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On a Class of Extremal Trees for Various Indices

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Abstract

It was recently shown that an interesting class of trees maximizes the Merrifield-Simmons index and minimizes the Hosoya index and energy among all trees with given number of vertices and maximum degree. In this paper, we describe how these trees (which we will call F-trees) can be constructed algorithmically by means of so-called F-expansions, which are very similar to ordinary base-d digital expansions. Our algorithms are illustrated by various examples. Furthermore, some more properties of F-trees are described and numerical data is provided.

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1 Introduction

The Merrifield-Simmons index, defined as the number of independent vertex subsets of a graph, and the Hosoya index, the number of matchings (independent edge subsets) of a graph, are two of the most popular topological indices that serve as molecular descriptors, see [6, 19, 22]. In view of the similar definitions, it is not surprising that there are many interesting connections between the two. One of the most important questions in the study of such indices is the extremal problem, i.e., the problem of determining the graphs within a prescribed class that maximize or minimize the index. There is a vast amount of recent literature on the extremal problem for the Merrifield-Simmons index as well as the Hosoya index: since acyclic systems are often of particular interest, a lot of work has been done on trees. It is a long-known fact [6, 21] that among all trees of a given size, the star has maximum Merrifield-Simmons index and minimum Hosoya index, while the path maximizes the Hosoya index and minimizes the Merrifield-Simmons index. The fact that the star and the path are extremal among all trees is actually the typical behavior for all topological indices.

In order to obtain a deeper understanding of the Merrifield-Simmons index and the Hosoya index of trees, the extremal problem has been investigated for trees with certain restrictions, such as given diameter [17, 20], given size of largest matching [12] or given number of leaves [20, 26, 27, 30]. For trees without restrictions, not only the largest or smallest possible values are known, but also further values, see [14, 15, 23].

Furthermore, graphs with a bounded number of cycles, in particular unicyclic and bicyclic graphs [3, 16, 24, 25, 28, 29], can be treated along essentially the same lines, and again, several restrictions (e.g. fixed girth) can be included in the study as well. Other structures that have been investigated include hexagonal chains [31], which are very natural objects considering the chemical background. Typically, the graphs within a given class that minimize one of the two indices maximize the other, and vice versa, even though there are notable exceptions (see [2]). This is quite intuitive in view of the similar definitions, while it is a less intuitive fact that the trees which minimize the Hosoya index usually also minimize the energy (see for instance [13, 27]), i.e., the sum of the absolute values of all eigenvalues (of the adjacency matrix). This is due to a relation between the characteristic polynomial and matchings of a tree, which gives rise to a formula for the energy via a so-called Coulson integral [6]:

$$E(T) = \frac{2}{\pi} \int_0^\infty x^{-2} \log \left(\sum_k m(T,k) x^{2k} \right) dx, \tag{1}$$

where $m(T,k)$ is the number of matchings of size k of a tree T. This relation was used in many instances to show that the extremal trees with respect to energy and Hosoya index coincide, see [5] for the earliest instance.

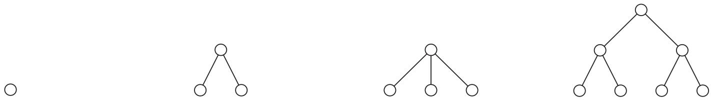
A very natural class of graphs that arises from the chemical applications is the class of chemical trees, i.e., trees with maximum degree at most 4. The minimum Hosoya index and energy of chemical trees were determined in [4] for a small number of vertices, and it was also conjectured in this paper that the extremal chemical trees for the two are always the same. This conjecture was proven recently in [8], where it was shown that the extremal chemical trees for the energy have the same shape as those that had been shown earlier to maximize the Merrifield-Simmons index and minimize the Hosoya index, see [9]. In the proof, the aforementioned Coulson integral representation plays a significant role.

The results for chemical trees are actually just special cases of more general theorems for trees with given maximum degree. An earlier result in this context is due to Lv and Yu [18], where the maximum degree is assumed to be relatively large. The extremal trees with given number of vertices and maximum degree form a very interesting class of trees that we treat in the current paper in some more depth. First, we define them and summarize all known results. Section 2 deals with an associated digital system which we call the F-system; the F-expansion associated to a given integer n can be determined by a short algorithm (Section 3) that also allows us to generate the trees (Section 4), which is exhibited for several examples (Section 5). Finally, we state a few more properties of our class of trees and provide some numerical data.

Before defining the class of trees under consideration, we fix our notations on complete trees. Throughout the paper, d is a fixed integer ≥ 2. The complete d-ary tree of height $h-1$ is denoted by C_h, i.e., C_1 is a single vertex and C_h has d branches $C_{h-1}, \ldots, C_{h-1}$, cf. Figure 1. It is convenient to set C_0 to be the empty graph.

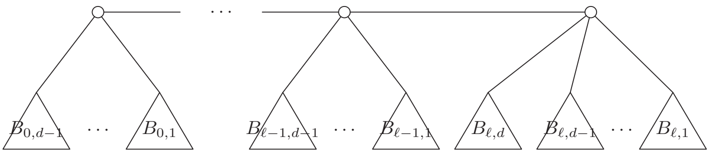
As the shape of the trees under consideration is somewhat reminiscent of a festoon, we call the trees *festoon trees* or F-trees for short.

Definition 1.1 An *F-tree* is a tree of the form



(a) C_1 for all d (b) C_2 for $d = 2$ (c) C_2 for $d = 3$ (d) C_3 for $d = 2$

Figure 1: Complete d-ary trees



with $B_{k,1}, \ldots, B_{k,d-1} \in \{C_k, C_{k+2}\}$ for $0 \le k < \ell$ and

- either $B_{\ell,1} = \cdots = B_{\ell,d} = C_{\ell-1}$
- or $B_{\ell,1} = \cdots = B_{\ell,d} = C_\ell$
- or $B_{\ell,1}, \ldots, B_{\ell,d} \in \{C_\ell, C_{\ell+1}, C_{\ell+2}\}$, where at least two of $B_{\ell,1}, \ldots, B_{\ell,d}$ equal $C_{\ell+1}$.

It is not obvious from the definition that such a tree exists for arbitrary order n and d and that it is unique. The existence has been proved implicitly (in the proof of their extremality with respect to the Merrifield-Simmons index and the Hosoya index) in [9].

Theorem 1 ([9]) *For every $d \ge 2$ and $n \ge 1$, there is a unique F-tree of order n, denoted by $T^*_{n,d}$.*

More specifically, let r_k be the number of copies of C_{k+2} among the subtrees $B_{k,j}$ for $k < \ell$, set $a_k = (d-1)(1+(d+1)r_k)$ and

- *$a_\ell = 1$, if $B_{\ell,1} = \cdots = B_{\ell,d} = C_{\ell-1}$,*
- *or $a_\ell = d$, if $B_{\ell,1} = \cdots = B_{\ell,d} = C_\ell$,*
- *or $a_\ell = d + (d-1)q_\ell + (d^2-1)r_\ell$, where $q_\ell \ge 2$ is the number of copies of $C_{\ell+1}$ and r_ℓ the number of copies of $C_{\ell+2}$ among the subtrees $B_{\ell,j}$.*

Then we have

$$(d-1)n + 1 = \sum_{k=0}^{\ell} a_k d^k. \tag{2}$$

In fact, (2) is the result of simply counting the vertices of the various branches of $T^*_{n,d}$, taking into account that C_h has precisely $\frac{d^h-1}{d-1}$ vertices.

The proof in [9] proves the existence of an F-tree of order n by starting with an extremal tree with respect to the Merrifield-Simmons index, deriving that this is an F-tree, and then using the counting argument to deduce (2). Uniqueness is then shown by establishing that (2) (together with the obvious restrictions $0 \le r_k < d$, $0 \le r_\ell$, $0 \le r_\ell + q_\ell \le d$) determines r_k, q_ℓ, r_ℓ completely. It is, however, not explained how to determine these quantities, and therefore $T^*_{n,d}$, from the knowledge of n and d. This gap is filled in the present paper: we provide an explicit short algorithm (Algorithm 2) to compute the auxiliary quantities and thus $T^*_{n,d}$ (Proposition 4.1). This is achieved by considering (2) as a d-ary digital expansion with slightly unusual digits. All this will motivate the definitions of Section 2.

The following properties of $T^*_{n,d}$ have been proven in [8, 9].

Theorem 2 ([9]) *Among all trees with n vertices and maximum degree $\le d+1$, the F-tree $T^*_{n,d}$ is the unique tree that maximizes the Merrifield-Simmons index and minimizes the Hosoya index.*

Theorem 3 ([8]) *Let $m(T,k)$ denote the number of matchings of size k of a tree T, and define the polynomial $M(T,x)$ by*

$$M(T,x) = \sum_{k\ge 0} m(T,k)x^k.$$

Then, for any fixed n and $x > 0$, the unique tree that minimizes $M(T,x)$ among all trees with n vertices and maximum degree $\le d+1$ is the F-tree $T^*_{n,d}$.

From the representation (1), one immediately obtains the following fact:

Theorem 4 ([8]) *The F-tree $T^*_{n,d}$ is the unique tree with n vertices and maximum degree $\le d+1$ that minimizes the energy.*

Furthermore, it is possible to describe the asymptotic behavior of the extremal values, i.e., the Merrifield-Simmons index, the Hosoya index and the energy of $T^*_{n,d}$, see [8, 10] for details.

Theorem 5 ([10]) *The Merrifield-Simmons index of the F-tree $T^*_{n,d}$ is given by*

$$\sigma(T^*_{n,d}) = \rho_n \beta^n,$$

where $\beta = \beta(d)$ only depends on d, and ρ_n is bounded above and below by positive constants which depend only on d.

Both $\beta(d)$ and the upper and lower bounds for ρ_n can be computed numerically. Similarly, one has an analogous theorem for the Hosoya index:

Theorem 6 ([10]) *The Hosoya index of the F-tree $T^*_{n,d}$ is given by*

$$Z(T^*_{n,d}) = \tau_n \gamma^n,$$

where $\gamma = \gamma(d)$ only depends on d, and τ_n is bounded above and below by positive constants which depend only on d.

Finally, it can be shown that the energy of an F-tree $T^*_{n,d}$ grows linearly in the number of vertices for fixed d. This is made explicit in the following theorem:

Theorem 7 ([8]) *The energy of $T^*_{n,d}$ is asymptotically*

$$E(T^*_{n,d}) = \alpha n + O(\log n),$$

where

$$\alpha = \alpha(d) = 2\sqrt{d}(d-1)^2 \left(\sum_{\substack{j \geq 1 \\ j \equiv 0 \mod 2}} d^{-j} \left(\cot \frac{\pi}{2j} - 1 \right) + \sum_{\substack{j \geq 1 \\ j \equiv 1 \mod 2}} d^{-j} \left(\csc \frac{\pi}{2j} - 1 \right) \right)$$

is a constant that only depends on d.

2 F-expansions

The equation (2) provides the starting point for an algorithm that constructs $T^*_{n,d}$ (given n and d) and motivates the following definitions. Note that the right hand side is essentially a digital expansion (base-d expansion), the only difference being the fact that the "digits" a_k are not contained in the set $\{0, 1, \dots, d-1\}$, but in a somewhat different set (the final one, a_ℓ, is particularly exceptional). Hence, we introduce the concept of an *F-expansion.*

In the following, we write $m + d\mathbb{Z}$ for the residue class of m modulo d, i.e., $m + d\mathbb{Z} = \{m + kd \mid k \in \mathbb{Z}\}$, where m and $d > 0$ are integers. Furthermore, we write $m \bmod d$ for the unique integer in $m + d\mathbb{Z}$ in the range $\{0, \dots, d-1\}$.

Let $d \geq 2$ be a fixed integer. We set

$$\mathcal{D} := \{(d-1) + (d^2-1)r \mid 0 \leq r \leq d-1\},$$
$$\mathcal{D}_f := \{1, d\} \cup \{d + (d-1)q + (d^2-1)r \mid q \geq 2, r \geq 0, r+q \leq d\}.$$

The elements of $\mathcal{D}$ and $\mathcal{D}_f$ are called the *F-digits* and *final F-digits*, respectively. Note that $a_k \in \mathcal{D}$ for $k < \ell$ in our identity (2) and that $a_\ell \in \mathcal{D}_f$. We are considering digital expansions to the base d with those digits.

Example 2.1 We give $\mathcal{D}$ and $\mathcal{D}_f$ for small values of d in Table 1.

d	$\mathcal{D}$	$\mathcal{D}_f$
2	$\{1, 4\}$	$\{1, 2, 4\}$
3	$\{2, 10, 18\}$	$\{1, 3, 7, 9, 15\}$
4	$\{3, 18, 33, 48\}$	$\{1, 4, 10, 13, 16, 25, 28, 40\}$
5	$\{4, 28, 52, 76, 100\}$	$\{1, 5, 13, 17, 21, 25, 37, 41, 45, 61, 65, 85\}$

Table 1: F-digits

A *d-ary F-expansion* of a positive integer N is a sequence $(a_\ell, a_{\ell-1}, \ldots, a_0)$ with $a_\ell \in \mathcal{D}_f$ and $a_j \in \mathcal{D}$ for $0 \leq j < \ell$ such that

$$N = \mathsf{value}(a_\ell, a_{\ell-1}, \ldots, a_0) = \sum_{j=0}^{\ell} a_j d^j.$$

Example 2.2 The sequence $(3, 2, 10, 10)$ is a ternary (i.e., 3-ary) F-expansion of $N = 139$: Obviously, the digits belong to the correct digit sets, and we have

$$3 \cdot 3^3 + 2 \cdot 3^2 + 10 \cdot 3^1 + 10 \cdot 1 = 139.$$

We need the following information on the set $\mathcal{D}$ in order to compute F-expansions.

Lemma 2.3 *Let $m \in \mathbb{Z}$. Then there is exactly one $a \in \mathcal{D}$ such that $m \equiv a \pmod{d}$, which will be denoted by $\varepsilon(m)$. We have*

$$\varepsilon(m) = (d-1) + (d^2-1)\,(-m-1 \bmod d)\,.$$

Example 2.4 For $d = 3$, we have $\varepsilon(139) = 2 + 8 \cdot (-140 \bmod 3) = 10$.

Proof: We have $m \equiv (d-1) + (d^2-1)r \pmod{d}$ for some $0 \le r < d$ if and only if $r \equiv -m-1 \pmod{d}$. Thus we have to choose $r = (-m-1 \bmod d)$. ■

Next, we give an alternative description of the set of final digits. It is obvious that all final digits are congruent to 1 modulo $d-1$.

Example 2.5 For $d = 5$, the intersections of the sets $\mathcal{D}_f$ and $\mathcal{D}$ with the residue classes modulo 5 are given in Table 1.

$\cap$	$\mathcal{D}_f$	$\mathcal{D}$
$0+5\mathbb{Z}$	$\{5,25,45,65,85\}$	$\{100\}$
$1+5\mathbb{Z}$	$\{1,21,41,61\}$	$\{76\}$
$2+5\mathbb{Z}$	$\{17,37\}$	$\{52\}$
$3+5\mathbb{Z}$	$\{13\}$	$\{28\}$
$4+5\mathbb{Z}$	$\emptyset$	$\{4\}$

Table 2: Intersections of $\mathcal{D}_f$ and $\mathcal{D}$ with the residue classes modulo 5 for $d = 5$

In Example 2.5, it is shown that the intersection of $\mathcal{D}_f$ with some residue class $m + 5\mathbb{Z}$ consists of those positive numbers congruent to 1 modulo $d-1 = 4$ and congruent to m modulo $d = 5$ which are less than (or equal to) the unique representative $\varepsilon(m)$ of the residue class in the set of digits $\mathcal{D}$. In the following lemma, we prove that this is true in general.

Lemma 2.6 *Let $m \in \mathbb{Z}$. Then*

$$\mathcal{D}_f \cap (m + d\mathbb{Z}) = \{a \in \mathbb{Z} \mid 0 < a \le \varepsilon(m),\ a \equiv 1 \pmod{d-1},\ a \equiv m \pmod{d}\}. \quad (3)$$

Furthermore, $a = \varepsilon(m)$ can only happen for $d = 2$.

Proof: We claim that

$$\mathcal{D}_f = \{a \in \mathbb{Z} \mid \exists k \in \mathbb{Z} : 0 < a \le \varepsilon(k),\ a \equiv 1 \pmod{d-1},\ a \equiv k \pmod{d}\}. \quad (4)$$

While proving this claim, we denote the set on the right hand side of (4) by S.

The congruence $a \equiv k \pmod{d}$ is equivalent to $a \equiv \varepsilon(k) \pmod{d}$ and to $a = \varepsilon(k) - sd$ for an appropriate $s \in \mathbb{Z}$. Thus in a first step we can rewrite S as

$$S = \{a = \varepsilon(k) - sd \mid a \ge 1,\ s \ge 0,\ a \equiv 1 \pmod{d-1},\ k \in \mathbb{Z}\}.$$

As $\varepsilon(k) \in \mathcal{D}$, we have $\varepsilon(k) \equiv 0 \pmod{d-1}$, so the condition $a \equiv 1 \pmod{d-1}$ translates to $s \equiv -1 \pmod{d-1}$, so we may write $s = -d + q(d-1)$ for an appropriate $q \in \mathbb{Z}$. The condition $s \geq 0$ then translates to $q \geq 2$. This gives

$$S = \{a = \varepsilon(k) + d^2 - qd(d-1) \mid a \geq 1,\ q \geq 2, k \in \mathbb{Z}\}.$$

Next, we replace $\varepsilon(k)$ by $(d-1) + (d^2-1)R$ for some $0 \leq R \leq d-1$ and obtain

$$\begin{aligned} S &= \{a = d^2 + d - 1 + (d^2-1)R - qd(d-1) \mid a \geq 1,\ q \geq 2,\ 0 \leq R \leq d-1\} \\ &= \{a = d + (d-1)q + (d^2-1)(R-q+1) \mid a \geq 1,\ q \geq 2,\ 0 \leq R \leq d-1\}. \end{aligned}$$

Setting $R - q + 1 = r$, we get the alternative expression

$$S = \left\{a = d + (d-1)q + (d^2-1)r \,\middle|\, 1 \leq r + q \leq d,\ q \geq 2,\ r \geq -\frac{1+q+r}{d}\right\}. \tag{5}$$

We note that $r + q \leq d$ implies $(1+q+r)/d \leq 1 + 1/d < 2$, and so these inequalities imply $r \geq -1$. Thus the lower bound $r + q \geq 1$ is redundant and can be removed. On the other hand, the lower bound for r is certainly negative. Thus we separately consider the two cases $r \geq 0$ and $r = -1$ in (5) and obtain

$$\begin{aligned} S = \{a = d + (d-1)q + (d^2-1)r \mid q \geq 2,\ r \geq 0,\ r + q \leq d\} \\ \cup \{a = d + 1 - d^2 + (d-1)q \mid 2 \leq q \leq d+1,\ q \geq d\}. \end{aligned} \tag{6}$$

In the second set, the lower bound $q \geq 2$ is redundant. Actually, we have

$$\{a = d + 1 - d^2 + (d-1)q \mid 2 \leq q \leq d+1,\ q \geq d\} = \{1, d\}, \tag{7}$$

as the only remaining choices for q are d and $d+1$. Combining (6) and (7) and comparing with the definition of $\mathcal{D}_f$ exactly gives $S = \mathcal{D}_f$, which concludes the proof of (4).

Intersecting (4) with $m + d\mathbb{Z}$ immediately yields (3).

As $\varepsilon(m) \equiv 0 \pmod{d-1}$ and all final digits $a \in \mathcal{D}_f$ satisfy $a \equiv 1 \pmod{d-1}$, $\varepsilon(m) = a$ implies that $(d-1)$ divides 1, i.e., $d = 2$. ■

We can now classify the integers admitting a F-expansion, prove uniqueness of the expansion, and give an algorithm to compute it.

Theorem 8 *If $N \not\equiv 1 \pmod{d-1}$, then N does not admit a F-expansion.*

If $N \equiv 1 \pmod{d-1}$, then N admits a unique F-expansion and it can be computed by Algorithm 1.

Algorithm 1 Computing the F-expansion

Input: Positive integer N with $N \equiv 1 \pmod{d-1}$

Output: The F-expansion $(a_\ell, a_{\ell-1}, \dots, a_0)$ of N

```
j ← −1
m ← N
while m ≠ 0 do
  j ← j + 1
  ε ← ε(m) = (d − 1) + (d² − 1)(−m − 1 mod d)
  if ε < m then
    a_j ← ε
    m ← (m − a_j)/d
    {We have m ≡ 1 (mod d − 1).}
  else
    a_j ← m
    m ← 0
  end if
  {We have N = m d^(j+1) + Σ_{k=0}^{j} a_k d^k.}
end while
return (a_j, a_{j−1}, ..., a_0).
```

Proof of Theorem 8: First, we prove that $N \equiv 1 \pmod{d-1}$ is necessary for the existence of an F-expansion of N: Assume that a positive integer N admits an F-expansion. Then

$$N = \sum_{j=0}^{\ell} a_j d^j \equiv a_\ell d^\ell \equiv 1 \cdot 1^\ell = 1 \pmod{d-1},$$

because $a \equiv 0 \pmod{d-1}$ for $a \in \mathcal{D}$ and $a \equiv 1 \pmod{d-1}$ for $a \in \mathcal{D}_f$.

Next, we prove uniqueness of the F-expansion via an indirect proof that was also used in [9]. Let N be the least positive integer which admits two different F-expansions. Let $(a_\ell, \dots, a_0)$ and $(b_{\ell'}, \dots, b_0)$ be two different F-expansions of N.

If we had $a_0 = b_0$, then $(N - a_0)/d = (N - b_0)/d$ would have two different F-expansions $(a_\ell, \dots, a_1)$ and $(b_{\ell'}, \dots, b_1)$, which is a contradiction to the minimality of N.

Thus we have $a_0 \neq b_0$. Considering $\sum_{j=0}^{\ell} a_j d^j = \sum_{j=0}^{\ell'} b_j d^j$ modulo d immediately yields $a_0 \equiv b_0 \pmod{d}$. As two different elements of $\mathcal{D}$ are incongruent modulo d (Lemma 2.3), we conclude that one of a_0 and b_0 is an element of $\mathcal{D}_f$. Without loss of generality, we may assume that $b_0 \in \mathcal{D}_f$, which implies that $\ell' = 0$ and $N = b_0$.

As $b_0 = N = \sum_{j=0}^{\ell} a_j d^j$ and $a_0 \neq b_0$, we conclude that $\ell > 0$. This implies that $a_0 < N$ and $a_0 \in \mathcal{D}$, which in turn shows that $a_0 = \varepsilon(N)$ (by Lemma 2.3) and $b_0 > \varepsilon(N)$. But this is a contradiction to Lemma 2.6, which concludes the proof of the uniqueness of the F-expansion.

To prove that $N \equiv 1 \pmod{d-1}$ is indeed sufficient for the existence of a F-expansion of N only requires to show that Algorithm 1 terminates and is correct.

To see termination, we simply note that $0 < a_j \leq m$ in every step, which implies that m strictly decreases in every step and is always a non-negative integer.

The invariants stated as comments in the algorithm are easily proved by induction. If $\varepsilon \leq m$, then the algorithm chooses $a_j = \varepsilon \in \mathcal{D}$. In the final step, when $\varepsilon > m$, we have $\varepsilon = \varepsilon(m) \equiv m \pmod{d}$ by construction. Furthermore, we have $m \equiv 1 \pmod{d-1}$ by the loop invariants. From Lemma 2.6 we conclude that $m \in \mathcal{D}_f$, as required. ■

Example 2.7 We come back to Example 2.2, where the ternary F-expansion of $N = 139$ has been given without any explanation. We now compute this expansion using Algorithm 1.

As noted in Example 2.4, we have $\varepsilon(139) = 2 + 8 \cdot 1 = 10$. As $10 < \varepsilon(139)$, we set $a_0 = 10$ and continue with $m = (139 - 10)/3 = 43$. Again, we have $\varepsilon(43) = 10$, set $a_1 = 10$ and continue with $m = 11$. Now, we have $\varepsilon(11) = 2$, which is still less than 11, so we get $a_2 = 2$ and $m = 3$. We obtain $\varepsilon(3) = 2 + 8 \cdot 2 = 18$, which is too large. Thus we have to set $a_3 = m = 3$ and are done: We obtained $\ell = 3$ and the F-expansion $(3, 2, 10, 10)$. The proof of Theorem 8 shows that the fact that the final $m = 3$ was an admissible final digit is not a coincidence.

3 F-coefficients

For our application, our interest is not focused on the digits a_j of the F-expansion, but rather on the auxiliary variables q and r used in the definition of $\mathcal{D}$ and $\mathcal{D}_f$.

For an $a \in \mathcal{D}$ with $a = (d-1) + (d^2-1)r$ and $0 \leq r \leq d-1$, we call r the corresponding *F-coefficient*. For a final digit $a = d + (d-1)q + (d^2-1)r$ with $q \geq 2$, $r \geq 0$, and $r + q \leq d$, the pair (q, r) is called the corresponding final F-coefficient. The final F-coefficients for $a = 1$ and $a = d$ are defined to be $(-1, 0)$ and $(0, 0)$, respectively, such that the relation

$a = d + (d-1)q + (d^2-1)r$ also holds in these special cases.

It is obvious that the F-coefficient of a digit $a \in \mathcal{D}$ is defined uniquely. We claim that this is also true for the final F-coefficient of a final digit.

Lemma 3.1 *Let $a \in \mathcal{D}_f$. Then there is a unique final F-coefficient (q, r) corresponding to a, namely*

$$q = \begin{cases} -1, & \text{if } a = 1, \\ \frac{a-d}{d-1} \bmod (d+1), & \text{if } a > 1, \end{cases}$$

and

$$r = \frac{a-d}{d^2-1} - \frac{q}{d+1}. \tag{8}$$

Proof: If $a = 1$, we get $q = -1$ and $r = -1/(d+1)+1/(d+1) = 0$, as requested. Similarly, if $a = d$, we obtain $q = 0$ and $r = 0$. So we are left with the case

$$a = d + (d-1)q + (d^2-1)r \tag{9}$$

for some $q \geq 2$. We obtain

$$\frac{a-d}{d-1} \bmod (d+1) = (q + (d+1)r) \bmod (d+1) = q \bmod (d+1) = q,$$

because $2 \leq q \leq d$ holds by assumption. Obviously, (8) is equivalent to (9). ■

Let N be a positive integer with F-expansion $(a_\ell, \ldots, a_0)$. The F-coefficients corresponding to the digits a_j, $0 \leq j < \ell$, are denoted by r_j, $0 \leq j < \ell$. The final F-coefficient of the final F-digit a_ℓ is denoted by (q_ℓ, r_ℓ). Then the *d-ary F-sequence of N* is defined to be r_0, r_1, $\ldots$, $r_{\ell-1}$, (q_ℓ, r_ℓ).

Example 3.2 We calculate the ternary F-sequence of 139. In Example 2.7, the F-expansion of 139 has been calculated as $(3, 2, 10, 10)$. Since $10 = 2+8\cdot 1$ and $2 = 2+8\cdot 0$, we have $r_0 = 1$, $r_1 = 1$ and $r_2 = 0$. For the final digit $a_3 = 3$, we have $q_3 = 0 \bmod 4 = 0$ and obtain $r_3 = 0$. Thus the F-sequence of 139 is $1, 1, 0, (0, 0)$.

For the convenience of the reader, we include a version of Algorithm 1 computing the F-sequence of a given integer N as Algorithm 2. It is simply a combination of Algorithm 1, Lemma 2.3 and Lemma 3.1.

Algorithm 2 Computing the F-sequence

Input: Positive integer N with $N \equiv 1 \pmod{d-1}$

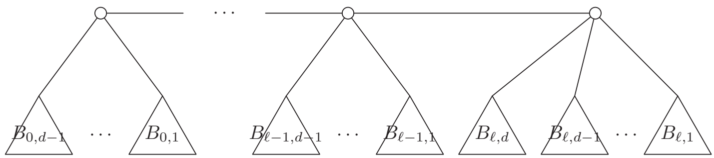
Output: The F-sequence $r_0, r_1, \ldots, r_{\ell-1}, (q_\ell, r_\ell)$ of N

```
j ← −1
m ← N
while m ≠ 0 do
    j ← j + 1
    R ← (−m − 1 mod d)
    ε ← (d − 1) + (d² − 1)R
    if ε < m then
        r_j ← R
        m ← (m − ε)/d
    else
        if m = 1 then
            q_j ← −1
        else
            q_j ← (m−d)/(d−1) mod (d + 1)
        end if
        r_j ← (m−d)/(d²−1) − q_j/(d+1)
        return (r_0, r_1, ..., r_{ℓ−1}, (q_ℓ, r_ℓ))
    end if
end while
```

4 F-trees

The considerations of the previous sections enable us to give the following constructive variant of Theorem 1.

Proposition 4.1 *Let n be a positive integer and $r_0, r_1, \ldots, r_{\ell-1}, (q_\ell, r_\ell)$ be the F-sequence of $N = (d-1)n+1$ (as computed by Algorithm 2). Then $T^*_{n,d}$ is the tree of the form*



with

- $B_{j,1} = \cdots = B_{j,r_j} = C_{k+2}$ *and* $B_{j,r_j+1} = \cdots B_{j,d-1} = C_k$ *for* $0 \le j \le \ell - 1$,
- *If* $q_\ell = -1$, *then* $B_{\ell,1} = \ldots = B_{\ell,d} = C_{\ell-1}$,
- *If* $q_\ell \ge 0$, *then* $B_{\ell,1} = \ldots = B_{\ell,r_\ell} = C_{\ell+2}$, $B_{\ell,r_\ell+1} = \ldots = B_{\ell,r_\ell+q_\ell} = C_{\ell+1}$ *and* $B_{\ell,r_\ell+q_\ell+1} = \cdots = B_{\ell,d} = C_\ell$.

Example 4.2 We construct $T^*_{69,3}$. To this aim, we need the F-sequence of $N = 2 \cdot 69 + 1 = 139$, which has been computed in Example 3.2 as $1, 1, 0, (0, 0)$. Thus we start with a path of 4 vertices v_0, v_1, v_2, v_3.

- We attach $r_0 = 1$ copy of $C_{0+2} = C_2$ and $d - 1 - r_0 = 1$ copy of $C_{0+0} = C_0$ at vertex v_0.
- We attach $r_1 = 1$ copy of $C_{1+2} = C_3$ and $d - 1 - r_1 = 1$ copy of $C_{1+0} = C_1$ at vertex v_1.
- We attach no ($r_2 = 0$) copy of $C_{2+2} = C_4$ and $d - 1 - r_2 = 2$ copies of $C_{2+0} = C_2$ at vertex v_2.
- Finally, we attach no ($r_3 = 0$) copy of $C_{3+2} = C_5$, no ($q_3 = 0$) copy of $C_{3+1} = C_4$ and $d - r_3 - q_3 = 3$ copies of $C_{3+0} = C_3$ at vertex v_4.

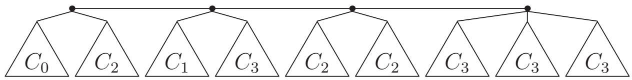


Figure 2: $T^*_{69,3}$ in decomposed form. An explicit version is shown in Figure 3

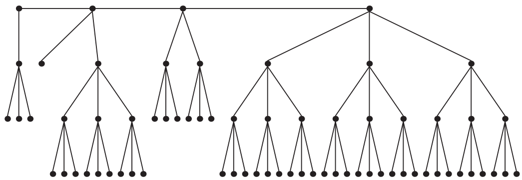


Figure 3: $T^*_{69,3}$, explicit version

The result is shown in Figures 2 and 3, once in the decomposition as in the definition and once in explicit form.

Example 4.3 In the same way, we construct $T^*_{69,2}$ now. The corresponding F-sequence (obtained from the binary F-expansion of 70) is easily found to be $1, 0, 1, 1, (-1, 0)$ in this case. Note that only one complete binary tree is attached to each of the vertices of the base-path $v_0v_1v_2v_3v_4$, except for the very last one. This complete binary tree is C_{j+2} if $r_j = 1$ and C_j otherwise. Note also that this example illustrates the special case when the final F-coefficient is $(-1, 0)$, so that we have to attach two copies of C_3 to the terminal vertex v_4 of the base path. The result is shown in Figures 4 and 5, as in the previous example.

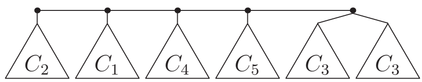


Figure 4: $T^*_{69,2}$ in decomposed form. An explicit version is shown in Figure 5

Example 4.4 Our last example in this section shows an instance where three different types of complete d-ary trees are attached to the terminal vertex of the base path, namely the F-tree $T^*_{44,4}$. The corresponding F-expansion is found to be $2, (2, 1)$ in this case, and so we have $\ell = 1$, meaning that we have to start with a path v_0v_1 and attach two copies of C_2 to v_0 (and one copy of C_0, which does not actually change anything) and one copy of C_1, two copies of C_2 and one copy of C_3 to v_1, see Figures 6 and 7.

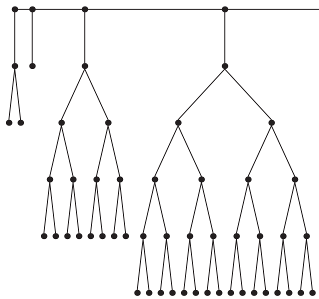


Figure 5: $T^*_{69,2}$, explicit version

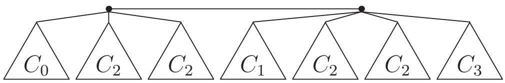


Figure 6: $T^*_{44,4}$ in decomposed form. An explicit version is shown in Figure 7

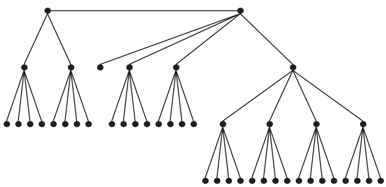


Figure 7: $T^*_{44,4}$, explicit version

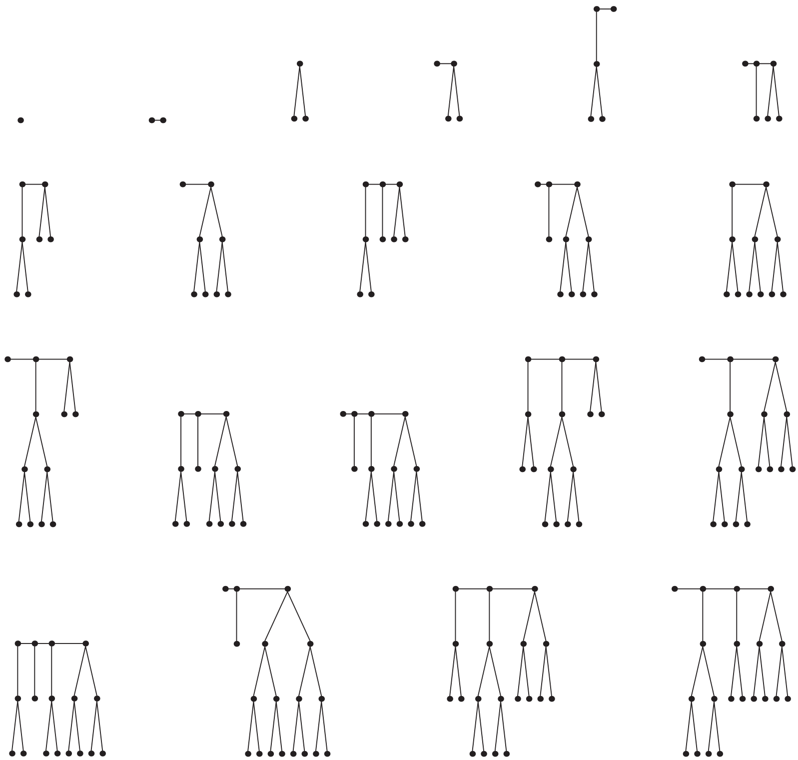


Figure 8: The F-trees $T^*_{n,2}$ for $1 \leq n \leq 20$

5 Further examples

In addition to the examples discussed in the previous section, we show complete lists of the F-trees $T^*_{n,d}$ for small values of n and d, specifically for $1 \leq n \leq 20$ and $2 \leq d \leq 4$. These are shown in Figures 8 to 10. All of these figures, including the ones in Section 4, were created automatically by means of an Asymptote [1] package that can be downloaded from [11]. On this webpage, all necessary files for creating pictures of F-trees of arbitrary size and degree are provided together with samples containing all F-trees up to 100 vertices for $d \leq 5$.

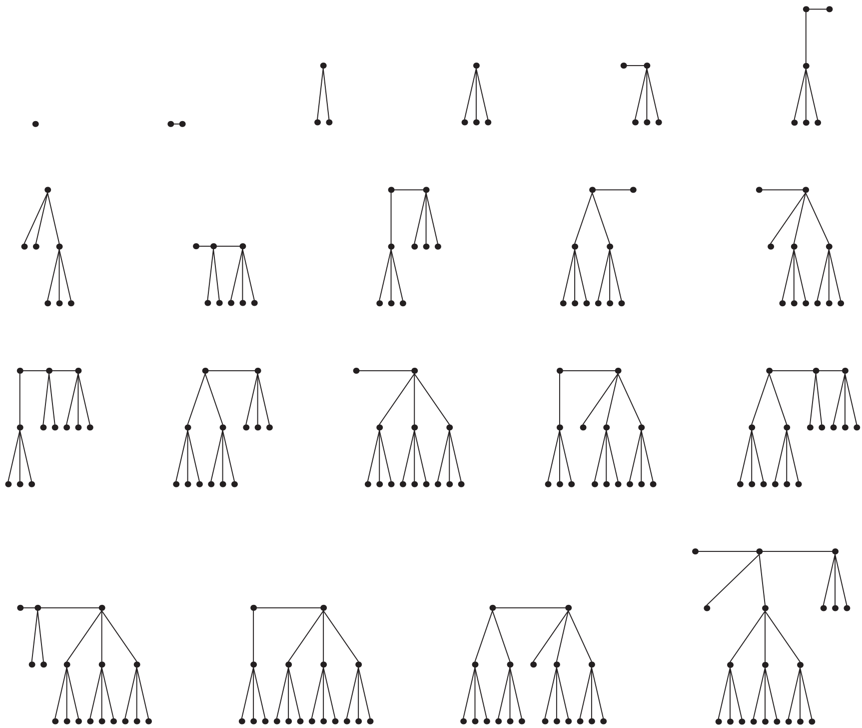


Figure 9: The F-trees $T^*_{n,3}$ for $1 \le n \le 20$

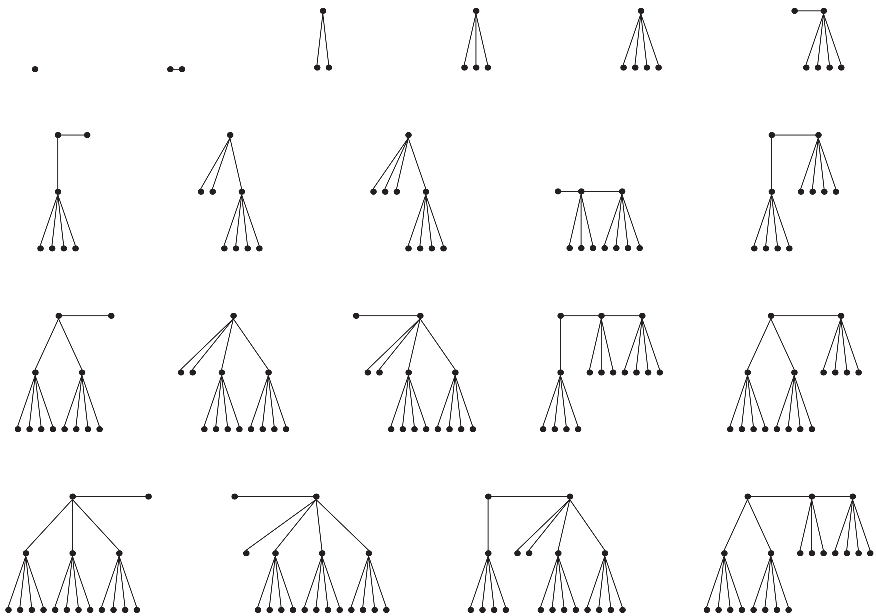


Figure 10: The F-trees $T^*_{n,4}$ for $1 \leq n \leq 20$

6 Further properties and numerical data

Various structural parameters of F-trees can be determined directly from the F-coefficients. For instance, it is not difficult to see that all vertices, with at most one exception, in an F-tree $T^*_{n,d}$ have degree 1 or $d+1$. The degree of the exceptional vertex is given by $1+r_0$, provided that $\ell > 0$. Since the sum of all degrees is known to be twice the number of edges, a simple counting argument yields a formula for the number of leaves of $T^*_{n,d}$:

Proposition 6.1 *For $n > 1$, the F-tree $T^*_{n,d}$ has exactly*

$$L = L(n,d) = \left\lfloor \frac{(d-1)n+2}{d} \right\rfloor$$

leaves.

Proof: Assume that $\ell > 0$. If $r_0 = 0$, every vertex has degree 1 or $d+1$, and one obtains

$$L + (d+1)(n-L) = 2(n-1),$$

which simplifies to

$$L = \frac{(d-1)n+2}{d}.$$

If $r_0 > 0$, then there is an additional vertex of degree $1+r_0$, which leads to

$$L + (1+r_0) + (d+1)(n-L-1) = 2(n-1),$$

or

$$L = \frac{(d-1)n+2+r_0-d}{d},$$

and since $0 < r_0 < d$, this simplifies to the desired identity. In case that $\ell = 0$, one simply has to replace r_0 by $q_0 + r_0$. ■

It is somewhat trickier to provide a formula for the diameter. Roughly stated, the diameter of $T^*_{n,d}$ is close to the minimum diameter for any tree with n vertices and maximum degree $\leq d+1$, i.e.,

Proposition 6.2 *The diameter of the F-tree $T^*_{n,d}$ is $2\log_d n + O(1)$.*

More specifically, the diameter can be expressed explicitly in terms of the F-expansion as follows:

Proposition 6.3 *The diameter of the F-tree $T^*_{n,d}$ is given by $2\ell + \delta$, where $-1 \leq \delta \leq 4$ is specified as follows:*

- *If $r_\ell \geq 2$, then $\delta = 4$.*
- *If $r_\ell = 1$, then*

$$\delta = \begin{cases} 3 & \ell = 0 \text{ or } r_k = 0 \text{ for all } k < \ell, \\ 4 & \text{otherwise.} \end{cases}$$

- *If $r_\ell = 0$ and $q_\ell \geq 2$, then*

$$\delta = \begin{cases} 2 & \ell = 0 \text{ or } r_k = 0 \text{ for all } k < \ell, \\ 3 & \text{otherwise.} \end{cases}$$

- *If $r_\ell = 0$ and $q_\ell = 0$, then*

$$\delta = \begin{cases} 0 & \ell = 0 \text{ or } r_k = 0 \text{ for all } k < \ell, \\ 2 & \text{otherwise.} \end{cases}$$

- *If $r_\ell = 0$ and $q_\ell = -1$, then*

$$\delta = \begin{cases} 2 & r_{\ell-1} \geq 2 \text{ or } r_{\ell-1} = 1 \text{ and } r_k \neq 0 \text{ for some } k < \ell - 1, \\ -1 & r_k = 0 \text{ for all } k < \ell \\ 1 & \text{otherwise.} \end{cases}$$

Proof: Note first that the diameter of any tree is the maximum distance between two of its leaves. If $H(B_{i,j}) - 1$ denotes the height of a subtree $B_{i,j}$ (i.e. $H(B_{i,j}) = h$ if $B_{i,j}$ is a C_h), then two leaves of the subtrees B_{i_1,j_1} and B_{i_2,j_2} have a distance of

$$|i_1 - i_2| + H(B_{i_1,j_1}) + H(B_{i_2,j_2}),$$

unless $(i_1, j_1) = (i_2, j_2)$, in which case the distance is at most $2H(B_{i_1,j_1}) - 2$. Now all that needs to be done is to distinguish all the cases mentioned in the statement of the problem and determine the maximum distance between leaves in each case. For instance, if $r_\ell \geq 2$, then $B_{\ell,1}$ and $B_{\ell,2}$ are both isomorphic to $C_{\ell+2}$, and so the distance between leaves of these two subtrees is $2(\ell + 2) = 2\ell + 4$. It is easy to see that there cannot be a larger distance between leaves, since

$$|i_1 - i_2| + H(B_{i_1,j_1}) + H(B_{i_2,j_2}) \leq |i_1 - i_2| + i_1 + 2 + i_2 + 2 = 2\max(i_1, i_2) + 4.$$

If $r_\ell = 1$, then the largest distance between leaves occurs for leaves of the two subtrees $B_{\ell,1}$ and $B_{\ell,2}$, which are isomorphic to $C_{\ell+2}$ and $C_{\ell+1}$ respectively (yielding a distance of $2\ell+3$), unless there is some $k < \ell$ for which $r_k > 0$. In this case, $B_{k,1}$ is a C_{k+2}, so that the distance between a leaf of $B_{k,1}$ and a leaf of $B_{\ell,1}$ is

$$(\ell - k) + \ell + 2 + k + 2 = 2\ell + 4.$$

Hence, we obtain the formula stated in the second case; the remaining cases are similar. Finally, it is not difficult to see that $\ell = \log_d n + O(1)$, yielding Proposition 6.2. This follows from the fact that

$$(d-1)n + 1 = \sum_{k=0}^{\ell} a_k d^k \geq (d-1)\sum_{k=0}^{\ell-1} d^k + d^\ell = 2d^\ell - 1$$

by (2) and similarly

$$(d-1)n + 1 = \sum_{k=0}^{\ell} a_k d^k \leq (d-1)d^2 \sum_{k=0}^{\ell-1} d^k + (d^3 - 2d^2 + 2d)d^\ell = (d^2 - d + 2)d^{\ell+1} - d^2.$$

Much more detailed asymptotic information on ℓ is contained in [7]. ■

Finally, we provide some numerical data; the following tables (Table 3 to Table 5) list the values of the Merrifield-Simmons index, the Hosoya index and the energy in the cases $d = 2$, $d = 3$, $d = 4$ for small values of n. The values have been computed using Mathematica® routines which are also available on the accompanying web site [11].

Table 6 lists the aforementioned polynomials $M(T^*_{n,d}, x)$ whose coefficients are exactly the numbers of k-matchings. We conjecture that the following strong result holds:

Conjecture 1 *For given positive integers n, d and k, the F-tree $T^*_{n,d}$ minimizes the number of k-matchings (i.e. matchings of cardinality k) among trees with n vertices and maximum degree $\leq d+1$.*

The same might also be true for independent vertex subsets:

Conjecture 2 *For given positive integers n, d and k, the F-tree $T^*_{n,d}$ maximizes the number of independent sets of cardinality k among trees with n vertices and maximum degree $\leq d+1$.*

The asymptotic behavior of the Merrifield-Simmons index, the Hosoya index and the energy is stated in Theorems 5 to 7; these results were proved in references [10] and [8] respectively, where numerical values of the involved constants were provided as well. We list these values again for completeness (Table 7).

n	$\sigma(T^*_{n,2})$	$\sigma(T^*_{n,3})$	$\sigma(T^*_{n,4})$
1	2	2	2
2	3	3	3
3	5	5	5
4	9	9	9
5	14	17	17
6	24	26	33
7	41	44	50
8	66	80	84
9	110	145	152
10	189	226	288
11	305	388	545
12	510	684	834
13	863	1241	1412
14	1425	1970	2568
15	2345	3330	4760
16	3987	5868	9009
17	6515	10657	13922
18	10905	17001	23748
19	18254	28674	42500
20	30135	50508	78744

Table 3: The Merrifield-Simmons index of F-trees $T^*_{n,d}$ for $1 \leq n \leq 20$ and $2 \leq d \leq 4$

n	$z(T^*_{n,2})$	$z(T^*_{n,3})$	$z(T^*_{n,4})$
1	1	1	1
2	2	2	2
3	3	3	3
4	4	4	4
5	7	5	5
6	10	9	6
7	15	13	11
8	24	17	16
9	37	24	21
10	54	40	26
11	87	56	35
12	132	81	60
13	201	112	85
14	306	176	110
15	483	264	151
16	720	376	200
17	1137	512	325
18	1710	816	450
19	2655	1216	635
20	4068	1712	860

Table 4: The Hosoya index of F-trees $T^*_{n,d}$ for $1 \leq n \leq 20$ and $2 \leq d \leq 4$

n	$E(T^*_{n,2})$	$E(T^*_{n,3})$	$E(T^*_{n,4})$
1	0	0	0
2	2	2	2
3	2.82843	2.82843	2.82843
4	3.46410	3.46410	3.46410
5	5.22625	4	4
6	6	5.81863	4.47214
7	6.82843	6.60272	6.32456
8	8.42429	7.21110	7.11529
9	9.33533	7.93624	7.72741
10	10.1290	9.61686	8.24621
11	11.6857	10.3631	8.89898
12	12.6171	11.1349	10.6332
13	13.4801	11.8272	11.3910
14	14.9113	13.3979	11.9820
15	15.9244	14.2651	12.6664
16	16.7721	15.0171	13.2915
17	18.2517	15.6838	14.9282
18	19.1867	17.2461	15.6569
19	20.1045	18.1316	16.3921
20	21.5369	18.8673	17.0539

Table 5: The energy of F-trees $T^*_{n,d}$ for $1 \leq n \leq 20$ and $2 \leq d \leq 4$

n	$M(T^*_{n,2},x)$	$M(T^*_{n,3},x)$	$M(T^*_{n,4},x)$
1	1	1	1
2	$x+1$	$x+1$	$x+1$
3	$2x+1$	$2x+1$	$2x+1$
4	$3x+1$	$3x+1$	$3x+1$
5	$2x^2+4x+1$	$4x+1$	$4x+1$
6	$4x^2+5x+1$	$3x^2+5x+1$	$5x+1$
7	$8x^2+6x+1$	$6x^2+6x+1$	$4x^2+6x+1$
8	$4x^3+12x^2+7x+1$	$9x^2+7x+1$	$8x^2+7x+1$
9	$10x^3+18x^2+8x+1$	$15x^2+8x+1$	$12x^2+8x+1$
10	$20x^3+24x^2+9x+1$	$9x^3+21x^2+9x+1$	$16x^2+9x+1$
11	$8x^4+36x^3+32x^2+10x+1$	$18x^3+27x^2+10x+1$	$24x^2+10x+1$
12	$24x^4+56x^3+40x^2+11x+1$	$33x^3+36x^2+11x+1$	$16x^3+32x^2+11x+1$
13	$52x^4+86x^3+50x^2+12x+1$	$54x^3+45x^2+12x+1$	$32x^3+40x^2+12x+1$

Table 6: Polynomials $M(T^*_{n,d},x)$ for $1 \leq n \leq 13$ and $2 \leq d \leq 4$

d	$\beta(d)$	$\gamma(d)$	$\alpha(d)$
2	1.663458397072	1.537176717182	1.102947505597
3	1.711047716866	1.467929313206	0.970541979946
4	1.752772283509	1.413925936186	0.874794345784
5	1.786638067241	1.371550869136	0.802215758706
10	1.877945384383	1.250294688426	0.597794680849
20	1.935063600987	1.157772471129	0.434553264777
50	1.973001642192	1.080428182842	0.279574397741
100	1.986321304317	1.046824956103	0.198836515295

Table 7: Numerical values of the constants $\beta(d)$, $\gamma(d)$ and $\alpha(d)$ that occur in Theorems 5 to 7. The Merrifield-Simmons index of an F-tree $T^*_{n,d}$ grows like $\beta(d)^n$, the Hosoya index like $\gamma(d)^n$, and the energy like $\alpha(d) \cdot n$.

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