FPSAC 2008, Valparaiso-Viña del Mar, Chile DMTCS proc. **AJ**, 2008, 247–258

New combinatorial computational methods arising from pseudo-singletons

Gilbert Labelle†

Laboratoire de Combinatoire et d'Informatique Mathématique, Université du Québec à Montréal,CP 8888, Succ. Centre-ville, Montréal (QC) Canada H3C3P8

Abstract. Since singletons are the connected sets, the species X of singletons can be considered as the combinatorial logarithm of the species $E(X)$ of finite sets. In a previous work, we introduced the (rational) species $\widehat{X}$ of pseudo-singletons as the analytical logarithm of the species of finite sets. It follows that $E(X) = \exp(\widehat{X})$ in the context of rational species, where $\exp(T)$ denotes the classical analytical power series for the exponential function in the variable T. In the present work, we use the species $\widehat{X}$ to create new efficient recursive schemes for the computation of molecular expansions of species of rooted trees, of species of assemblies of structures, of the combinatorial logarithm species, of species of connected structures, and of species of structures with weighted connected components.

Résumé. Puisque les singletons sont les ensembles connexes, l'espèce X des singletons peut être considérée comme le logarithme combinatoire de l'espèce $E(X)$ des ensembles finis. Dans un travail antérieur, nous avons introduit l'espèce (rationnelle) $\widehat{X}$ des pseudo-singletons comme étant le logarithme analytique de l'espèce des ensembles finis. Il en découle que $E(X) = \exp(\widehat{X})$ dans le contexte des espèces rationnelles, où $\exp(T)$ désigne la série de puissances analytique classique de la fonction exponentielle dans la variable T. Dans le présent travail, nous utilisons l'espèce $\widehat{X}$ pour créer de nouveaux schémas computationnels récursifs efficaces pour le calcul du développement moléculaire de l'espèce des arborescences, d'espèces d'assemblées de structures, de l'espèce du logarithme combinatoire, d'espèces de structures connexes, et d'espèces de structures à composantes connexes pondérées.

Keywords: theory of species, formal power series, molecular expansions.

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1 Preliminary notions

A class of labelled weighted structures which is closed under relabellings induced by a bijection between their underlying sets is called a (weighted) *species of structures*(i), in the sense of Joyal (1981). For example, let u and v be formal variables. Then, the class of all trees, where the weight

†With the support of NSERC(Canada).

(i) Formally, a species is a functor from the category of finite sets and bijections to the category of summable weighted sets of a tree τ is $u^{\#\text{ leaves in }\tau}v^{\#\text{ internal nodes in }\tau}$, forms a weighted species of structures since this class is obviously closed under relabellings. By convention, the weight of a structure is a unitary monomial in some weight-variables. Relabellings do not affect weights. A structure belonging to a species F is called an *F-structure*. If the species F is weighted by w, we write $F = F_w$. Two F_w-structures s_1 and s_2 are said to be *isomorphic* if one can be obtained from the other one by a relabelling induced by a bijection between their underlying sets. An isomorphism class of F_w-structures is called an *unlabelled* F_w-structure. By definition, the weight of an unlabelled F_w-structure is the weight of (any) one of its representatives. We say that a species F is *ordinary*, or *unweighted*, if the weight of any of its structure is equal to 1 (the trivial monomial). Species can be added, multiplied, substituted one into another and differentiated.

We now recall the notion of molecular species. A *molecular species* M is an ordinary species having only one type of isomorphy. In others words, any two M-structures are always isomorphic. We can characterize a molecular species by the fact that it is indecomposable under the combinatorial sum. For instance, if $\mathcal{M}$ denotes the (countable) set of all molecular species, we have, up to degree three, $\mathcal{M} = \{1, X, E_2, X^2, E_3, C_3, XE_2, X^3, \ldots\}$, where X^n is the species of n-lists, C_n is the species of oriented n-cycles, and E_n is the species of n-sets. Each molecular species M is completely determined by the stabilizer $H = \mathrm{Stab}(s)$ of one of its structures, say s on $[n]$, where n is the degree of M and $[n] = \{1, 2, \ldots, n\}$. We write $M(X) = X^n/H$. In particular, we have $X^n = X^n/\{1\}$, $\quad E_n = X^n/S_n$, $\quad C_n = X^n/\langle\rho\rangle$, where S_n denotes the symmetric group on $[n]$ and ρ generates a cyclic subgroup of order n of S_n.

Let now F be any unweighted species, not necessarily molecular. Then, we can always write F as a linear combination with nonnegative integer coefficients of molecular species,

$$F = \sum_{M\in\mathcal{M}} f_M M, \tag{1}$$

where $f_M \in \mathbb{N}$ denotes the number of subspecies of F isomorphic to M. This expansion is unique and is called the *molecular expansion* of the species F. This expansion is very strong since it is a common refinement of the classical generating series $F(x), \widetilde{F}(x), Z_F(p_1, p_2, \cdots)$ associated to the species F. For an example of molecular expansion, consider the well-known (unweighted) species A of rooted trees, defined by the functional equation $A = XE(A)$, where E denotes the species of sets (E for French *ensembles*). Its molecular expansion can be seen as an explicit description of the species. Up to degree (size) 6, we have (see Bergeron et al. (1998) for example)

$$\begin{aligned} A = {} & X + X^2 + XE_2(X) + X^3 + XE_3(X) + 2X^4 + X^2E_2(X) + XE_4(X) + 3X^3E_2(X) \\ & + XE_2(X^2) + 3X^5 + X^2E_3(X) + X^2E_4(X) + 6X^4E_2(X) + 2X^2E_2(X^2) + 3X^3E_3(X) \\ & + X^2E_2(X)^2 + XE_5(X) + 6X^6 + \cdots . \end{aligned} \tag{2}$$

In the weighted case, the molecular expansion of a species F_w is of the form

$$F_w = \sum_{M\in\mathcal{M}} f_M(w) M, \tag{3}$$

where $f_M(w)$ is a power series in the weight-variables. Molecular expansions of the form (3) are considered to be in the ring of weighted complex species, that is the ring of formal power series

$$\mathbb{C}\,[[v_1, v_2, v_3, \cdots]][[X, E_2, E_3, C_3, \ldots]] = \mathbb{C}\,[[\vec{v}, \mathcal{A}]], \tag{4}$$

where $\mathbb{C}$ is the complex field, $\vec{v} = v_1, v_2, \ldots$ is a sequence of some weight-variables and $\mathcal{A} = X, E_2, E_3, C_3, \ldots$ is the sequence of *atomic species*; that is those molecular species which are irreducible under product. The above operations on species have been defined on this ring (see Joyal (1986), Yeh (1986), Labelle and Lamathe (2004)). If $\mathbb{C}$ in (4) is replaced by $\mathbb{R}, \mathbb{Q}, \mathbb{Z}$ or $\mathbb{N}$, we speak of weighted *real, rational, virtual* or *ordinary* species.

To illustrate the meaning of the coefficients $f_M(w)$ in expressions such as (3), consider the species of rooted trees, weighted by v for each internal node (root included) and by u for each leaf. Figure 1 shows three *non isomorphic* such rooted trees on five vertices. The first two of

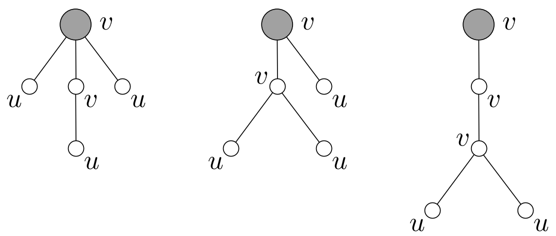

Fig. 1: Illustration of $(2u^3v^2 + u^2v^3)X^3E_2(X)$

these rooted trees have the weight u^3v^2 and the third has the weight u^2v^3. Leaving apart the weights, each one of these three trees belongs to the same molecular species $X^3E_2(X)$, where X represents the species of singletons (vertices). Thus, the molecular expansion of the species of rooted trees, weighted as indicated above, contains the term $\cdots + (2u^3v^2 + u^2v^3)X^3E_2(X) + \cdots$. The coefficient 2 is called the *multiplicity* of the weighted molecular species $u^3v^2X^3E_2(X)$.

Let F be an arbitrary (weighted or unweighted) species. For each $n \geq 0$ we can extract a subspecies F_n of F by collecting all those F-structures having an underlying set of cardinality n. If $F = F_n$, we say that F is concentrated on the cardinality n. In the general situation, we obviously have a countable decomposition

$$F = F_0 + F_1 + F_2 + \cdots + F_n + \cdots , \tag{5}$$

called the *canonical expansion* of F. The species F_n is often called the *homogeneous component of degree n of F*. For example, the homogeneous component of degree 5 of the above molecular expansion of the species A is given by $A_5 = XE_4(X) + 3X^3E_2(X) + XE_2(X^2) + 3X^5 + X^2E_3(X)$. These terms are illustrated in Figure 2. Let t be an extra variable not beloning to $\vec{v} = (v_1, v_2, \ldots)$. Substituting the species tX of singletons of weight t into F, we obtain the useful formula

$$F(tX) = F_0 + tF_1 + t^2F_2 + \cdots + t^nF_n + \cdots , \tag{6}$$

from which we can express the homogeneous component F_n of F by a simple coefficient extraction $F_n = [t^n]F(tX)$, in the augmented ring $\mathbb{C}\,[[t, \vec{v}, \mathcal{A}]] = \mathbb{C}\,[[\vec{v}, \mathcal{A}]][[t]]$.

In the present work, we use the species $\widehat{X}$ of pseudo-singletons (defined in Section 2) to create new efficient recursive schemes (in Section 3) for the computation of molecular expansions of the species of rooted trees, of species of assemblies of structures, of the combinatorial logarithm species, of species of connected structures, and of species of structures with weighted connected components.

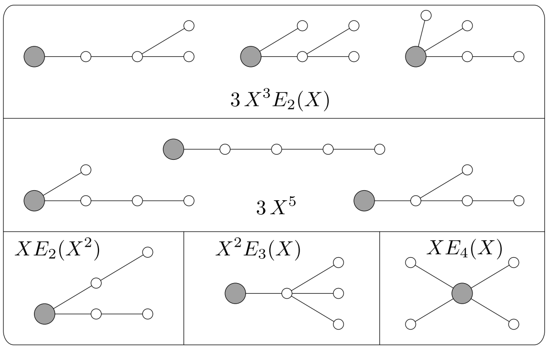

Fig. 2: Molecular terms in A_5

2 Pseudo-singletons and combinatorial power sums species

2.1 Basic definitions and notations

The classical analytical logarithmic function $\log(1+X)$ can be defined by the power series

$$\log(1+X) = X - \frac{1}{2}X^2 + \frac{1}{3}X^3 - \frac{1}{4}X^4 + \cdots \in \mathbb{Q}[[X]] \subset \mathbb{C}[[\vec{v}, \mathcal{A}]] \tag{7}$$

This is an unweighted rational species (or $\mathbb{Q}$-species), since the coefficients of the molecular species X^n are all rational number. The rational species of pseudo-singletons is defined by substituting the species of non-empty sets $E_+ = E_1 + E_2 + E_3 + \cdots$ for X in (7). The resulting rational species can be considered as the *analytical logarithm* of the species E of all finite sets since $E = 1 + E_+$. More precisely, we have the following definition.

Definition 1 *Labelle (1989, 1990) Let $E_+ = E_+(X)$ be the species of all non-empty (finite) sets. The $\mathbb{Q}$-species $\widehat{X}$ of pseudo-singletons is the infinite summable series*

$$\begin{aligned}
\widehat{X} &= E_+ - \frac{1}{2}(E_+)^2 + \frac{1}{3}(E_+)^3 - \frac{1}{4}(E_+)^4 + \cdots \\
&= X + (E_2 - \frac{1}{2}{E_1}^2) + (E_3 - E_1E_2 + \frac{1}{3}{E_1}^3) + \cdots \\
&+ \Big(\sum (-1)^{\nu_1+\nu_2+\cdots-1}((\nu_1+\nu_2+\cdots-1)!/\nu_1!\nu_2!\cdots){E_1}^{\nu_1}{E_2}^{\nu_2}\cdots\Big) + \cdots
\end{aligned} \tag{8}$$

where for each $n \geq 3$, the sum in the general term is extended over $\nu_1 + 2\nu_2 + 3\nu_3 + \cdots = n$.

Hence, we can write $\widehat{X} = \log(1+E_+) = \log(E)$ or, equivalently, $E = \exp(\widehat{X})$. The $\mathbb{Q}$-species $\log(1+X)$ should not be confused with the *combinatorial logarithm*, defined by Joyal (1986), which is a $\mathbb{Z}$-species $\mathrm{Lg}(1+X)$ satisfying $\mathrm{Lg}(1+E_+) = \mathrm{Lg}(E) = X$. The species $\widehat{X}$ gives rize to an infinite family $(P_n)_{n\geq 1}$ of $\mathbb{Z}$-species which are new combinatorial liftings of the classical power sum functions p_n as the following proposition shows.

Proposition 1 *There exists a unique family $(P_n)_{n\geq 1}$ of $\mathbb{Z}$-species such that* $\deg P_n = n$ *and*

$$\widehat{X} = P_1 + \frac{1}{2}P_2 + \frac{1}{3}P_3 + \cdots . \tag{9}$$

Moreover, the species P_n satisfy the combinatorial recursion

$$P_1 = X, \quad P_n = nE_n - E_1P_{n-1} - E_2P_{n-2} - \cdots - E_{n-1}P_1, \quad n \geq 2. \tag{10}$$

Finally, for the cycle index series (i.e. underlying symmetric function), we have,

$$Z_{P_n} = p_n, \quad Z_{\widehat{X}} = p_1 + \frac{1}{2}p_2 + \frac{1}{3}p_3 + \cdots \tag{11}$$

Proof. We simply adapt to the ring of $\mathbb{C}$-species the classical argument which recursively expresses the power sums symmetric functions p_n in terms of the complete ones h_n. Let t be an extra variable, as above. Taking, in the augmented ring $\mathbb{C}[[\vec{v}, \mathcal{A}]][[t]]$, the analytical logarithm on both sides of the equality $E(tX) = E_0 + tE_1 + t^2E_2 + \cdots + t^nE_n + \cdots$, we see that there exists a unique family of coefficients P_n in the original ring $\mathbb{C}[[\vec{v}, \mathcal{A}]]$ such that

$$\log(E(tX)) = \log(\sum_{n\geq 0} t^nE_n) = \sum_{n\geq 1} \frac{1}{n}t^nP_n \tag{12}$$

Of course, $P_1 = X$. Differentiating with respect to t and multiplying by t we get the recursive scheme (10) by cross multiplication and comparing similar powers of t. It immediately follows that each P_n is a $\mathbb{Z}$-species since the coefficients in the right side of the recursion are integers. Formula (9) for $\widehat{X}$ follows by taking $t = 1$. The corresponding formulas (11) for the underlying cycle index series follows from the well-known fact that $\mathbb{Z}_{E(tX)}(p_1, p_2, p_3, \cdots) = \exp(tp_1 + \frac{1}{2}t^2p_2 + \frac{1}{3}t^2p_3 + \cdots)$ where p_n denotes the classical power sum symmetric function of degree n. ■

Note the following equalities in the context of power series in x associated to $\widehat{X}$ and P_n : $\widehat{x} = \widetilde{\widehat{x}} = P_1(x) = \widetilde{P_1}(x) = x, \quad P_n(x) = \widetilde{P_n}(x) = 0 \quad$ if $n > 1$. The molecular expansion of the first few species P_n are given in Table 1 of the Appendix.

2.2 Combinatorial plethystic linearity

In order to analyse further the properties of the species $\widehat{X}$ and P_n, we recall some plethystic notations and introduce a new combinatorial notion of plethystic linearity for species.

Let $\xi = c_1\mu_1 + c_2\mu_2 + \cdots \in \mathbb{C}[[\vec{v}]]$ denote a power series in the variables $v_1, v_2, \cdots$ where $c_1, c_2, \cdots$ are complex numbers and $\mu_1, \mu_2, \cdots$ are unitary monomials in the v_i's. Given an integer $k \geq 1$, we use the following plethystic notation borrowed from the theory of symmetric functions (Macdonald (1995)):

$$\xi_k = c_1\mu_1^k + c_2\mu_2^k + \cdots \in \mathbb{C}[[\vec{v}]] \tag{13}$$

which amounts to replace each v_i by v_i^k in ξ. More generally, given an integer partition $\lambda = (\lambda_1 \geq \lambda_2 \geq \lambda_3 \geq \cdots)$ and a species F, we write $\xi_\lambda = \xi_{\lambda_1}\xi_{\lambda_2}\xi_{\lambda_3}\cdots$ and $F_\lambda = F_{\lambda_1}F_{\lambda_2}F_{\lambda_3}\cdots$.

Definition 2 (Plethystic linearity) *A species F is n-plethystic linear if $F(\alpha G+\beta H+\cdots)=\alpha_n F(G)+\beta_n F(H)+\cdots$ for every finite or infinite (summable) linear combination of species $G, H, \cdots$ with coefficients $\alpha, \beta, \cdots$ in the ring $\mathbb{C}[[\vec{v}]]$.*

Proposition 2 *For every n, the combinatorial power-sum species P_n is n-plethystic linear. Moreover, given any ξ in the ring $\mathbb{C}[[\vec{v}]]$, the following relation holds in the ring $\mathbb{C}[[\vec{v}, \mathcal{A}]]$:*

$$E(\xi X)=\exp(\xi_1 P_1+\frac{1}{2}\xi_2 P_2+\frac{1}{3}\xi_3 P_3+\cdots \frac{1}{n}\xi_n P_n+\cdots)=\sum_\lambda \frac{\xi_\lambda}{z_\lambda}P_\lambda \tag{14}$$

where $E(X)$ denotes the species of finite sets and $z_\lambda = 1^{d_1}d_1!2^{d_2}d_2!3^{d_3}d_3!\cdots$, where d_i is the number of parts of length i in λ.

Proof. The special case $\xi=\mu$ in (14) where $\mu \in \mathbb{C}[[\vec{v}]]$ is an unitary monomial follows by substituting μ for t in formula (12) of the proof of Proposition 1. The general case $\xi = c_1\mu_1 + c_2\mu_2+\cdots$ of a $\mathbb{C}-$linear combination of such monomials is a consequence of the classical addition formula for the species E of sets

$$E(c_1X_1+c_2X_2+\cdots)=(E(X_1))^{c_1}(E(X_2))^{c_2}\cdots \tag{15}$$

(see Bergeron et al. (1998) and Auger et al. (2002)) where $c_1, c_2, \cdots$ are complex numbers and $X_1, X_2, \cdots$ are arbitrary sorts of elements. Indeed, this gives $E(\xi X)=E(c_1\mu_1X+c_2\mu_2X+\cdots)=(E(\mu_1X))^{c_1}(E(\mu_2X))^{c_2}\cdots$ which implies (14) using the special case $\xi=\mu$ above. The plethystic linearity of the species P_n follows by introducing an extra variable t and then comparing the coefficient of t^n in the rightmost members of the following two sets of equalities:

$$E(t\alpha F+t\beta G+\cdots)=E(t(\alpha F+\beta G+\cdots))=\exp(\sum_n \frac{1}{n}t^nP_n(\alpha F+\beta G+\cdots)), \tag{16}$$

$$\begin{aligned} E(t\alpha F+t\beta G+\cdots)=E(t\alpha F)E(t\beta G)\cdots &=\exp(\sum_n \frac{1}{n}t^n\alpha_nP_n(F))\exp(\sum_n \frac{1}{n}t^n\beta_nP_n(G))\cdots \\ &=\exp(\sum_n \frac{1}{n}t^n(\alpha_nP_n(F)+\beta_nP_n(G)+\cdots)). \end{aligned} \tag{17}$$

■

Note that (14) is not a symmetric function identity in the ring $\mathbb{C}[[\vec{v}]]$. It is an algebraic-combinatorial identity in the ring $\mathbb{C}[[\vec{v}, \mathcal{A}]]$. The substitution $X=1$, in (14), which amounts to unlabel the underlying elements in structures, reduces to the cycle index formula $E(\xi)=Z_E(\xi_1,\xi_2,\cdots)$ (see, for example, the two papers by Labelle and Lamathe (2004) for further explanations).

The difference between the classical power sums, p_n, and their combinatorial counterparts, P_n, is also emphasized by the fact that for $m, n \geq 1$,

$$p_m\circ p_n = p_{mn}, \quad \text{while} \quad P_m\circ P_n \neq P_{mn} \quad \text{in general} \tag{18}$$

since, for example (using Table 1) $P_2 \circ P_2 = 4E_2 \circ E_2 - 2E_2^2 - 2E_2 \circ X^2 + X^4 \neq P_4$.
However,

$$\begin{aligned} P_m \circ P_n(\alpha F + \beta G + \cdots) &= \alpha_{mn} P_m \circ P_n(F) + \beta_{mn} P_m \circ P_n(G) + \cdots \\ P_{mn}(\alpha F + \beta G + \cdots) &= \alpha_{mn} P_{mn}(F) + \beta_{mn} P_{mn}(G) + \cdots \end{aligned} \tag{19}$$

Formula (14) for $E(\xi X)$ and the plethystic linearity of P_n are central in the present paper since they can easily be implemented in computer algebra systems and give rize to new efficient combinatorial computational schemes which we now describe. The first few homogeneous components $E_n(\xi X)$ of $E(\xi X)$ are given in Table 2 of the Appendix.

3 Applications to new computational methods for molecular expansions

3.1 Applications to rooted trees

Recall that the well-known (unweighted) species $A = A(X)$ of rooted trees[ii] is characterized by the classical combinatorial equation

$$A = XE(A) \tag{20}$$

where E is the species of finite sets (see Pólya and Read (1987), Bergeron et al. (1998)). The usual method to compute its molecular expansion is by successive approximations and can be described as follows (see Auger et al. (2003)). Let $A_0 = 0$ and successively compute, for $n = 1, 2, \cdots$ the molecular expansion of the homogeneous component A_n of A by the formula

$$A_n = XE(A_0 + A_1 + \cdots + A_{n-1})|_n \tag{21}$$

where $*|_n$ denotes the homogeneous component of degree n of $*$. This computation is done by expanding the formula

$$XE(A_0 + A_1 + \cdots + A_{n-1}) = XE(A_0)E(A_1)\cdots E(A_{n-1}). \tag{22}$$

However, this is quite expensive in computer time. Indeed, let

$$A_k = \sum_{M \in \mathcal{M}_k} a_M M, \quad a_M \in \mathbb{N} \tag{23}$$

be the (already computed) molecular expansion of A_k, where $k < n$ and $\mathcal{M}_k$ is the set of molecular species of degree k. Then, by the addition formula (15),

$$E(A_k) = \prod_{M \in \mathcal{M}_k} E(M)^{a_M}, \quad \text{where} \quad E(M) = 1 + M + E_2(M) + E_3(M) + \cdots. \tag{24}$$

We propose the following alternative approach based on Proposition 2.

[ii] A stands for *arborescence*, in french

Proposition 3 *The homogeneous components A_n of the species $A = XE(A)$ of rooted trees satisfy $A_0 = 0$, $A_1 = X$ and for $n > 1$*

$$A_n = \frac{1}{n-1}(A_{n-1}B_1 + A_{n-2}B_2 + \cdots + A_1B_{n-1}), \quad \text{where} \quad B_j = \sum_{d|j} dP_{j/d}(A_d). \tag{25}$$

Proof. Of course, $A_0 = 0$ and $A_1 = X$. Let t be a weight-variable, then $A(tX) = tA_1 + t^2A_2 + t^3A_3 + \cdots$. Substituting tX for X in (20) and using Proposition 2, we can write

$$\begin{aligned}\sum_{n\geq 1} t^n A_n = tXE(\sum_{d\geq 1} t^d A_d) &= tX \exp(\sum_{k\geq 1} \frac{1}{k} P_k(\sum_{d\geq 1} t^d A_d)) \\ &= tX \exp(\sum_{k,d\geq 1} \frac{t^{kd}}{k} P_k(A_d)) \\ &= tX \exp(\sum_{j\geq 1}(\sum_{d|j} dP_{j/d}(A_d))\frac{t^j}{j}).\end{aligned} \tag{26}$$

Applying the operator $t\frac{d}{dt}$ we get

$$\sum_{n\geq 1} nt^n A_n = \sum_{n\geq 1} t^n A_n + (\sum_{i\geq 1} t^i A_i)(\sum_{j\geq 1} t^j B_j). \tag{27}$$

The result follows by extracting the coefficient of t^n on both sides of this last equation. ∎

The strength of recursive scheme of Proposition 3 lies in its simplicity and the fact that the computation of B_j in (25) can be greatly simplified using the linearity of $P_{j/d}$, since the species A is unweighted. Tables of the species A_n for high values of n can easily be made using computer algebra and a precomputed table of the linear species P_k.

Recursive schemes for the computation of the series $Z_A(p_1, p_2, \cdots)$, $\widetilde{A}(x)$ and $A(x)$ can also be obtained using Proposition 3. For example, for the series $\widetilde{A}(x) = \sum_{n\geq 1} \widetilde{a}x^n$ that counts unlabelled rooted trees, we get the well known result (see for example Bergeron et al. (1998)),

$$\widetilde{a}_n = \frac{1}{n-1}(\widetilde{a}_{n-1}b_1 + \cdots + \widetilde{a}_1 b_{n-1}), \quad b_j = \sum_{d|j} d\widetilde{a}_d, \quad j = 1, \cdots, n-1. \tag{28}$$

It is easy to adapt Proposition 3 and its proof to many classes of weighted rooted trees. For example, for the species $A = A_w$ of rooted trees with weight counters u for leaves and v for internal nodes, the equation is

$$A = (u - v)X + vXE(A) \tag{29}$$

and the recursive scheme of Proposition 3 becomes $A_0 = 0, A_1 = uX$ and, for $n > 1$

$$A_n = \frac{1}{n-1}\{A_{n-1}B_1 + A_{n-2}B_2 + \cdots + A_2B_{n-2} + vB_{n-1}\} \tag{30}$$

with B_j given by (25), In this case the plethystic linearity of $P_{j/d}$ must be used instead of simple linearity since the species A_n are weighted.

3.2 Applications to assemblies of weighted structures

Given a (weighted or unweighted) species G, $G(0) = 0$, one can form another species $F = E(G)$ whose structures are called *assemblies* of G-structures (see Joyal (1981)). Suppose that the molecular expansion of each homogeneous components G_n of G are known, then the molecular expansion of F can be recursively computed as follows.

Proposition 4 *Let $F = E(G)$ with $G = G_1 + G_2 + \cdots$ then $F = F_0 + F_1 + F_2 + \cdots$ where $F_0 = 1$ and, for $n > 0$,*

$$F_n = \frac{1}{n}(F_{n-1}H_1 + F_{n-2}H_2 + \cdots + F_0H_n), \quad \text{where} \quad H_j = \sum_{d|j} dP_{j/d}(G_d). \tag{31}$$

Proof. Again, $F(tX) = \sum_{n\geq 0} t^n F_n = E(\sum_{d\geq 1} t^d G_d)$. This implies, by Proposition 2, that

$$\sum_{n\geq 0} t^n F_n = \exp(\sum_{j\geq 1}(\sum_{d|j} dP_{j/d}(G_d))t^j/j). \tag{32}$$

Applying $t\frac{d}{dt}$ on both sides we get $\sum_{n\geq 1} nt^n F_n = (\sum_{i\geq 0} t^i F_i)(\sum_{j\geq 1} H_j t^j)$. ∎

Once again, the computations can be greatly simplified by making use of the plethystic linearity of the power sums P_k. Molecular expansions of various species such as the species $E(uE_+)$ of partitions weighted according to their number of parts or the species $E(A)$ of acyclic endofunctions can be computed to high degrees using this method.

3.3 Applications to connected components and combinatorial algorithm

Given a (weighted or unweighted) species F, with $F(0) = 1$, the equation $F = E(G)$ uniquely defines a cooresponding species G, denoted F^c, of connected F-structures (see Joyal (1986)). In fact,

$$F^c = \mathrm{Lg}(F) = \mathrm{Lg}(1 + F_+) \tag{33}$$

where $\mathrm{Lg}(1 + X)$ is the combinatorial logarithm mentioned in Section 2. Reversing the computational scheme of Propositon 4 we easily get the following.

Proposition 5 *Let $F = 1 + F_+ = 1 + F_1 + F_2 + \cdots$, then $F^c = F_0^c + F_1^c + F_2^c + \cdots$ where $F_0^c = 0$ and, for $n > 0$,*

$$F_n^c = F_n - \frac{1}{n}\left(\sum_{d|n,d<n} dP_{j/d}(F_d^c) + F_{n-1}H_1 + F_{n-2}H_2 + \cdots + F_1H_{n-1}\right) \tag{34}$$

where H_j is given by $\sum_{d|j} dP_{j/d}(F_d^c)$.

The molecular expansion of the combinatorial logarithm itself can be computed as follows.

Proposition 6 *Let* $\mathrm{Lg}(1+X) = \Omega = \Omega_0 + \Omega_1 + \Omega_2 + \cdots$ *then* $\Omega_0 = 0$, $\Omega_1 = X$ *and, for* $n > 1$,

$$\Omega_n = \frac{1}{n}\left((-1)^{n-1}X^n - \sum_{d|n, d<n} dP_{n/d}(\Omega_d)\right). \tag{35}$$

Proof. One must solve $E_+(\Omega) = X$, or, equivalently, $E(\Omega) = 1 + X$. Since $E(\Omega(tX)) = \exp(\sum_{k\geq 1} \frac{1}{k} P_k(\sum_{d\geq 1} t^d\Omega_d)) = \exp(\sum_{k,d\geq 1} \frac{t^{kd}}{k} P_k(\Omega_d)) = 1 + tX$, we get, taking the analytical logarithm,

$$\sum_{n\geq 1}\left(\sum_{d|n} dP_{n/d}(\Omega_d)\right)\frac{t^n}{n} = \sum_{n\geq 1}(-1)^{n-1}\frac{t^nX^n}{n} \tag{36}$$

From which (35) follows immediately. ∎

The first few homogeneous components of the combinatorial logarithm are given in Table 3 of the Appendix. Since $(\mathrm{Lg}(1+X)) \circ E_+ = X$, the combinatorial logarithm can be considered to the combinatorial substitutional inverse $E_+^{<-1>}$ of the species E_+ of non empty sets. Let u be a weight variable. In (Labelle and Leroux (1996)) we introduced a virtual weighted species $\Lambda^{[u]} = E(uE_+^{<-1>})$ which satisfies

$$\Lambda^{[u]} \circ F_+ = E(uE_+^{<-1>}(F_+)) = E(uF^c), \tag{37}$$

for $F = 1 + F_+$. Hence, the species $\Lambda^{[u]} \circ F_+$ assigns an extra weight counter u for each connected component in F-structure.

For $\xi \in \mathbb{C}[[\vec{v}]]$, the molecular expansion of the more general species $\Lambda^{[\xi]} = E(\xi E_+^{<-1>})$ can be recursively computed to high degrees by combining Proposition 4 and 6. Using Moebius inversion techniques, the reader can check that the cycle index series of $\Lambda^{[\xi]}$ satisfies

$$Z_{\Lambda^{[\xi]}}(p_1, p_2, \cdots) = \prod_{n\geq 1}(1 + p_n)^{\frac{1}{n}\sum_{d|n}\mu(n/d)\xi_d}. \tag{38}$$

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APPENDIX

$P_1 = X$
$P_2 = 2\,E_2 - X^2$
$P_3 = -3\,XE_2 + 3\,E_3 + X^3$
$P_4 = -2\,{E_2}^2 + 4\,X^2E_2 - 4\,XE_3 + 4\,E_4 - X^4$
$P_5 = -5\,E_3E_2 + 5\,X^2E_3 - 5\,XE_4 + 5\,E_5 + 5\,X{E_2}^2 - 5\,X^3E_2 + X^5$
$P_6 = -6\,E_4E_2 + 6\,X^2E_4 + 6\,E_6 - 6\,XE_5 + 12\,XE_3E_2 - 3\,{E_3}^2 - 6\,X^3E_3 + 2\,{E_2}^3 - 9\,X^2{E_2}^2$ $+6\,X^4E_2 - X^6$

Tab. 1: The molecular expansion of the power sum species $P_n(X)$ for $n = 1$ to 6.

$E_0(\xi\,X) = 1$
$E_1(\xi\,X) = \xi_1 X$
$E_2(\xi\,X) = (-\frac{1}{2}\,\xi_2 + \frac{1}{2}\,{\xi_1}^2)X^2 + \xi_2 E_2$
$E_3\,(\xi\,X) = (-\xi_3 + \xi_1\xi_2)XE_2 + (\frac{1}{3}\,\xi_3 - \frac{1}{2}\,\xi_1\xi_2 + \frac{1}{6}\,{\xi_1}^3)X^3 + \xi_3 E_3$
$E_4(\xi\,X) = (-\frac{1}{4}\,\xi_4 + \frac{1}{8}\,{\xi_2}^2 + \frac{1}{3}\,\xi_1\xi_3 - \frac{1}{4}\,\xi_2{\xi_1}^2 + \frac{1}{24}\,{\xi_1}^4)X^4$ $+ (\xi_4 - \xi_1\xi_3 + \frac{1}{2}\,\xi_2{\xi_1}^2 - \frac{1}{2}\,{\xi_2}^2)X^2E_2 + (-\xi_4 + \xi_1\xi_3)XE_3$ $+(\frac{1}{2}\,{\xi_2}^2 - \frac{1}{2}\,\xi_4){E_2}^2 + \xi_4 E_4$
$E_5(\xi\,X) = (-\frac{1}{6}\,\xi_3\xi_2 + \frac{1}{5}\,\xi_5 + \frac{1}{120}\,{\xi_1}^5 + \frac{1}{6}\,\xi_3{\xi_1}^2 - \frac{1}{4}\,\xi_1\xi_4 - \frac{1}{12}\,\xi_2{\xi_1}^3$ $+\frac{1}{8}\,\xi_1{\xi_2}^2)X^5 + (\xi_1\xi_4 + \frac{5}{6}\,\xi_3\xi_2 - 1/2\,\xi_3{\xi_1}^2 - \xi_5 - \frac{1}{2}\,\xi_1{\xi_2}^2 + \frac{1}{6}\,\xi_2{\xi_1}^3)X^3E_2$ $+ (-\frac{1}{2}\,\xi_3\xi_2 - \xi_1\xi_4 + \frac{1}{2}\,\xi_3{\xi_1}^2 + \xi_5)X^2E_3 + (\xi_5 + \frac{1}{2}\,\xi_1{\xi_2}^2 - 1/2\,\xi_1\xi_4 - \xi_3\xi_2)X{E_2}^2$ $+ (\xi_1\xi_4 - \xi_5)XE_4 + (\xi_3\xi_2 - \xi_5)E_3E_2 + \xi_5 E_5$

Tab. 2: Homogeneous components $E_n\,(\xi\,X)$ of the species $E\,(\xi\,X)$ for $n = 0$ to 5.

$\mathrm{Lg}(1+X)_1 = X$
$\mathrm{Lg}(1+X)_2 = -E_2$
$\mathrm{Lg}(1+X)_3 = XE_2 - E_3$
$\mathrm{Lg}(1+X)_4 = -X^2E_2 + XE_3 + E_2 \circ E_2 - E_4$
$\mathrm{Lg}(1+X)_5 = -X{E_2}^2 + E_2E_3 + X^3E_2 - X^2E_3 + XE_4 - E_5$
$\mathrm{Lg}(1+X)_6 = 2\,X^2{E_2}^2 - 2\,XE_2E_3 + E_2E_4 - (E_2 \circ E_2)E_2 - X^4E_2 + X^3E_3 - X^2E_4 + E_3 \circ E_2$ $-E_2 \circ (XE_2) + E_2 \circ E_3 + XE_5 - E_6$

Tab. 3: Homogeneous components $\mathrm{Lg}(1+X)_n$ of the combinatorial logarithm $\mathrm{Lg}(1+X)$ for $n = 1$ to 6.