Labelled and unlabelled enumeration of k-gonal 2-trees*

Gilbert Labelle, Cédric Lamathe and Pierre Leroux

December 22, 2003

Abstract

In this paper[1], we generalize 2-trees by replacing triangles by quadrilaterals, pentagons or k-sided polygons (k-gons), where $k \geq 3$ is given. This generalization, to k-gonal 2-trees, is natural and is closely related, in the planar case, to some specializations of the cell-growth problem. Our goal is the labelled and unlabelled enumeration of k-gonal 2-trees according to the number n of k-gons. We give explicit formulas in the labelled case, and, in the unlabelled case, recursive and asymptotic formulas.

1 Introduction

Essentially, a 2-*tree* (or *bidimensional tree*) is a connected simple graph composed of triangles glued along their edges in a tree-like fashion, that is, without cycles (of triangles). This definition can be extended by replacing the triangles by quadrilaterals, pentagons or k-sided polygons (k-gons), where $k \geq 3$ is fixed. Such 2-trees, built on k-gons, are called *k-gonal 2-trees*. Figures 1a, 1b, and 2a show examples of k-gonal 2-trees, for $k = 3, 5$ and 4, respectively. Of course the usual 2-trees correspond to $k = 3$.

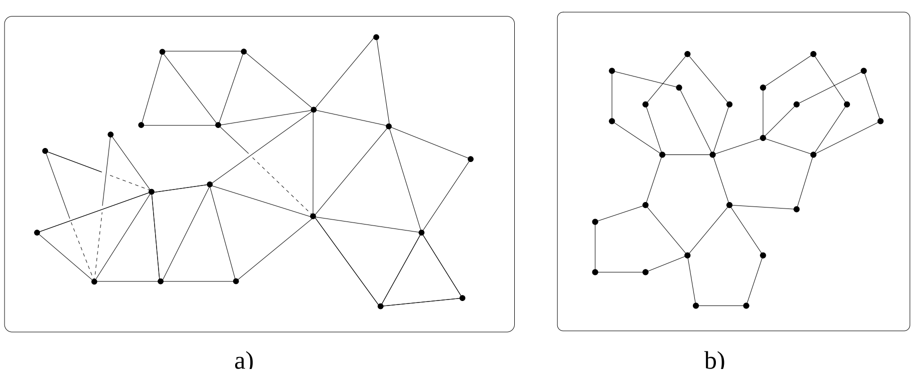


Figure 1: k-gonal 2-trees with $k = 3$ and $k = 5$

The enumeration of 2-trees is extensively studied in the literature. The first results in this direction are found in 1970, in Palmer [22] for the labelled enumeration of 2-trees (see also Beineke and Moon [2]) and in Harary and Palmer [9] (1973) for the unlabelled enumeration. During the same period, Palmer and Read [23] enumerated labelled and unlabelled *outerplanar* 2-trees, that is, 2-trees which can be embedded in the plane in such a way that each vertex belongs to the external face. The term *planar* is also used in this sense. See also Labelle, Lamathe and Leroux [17, 18].

*With the support of FCAR (Québec) and NSERC (Canada).

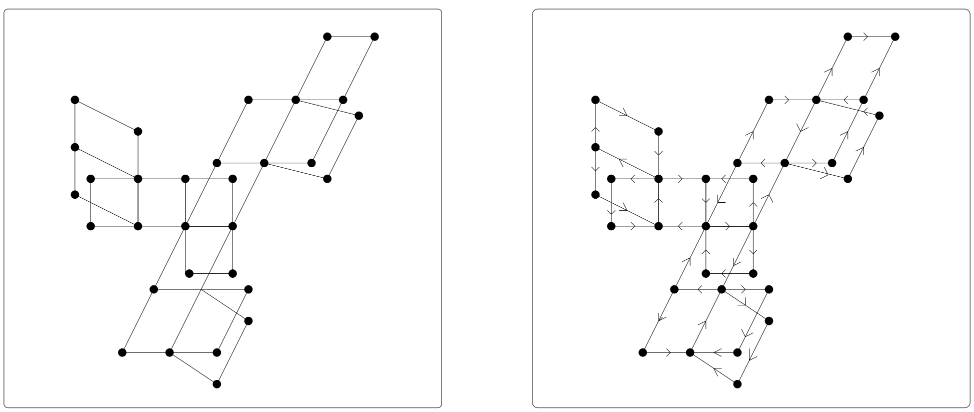
[1]This is the full version of a paper presented at the International Colloquium on "Mathematics and Computer Science" held in Versailles, France, in September 2002 (see [19]).

Two years later, together with Harary, these authors generalized their results in [10] by considering for the first time k-gonal 2-trees and enumerating them in the outerplanar case, in the context of a cell-growth problem.

In his 1993 Ph.D. Thesis [13, 14], Ton Kloks enumerated unlabelled *biconnected partial 2-trees*, that is, 2-trees in which some edges have been deleted without however losing the 2-connectedness. He calls these graphs *2-partials*. This class strictly contains that of k-gonal 2-trees since, in a 2-partial, polygons of different sizes can occur and some edges can be missing, provided that they are incident to at least three polygons. In principle Kloks' method, which extends the traditional *dissimilarity characteristic* of Otter [21] to 2-partials, could be used to enumerate k-gonal 2-trees (with k fixed). However, to our knowledge, this work has not been done.

More recently, in 2000, Fowler, Gessel, Labelle and Leroux [7, 8], have proposed some new functional equations for the class of (ordinary) 2-trees, which yield recurrences and asymptotic formulas for their unlabelled enumeration. Their approach, which is based on the theory of combinatorial species of Joyal (see [12, 4]), is more structural, replacing a potential dissimilarity characteristic formula for each individual 2-tree by a Dissymmetry Theorem for the species of 2-trees. Such a theorem can be formulated for most classes of tree-like stuctures, for example ordinary (one-dimensional, Cayley) trees or more generaly simple graphs, all of whose 2-connected components are in a given class (see [4]), plane embedded trees (see [16]), various classes of cacti (see [5], etc.

In the present paper, we extend to k-gonal 2-trees the work of Fowler et als, which corresponds to the case $k = 3$. In particular, we label the 2-trees at their k-gons. Our goal is their labelled and unlabelled enumeration, according to the number of k-gons. We will give explicit formulas in the labelled case and recursive and asymptotic formulas in the unlabelled case, emphasizing the dependency on k. Special attention must be given to the cases where k is even.



a) b)

Figure 2: Unoriented and oriented 4-gonal 2-trees

We say that a k-gonal 2-tree is *oriented* if its edges are oriented in such a way that each k-gon forms an oriented cycle; see Figure 2 b). In fact, for any k-gonal 2-tree s, the orientation of any one of its edges can be extended uniquely to all of s by first orienting all the polygons to which the edge belongs and then continuing recursively on all adjacent polygons. The coherence of the extension is ensured by the arborescent (acyclic) nature of 2-trees.

We denote by a and a_o the species of k-gonal 2-trees and of oriented k-gonal 2-trees. For these species, we use the symbols $-$, $\diamond$ and $\underline{\diamond}$ as upper indices to indicate that the structures are pointed at an edge, at a k-gon, and at a k-gon having itself a distinguished edge, respectively.

A first step is the extension to the k-gonal case of the Dissymmetry Theorem for 2-trees, which links together these various pointed species. The proof is similar to the case $k = 3$ and is omitted (see [7, 8]).

Theorem 1. Dissymmetry theorem for k-gonal 2-trees. The species $\mathcal{a}_o$ and $\mathcal{a}$ of oriented and unoriented k-gonal 2-trees, respectively, satisfy the following isomorphisms of species:

$$\mathcal{a}_o^- + \mathcal{a}_o^\diamond = \mathcal{a}_o + \mathcal{a}_o^{\underset{-}{\diamond}}, \tag{1}$$

$$\mathcal{a}^- + \mathcal{a}^\diamond = \mathcal{a} + \mathcal{a}^{\underset{-}{\diamond}}. \tag{2}$$

There is yet another species to introduce, which plays an essential role in the process. It is the species $B = \mathcal{a}^{\rightarrow}$ of oriented-edge rooted (k-gonal) 2-trees, that is of 2-trees where an edge is selected and oriented. As mentionned above, the orientation of the rooted edge can be extended uniquely to an orientation of the 2-tree so that there is a canonical isomorphism $B = \mathcal{a}_o^-$. However, it is often useful not to perform this extension and to consider that only the rooted edge is oriented.

In the next section, we characterize the species $B = \mathcal{a}^{\rightarrow}$ by a combinatorial functional equation and give some of its consequences. The goal is then to express the various pointed species occuring in the Dissymmetry Theorem in terms of B and to deduce enumerative results for the species $\mathcal{a}_o$ and $\mathcal{a}$. The oriented case is simpler and carried out first, in Section 3. The unoriented case is analyzed in Section 4, where $\mathcal{a}$ is viewed as a quotient species of $\mathcal{a}_o$ and two cases are distinguished, according to the parity of the integer k. Finally, asymptotic results are presented in Section 5.

For our purposes, the main tool of species theory is the Pólya-Robinson-Joyal Composition Theorem which can be stated as follows (see [4], Th. 1.4.2): let the species F be the (partitionnal) composition of two species, $F = G \circ H = G(H)$. Then, the exponential generating function

$$F(x) = \sum_{n\geq 0} f_n \frac{x^n}{n!},$$

where $f_n = |F[n]|$ is the number of labelled F-structures over a set of cardinality n, and the *tilde* generating function

$$\widetilde{F}(x) = \sum_{n\geq 0} \widetilde{f}_n x^n,$$

where $\widetilde{f}_n = |F[n]/\mathbb{S}_n|$ is the number of unlabelled F-structures of order n, satisfy the following equations:

$$F(x) = G(H(x)), \tag{3}$$

$$\widetilde{F}(x) = Z_G(\widetilde{H}(x), \widetilde{H}(x^2), \ldots), \tag{4}$$

where $Z_G(x_1, x_2, \ldots)$ is the cycle index series of G. Moreover, we have

$$Z_F(x_1, x_2, \ldots) = Z_G \circ Z_H = Z_G(Z_H(x_1, x_2, \ldots), Z_H(x_2, x_4, \ldots), \ldots). \tag{5}$$

Here the operation $\circ$ is the *plethystic composition* of symmetric functions when the $x_1, x_2, \ldots$ are interpreted as *power sum* symmetric functions in some other set of variables $\mathbf{s} = (s_1, s_2, s_3, \ldots)$: $x_i = p_i = p_i(s_1, s_2, \ldots) := \sum_{j\geq 1} s_j^i$.

This interpretation of the cycle index series as symmetric functions can be taken as an alternate definition, as follows (see [4], Example 2.3.15 and Rem. 4.3.8). An F-structure is said to be *colored* if the elements of its underlying set are assigned colors in the set $\{1, 2, 3, \ldots\}$. Such a colored structure has a weight w given by its color distribution monomial in the variables $\mathbf{s} = (s_1, s_2, s_3, \ldots)$. Let us denote by $F(1_\mathbf{s})$ the weighted set of unlabelled colored F-structures. Its total weight (or *inventory*) $|F(1_\mathbf{s})|_w$ is a symmetric function in the variables $\mathbf{s}$ and thus has a unique expression in terms of the power sums $x_i = p_i(s_1, s_2, \ldots)$ given precisely by Z_F:

$$|F(1_\mathbf{s})|_w = Z_F(x_1, x_2, \ldots). \tag{6}$$

For example, for the species E_2, of 2-element sets, and E, of sets, we have

$$Z_{E_2}(x_1, x_2, \ldots) = \sum_{i<j} s_i s_j + \sum_i s_i^2 = \frac{1}{2}\left((\sum_i s_i)^2 + \sum_i s_i^2\right) = \frac{1}{2}(x_1^2 + x_2) \tag{7}$$

and

$$Z_E(x_1, x_2, \ldots) = h(s_1, s_2, \ldots) = \exp\left(\sum_{i\geq 1} \frac{x_i}{i}\right), \tag{8}$$

where $h = \sum_{n\geq 0} h_n$ denotes the complete homogeneous symmetric function.

2 The species B of oriented-edge rooted 2-trees

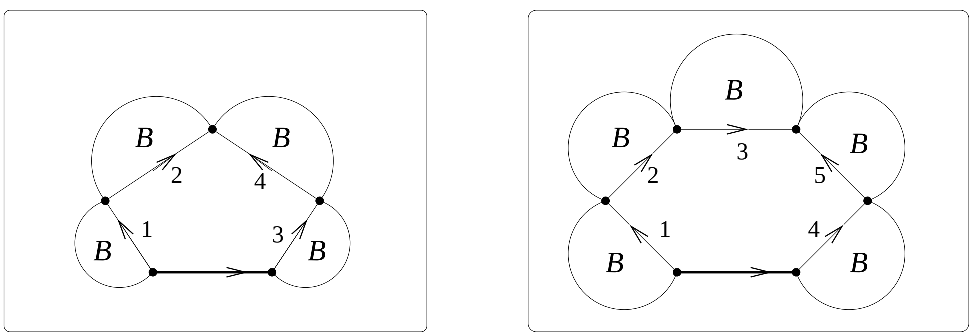
The species $B = a^{\rightarrow}$ plays a central role in the study of k-gonal 2-trees. The following theorem is an extension to a general k of the case $k = 3$. Note that formula (9) below also makes sense for $k = 2$ and corresponds to edge-labelled (ordinary) rooted trees.

Theorem 2. The species $B = a^{\rightarrow}$ of oriented-edge rooted k-gonal 2-trees satisfies the following functional equation (isomorphism):

$$B = E(XB^{k-1}), \tag{9}$$

where E represents the species of sets and X is the species of singleton k-gons.

Proof. We decompose an $a^{\rightarrow}$-structure as a set of *pages*, that is, of maximal subgraphs sharing only one k-gon with the rooted edge. For each page, the orientation of the rooted edge permits to define a linear order and an orientation on the $k-1$ remaining edges of the polygon having this edge, in some conventional way, for example in the fashion illustrated in Figure 3a, for the odd case, and 3b, for the even case. These edges being oriented, we can glue on them some B-structures. We then deduce relation (9). ■



a) b)

Figure 3: A page of an oriented-edge rooted 2-tree, for a) $k = 5$, b) $k = 6$

Among the possible edge orientations of an oriented-edge rooted k-gon, the one illustrated in Figure 3a, "away from the root edge", has the advantage of remaining valid if the root edge is not oriented, for k odd. If k is even, we see a difference caused by the existence of an opposite edge whose orientation will remain ambiguous.

We can easily relate the species $B = a^{\rightarrow}$ to that of (ordinary) rooted trees, denoted by A, characterized by the functional equation $A = XE(A)$, where X now represents the sort of vertices. Indeed from (9), we deduce

$$(k-1)XB^{k-1} = (k-1)XE((k-1)XB^{k-1}), \tag{10}$$

knowing that $E^m(X) = E(mX)$. By the Implicit Species Theorem of Joyal (see [4]), there exists a unique (up to isomorphism) species Y such that $Y = (k-1)XE(Y)$, namely $Y = A((k-1)X)$. It follows that

$$(k-1)XB^{k-1} = A((k-1)X) \tag{11}$$

and

$$B^{k-1} = \frac{A((k-1)X)}{(k-1)X}. \tag{12}$$

In analogy with formal power series, it can be shown that for any rational number $r \neq 0$, any species F with constant term equal to 1 (that is $F(0) = 1$) admits a *unique* r^{th}-root with constant term 1, that is a unique species G such that $G^r = F$ and $G(0) = 1$; here G may be a virtual species, with rational coefficients (see Rem. 2.6.16 of [4]). In the present case, since both B and $A((k-1)X)/(k-1)X$ have constant term 1, we obtain the following expression for the species B in terms of the species of rooted trees. This expression can be used to compute the first terms of the molecular expansion of B, using Newton's Binomial Theorem; see [1].

Proposition 1. The species $B = \mathcal{a}^{\rightarrow}$ of oriented-edge-rooted k-gonal 2-trees satisfies

$$B = \sqrt[k-1]{\frac{A((k-1)X)}{(k-1)X}}. \tag{13}$$

Corollary 1. The numbers $a_n^{\rightarrow}$, $a_{n_1,n_2,\ldots}^{\rightarrow}$, and $b_n = \widetilde{a}_n^{\rightarrow}$ of k-gonal 2-trees pointed at an oriented edge and having n k-gons, respectively labelled, fixed by a permutation of cycle type $1^{n_1}2^{n_2}\ldots$ and unlabelled, satisfy the following formulas and recurrence:

$$a_n^{\rightarrow} = ((k-1)n+1)^{n-1} = m^{n-1}, \tag{14}$$

where $m = (k-1)n+1$ is the number of edges,

$$a_{n_1,n_2,\ldots}^{\rightarrow} = \prod_{i=1}^{\infty}(1+(k-1)\sum_{d|i} dn_d)^{n_i-1}(1+(k-1)\sum_{d|i,d<i} dn_d), \tag{15}$$

and

$$b_n = \frac{1}{n}\sum_{1\leq j\leq n}\sum_{\alpha}(|\alpha|+1)b_{\alpha_1}b_{\alpha_2}\ldots b_{\alpha_{k-1}}b_{n-j}, \qquad b_0 = 1, \tag{16}$$

the last sum running over $(k-1)$-tuples of integers $\alpha = (\alpha_1, \alpha_2, \ldots, \alpha_{k-1})$ such that $|\alpha|+1$ divides the integer j, where $|\alpha| = \alpha_1 + \alpha_2 + \cdots + \alpha_{k-1}$.

Proof. Formulas (14) and (15) are obtained by specializing with $\mu = (k-1)^{-1}$ the following formulas, given by Fowler et al. in [7, 8],

$$\left(\frac{A(x)}{x}\right)^{\mu} = \sum_{n\geq 0}\mu(\mu+n)^{n-1}\frac{x^n}{n!}, \tag{17}$$

$$Z_{\left(\frac{A(X/\mu)}{X/\mu}\right)^{\mu}} = \sum_{n_1,n_2,\ldots}\frac{x_1^{n_1}x_2^{n_2}\ldots}{1^{n_1}n_1!2^{n_2}n_2!\ldots}\prod_{i=1}^{\infty}(1+\frac{1}{\mu}\sum_{d|i} dn_d)^{n_i-1}(1+\frac{1}{\mu}\sum_{d|i,d<i} dn_d). \tag{18}$$

Formula (14) can also be established by a Prüfer-like bijection; see [24, 20]. To obtain the recurrence (16), it suffices to take the logarithmic derivative of the equation

$$\widetilde{B}(x) = \exp\left(\sum_{i\geq 1}\frac{x^i\widetilde{B}^{k-1}(x^i)}{i}\right), \tag{19}$$

where $\widetilde{B}(x) = \sum_{n\geq 0} b_n x^n$, which follows from relation (9), using (4) and (8). ∎

The sequences $\{b_n\}_{n\in\mathbb{N}}$, for $k = 2, 3, 4, 5, 6$, are listed in the Encyclopedia of Integer Sequences [25, 26]. Respectively: A000081, for the number of rooted trees with n nodes, A005750, in relation with planted matched trees with n nodes and 2-trees, A052751, A052773, A052781, in relation with equation (19). Also, equation (9), is referenced in the Encyclopedia of Combinatorial Structures [11].

Observe that for each $n \geq 1$, b_n is a polynomial in k of degree $n-1$. This follows from (15) and the following explicit formula for b_n,

$$b_n = \sum_{n_1+2n_2+\cdots=n} \frac{a^{\rightarrow}_{n_1,n_2,\ldots}}{1^{n_1}n_1!2^{n_2}n_2!\ldots}, \tag{20}$$

which is a consequence of Burnside's lemma. The asymptotic behavior of the numbers b_n as $n \to \infty$, is studied, in particular as a function of k, in Section 7.

3 Oriented k-gonal 2-trees

We begin by determining relations for the pointed species appearing in the Dissymmetry Theorem. These relations are quite direct and the proof is left to the reader.

Proposition 2. The species a_o^{-}, $a_o^{\diamond}$, and $a_o^{\underline{\diamond}}$ are characterized by the following isomorphisms:

$$a_o^{-} = B, \quad a_o^{\diamond} = XC_k(B), \quad a_o^{\underline{\diamond}} = XB^k, \tag{21}$$

where $B = a^{\rightarrow}$ and C_k represents the species of oriented cycles of length k.

Recall that the cycle index series of C_k is given by $Z_{C_k} = \frac{1}{k}\sum_{d|k}\phi(d)x_d^{n/d}$ where ϕ is the Euler function. The Dissymmetry Theorem then permits us to express the ordinary (tilde) generating series $\widetilde{a}_o(x)$ of unlabelled oriented k-gonal 2-trees in terms of the corresponding series for the rooted species:

$$\widetilde{a}_o(x) = \widetilde{a}_o^{-}(x) + \widetilde{a}_o^{\diamond}(x) - \widetilde{a}_o^{\underline{\diamond}}(x). \tag{22}$$

By Proposition 2, we can now express $\widetilde{a}_o(x)$ as function of $\widetilde{B}(x) = \widetilde{a}^{\rightarrow}(x)$.

Proposition 3. The ordinary generating series $\widetilde{a}_o(x)$ of unlabelled oriented k-gonal 2-trees is given by

$$\widetilde{a}_o(x) = \widetilde{B}(x) + \frac{x}{k}\sum_{\substack{d|k\\ d>1}}\phi(d)\widetilde{B}^{\frac{k}{d}}(x^d) - \frac{k-1}{k}x\widetilde{B}^k(x). \tag{23}$$

Corollary 2. The numbers $a_{o,n}$ and $\widetilde{a}_{o,n}$ of oriented k-gonal 2-trees labelled and unlabelled, over n k-gons, respectively, are given by

$$a_{o,n} = ((k-1)n+1)^{n-2} = m^{n-2}, \quad n \geq 2, \tag{24}$$

$$\widetilde{a}_{o,n} = b_n - \frac{k-1}{k}b_{n-1}^{(k)} + \frac{1}{k}\sum_{\substack{d|k\\ d>1}}\phi(d)b_{\frac{n-1}{d}}^{(\frac{k}{d})}, \tag{25}$$

where

$$b_i^{(j)} = [x^i]\widetilde{B}^j(x) = \sum_{i_1+\cdots+i_j=i} b_{i_1}b_{i_2}\ldots b_{i_j},$$

denotes the coefficient of x^i in the series $\widetilde{B}^j(x)$, with $b_r^{(j)} = 0$ if r is non-integral or negative.

Proof. For the labelled case, it suffices to remark that $a_n^{\rightarrow} = ma_{o,n}$. In the unlabelled case, equation (25) is directly obtained from (23). ■

4 Unoriented k-gonal 2-trees

For the enumeration of (unoriented) k-gonal 2-trees, we consider quotient species of the form $F/\mathbb{Z}_2$, where F is a species of "oriented" structures, $\mathbb{Z}_2 = \{1, \tau\}$, is a group of order 2 and the action of τ is to reverse the structure orientations. A structure of such a quotient species then consists in an orbit $\{s, \tau \cdot s\}$ of F-structures under the action of $\mathbb{Z}_2$.

For instance, the different pointed species of unoriented k-gonal 2-trees a^{-}, $a^{\diamond}$ and $a^{\hat{\diamond}}$, can be expressed as quotient species of the corresponding species of oriented k-gonal 2-trees:

$$a^{-} = \frac{a^{\rightarrow}}{\mathbb{Z}_2}, \quad a^{\diamond} = \frac{a_o^{\diamond}}{\mathbb{Z}_2} = \frac{XC_k(B)}{\mathbb{Z}_2}, \quad a^{\hat{\diamond}} = \frac{a_o^{\hat{\diamond}}}{\mathbb{Z}_2} = \frac{XB^k}{\mathbb{Z}_2}. \tag{26}$$

The three basic generating series associated to such a quotient species, are given by

$$(F/\mathbb{Z}_2)(x) = \frac{1}{2}(F(x) + \sum_{n\geq 0} |\mathrm{Fix}_{F_n}(\tau)| \frac{x^n}{n!}), \tag{27}$$

$$(F/\mathbb{Z}_2)^{\sim}(x) = \frac{1}{2}(\widetilde{F}(x) + \sum_{n\geq 0} |\mathrm{Fix}_{\widetilde{F}_n}(\tau)| x^n), \tag{28}$$

where $\mathrm{Fix}_{F_n}(\tau)$ and $\mathrm{Fix}_{\widetilde{F}_n}(\tau)$ denote the sets of labelled and unlabelled, respectively, F-structures left fixed by the action of τ, that is, by orientation reversal, and

$$Z_{F/\mathbb{Z}_2}(x_1, x_2, \ldots) = \frac{1}{2}(Z_F(x_1, x_2, \ldots) + |\mathrm{Fix}_{F(1_{\mathbf{s}})}(\tau)|_w), \tag{29}$$

where $\mathrm{Fix}_{F(1_{\mathbf{s}})}(\tau)$ is the set of unlabelled colored F-structures left fixed by τ, weighted by the color distribution monomials in the variables $\mathbf{s} = (s_1, s_2, s_3, \ldots)$ and where the inventory $|\mathrm{Fix}_{F(1_{\mathbf{s}})}(\tau)|_w$, being a symmetric function in $\mathbf{s}$, is expressed in terms of the power sums $x_i = p_i(\mathbf{s})$. A simple example is given by the species $E_2 = X^2/\mathbb{Z}_2$, the species of 2-element sets, where formula (29) yields immediately $Z_{E_2} = \frac{1}{2}(x_1^2 + x_2)$.

However, some important differences appear in the computations, according to the parity of k. The main difference comes from the existence of *opposite* edges in k-gons, when k is even. Accordingly, it is better to treat the two cases separately.

4.1 Case k odd

If k is odd, it is quite simple to extend the method of Fowler et als [7, 8] where $k = 3$. For example, the only labelled oriented k-gonal 2-tree left fixed by an orientation reversal, for a given number of polygons, is the one in which all polygons share one common edge. Hence, from (27) and the fact that $a = a_o/\mathbb{Z}_2$, we deduce directly the following.

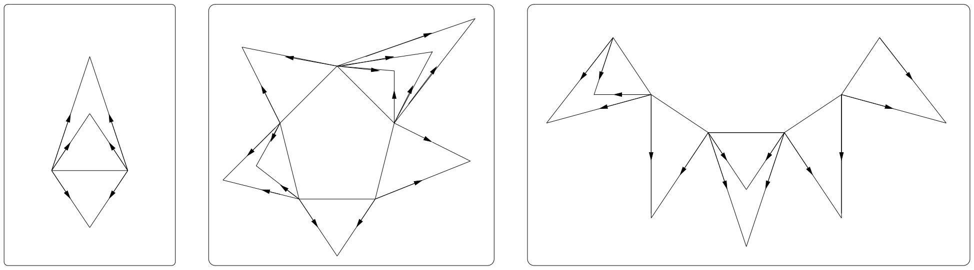
Proposition 4. If k is odd, the number a_n of labelled k-gonal 2-trees on n k-gons is given by

$$a_n = \frac{1}{2}\left(m^{n-2} + 1\right), \qquad n \geq 2, \tag{30}$$

where $m = (k-1)n + 1$ is the number of edges.

For the unlabelled enumeration, notice from Figure 3a that in every k-gon containing the pointed (but not oriented) edge of an a^{-}-structure, it is possible to orient the $k-1$ other edges in a canonical direction, "away from the root edge", when k is odd (but there remains an ambiguous opposite edge if k is even). This phenomenon permits us to introduce *skeleton* species, when k is odd, in analogy with the approach of Fowler et al. They are the two-sort quotient species $Q(X, Y)$, $S(X, Y)$ and $U(X, Y)$, where X represents the sort of k-gons and Y the sort of oriented edges, defined by Figures 4a, b and c, where $k = 5$.

In analogy with the case $k = 3$, we get the following propositions.



a) b) c)

Figure 4: Skeleton species a) $Q(X,Y)$, b) $S(X,Y)$ and c) $U(X,Y)$

Proposition 5. The skeleton species Q, S and U admit the following expressions in terms of quotients species

$$\begin{aligned} Q(X,Y) &= E(XY^2)/\mathbb{Z}_2, && (31)\\ S(X,Y) &= C_k(E(XY^2))/\mathbb{Z}_2, && (32)\\ U(X,Y) &= (E(XY^2))^k/\mathbb{Z}_2. && (33)\end{aligned}$$

Proposition 6. For k odd, $k \geq 3$, we have the following expressions for the pointed species of k-gonal 2-trees, where $B = \mathfrak{a}^{\to}$:

$$\mathfrak{a}^{-} = Q(X, B^{\frac{k-1}{2}}), \quad \mathfrak{a}^{\diamond} = X \cdot S(X, B^{\frac{k-1}{2}}), \quad \mathfrak{a}^{\hat{\diamond}} = X \cdot U(X, B^{\frac{k-1}{2}}). \tag{34}$$

In order to obtain enumerative formulas, we have to compute the cycle index series of the species Q, S and U.

Proposition 7. The cycle index series of the species $Q(X,Y)$, $S(X,Y)$ and $U(X,Y)$ are given by

$$\begin{aligned} Z_Q &= \frac{1}{2}\left(Z_{E(XY^2)} + q\right), && (35)\\ Z_S &= \frac{1}{2}\left(Z_{C_k(E(XY^2))} + q \cdot (p_2 \circ Z_{E(XY^2)})^{\frac{k-1}{2}}\right), && (36)\\ Z_U &= \frac{1}{2}\left(Z_{(E(XY^2))^k} + q \cdot (p_2 \circ Z_{E(XY^2)})^{\frac{k-1}{2}}\right), && (37)\end{aligned}$$

where

$$q = h \circ (x_1 y_2 + p_2 \circ (x_1 \frac{y_1^2 - y_2}{2})), \tag{38}$$

p_2 represents the power sum symmetric function of degree two, h the homogeneous symmetric function and $\circ$, the plethystic substitution.

Proof. We use a two-sort extension of formula (29) but the sort Y is the important one here. The variables $\mathbf{s}$ will keep track of the colored triangles and new variables $\mathbf{t} = (t_1, t_2, \ldots)$, of the colored oriented edges and we seek to express the inventory in terms of the power sums $x_i = p_i(\mathbf{s})$ and $y_i = p_i(\mathbf{t})$. Hence the second terms of the right-hand-sides of formulas (35)–(37), represent the τ-symmetric unlabelled colored $F(X,Y)$-structures. For example, for (35), the given formula (38) simply expresses the fact that a τ-symmetric unlabelled colored $Q(X,Y)$-structure consists of a set of *pages*, where the τ symmetry comes either from a page with identically colored oriented edges or from pairs of pages whose oriented edges are oppositely colored. See [7, 8] for more details.

In the case of S, we have to leave fixed an unlabelled colored $C_k(E(XY^2))$-structure. For this, the cycle of length k must possess (at least) one symmetry axis passing through the middle of one of its sides. The attached structure on this distinguished edge must be globally left fixed; this gives the factor q. On each side of the axis, each colored $E(XY^2)$-structure must have its mirror image; this contributes the factor $(p_2 \circ Z_{E(XY^2)})^{\frac{k-1}{2}}$. It can be seen that in the case of higher degree of symmetry, the choice of the symmetry axis is arbitrary. The reasoning is very similar for the species U and in fact the τ-symmetric term is the same as in the previous case. ■

It is now a simple matter to combine the Dissymmetry Theorem with Propositions 6 and 7 and the substitution rules of unlabelled enumeration in order to obtain $\widetilde{a}(x)$. Note that the first terms of formulas (35)–(37) will give rise to $\widetilde{a}_o(x)$ and that a cancellation will occur in the τ-symmetric terms, leaving only $q(x_i \mapsto x^i, y_i \mapsto \widetilde{B}^{\frac{k-1}{2}}(x^i))$ to compute.

Proposition 8. Let $k \geq 3$ be an odd integer. The ordinary generating series $\widetilde{a}(x)$ of unlabelled k-gonal 2-trees is given by

$$\widetilde{a}(x) = \frac{1}{2}\Bigg(\widetilde{a}_o(x) + \exp\Big(\sum_{i\geq 1} \frac{1}{2i}(2x^i\widetilde{B}^{\frac{k-1}{2}}(x^{2i}) + x^{2i}\widetilde{B}^{k-1}(x^{2i}) - x^{2i}\widetilde{B}^{\frac{k-1}{2}}(x^{4i})\Big)\Bigg). \tag{39}$$

Corollary 3. For $k \geq 3$, odd, the number $\widetilde{a}_n$ of unlabelled k-gonal 2-trees over n k-gons, satisfy the following recurrence

$$\widetilde{a}_n = \frac{1}{2n}\sum_{j=1}^{n}\Bigg(\sum_{l|j} l\omega_l\Bigg)\Big(\widetilde{a}_{n-j} - \frac{1}{2}\widetilde{a}_{o,n-j}\Big) + \frac{1}{2}\widetilde{a}_{o,n}, \quad \widetilde{a}_0 = 1, \tag{40}$$

where, for all $n \geq 1$,

$$\omega_n = 2b_{\frac{n-1}{2}}^{(\frac{k-1}{2})} + b_{\frac{n-2}{2}}^{(k-1)} - b_{\frac{n-2}{4}}^{(\frac{k-1}{2})}, \tag{41}$$

and $b_i^{(j)}$ is defined in Corollary 2.

4.2 Case k even

The case k even is more delicate. For example, as observed by one of the anonymous referees, there are more than one labelled oriented k-gonal 2-tree left fixed by an orientation reversal. They can be obtained by taking an edge labelled ordinary tree and replacing edges by k-gons attached at opposite edges. These k-gonal 2-trees have no *side decoration* and this explains their symmetry with respect to orientation. It is known (and follows from (14) for $k = 2$) that the number of edge-labelled trees with n edges is $(n+1)^{n-2}$. Hence we have the following:

Proposition 9. If k is even, the number a_n of labelled k-gonal 2-trees on n k-gons is given by

$$a_n = \frac{1}{2}\left(m^{n-2} + (n+1)^{n-2}\right), \qquad n \geq 2, \tag{42}$$

where $m = (k-1)n + 1$ is the number of edges.

For the unlabelled enumeration of the three species a^-, $a^\diamond$ and $a^{\hat{-}}$, we apply relation (28) to formulas (26). For the species $a^- = a^{\rightarrow}/\mathbb{Z}_2$, the action of τ consists in reversing the orientation of the rooted edge. we have

$$\widetilde{a}^-(x) = \frac{1}{2}(\widetilde{a}^{\rightarrow}(x) + \widetilde{a}_\tau^{\rightarrow}(x)), \tag{43}$$

where $\widetilde{a}_\tau^{\rightarrow}(x)$ is the tilde generating series of τ-symmetric (unlabelled) oriented-edge-rooted 2-trees. Let a_S denote the subspecies of $B = a^{\rightarrow}$ consisting of $a^{\rightarrow}$-structures s which are isomorphic to their image $\tau \cdot s$. We have to compute $\widetilde{a}_S(x) = \widetilde{a}_\tau^{\rightarrow}(x)$.

Let us introduce some auxiliary subspecies of $\mathcal{A}_{\mathrm{S}}$ which appear when we analyse these τ-symmetric structures in terms of their *pages* that is their maximal sub-2-trees containing a unique triangle adjacent to the rooted edge. We say that there is some *crossed symmetry* if we can find, inside the 2-tree, two *alternated* pages, that is pages of the form $\{s, \tau \cdot s\}$, where s is not itself τ-symmetric, attached to the same root edge. See Figure 5a Let P_{AL} denote the subspecies of pairs of alternated pages. A *mixed page* is a symmetric page having at least one crossed symmetry. See Figure 5b. Let P_{M} denote the species of mixed pages.

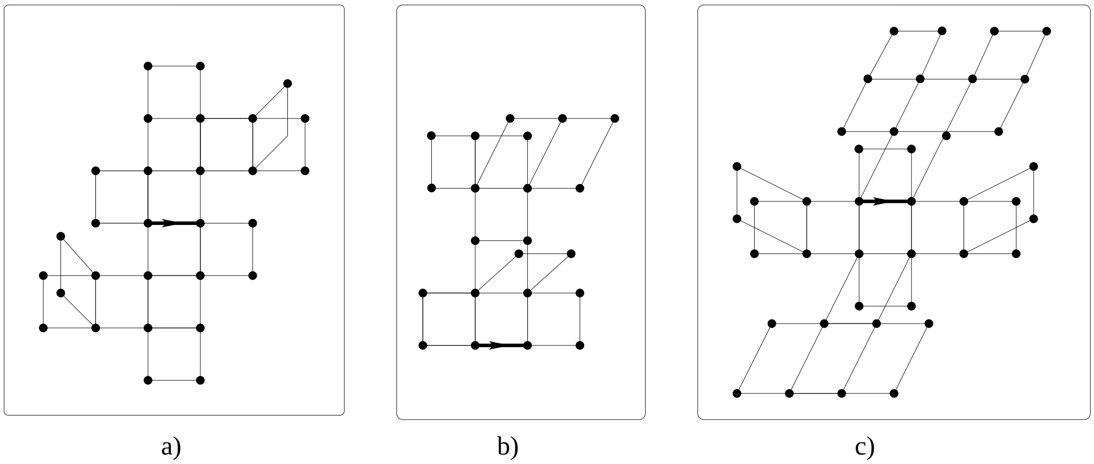


Figure 5: a) A pair of alternated pages, b) a mixed page, c) a totally symmetric $\mathcal{A}^{\rightarrow}$-structure

Finally, we say that a page is *totally symmetric* or *vertically symmetric* if it contains no crossed symmetries. Let P_{TS} denote the species of totally symmetric pages and set

$$\mathcal{A}_{\mathrm{TS}} = E(P_{\mathrm{TS}}), \tag{44}$$

the subspecies of *totally symmetric* $\mathcal{A}^{\rightarrow}$-structures. See Figure 5c. We can characterize all these species and their tilde generating series by functional equations. First, we have

$$P_{\mathrm{TS}} = X \cdot X^2_{=} < B^{\frac{k-2}{2}} > \cdot \mathcal{A}_{\mathrm{TS}}, \tag{45}$$

where $X^2_{=} < F >$ represents the species of ordered pairs of isomorphic F-structures. Note that $(X^2_{=} < F >)^{\sim}(x) = \widetilde{F}(x^2)$. Translating equations (44) and (45) in terms of tilde generating series, we get

$$\widetilde{\mathcal{A}}_{\mathrm{TS}}(x) = \exp\left(\sum_{j\geq 1} \widetilde{P}_{\mathrm{TS}}(x^j)\right) \tag{46}$$

and

$$\widetilde{P}_{\mathrm{TS}}(x) = x\ \widetilde{B}^{\frac{k-2}{2}}(x^2)\widetilde{\mathcal{A}}_{\mathrm{TS}}(x). \tag{47}$$

Proposition 10. The numbers $\pi_n = |\widetilde{P}_{\mathrm{TS}}[n]|$ and $\beta_n = |\widetilde{\mathcal{A}}_{\mathrm{TS}}[n]|$ of unlabelled totally symmetric pages and $\mathcal{A}^{\rightarrow}$-structures, respectively, on n polygons, satisfy the following system of recurrences: $\beta_0 = 1$ and, for $n \geq 1$,

$$\pi_n = \sum_{\substack{i+j=n-1 \\ i\ even}} b^{(\frac{k-2}{2})}_{\frac{i}{2}} \beta_j, \tag{48}$$

$$\beta_n = \frac{1}{n}\sum_{j=0}^{n-1} \beta_j \sum_{d|n-j} d\pi_d. \tag{49}$$

Proof. Formula (48) is obvious. For (49), it suffices to take x times the logarithmic derivative of (46). ■

Now, from the definition of the species P_{AL} of pairs of alternated pages, we have

$$P_{\mathrm{AL}} = \Phi_2 < XB^{k-1} - (P_{\mathrm{TS}} + P_{\mathrm{M}}) >, \tag{50}$$

where $\Phi_2 < F >$ represents the species of unordered pairs of F-structures of the form $\{s, \tau \cdot s\}$. Note that $\Phi_2 < F >^{\sim}(x) = \frac{1}{2}\widetilde{F}(x^2)$ whenever the structures s and $\tau \cdot s$ are guaranteed not to be isomorphic, so that

$$\widetilde{P}_{\mathrm{AL}}(x) = \frac{1}{2}\big(x^2 \widetilde{B}^{k-1}(x^2) - \widetilde{P}_{\mathrm{TS}}(x^2) - \widetilde{P}_{\mathrm{M}}(x^2)\big). \tag{51}$$

Also by definition, the species P_{M} of mixed pages satisfies

$$\begin{aligned} P_{\mathrm{M}} &= X \cdot X^2_{=} < B^{\frac{k-2}{2}} > \cdot (a_{\mathrm{S}} - a_{\mathrm{TS}}) \\ &= X \cdot X^2_{=} < B^{\frac{k-2}{2}} > \cdot a_{\mathrm{S}} - P_{\mathrm{TS}}, \end{aligned} \tag{52}$$

so that

$$\widetilde{P}_{\mathrm{M}}(x) = x\widetilde{B}^{\frac{k-2}{2}}(x^2)\widetilde{a}_{\mathrm{S}}(x) - \widetilde{P}_{\mathrm{TS}}(x). \tag{53}$$

Finally, for the tilde generating series $\widetilde{a}_{\mathrm{S}}(x)$ of unlabelled τ-symmetric $a^{\rightarrow}$-structures, we have (see Figure 6)

$$\widetilde{a}_{\mathrm{S}}(x) = E(P_{\mathrm{TS}} + P_{\mathrm{AL}} + P_{\mathrm{M}})^{\sim}(x), \tag{54}$$

$$= \exp\left(\sum_{i\geq 1} \frac{1}{i}(\widetilde{P}_{\mathrm{TS}}(x^i) + \widetilde{P}_{\mathrm{AL}}(x^i) + \widetilde{P}_{\mathrm{M}}(x^i))\right). \tag{55}$$

From equations (51), (53) and (55) we deduce the following.

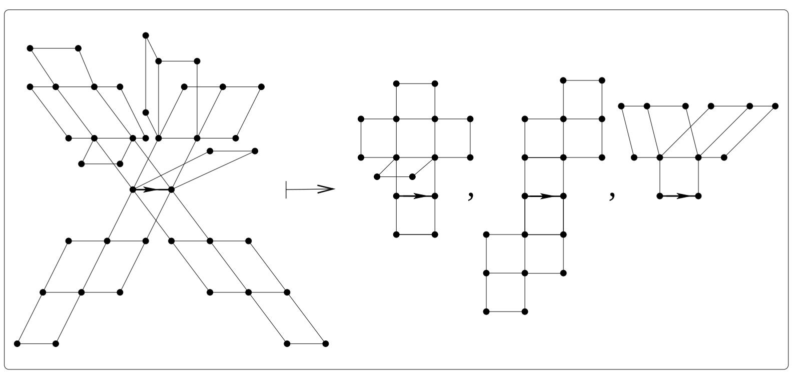


Figure 6: Decomposition of a τ-symmetric $\widetilde{a}^{\rightarrow}$-structure

Proposition 11. The numbers $\alpha_n = \widetilde{a}_{\mathrm{S},n}$ of unlabelled τ-symmetric $a^{\rightarrow}$-structures, $\widetilde{P}_{\mathrm{AL},n}$, of pairs of alternated pages and $\widetilde{P}_{\mathrm{M},n}$ of mixed pages, on n k-gons are characterized by the following system of recurrences: $\alpha_0 = 1$, and for $n \geq 1$,

$$\widetilde{P}_{\mathrm{M},n} = \sum_{i=0}^{n-1} b_{\frac{i}{2}}^{(\frac{k-2}{2})}\alpha_{n-1-i} - \pi_n, \tag{56}$$

$$\widetilde{P}_{\mathrm{AL},n} = \frac{1}{2}\left(b_{\frac{n-2}{2}}^{(k-1)} - \pi_{n/2} - \widetilde{P}_{\mathrm{M},n/2}\right), \tag{57}$$

$$\alpha_n = \frac{1}{n}\sum_{i=1}^{n}\left(\sum_{d|i} d\omega_d\right)\alpha_{n-i}, \tag{58}$$

where $\pi_n = \widetilde{P}_{\mathrm{TS},n}$ is given by Propositon 10 and

$$\omega_k = \pi_k + \widetilde{P}_{\mathrm{AL},k} + \widetilde{P}_{\mathrm{M},k}. \tag{59}$$

Proposition 12. If k is an even integer, then the number of unlabelled (unoriented) edge rooted k-gonal 2-trees over n k-gons is given by

$$\widetilde{a}_n^{-} = \frac{1}{2}(b_n + \alpha_n). \tag{60}$$

Let us now turn to the species $\mathcal{a}^{\diamond}_{-}$ of k-gonal 2-trees rooted at an edge-pointed k-gon.

Proposition 13. We have

$$\widetilde{\mathcal{a}}^{\diamond}_{-}(x) = \frac{1}{2}\left(\widetilde{\mathcal{a}}^{\diamond}_{\overset{-}{o}}(x) + \widetilde{\mathcal{a}}^{\diamond}_{\overset{-}{o},\tau}(x)\right), \tag{61}$$

where

$$\widetilde{\mathcal{a}}^{\diamond}_{\overset{-}{o},\tau}(x) = x\widetilde{\mathcal{a}}^{2}_{\mathrm{S}}(x)\widetilde{B}^{\frac{k-2}{2}}(x^2).$$

Proof. An unlabelled τ-symmetric $\mathcal{a}^{\diamond}_{\overset{-}{o}}$-structure possesses an axis of symmetry which is, in fact, the mediatrix of the distinguished edge of the root polygon, and also the mediatrix of its opposite edge; see Figure 7. The two structures s and t glued on these two edges are thus symmetric, which leads to the term $(\widetilde{\mathcal{a}}_{\mathrm{S}}(x))^2$. Then, on each side of the axis, are found two $B^{\frac{k-2}{2}}$-structures α and β, which by symmetry satisfy $\beta = \tau\cdot\alpha$, contributing to the factor $\widetilde{B}^{\frac{k-2}{2}}(x^2)$. ■

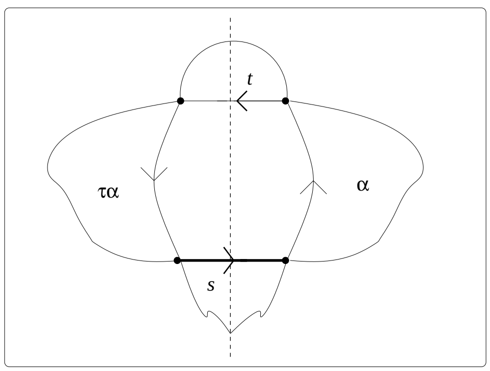


Figure 7: A τ-symmetric unlabelled $\mathcal{a}^{\diamond}_{\overset{-}{o}}$-structures

Corollary 4. We have the following expression for the number $\widetilde{a}^{\diamond}_{\overset{-}{n}}$ of unlabelled $\mathcal{a}^{\diamond}_{-}$-structures,

$$\widetilde{a}^{\diamond}_{\overset{-}{n}} = \frac{1}{2}\left(\widetilde{a}^{\diamond}_{\overset{-}{o},n} + \sum_{i+j=n-1}\alpha_i^{(2)}\cdot b_{\frac{j}{2}}^{(\frac{k-2}{2})}\right), \tag{62}$$

where $\alpha_i^{(2)} = [x^i]\widetilde{\mathcal{a}}^{2}_{S}(x)$. □

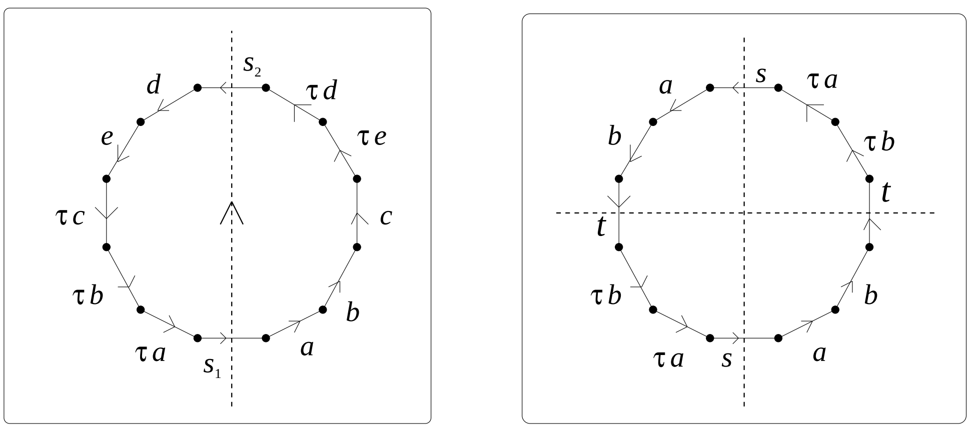
We proceed in a similar way for the species $\mathcal{a}^{\diamond}$, of k-gon rooted k-gonal 2-trees. Once again, we use relation (28), giving

$$\widetilde{\mathcal{a}}^{\diamond}(x) = \frac{1}{2}\left(\widetilde{\mathcal{a}}^{\diamond}_{o}(x) + \widetilde{\mathcal{a}}^{\diamond}_{o,\tau}(x)\right). \tag{63}$$

Proposition 14. Let $\widetilde{a}^{\diamond}_{o,\tau}(x)$ be the generating series of unlabelled $a^{\diamond}_{o}$-structures which are left fixed by orientation reversing. Then, we have

$$\widetilde{a}^{\diamond}_{o,\tau}(x) = \frac{x}{2}\widetilde{a}^{2}_{\mathrm{S}}(x)\widetilde{B}^{\frac{k-2}{2}}(x^2) + \frac{x}{2}\widetilde{B}^{\frac{k}{2}}(x^2). \tag{64}$$

Proof. Notice first that in order to be left fixed by orientation reversing, an $a^{\diamond}_{o}$-structure must admit a reflective symmetry, along an axis which can either pass through the middle of two opposite edges, or pass through opposite vertices of the pointed polygon. The enumeration is carried out by first orienting the axis of symmetry. The first term of (64) then corresponds to an edge–edge symmetry, and the second term to a vertex–vertex symmetry. The structures having both symmetries are precisely those which are counted one half time in both of these terms. This is established for a general k by considering the unique power of 2, 2^m, such that $k/2^m$ is odd. We illustrate the proof in the following lines with $k = 12$; the reader will easily convince himself of the validity of this argument for any k.



a) b)

Figure 8: $\widetilde{a}^{\diamond}_{o,\tau}$-structures with an edge–edge symmetry

For $k = 12$, a general unlabelled τ-symmetric polygon-rooted oriented k-gonal 2-tree with an oriented edge–edge axis will be of the form illustrated in Figure 8 a), where s_1 and s_2 represent unlabelled a_{S}-structures, a, b, c, d and e are general unlabelled B-structures and τx represents the opposite of the B-structures x, obtained by reversing their orientation. Most of these structures are enumerated exactly by $\frac{1}{2}x\widetilde{a}^{2}_{\mathrm{S}}(x)\widetilde{B}^{5}(x^2)$. Indeed, the factor $x\widetilde{a}^{2}_{\mathrm{S}}(x)\widetilde{B}^{5}(x^2)$ is obtained in the same way as for $a^{\diamond}_{\bar{o},\tau}$-structures and the division by two is justified in the following cases:

1. $s_1 \neq s_2$ (two orientations of the axis),
2. $s_1 = s_2 = s$, $(a, b, c) \neq (d, e, \tau \cdot c)$ (two orientations),
3. $s_1 = s_2 = s$, $(a, b, c) = (d, e, \tau \cdot c)$, so that $c = \tau \cdot c = t \in \widetilde{a}_{\mathrm{S}}$, and either $s \neq t$ or $s = t$ and $(a, b) \neq (\tau \cdot b, \tau \cdot a)$ (two choices for the symmetry axis, see Figure 8 b)),

However, the structures with $s = t$ and $b = \tau \cdot a$ (see Figure 9) will occur only once and are counted only one half time in the formula. But, notice that these structures also admit a vertex–vertex symmetry axis and, as it will turn out, are also counted one half time in the second term of (64).

Similarly, an unlabelled $a^{\diamond}_{o,\tau}$-structure with an oriented vertex–vertex symmetry axis will be of the form illustrated in Figure 10 a), where a, b, …, f are arbitrary unlabelled B-structures. Most of these terms are enumerated exactly by $\frac{1}{2}x\widetilde{B}^{6}(x^2)$, the division by two being justified in the following cases:

1. $(a, b, c) \neq (d, e, f)$ (two orientations of the symmetry axis),

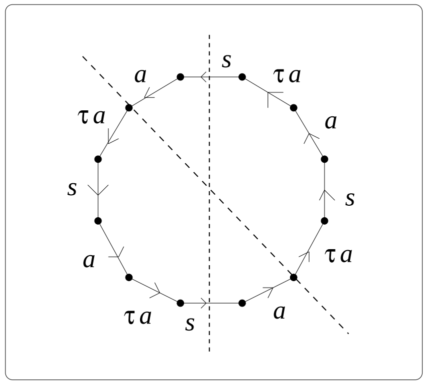
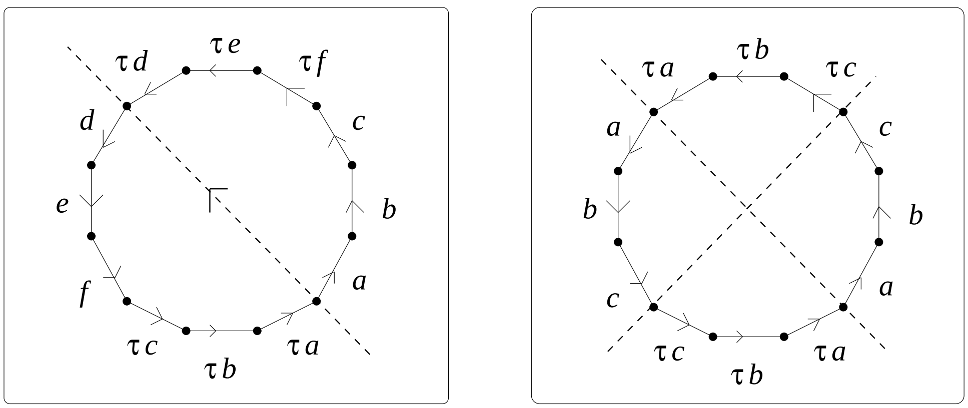


Figure 9: An $\widetilde{\mathcal{a}}^{\diamond}_{o,\tau}$-structure with edge–edge and vertex–vertex symmetries

2. $(a,b,c) = (d,e,f)$ and $(a,b,c) \neq (\tau \cdot c, \tau \cdot b, \tau \cdot a)$ (two choices for the symmetry axis, see Figure 10 b)),



a) b)

Figure 10: $\widetilde{\mathcal{a}}^{\diamond}_{o,\tau}$-structures with a vertex–vertex symmetry axis

However, the structures with $(a,b,c) = (d,e,f)$, $c = \tau \cdot a$ and $b = \tau \cdot b = s \in \widetilde{\mathcal{a}}_{\mathrm{S}}$ appear only once and are counted one half time here. But they also have an edge-edge symmetry axis and were also counted one half time in the first term of (64) (exchange a and $\tau \cdot a$ in Figure 9). ∎

The Dissymmetry Theorem yields, for k even,

$$\widetilde{\mathcal{a}}(x) = \frac{1}{2}\widetilde{\mathcal{a}}_o(x) + \frac{1}{2}\widetilde{\mathcal{a}}_{\mathrm{S}}(x) + \frac{1}{2}\widetilde{\mathcal{a}}^{\diamond}_{o,\tau}(x) - \frac{1}{2}\widetilde{\mathcal{a}}^{\underline{\diamond}}_{o,\tau}(x), \tag{65}$$

and we have the following result.

Proposition 15. Let k be an even integer, $k \geq 4$. Then the generating series $\widetilde{\mathcal{a}}(x)$ of unlabelled k-gonal 2-trees is given by

$$\widetilde{\mathcal{a}}(x) = \frac{1}{2}\widetilde{\mathcal{a}}_o(x) + \frac{1}{2}\widetilde{\mathcal{a}}_{\mathrm{S}}(x) + \frac{x}{4}(\widetilde{B}^{\frac{k}{2}}(x^2) - \widetilde{\mathcal{a}}^2_{\mathrm{S}}(x)\widetilde{B}^{\frac{k-2}{2}}(x^2)). \tag{66}$$

Corollary 5. Let k be an even integer, $k \geq 4$. Then the number of unlabelled k-gonal 2-trees over n k-gons is given by

$$\widetilde{a}_n = \frac{1}{2}\widetilde{a}_{o,n} + \frac{1}{2}\alpha_n + \frac{1}{4}b^{(\frac{k}{2})}_{\frac{n-1}{2}} - \frac{1}{4}\sum_{i+j=n-1} \alpha^{(2)}_i \cdot b^{(\frac{k-2}{2})}_{\frac{j}{2}}, \tag{67}$$

where

$$b_l^{(m)} = [x^l]\widetilde{B}^m(x), \quad \alpha_i^{(2)} = [x^i]\,\widetilde{a}_{\mathrm{S}}^2(x).$$

Note that the case $k = 2$ corresponds to ordinary trees with n edges and that the formulas given here are also valid when properly interpreted. Table 1 gives the exact values of the numbers $\widetilde{a}_n$ of unlabelled k-gonal 2-trees with n k-gons, for k from 2 up to 12 and for $n = 0, 1, \ldots, 20$.

$\boldsymbol{k = 2}$
1, 1, 1, 2, 3, 6, 11, 23, 47, 106, 235, 551, 1301, 3159, 7741, 19320, 48629, 123867, 317955, 823065, 2144505
$\boldsymbol{k = 3}$
1, 1, 1, 2, 5, 12, 39, 136, 529, 2171, 9368, 41534, 188942, 874906, 4115060, 19602156, 94419351, 459183768, 2252217207, 11130545494, 55382155396
$\boldsymbol{k = 4}$
1, 1, 1, 3, 8, 32, 141, 749, 4304, 26492, 169263, 1115015, 7507211, 51466500, 358100288, 2523472751, 17978488711, 129325796854, 938234533024, 6858551493579, 50478955083341
$\boldsymbol{k = 5}$
1, 1, 1, 3, 11, 56, 359, 2597, 20386, 167819, 1429815, 12500748, 111595289, 1013544057, 9340950309, 87176935700, 822559721606, 7836316493485, 75293711520236, 728968295958626, 7105984356424859
$\boldsymbol{k = 6}$
1, 1, 1, 4, 16, 103, 799, 7286, 71094, 729974, 7743818, 84307887, 937002302, 10595117272, 121568251909, 1412555701804, 16594126114458, 196829590326284, 2354703777373055, 28385225424840078, 344524656398655124
$\boldsymbol{k = 7}$
1, 1, 1, 4, 20, 158, 1539, 16970, 199879, 2460350, 31266165, 407461893, 5420228329, 73352481577, 1007312969202, 14008437540003, 196963172193733, 2796235114720116, 40038505601111596, 577693117173844307, 8392528734991449808
$\boldsymbol{k = 8}$
1, 1, 1, 5, 26, 245, 2737, 35291, 483819, 6937913, 102666626, 1558022255, 24133790815, 380320794122, 6081804068869, 98490990290897, 1612634990857755, 26660840123167203, 444560998431678554, 7469779489114328514, 126375763235359105446
$\boldsymbol{k = 9}$
1, 1, 1, 5, 32, 343, 4505, 66603, 1045335, 17115162, 289107854, 5007144433, 88516438360, 1591949961503, 29053438148676, 536972307386326, 10034276171127780, 189331187319203010, 3603141751525175854, 69097496637591215442, 1334213677527481808220
$\boldsymbol{k = 10}$
1, 1, 1, 6, 39, 482, 7053, 117399, 2070289, 38097139, 723169329, 14074851642, 279609377638, 5651139037570, 115901006038377, 2407291353219949, 50553753543016719, 1071971262516091572, 22926544048209731554, 494103705426160765546, 10722146465907412669810
$\boldsymbol{k = 11}$
1, 1, 1, 6, 46, 636, 10527, 194997, 3823327, 78118107, 1646300388, 35570427615, 784467060622, 17601062294302, 400750115756742, 9240636709048733, 215435023547580882, 5071520482516388865, 120417032326341878672, 2881134828445365441407, 69410468220307148620226
$\boldsymbol{k = 12}$
1, 1, 1, 7, 55, 840, 15189, 309607, 6671842, 149850849, 3471296793, 82442359291, 1998559329142, 49290785442796, 1233639304644946, 31268489727956101, 801335133177932829, 20736286803363051714, 541224489038545084067, 14234799536039481373552, 376974819516101224941091

Table 1: Values of $\widetilde{a}_n$ for $k = 2, \ldots, 12$ and $n = 0, \ldots, 20$

5 Asymptotics

Thanks to the Dissymmetry Theorem and to the various combinatorial equations related to it, the asymptotic enumeration of unlabelled k-gonal 2-trees depends essentially on the asymptotic enumeration of B-structures where B is the auxiliary species characterized by the functional equation (9).

We first give the following result, which is a consequence of the classical theorem of Bender (see [3]) and is inspired from the approach of Fowler et al. for 2-trees (see [7, 8]).

Proposition 16. Let $p = k - 1$. Let us write $b(x) = \widetilde{B}(x) = \sum b_n(p)x^n$. Let ξ_p be the smallest root of the equation

$$\xi = \frac{1}{ep}\omega^{-p}(\xi), \tag{68}$$

where $\omega(x)$ is defined by

$$\omega(x) = \mathrm{e}^{\frac{1}{2}x^2 b^p(x^2) + \frac{1}{3}x^3 b^p(x^3) + \cdots}. \tag{69}$$

Then, there exist constants α_p and β_p such that

$$b_n(p) \sim \alpha_p \beta_p^n n^{-3/2}, \qquad \text{as } n \to \infty. \tag{70}$$

Moreover,

$$\alpha_p = \alpha(\xi_p) = \frac{1}{\sqrt{2\pi}} \frac{1}{p^{1+\frac{1}{p}}} \xi_p^{-\frac{1}{p}} \left(1 + \frac{p\xi_p \omega'(\xi_p)}{\omega(\xi_p)}\right)^{\frac{1}{2}} \tag{71}$$

and

$$\beta_p = \frac{1}{\xi_p}, \tag{72}$$

Proof. The functional equation (19) implies that $y = b(x)$ satisfies the relation

$$y = e^{xy^p} \omega(x). \tag{73}$$

By Bender's theorem applied to the function $f(x, y) = y - e^{xy^p}\omega(x)$, we have to find a solution (ξ_p, τ_p) of the system

$$f(x, y) = 0 \qquad \text{and} \qquad f_y(x, y) = 0. \tag{74}$$

It is equivalent to say that ξ_p is solution of (68) and that $p\xi_p\tau_p^p = 1$. In fact, ξ_p is the radius of convergence of $b(x)$ and $\sqrt{\xi_p}$ is radius of convergence of $\omega(x)$. It can be shown that $0 < \xi_p < 1$ so that $0 < \xi_p < \sqrt{\xi_p} < 1$. Indeed, if ρ_p is the radius of convergence of the algebraic function $\theta(x)$ defined by $\theta = 1 + x\theta^p$, then, using Lagrange Inversion Formula and Stirling's Formula, we obtain $\rho_p = (p-1)^{p-1}/p^p < 1$, for $p \geq 2$. Now, take a small fixed $x > 0$ and consider the two curves $z = \varphi_1(y) = 1 + xy^p$ and $z = \varphi_2 = e^{xy^p}\omega(x)$ in the (y, z)-plane. Since $\varphi_1(y) < \varphi_2(y)$, for $y > 0$, and $\theta(x) = \varphi_1(\theta(x))$ and $b(x) = \varphi_2(b(x))$, we have that $\theta(x) < b(x)$. If $x_0 > \rho_p$, we must have $b(x_0) = \infty$ since $\theta(x_0) = \infty$. This implies that $\xi_p \leq \rho_p$. For $p = 1$ ($k = 2$), a similar argument with $\varphi_1(y) = 1 + xy + xy^2/2$ shows that $\xi_1 \leq \sqrt{2} - 1$. Note also that from the recurrence (16) it follows that $b_n(p)$ is bounded by the coefficient c_n of the function $c(x)$ defined by $c = 1 + xc^k$, so that we have $\xi_p \geq \rho_{p+1} = p^p/(p+1)^{p+1}$, for $p \geq 1$.

Since $f_{yy}(\xi_p, \tau_p) \neq 0$, ξ_p is an algebraic singularity of degree 2 of $b(x)$ and, for x near ξ_p, we have an expression of the form

$$b(x) = \tau_{p,0} + \tau_{p,1}(1 - \frac{x}{\xi_p})^{\frac{1}{2}} + \tau_{p,2}(1 - \frac{x}{\xi_p}) + \tau_{p,3}(1 - \frac{x}{\xi_p})^{\frac{3}{2}} + \cdots \tag{75}$$

where

$$\tau_{p,0} = \tau_p = b(\xi_p) = \left(\frac{1}{p\xi_p}\right)^{\frac{1}{p}}, \tag{76}$$

$$\tau_{p,1} = -\frac{\sqrt{2}}{p^{1+\frac{1}{p}}} \xi_p^{-\frac{1}{p}} \left(1 + \frac{p\xi_p\omega'(\xi_p)}{\omega(\xi_p)}\right)^{\frac{1}{2}}, \tag{77}$$

$$\tau_{p,2} = \frac{1}{3p^{2+\frac{1}{p}}} \xi_p^{-\frac{1}{p}} \left((2p+3) - p(p-3)\frac{\xi_p\omega'(\xi_p)}{\omega(\xi_p)}\right). \tag{78}$$

The asymptotic formula (70) with α_p and β_p given by (71) and (72) then follow from the fact that the main term of the asymptotic behavior of the coefficients $b_n(p)$ of x^n in (75) depends only on the term $\tau_{p,1}(1 - \frac{x}{\xi_p})^{\frac{1}{2}}$ in (75) and is given by

$$b_n(p) \sim \binom{\frac{1}{2}}{n} \tau_{p,1} (-1)^n \frac{1}{\xi_p^n} \sim \alpha_p \beta_p^n n^{-\frac{3}{2}} \quad \text{as} \quad n \to \infty. \tag{79}$$

■

Note that numerical approximations of ξ_p, for fixed p, can be computed by iteration using (68), and a suitable truncated polynomial approximation of $b(x)$. We now state our main asymptotic result.

Proposition 17. Let $p = k-1$. Then, the number $\widetilde{a}_n$ of k-gonal 2-trees on n unlabelled k-gons satisfy

$$\widetilde{a}_n \sim \frac{1}{2}\widetilde{a}_{o,n}, \quad n \to \infty, \tag{80}$$

where $\widetilde{a}_{o,n}$ is the number of oriented k-gonal 2-trees over n unlabelled polygons. Moreover,

$$\widetilde{a}_{o,n} \sim \overline{\alpha}_p \beta_p^n n^{-5/2}, \quad n \to \infty, \tag{81}$$

where

$$\overline{\alpha_p} = 2\pi p^{1+\frac{2}{p}} \xi_p^{\frac{2}{p}} \alpha_p^3, \tag{82}$$

$$= \frac{1}{\sqrt{2\pi}} \frac{1}{p^{2+\frac{1}{p}}} \xi_p^{-\frac{1}{p}} \left(1 + p\frac{\omega^{'}(\xi_p)}{\omega(\xi_p)}\right)^{\frac{3}{2}}, \tag{83}$$

and $\beta_p = \frac{1}{\xi_p}$ is the same growth as in Proposition 16.

Proof. The asymptotic formula (80) follows from the fact that the radius of convergence, ξ_p, of $\widetilde{a}(x)$ is equal to the radius of convergence of the dominating term $\frac{1}{2}\widetilde{a}_o(x)$. This is due to the easily checked fact that all terms in (39) and (66), except $\frac{1}{2}\widetilde{a}_o(x)$, have a radius of convergence greater or equal to $\sqrt{\xi_p} > \xi_p$. To establish (81), note first that, because of equation (23), the radius of convergence of $\widetilde{a}_o(x)$ is equal to the radius of convergence, ξ_p, of

$$b(x) - \frac{k-1}{k} x b^k(x), \tag{84}$$

where $b(x) = \widetilde{B}(x)$ and $k = p+1$. This implies that the asymptotic behavior of the coefficients $\widetilde{a}_{o,n}$ of $\widetilde{a}_o(x)$ is completely determined by that of (84). Substituting (75) into (84) and making use of (78) gives the following expansion

$$b(x) - \frac{k-1}{k} x b^k(x) = \overline{\tau}_{p,0} + \overline{\tau}_{p,1}\left(1 - \frac{x}{\xi_p}\right)^{\frac{1}{2}} + \overline{\tau}_{p,2}\left(1 - \frac{x}{\xi_p}\right) + \overline{\tau}_{p,3}\left(1 - \frac{x}{\xi_p}\right)^{\frac{3}{2}} + \cdots \tag{85}$$

where

$$\overline{\tau}_{p,0} = \frac{p}{p+1}\tau_{p,0}, \tag{86}$$

$$\overline{\tau}_{p,1} = 0, \tag{87}$$

$$\overline{\tau}_{p,2} = -\frac{1}{2}\frac{p(p+1)\tau_{p,1}^2 - 2\tau_{p,0}^2}{(p+1)\tau_{p,0}}, \tag{88}$$

$$\overline{\tau}_{p,3} = -\frac{1}{6}\frac{\tau_{p,1}(6p\tau_{p,0}\tau_{p,2} + p(p-1)\tau_{p,1}^2 - 6\tau_{p,0}^2)}{\tau_{p,0}^2}, \tag{89}$$

$$= -\frac{p}{3}\frac{\tau_{p,1}^3}{\tau_{p,0}^2}. \tag{90}$$

This implies that the dominating term for the asymptotic behavior of the coefficients $\widetilde{a}_{n,o}$ of x^n in $\widetilde{a}_o(x)$ depends only on the term $\overline{\tau}_{p,3}\left(1 - \frac{x}{\xi_p}\right)^{\frac{3}{2}}$ in (85) and is given by

$$\widetilde{a}_{n,o} \sim \binom{\frac{3}{2}}{n}\overline{\tau}_{p,3}(-1)^n \frac{1}{\xi_p^n} \sim \overline{\alpha}_p \beta_p n^{-\frac{5}{2}}, \quad \text{as } n \to \infty. \tag{91}$$

Computations making use of (90), (76) and (77), show that $\overline{\alpha}_p$ is indeed given by (82) and (83). ∎

Our final result gives an explicit formula in terms of integer partitions for the common radius of convergence ξ_p of the series $\widetilde{B}(x)$, $\widetilde{a}(x)$ and $\widetilde{a}_o(x)$ from which the growth constant $\beta_p = \frac{1}{\xi_p}$ is obtained. We need the following special notations. If $\lambda = (\lambda_1 \geq \lambda_2 \geq \ldots \geq \lambda_\nu)$ is a partition of an integer n in ν parts, we write $\lambda \vdash n$, $n = |\lambda|$, $\nu = l(\lambda)$, $m_i(\lambda) = |\{j : \lambda_j = i\}|$ = number of parts of size i in λ. Furthermore, we put

$$\sigma_i(\lambda) = \sum_{d|i} d m_d(\lambda), \quad \sigma_i^*(\lambda) = \sum_{d|i, d<i} d m_d(\lambda), \tag{92}$$

$$\widehat{\lambda} = 1 + |\lambda| + l(\lambda), \quad \widehat{z}(\lambda) = 2^{m_1(\lambda)} m_1(\lambda)! 3^{m_2(\lambda)} m_2(\lambda)! \ldots. \tag{93}$$

Proposition 18. We have the convergent expansion

$$\xi_p = \sum_{n=1}^{\infty} \frac{c_n}{p^n}, \tag{94}$$

where the coefficients c_n are constants, independent of p, explicitely given by

$$c_n = \sum_{\lambda \vdash n} \frac{e^{-\widehat{\lambda}}}{\widehat{\lambda} \widehat{z}(\lambda)} \prod_{i \geq 1} (\sigma_i(\lambda) - \widehat{\lambda})^{m_i(\lambda)-1} (\sigma_i^*(\lambda) - \widehat{\lambda}), \tag{95}$$

where λ runs over the set of partitions of n.

Proof. We establish the explicit formulas (94) and (95) by applying first Lagrange inversion to the equation $\xi = zR(\xi)$ where $z = \frac{1}{\mathrm{e}p}$ and $R(t) = \omega^{-p}(t)$, to get

$$\xi_p = \xi = \sum_{n \geq 1} \gamma_n \left(\frac{1}{\mathrm{e}p} \right)^n, \quad \text{and} \quad \gamma_n = \frac{1}{n} [t^{n-1}] \omega^{-np}(t). \tag{96}$$

Next, to explicitely evaluate $\omega^{-np}(x)$, we use Labelle's version ([15]) of the Good inversion formula in the context of cycle index series as follows. We begin with

$$\omega^p(x) = \exp(\frac{1}{2} p x^2 b^p(x^2) + \frac{1}{3} p x^3 b^p(x^3) + \cdots), \tag{97}$$

$$= \exp(\frac{1}{2} p x_2 + \frac{1}{3} p x_3 + \cdots) \circ Z_{XB^p(X)} \Big|_{x_i := x^i} \tag{98}$$

where the $\circ$ denotes the plethystic substitution. Using (11), we can then write $XB^p(X) = \frac{A(pX)}{p}$. This implies that

$$\omega^p(x) = \exp(\frac{1}{2} p x_2 + \frac{1}{3} p x_3 + \cdots) \circ \frac{Z_A(px_1, px_2, \ldots)}{p} \Big|_{x_i := x^i}, \tag{99}$$

and we get

$$\omega^{-np}(x) = \exp(-\frac{n}{2} p x_2 - \frac{n}{3} p x_3 - \cdots) \circ \left(\frac{1}{p} Z_A(px_1, px_2, \ldots) \right) \Big|_{x_i := x^i} \tag{100}$$

$$= \exp(-\frac{n}{2} x_2 - \frac{n}{3} x_3 - \cdots) \circ Z_A(x_1, x_2, \ldots) \Big|_{x_i := px^i}. \tag{101}$$

Then, using Labelle's inversion formula for cycle index series, we have, for any formal cycle index series $g(x_1, x_2, \ldots)$

$$[x_1^{n_1} x_2^{n_2} \ldots] \; g \circ Z_A(x_1, x_2, \ldots) = [t_1^{n_1} t_2^{n_2} \ldots] g(t_1, t_2, \ldots) \prod_{i=1}^{\infty} (1 - t_i) \exp(n_i (t_i + \frac{1}{2} t_{2i} + \cdots)), \tag{102}$$

and

$$\prod_{j=1}^{\infty}\exp(n_j(t_j+\frac{1}{2}t_{2j}+\cdots))=\prod_{i=1}^{\infty}\exp(\sum_{d|i}dn_d\frac{t_i}{i}). \tag{103}$$

Taking $g(x_1,x_2,\ldots)=\exp(-\frac{\nu}{2}px_2-\frac{\nu}{3}px_3-\cdots)$, gives, after some computations,

$$[x_1^{n_1}x_2^{n_2}\ldots]\left(\exp(-\frac{\nu}{2}x_2-\frac{\nu}{3}x_3-\cdots)\circ Z_A\right)=$$

$$\begin{cases} 0 & \text{if} \quad n_1>0, \\ \left(\dfrac{\prod\limits_{i\geq 2}(-\nu+\sum\limits_{d|i}dn_d)^{n_i-1}(-\nu+\sum\limits_{d|i,d<i}dn_d)}{2^{n_2}n_2!3^{n_3}n_3!\ldots}\right) & \text{if} \quad n_1=0. \end{cases} \tag{104}$$

Making the substitution $x_i:=px^i$, for $i=1,2,3,\ldots$, gives the explicit formula

$$\omega^{-\nu p}(x)=\sum_{n\geq 0}\left(\sum_{2n_2+3n_3+\cdots=n}p^{n_2+n_3+\cdots}\frac{\prod\limits_{i\geq 2}(-\nu+\sum\limits_{d|i}dn_d)^{n_i-1}(-\nu+\sum\limits_{d|i,d<i}dn_d)}{2^{n_2}n_2!3^{n_3}n_3!\ldots}\right)x^n.$$

This implies, taking $\nu=n$ and using (96), that

$$\begin{aligned}\xi_p &= \sum_{n\geq 1}\frac{1}{n}\left(\sum_{2n_2+3n_3+\cdots=n-1}p^{n_2+n_3+\cdots}\frac{\prod\limits_{i\geq 2}(1-n+\sum\limits_{d|i}dn_d)^{n_i-1}(1-n+\sum\limits_{d|i,d<i}dn_d)}{2^{n_2}n_2!3^{n_3}n_3!\ldots}\right)\left(\frac{1}{\mathrm{e}p}\right)^n, \\ &= \sum_{n\geq 1}\frac{c_n}{p^n},\end{aligned}$$

where the coefficients c_n, $n\geq 1$, are given by (95). ■

Here are the first few values of the universal constants c_n occuring in (94), for $n=1,\ldots,5$.

$$\begin{aligned} c_1 &= \frac{1}{\mathrm{e}} = 0.36787944117144232160, \\ c_2 &= -\frac{1}{2}\frac{1}{\mathrm{e}^3} = -0.024893534183931971 49, \\ c_3 &= \frac{1}{8}\frac{1}{\mathrm{e}^5}-\frac{1}{3}\frac{1}{\mathrm{e}^4} = -0.0052629695880257100 4, \\ c_4 &= -\frac{1}{48}\frac{1}{\mathrm{e}^7}+\frac{1}{\mathrm{e}^6}-\frac{1}{4}\frac{1}{\mathrm{e}^5} = 0.00077526788594593923, \\ c_5 &= \frac{1}{384}\frac{1}{\mathrm{e}^9}-\frac{4}{3}\frac{1}{\mathrm{e}^8}+\frac{49}{72}\frac{1}{\mathrm{e}^7}-\frac{1}{5}\frac{1}{\mathrm{e}^6} = 0.00032212622183609932. \end{aligned} \tag{105}$$

Table 2 gives, to 12 decimal places, the constants ξ_p, α_p, $\overline{\alpha}_p$ and $\beta_p=\frac{1}{\xi_p}$ for $p=1,\ldots,12$.

Remark 1. The computations of this section are also valid for the case $k=2$ ($p=1$), corresponding to the class of ordinary rooted trees (*Cayley trees*) defined by the functional equation $A=XE(A)$. In this case, the growth constant $\beta=\beta_1$, in (70), is known as the Otter constant (see [21]). It is interesting to note that this constant takes the explicit form $\beta=\frac{1}{\xi_1}$, with

$$\xi_1=\sum_{n\geq 1}c_n. \tag{106}$$

p	ξ_p	α_p	$\overline{\alpha}_p$	β_p
1	0.338321856899	1.300312124682	1.581185475409	2.955765285652
2	0.177099522303	0.349261381742	0.349261381742	5.646542616233
3	0.119674100436	0.191997258650	0.067390781222	8.356026879296
4	0.090334539604	0.131073637349	0.034020667269	11.069962877759
5	0.072539192528	0.099178841365	0.020427915489	13.785651110085
6	0.060597948397	0.079660456931	0.013601784466	16.502208844693
7	0.052031135998	0.066517090385	0.009699566188	19.219261329064
8	0.045585869619	0.057075912245	0.007262873797	21.936622211299
9	0.040561059517	0.049970993036	0.005640546218	24.654188324989
10	0.036533820306	0.044433135893	0.004506504206	27.371897918664
11	0.033233950789	0.039996691773	0.003682863427	30.089711763681

Table 2: Numerical values of ξ_p, α_p, $\overline{\alpha}_p$ and β_p, $p = 1, \ldots, 12$

Acknowledgments

We thank the referees for correcting a mistake in Proposition 9 and for making many constructive suggestions.

References

[1] P. Auger, G. Labelle and P. Leroux, *Computing the molecular expansion of species with the Maple package Devmol*, Séminaire Lotharingien de Combinatoire, Article B49z (2003), 34 p. (http://euler.univ-lyon1.fr/home/slc)

[2] L. W. Beineke and J. W. Moon, *Several proofs of the number of labeled 2-dimensional trees*, in "Proof Techniques in Graph Theory" (F. Harary, Ed.), 11–20, Academic Press, New York, (1969).

[3] E. A. Bender *Asymptotic methods in enumeration*, SIAM Rev., **16**, 485–515, (1974).

[4] F. Bergeron, G. Labelle, and P. Leroux, *Combinatorial Species and Tree-like Structures*, Encyclopedia of Mathematics and its Applications, vol. **67**, Cambridge University Press, (1998).

[5] M. Bona, M. Bousquet, G. Labelle and P. Leroux, *Enumeration of m-ary cacti*, Discrete Mathematics, **157**, 227–240, (1996).

[6] L. Comtet, *Analyse Combinatoire*, tome premier, Presses Universitaires de France, (1970).

[7] T. Fowler, I. Gessel, G. Labelle and P. Leroux, *Specifying 2-trees*, Proceedings FPSAC'00, Moscow, June 26-30, 2000, D. Krob, A. A. Mikhalev, A. V. Mikhalev Eds, Springer-Verlag, 202–213.

[8] T. Fowler, I. Gessel, G. Labelle and P. Leroux, *The Specification of 2-trees*, Advances in Applied Mathematics, **28**, 145–168, (2002).

[9] F. Harary and E. Palmer, *Graphical Enumeration*, Academic Press, New York, (1973).

[10] F. Harary, E. Palmer and R. Read, *On the cell-growth problem for arbitrary polygons*, Discrete Mathematics, **11**, 371–389, (1975).

[11] INRIA, *Encyclopedia of combinatorial structures*, `http://algo.inria.fr/encyclopedia/index.html`.

[12] A. Joyal, *Une théorie combinatoire des séries formelles*, Advances in Mathematics, **42**, 1–82, (1981).

[13] T. Kloks, *Enumeration of biconnected partial 2-trees*, 26$^{\text{th}}$ Dutch Mathematical Conference, 1990.

[14] T. Kloks, *Treewidth*, Ph.D. Thesis, Royal University of Utrecht, Holland, (1993).

[15] G. Labelle, *Some new computational methods in the theory of species*, Combinatoire énumérative, Proceedings, Montréal, Québec, Lectures Notes in Mathematics, vol. 1234, Springer-Verlag, New-York/Berlin, 160–176, (1985).

[16] G. Labelle and P. Leroux, *Enumeration of (uni- or bi-colored) plane trees according to their degree distribution*, Discrete Mathematics, **157**, 227–240, (1996).

[17] G. Labelle, C. Lamathe and P. Leroux, *Développement moléculaire de l'espèce des 2-arbres planaires*, Proceedings GASCom'01, 41–46, (2001).

[18] G. Labelle, C. Lamathe and P. Leroux, *A classification of plane and planar 2-trees*, Theoretical Computer Science, **307**, 337–363, (2003).

[19] G. Labelle, C. Lamathe and P. Leroux, *Enumération des 2-arbres k-gonaux*, in Mathematics and Computer Science II, Edited by B. Chauvin, P. Flajolet D. Gardy and A. Mokkadem, Trends in Mathematics, Birkhäuser Verlag Basel Switzwerland, 95–109, (2002).

[20] G. Labelle, C. Lamathe and P. Leroux, *Dénombrement des 2-arbres k-gonaux selon leur taille et leur périmètre*, Annales des Sciences Mathématiques du Québec, submitted, (2003).

[21] R. Otter, *The number of trees*, Annals of Mathematics, **49**, 583–599, (1948).

[22] E. Palmer, *On the Number of Labeled 2-trees*, Journal of Combinatorial Theory, **6**, 206–207, (1969).

[23] E. Palmer and R. Read, *On the Number of Plane 2-trees*, Journal of London Mathematical Society, **6**, 583–592, (1973).

[24] H. Prüfer, *Neuer Beweis eines Satzes über Permutationen*, Arch. Math, Phys., **27**, 742–744, (1918).

[25] N. J. A. Sloane, *The On-Line Encyclopedia of Integer Sequences*, `http://www.research.att.com/~njas/sequences`

[26] N. J. A. Sloane and S. Plouffe, *The Encyclopedia of Integer Sequences*, Academic Press, San Diego, (1995).

E-mail adresses: [gilbert,leroux]@lacim.uqam.ca, lamathe@loria.fr