beta^{(d-1)\sum_{k=0}^{\ell}(1+(d+1)a_k)d^k}$$

with $\beta=\beta(d)$ as in Proposition 2.3. Then $\lambda(a_0,\dots,a_\ell)$ is uniformly bounded above and below by positive constants. Furthermore, for $d\le 4$, one can write

$$\lambda(a_0,\dots,a_m) = \sum_{k=0}^{m}\mu(a_0,\dots,a_k),$$

where

$$|\mu(a_0,\dots,a_k)| \le C_\sigma D_\sigma^k$$

holds for absolute constants $C_\sigma = C_\sigma(d) > 0$ and $0 < D_\sigma = D_\sigma(d) < 1$ depending only on d. Similarly,

$$Z(T(a_0,a_1,\dots,a_\ell)) = \zeta(a_0,\dots,a_\ell)\cdot\delta^{(d-1)\sum_{k=0}^{\ell}(1+(d+1)a_k)d^k}$$

with $\delta=\delta(d)$ as in Proposition 2.6, and the decomposition

$$\zeta(a_0,\dots,a_m) = \sum_{k=0}^{m}\xi(a_0,\dots,a_k),$$

holds for arbitrary d, where

$$|\xi(a_0,\dots,a_k)| \le C_Z D_Z^k$$

holds for absolute constants $C_Z = C_Z(d) > 0$ and $0 < D_Z = D_Z(d) < 1$ depending only on d.

Proof. We only give a proof for $\lambda(a_0,a_1,\dots,a_\ell)$, since the second part can be proved along the same lines (and is even easier). Noting that $\sigma_0(C_k) = \sigma(C_{k-1})^d$, Proposition 2.3, together with formula (3), shows that

$$\lambda(a_0,\dots,a_\ell)\cdot\beta^{(d-1)\sum_{k=0}^{\ell}(1+(d+1)a_k)d^k} \\ = \alpha_\ell^{d-1-a_\ell}\beta^{(d-1-a_\ell)d^\ell}\alpha_{\ell+2}^{a_\ell}\beta^{a_\ell d^{\ell+2}}\lambda(a_0,\dots,a_{\ell-1})\beta^{(d-1)\sum_{k=0}^{\ell-1}(1+(d+1)a_k)d^k} \\ + \alpha_{\ell-1}^{d-1-a_{\ell-1}}\beta^{(d-1-a_{\ell-1})d^{\ell-1}}\alpha_{\ell+1}^{a_{\ell-1}}\beta^{a_{\ell-1}d^{\ell+1}}\alpha_{\ell-1}^{d(d-1-a_\ell)}\beta^{(d-1-a_\ell)d^\ell}\alpha_{\ell+1}^{da_\ell}\beta^{a_\ell d^{\ell+2}} \\ \times\lambda(a_0,\dots,a_{\ell-2})\cdot\beta^{(d-1)\sum_{k=0}^{\ell-2}(1+(d+1)a_k)d^k}$$

or

$$\lambda(a_0,\dots,a_\ell) = \alpha_\ell^{d-1-a_\ell}\alpha_{\ell+2}^{a_\ell}\lambda(a_0,\dots,a_{\ell-1}) + \alpha_{\ell-1}^{d-1-a_{\ell-1}+d(d-1-a_\ell)}\alpha_{\ell+1}^{a_{\ell-1}+da_\ell}\lambda(a_0,\dots,a_{\ell-2}). \tag{8}$$

Next we show that $\lambda(a_0,a_1,\dots,a_{\ell-1})$ is bounded above and below by positive constants. Let us assume that $a_0,a_1,\dots$ is a given infinite sequence; using the abbreviations $x_m = \lambda(a_0,a_1,\dots,a_{2m-1})$, $y_m = \lambda(a_0,a_1,\dots,a_{2m})$ and

$$\begin{aligned}
r_{1,m} &= \alpha_{2m-1}^{d-1-a_{2m-1}}\alpha_{2m+1}^{a_{2m-1}},\\
r_{2,m} &= \alpha_{2m-2}^{d-1-a_{2m-2}+d(d-1-a_{2m-1})}\alpha_{2m}^{a_{2m-2}+da_{2m-1}},\\
r_{3,m} &= \alpha_{2m}^{d-1-a_{2m}}\alpha_{2m+2}^{a_{2m}},\\
r_{4,m} &= \alpha_{2m-1}^{d-1-a_{2m-1}+d(d-1-a_{2m})}\alpha_{2m+1}^{a_{2m-1}+da_{2m}},
\end{aligned}$$

one obtains

$$x_m = r_{1,m}y_{m-1} + r_{2,m}x_{m-1} \quad \text{and} \quad y_m = r_{3,m}x_m + r_{4,m}y_{m-1}.$$

Hence, if R_m is the matrix

$$R_m := \begin{pmatrix} r_{2,m} & r_{1,m} \\ r_{2,m}r_{3,m} & r_{1,m}r_{3,m} + r_{4,m} \end{pmatrix},$$

and $\mathbf{x}_m = (x_m, y_m)^T$, we have

$$\mathbf{x}_m = R_m\mathbf{x}_{m-1}.$$

From Proposition 2.3, it follows that

$$\begin{aligned}
r_{1,m} &= A_1^{d-1} + O(B^m),\\
r_{2,m} &= A_0^{d^2-1} + O(B^m),\\
r_{3,m} &= A_0^{d-1} + O(B^m),\\
r_{4,m} &= A_1^{d^2-1} + O(B^m),
\end{aligned}$$

where the implied constants are independent of $a_0,a_1,\dots$. It follows that

$$R_m = \begin{pmatrix} A_0^{d^2-1} & A_1^{d-1} \\ A_0^{d^2+d-2} & (A_0A_1)^{d-1} + A_1^{d^2-1} \end{pmatrix} + O(B^m).$$

The limit matrix $R = \lim_{m\to\infty} R_m$ has characteristic polynomial

$$t^2 - ((A_0A_1)^{d-1} + A_0^{d^2-1} + A_1^{d^2-1})t + (A_0A_1)^{d^2-1}.$$

Multiplying the equations for A_0 and A_1 in (2), we obtain

$$A_0A_1(1 - A_0^{d^2-1})(1 - A_1^{d^2-1}) = (A_0A_1)^d$$

or

$$1 - ((A_0A_1)^{d-1} + A_0^{d^2-1} + A_1^{d^2-1}) + (A_0A_1)^{d^2-1} = 0,$$

which shows that 1 is an eigenvalue of R. The other eigenvalue is $(A_0A_1)^{d^2-1}$, which lies between 0 and 1. Furthermore, note that R and all R_m have only positive entries. Therefore, there is a real number $\epsilon > 0$ such that the inequality

$$|R - R_m| < \epsilon B^m \cdot R$$

holds componentwise. Choose m_0 large enough such that $1-\epsilon B^m > 0$ for $m > m_0$. Then we have

$$(1 - \epsilon B^m)R \le R_m \le (1 + \epsilon B^m)R$$

for $m > m_0$ and therefore

$$\begin{aligned}\left(\prod_{k=m_0+1}^{m}(1-\epsilon B^k)\right) R^{m-m_0} R_{m_0}R_{m_0-1}\dots R_1\mathbf{x}_0 &\le R_mR_{m-1}\dots R_1\mathbf{x}_0 = \mathbf{x}_m \\ &\le \left(\prod_{k=m_0+1}^{m}(1+\epsilon B^k)\right) R^{m-m_0} R_{m_0}R_{m_0-1}\dots R_1\mathbf{x}_0,\end{aligned}$$

where the inequalities hold in both components again. Since the products are bounded and R^{m-m_0} converges to a positive limit matrix in view of its eigenvalues, this shows that the components of $\mathbf{x}_m$ can be bounded above and below by absolute positive constants independent of $a_0, a_1, \dots$ (and depending only on d).

For $d \le 4$, this can be refined as follows: we set $w_m = \lambda(a_0, a_1, \dots, a_m)$ and have

$$w_m = t_{1,m}w_{m-1} + t_{2,m}w_{m-2},$$

where

$$t_{1,m} = \alpha_m^{d-1-a_m}\alpha_{m+2}^{a_m}$$

and

$$t_{2,m} = \alpha_{m-1}^{d-1-a_{m-1}+d(d-1-a_m)}\alpha_{m+1}^{a_{m-1}+da_m}.$$

From Proposition 2.3, we know that $t_{1,m} = A^{d-1} + O(B^{m/2})$ and $t_{2,m} = A^{d^2-1} + O(B^{m/2})$. Therefore,

$$w_m - A^{d-1} w_{m-1} - A^{d^2-1} w_{m-2} = \eta_m, \tag{9}$$

where $\eta_m = (t_{1,m} - A^{d-1}) w_{m-1} + (t_{2,m} - A^{d^2-1}) w_{m-2} = O(B^{m/2})$ for $m \geq 2$. All estimates are uniform in $a_0, a_1, \ldots$ again. Additionally, we set $T_1 = A^{d-1}$, $T_2 = A^{d^2-1}$, $w_{-1} = w_{-2} = 0$, $\eta_0 = w_0$ and $\eta_1 = w_1 - T_1 w_0$, so that equation (9) is valid for all $m \geq 0$. In terms of the generating functions $W(t) = \sum_{m\geq 0} w_m t^m$ and $H(t) = \sum_{m\geq 0} \eta_m t^m$, the recurrence becomes

$$W(t) = \frac{H(t)}{1 - T_1 t - T_2 t^2}.$$

Note that the equations in (2) imply that $T_1 + T_2 = A^{d-1} + A^{d^2-1} = 1$ and $0 < T_1, T_2 < 1$. The partial fraction decomposition

$$\frac{1}{1 - T_1 t - T_2 t^2} = \frac{1}{1 + T_2} \left(\frac{1}{1-t} + \frac{T_2}{1 + T_2 t} \right)$$

yields

$$W(t) = \frac{H(t)}{(1+T_2)(1-t)} + \frac{T_2 H(t)}{(1+T_2)(1+T_2 t)}$$

or

$$w_m = \frac{1}{1+T_2} \sum_{k=0}^{m} \eta_k + \frac{T_2}{1+T_2} \sum_{k=0}^{m} (-T_2)^{m-k} \eta_k.$$

Therefore,

$$\mu(a_0, a_1, \ldots, a_m) := w_m - w_{m-1} = \sum_{k=0}^{m} (-T_2)^{m-k} \eta_k.$$

Since $0 < T_2 < 1$, and since η_k also decreases exponentially, we have

$$|\mu(a_0, a_1, \ldots, a_m)| \leq C_\sigma D_\sigma^m$$

for certain constants C_σ, D_σ. This finishes the proof of Proposition 3.2. □

Now, let n be a positive integer, and take $a_k \geq 0$ ($0 \leq k \leq \ell$) and $\tilde{a}_\ell \geq -1$ as in (1). Then, (7) translates to

$$\sigma(X_n) = \alpha_\ell^{d - a_\ell - \tilde{a}_\ell} \beta^{(d - a_\ell - \tilde{a}_\ell) d^\ell} \alpha_{\ell+1}^{\tilde{a}_\ell} \beta^{\tilde{a}_\ell d^{\ell+1}} \alpha_{\ell+2}^{a_\ell} \beta^{a_\ell d^{\ell+2}}$$

$$\begin{aligned}
&\times \lambda(a_0,\dots,a_{\ell-1})\beta^{(d-1)\sum_{k=0}^{\ell-1}(1+(d+1)a_k)d^k}\\
&+ \alpha_{\ell-1}^{d-1-a_{\ell-1}}\beta^{(d-1-a_{\ell-1})d^{\ell-1}}\alpha_{\ell+1}^{a_{\ell-1}}\beta^{a_{\ell-1}d^{\ell+1}}\\
&\times \alpha_{\ell-1}^{d(d-a_\ell-\tilde a_\ell)}\beta^{(d-a_\ell-\tilde a_\ell)d^\ell}\alpha_\ell^{d\tilde a_\ell}\beta^{\tilde a_\ell d^{\ell+1}}\alpha_{\ell+1}^{da_\ell}\beta^{a_\ell d^{\ell+2}}\\
&\times \lambda(a_0,\dots,a_{\ell-2})\beta^{(d-1)\sum_{k=0}^{\ell-2}(1+(d+1)a_k)d^k}\\
={}& \big(\alpha_\ell^{d-a_\ell-\tilde a_\ell}\alpha_{\ell+1}^{\tilde a_\ell}\alpha_{\ell+2}^{a_\ell}\lambda(a_0,\dots,a_{\ell-1})\\
&+ \alpha_{\ell-1}^{d-1-a_{\ell-1}}\alpha_{\ell+1}^{a_{\ell-1}}\alpha_{\ell-1}^{d(d-a_\ell-\tilde a_\ell)}\alpha_\ell^{d\tilde a_\ell}\alpha_{\ell+1}^{da_\ell}\lambda(a_0,\dots,a_{\ell-2})\Big)\beta^{(d-1)n+1} \qquad (10)
\end{aligned}$$

for $\tilde a_l \neq -1$. In the special case that $M_{\ell,1} = \dots = M_{\ell,d} = C_{\ell-1}$, $a_\ell = 0$ and $\tilde a_\ell = -1$, we obtain analogously

$$\begin{aligned}
\sigma(X_n) ={}& \Big(\alpha_{\ell-1}^{d}\lambda(a_0,\dots,a_{\ell-1}) + \alpha_{\ell-2}^{d^2}\alpha_{\ell-1}^{d-1-a_{\ell-1}}\alpha_{\ell+1}^{a_{\ell-1}}\lambda(a_0,\dots,a_{\ell-2})\Big)\\
&\times \beta^{(d-1)n+1}. \qquad (11)
\end{aligned}$$

Hence we have proved the following theorem:

Theorem 2. *The number of independent vertex subsets of the optimal tree X_n is*

$$\sigma(X_n) = \rho_n\beta^{(d-1)n}$$

with $\beta = \beta(d)$ as in Proposition 2.3, where ρ_n is bounded above and below by positive constants which depend only on d.

For $d \le 4$, this can be refined once again:

Theorem 3. *If $d \le 4$, the sequence ρ_n is Cesàro summable, i.e.,*

$$\lim_{N\to\infty}\frac{1}{N}\sum_{n=1}^{N}\rho_n$$

exists.

Proof. From formulas (10) and (11) for $\sigma(X_n)$, it follows that

$$\rho_n = \beta\left(A^d\lambda(a_0,\dots,a_{\ell-1}) + A^{d^2+d-1}\lambda(a_0,\dots,a_{\ell-2})\right) + O(B^{\ell/2}),$$

regardless of which of the two cases holds. Now, we make use of the sum representation for $\lambda(a_0,\dots,a_\ell)$:

$$\rho_n = \beta A^d\sum_{k=0}^{\ell-1}\mu(a_0,\dots,a_k) + \beta A^{d^2+d-1}\sum_{k=0}^{\ell-2}\mu(a_0,\dots,a_k) + O(B^{\ell/2}).$$

Note that $\ell = \log_d n + O(1)$. First of all, this means that the error term sums to

$$O\left(\sum_{n=1}^{N} B^{\log_d n/2}\right) = O\left(\sum_{n=1}^{N} n^{\log B/(2\log d)}\right) = O\left(N^{1+\log B/(2\log d)}\right) = o(N).$$

Now, set $L = \lfloor \frac{1}{2}\log_d N \rfloor$, and let N_1 be the largest number such that the representation of N_1 according to equation (1) has length $< L$. Furthermore, N_2 denotes the largest multiple of d^L less or equal to N. We divide the sum $\sum_{n=1}^{N} \rho_n$ into three parts:

- First of all,
$$\sum_{n=1}^{N_1} \rho_n \ll N_1 \ll d^L \ll \sqrt{N}.$$
- Moreover,
$$\sum_{n=N_2+1}^{N} \rho_n \ll d^L \ll \sqrt{N}.$$
- Finally, since $a_0, a_1, \ldots, a_{L-1}$ only depend on n modulo d^L, and since we know that $\mu(a_0, a_1, \ldots, a_k) = O(D_\sigma^k)$, we have
$$\begin{aligned}\sum_{n=N_1+1}^{N_2} \rho_n = \beta(A^d + A^{d^2+d-1})\frac{N_2}{d^L} \sum_{0\le a_0,a_1,\ldots,a_{L-1}<d} \sum_{k=0}^{L-1} \mu(a_0,\ldots,a_k) \\ + O(N_1) + O(N_2 D_\sigma^L).\end{aligned}$$

Combining all the estimates, we obtain

$$\begin{aligned}\frac{1}{N}\sum_{n=1}^{N} \rho_n &= \beta(A^d + A^{d^2+d-1})\frac{1}{d^L} \sum_{0\le a_0,a_1,\ldots,a_{L-1}<d} \sum_{k=0}^{L-1} \mu(a_0,\ldots,a_k) \\ &\quad + O(N^{-1/2} + D_\sigma^{\frac{1}{2}\log_d N} + N^{\log B/(2\log d)}) \\ &= \beta(A^d + A^{d^2+d-1}) \sum_{k=0}^{L-1} \frac{1}{d^{k+1}} \sum_{0\le a_0,a_1,\ldots,a_k<d} \mu(a_0,\ldots,a_k) \\ &\quad + O(N^{-1/2} + D_\sigma^{\frac{1}{2}\log_d N} + N^{\log B/(2\log d)}).\end{aligned}$$

Hence, as $N \to \infty$,

$$\lim_{N\to\infty} \frac{1}{N}\sum_{n=1}^{N} \rho_n = \beta(A^d + A^{d^2+d-1}) \sum_{k=0}^{\infty} \frac{1}{d^{k+1}} \sum_{0\le a_0,a_1,\ldots,a_k<d} \mu(a_0,\ldots,a_k). \quad (12)$$

$\square$

The same theorem holds (with an analogous proof) for $Z(X_n)$ (and arbitrary d):

Theorem 4. *The number of independent edge subsets of the optimal tree X_n is*

$$Z(X_n) = \tau_n \delta^{(d-1)n}$$

with $\delta = \delta(d)$ as in Proposition 2.6, where τ_n is bounded above and below by positive constants which depend only on d. Furthermore, τ_n is Cesàro summable.

Note that Theorem 3 is not correct for $d > 4$: this is due to the fact that $\tilde{a}_\ell$ and thus the most significant digit in the representation (1) is relevant (also from an asymptotic point of view) for the value of ρ_n, and this digit is, unlike the least significant digit, not uniformly distributed (cf. [6]). This phenomenon leads to tiny fluctuations in the Cesàro means; however, the restricted means over all n such that $\tilde{a}_\ell$ is fixed converge by almost the same argument (Proposition 3.2 has to be refined for this purpose as well) as in the proof of Theorem 3.

Equation (12) is useful for the proof of convergence, but not for actually computing the value of $\lim_{N\to\infty} \frac{1}{N}\sum_{n=1}^{n} \rho_n$. For this purpose, we rewrite it once again:

$$\begin{aligned}
\lim_{N\to\infty} \frac{1}{N}\sum_{n=1}^{N} \rho_n &= \beta(A^d + A^{d^2+d-1}) \lim_{L\to\infty} \sum_{k=0}^{L} \frac{1}{d^{k+1}} \sum_{0\le a_0,a_1,\dots,a_k<d} \mu(a_0,\dots,a_k) \\
&= \beta(A^d + A^{d^2+d-1}) \lim_{L\to\infty} d^{-L-1} \sum_{0\le a_0,a_1,\dots,a_L<d} \sum_{k=0}^{L} \mu(a_0,\dots,a_k) \\
&= \beta(A^d + A^{d^2+d-1}) \lim_{L\to\infty} d^{-L-1} \sum_{0\le a_0,a_1,\dots,a_L<d} \lambda(a_0,\dots,a_L).
\end{aligned}$$

Now, set $S_\ell := \sum_{0\le a_0,a_1,\dots,a_\ell<d} \lambda(a_0,\dots,a_\ell)$. Then we can deduce a recurrence formula for S_ℓ from (8):

$$\begin{aligned}
S_\ell = &\sum_{0\le a_0,a_1,\dots,a_\ell<d} \lambda(a_0,\dots,a_\ell) \\
= &\sum_{a_\ell=0}^{d-1} \sum_{0\le a_0,a_1,\dots,a_{\ell-1}<d} \alpha_\ell^{d-1-a_\ell} \alpha_{\ell+2}^{a_\ell} \lambda(a_0,\dots,a_{\ell-1}) \\
&+ \sum_{a_\ell=0}^{d-1} \sum_{a_{\ell-1}=0}^{d-1} \sum_{0\le a_0,a_1,\dots,a_{\ell-2}<d} \alpha_{\ell-1}^{d-1-a_{\ell-1}+d(d-1-a_\ell)} \alpha_{\ell+1}^{a_{\ell-1}+da_\ell} \lambda(a_0,\dots,a_{\ell-2})
\end{aligned}$$

$$= \sum_{a_\ell=0}^{d-1} \alpha_\ell^{d-1-a_\ell} \alpha_{\ell+2}^{a_\ell} S_{\ell-1} + \sum_{a_\ell=0}^{d-1} \alpha_{\ell-1}^{d(d-1-a_\ell)} \alpha_{\ell+1}^{da_\ell} \sum_{a_{\ell-1}=0}^{d-1} \alpha_{\ell-1}^{d-1-a_{\ell-1}} \alpha_{\ell+1}^{a_{\ell-1}} S_{\ell-2}$$

and finally

$$S_\ell = \frac{\alpha_\ell^d - \alpha_{\ell+2}^d}{\alpha_\ell - \alpha_{\ell+2}} S_{\ell-1} + \frac{\alpha_{\ell-1}^{d^2} - \alpha_{\ell+1}^{d^2}}{\alpha_{\ell-1} - \alpha_{\ell+1}} S_{\ell-2}. \tag{13}$$

This enables us to compute numerical values of the Cesàro means in an effective way; the result of the numerical computations in the case $d = 2$ is given in the following section. Note also that an analogous formula can be proved for $\sum_{0 \le a_0, a_1, \ldots, a_\ell < d} \zeta(a_0, \ldots, a_\ell)$.

4. Final remarks and numerical results

In this final section, we provide some numerical data for the most important constants given in the previous section, namely ρ_n, τ_n and their Cesàro means. Figure 2 shows a plot of ρ_n in the case $d = 2$ – the different branches that can be observed correspond to specific choices for the "least significant digits" $a_0, a_1, \ldots$

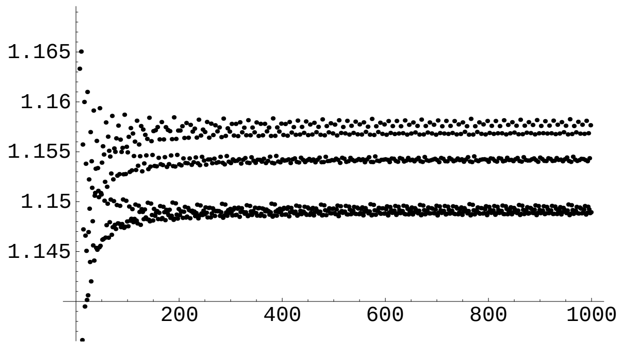

Figure 2. Plot of ρ_n in the case $d = 2$.

The subsequent plot (see Figure 3) gives the corresponding mean values $\frac{1}{N} \sum_{n=1}^{N} \rho_n$, which tend to a limit, as proved in Theorem 3. Its numerical value can be determined by means of the recurrence formula (13):

$$\lim_{N \to \infty} \sum_{n=1}^{N} \rho_n = 1.15247\ 35251\ 60637\ 47956\ 21404.$$

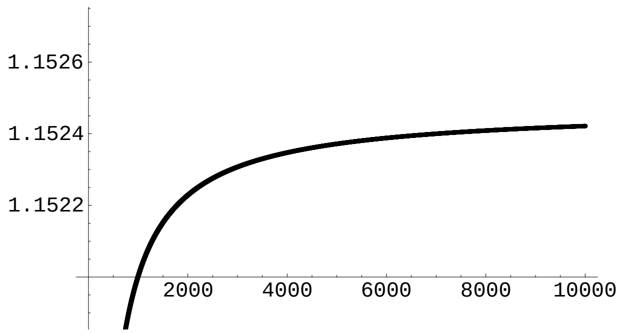

Figure 3. Plot of the Cesàro means $\frac{1}{N}\sum_{n=1}^{N}\rho_n$ in the case $d = 2$.

Let us also give the respective plots for τ_n in the case $d = 3$ (see Figures 4 and 5).

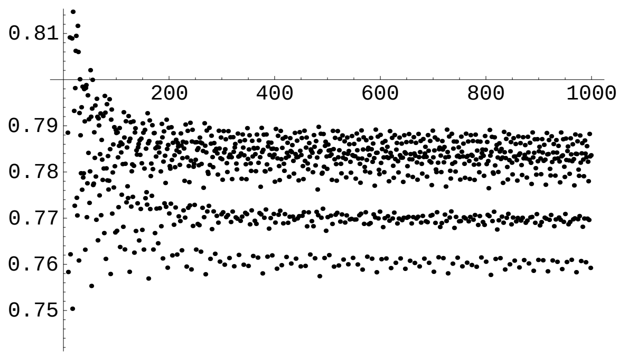

Figure 4. Plot of τ_n in the case $d = 3$.

However, the constants $\beta(d)^{d-1}$ and $\delta(d)^{d-1}$ are far more relevant for the growth of $\sigma(X_n)$ and $Z(X_n)$. From general considerations, it is clear that $\beta(d)^{d-1}$ lies between $\frac{1+\sqrt{5}}{2}$ and 2 (since the absolute minimum and maximum number of independent vertex subsets in a tree on n vertices are given by F_{n+2} and $2^{n-1}+1$ for the path and star respectively), and that $\beta(d)^{d-1}$ increases with d (since the restriction becomes weaker for increasing d) and tends to 2. Similarly, $\delta(d)^{d-1}$ lies between 1 and $\frac{1+\sqrt{5}}{2}$, is decreasing and tends to 1. Some numerical values are

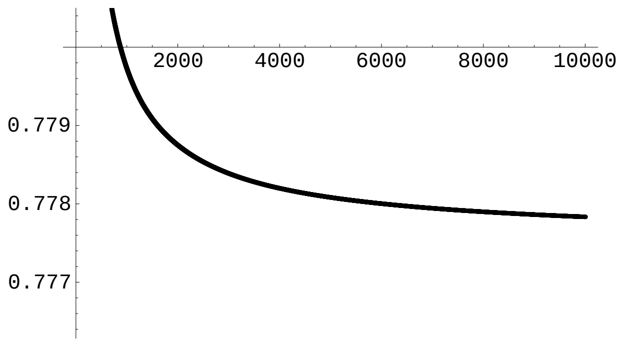

Figure 5. Plot of the Cesàro means $\frac{1}{N}\sum_{n=1}^{N}\tau_n$ in the case $d=3$.

given in the following table – it is not difficult to achieve a considerable precision for these constants.

d	$\beta(d)^{d-1}$	$\delta(d)^{d-1}$
2	1.66345 83970 72426 71400 29341	1.53717 67171 82357 94959 01403
3	1.71104 77168 65854 39252 73758	1.46792 93132 06252 26446 93247
4	1.75277 22835 08758 20411 33753	1.41392 59361 85955 94075 16282
5	1.78663 80672 40820 67508 45428	1.37155 08691 35932 33996 43430
10	1.87794 53843 82516 51109 09164	1.25029 46884 25647 29912 57823
20	1.93506 36009 86574 58856 21997	1.15777 24711 29443 56294 89233
50	1.97300 16421 91753 19422 92396	1.08042 81828 41889 98839 31038
100	1.98632 13043 16506 81563 84834	1.04682 49561 02834 62023 79355

Table 1. Numerical values for $\beta(d)$ and $\delta(d)$ in some special cases

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(Received November 3, 2008; revised January 31, 2010)