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Algorithmic and combinatoric aspects of multiple harmonic sums

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Ordinary generating series of multiple harmonic sums admit a full singular expansion in the basis of functions \( (1 - z)^\alpha \log^\beta (1 - z) \) near the singularity \( z = 1 \). A constructive proof of this result is given, and, by combinatoric aspects, an explicit evaluation of Taylor coefficients of functions in some polylogarithmic algebra is obtained. In particular, the asymptotic expansion of multiple harmonic sums is easily deduced.

Keywords: polylogarithms, polyzêtas, multiple harmonic sums, singular expansion, shuffle algebra, Lyndon words

1 Introduction

Hierarchical data structure occur in numerous domains, like computer graphics, image processing or biology (pattern matching). Among them, quadtrees, whose construction is based on a recursive definition of space, constitute a classical data structure for storing and accessing collection of points in multidimensional space. Their characteristics (depth of a node, number of nodes in a given subtree, number of leaves) are studied by Laforest [12], with probabilistic tools. In particular, she shows, for a quadtree of size \( N \) in a \( d \)-dimension space, that the probability \( \pi_{N,k} \) for the first subtree to have size \( k \) can be expressed as an algebraic combination of \( j \)-th order harmonic numbers \( H_j(N) \) and \( H_j(k), j \geq 1 \), defined by

\[
H_j(n) = \sum_{m=1}^{n} \frac{1}{mj}.
\]

For instance, for \( d = 3 \), one has

\[
\pi_{N,k} = \frac{[H_1(N) - H_1(k)]^2 + H_2(N) - H_2(k)}{2N}.
\]

Flajolet et al. [2] give this general expression for the splitting probability

\[
\pi_{N,k} = \sum_{N \geq i_1 \geq \cdots \geq i_{d-1} > k} \frac{1}{i_1 \cdots i_{d-1}}.
\]

The probability \( \pi_{N,k} \) appears as a particular case of the following sum \( A_s(N) \) associated to the multi-index \( s = (s_1, \ldots, s_r) \), which is strongly related to multiple harmonic sums \( H_s(N) \):

\[
A_s(N) = \sum_{N \geq n_1 \geq \cdots \geq n_r > 0} \frac{1}{n_1^{s_1} \cdots n_r^{s_r}} \quad \text{and} \quad H_s(N) = \sum_{N \geq n_1 \geq \cdots \geq n_r > 0} \frac{1}{n_1^{s_1} \cdots n_r^{s_r}}.
\]

Let us note that there exist explicit relations, given by Hoffman [10] between the \( A_s(N) \) and \( H_s(N) \). Indeed, let \( \text{Comp}(n) \) be the set of compositions of \( n \), i.e. sequences \( (i_1, \ldots, i_r) \) of positive integers summing to \( n \). If \( I = (i_1, \ldots, i_r) \) (resp. \( J = (j_1, \ldots, j_p) \)) is a composition of \( n \) (resp. of \( r \)) then \( J \circ I = (i_1 + \cdots + i_{j_1}, i_{j_1+1} + \cdots + i_{j_1+j_2}, \ldots, i_{j_p-j_{p-1}} + \cdots + i_k) \) is a composition of \( n \). By Möbius inversion, one has

\[
A_s(N) = \sum_{J \in \text{Comp}(r)} H_{s \circ J}(N) \quad \text{and} \quad H_s(N) = \sum_{J \in \text{Comp}(r)} (-1)^{l(J)-r} A_{s \circ J}(N),
\]

where \( l(J) \) is the number of parts of \( J \).
Example 1. For \( s = (1, 1, 1) \), since the set of compositions of 3 is \{ (1, 1, 1), (1, 2), (2, 1), (3) \}, we get
\[
A_{1,1,1}(N) = H_{1,1,1}(N) + H_{1,2}(N) + H_{2,1}(N) + H_{3}(N),
\]
\[
H_{1,1,1}(N) = A_{1,1,1}(N) - A_{1,2}(N) - A_{2,1}(N) + A_{3}(N).
\]

Therefore, the \( A_s(N) \) are \( \mathbb{Z} \)-linear combinations on \( H_s(N) \) (and vice versa). Thus, the remaining problem is to know the asymptotic behaviour of \( \pi_{N,k} \), for \( N \to \infty \) [11]. For that, in this work, we are interested in the combinatorial aspects of these sums by use of a symbolic encoding by words. This enables then to transfer shuffle relations on words into algebraic relations between multiple harmonic sums, or between polylogarithm functions, defined for a multi-index \( s = (s_1, \ldots, s_r) \) by
\[
\text{Li}_s(z) = \sum_{n_1 > \ldots > n_r > 0} \frac{z^{n_1}}{n_1^{s_1} \cdots n_r^{s_r}}, \quad \text{for } |z| < 1. \tag{6}
\]

These relations are recalled in Section 2. The reason to call upon polylogarithms is given in Section 3, since the generating function \( P_s(z) = \sum_{n \geq 0} H_s(n) z^n \) of \( \{H_s(n)\}_{n \geq 0} \), verifies
\[
P_s(z) = \frac{1}{1-z} \text{Li}_s(z). \tag{7}
\]

So, we set the polylogarithmic algebra of \( \{P_s\}_s \), with coefficients in \( C = \mathbb{C}[z, z^{-1}, (z-1)^{-1}] \), and we then establish exact transfer results between a function \( g \) in this algebra and its Taylor coefficients \( [z^n]g(z) \), in the \( C \)-algebra generated by \( \{N^k H_s(N)\}_{s, k \in \mathbb{Z}} \) in both directions. The main result of this paper is finally stated in Section 4, which gives a computation of the full singular expansion of \( g \), in the basis of functions \( \{(1 - z)^a \log^b (1 - z)\}_{a \in \mathbb{Z}, b \in \mathbb{N}} \), near the singularity \( z = 1 \). We deduce from this a full asymptotic expansion of its Taylor coefficients. These results are based on the analysis of the noncommutative generating series of functions of the form (7), in particular on its infinite factorization indexed by Lyndon words.

2 Background

2.1 Combinatorics on words

To the multi-index \( s \) we can canonically associate the word \( u = x_0^{s_1-1} x_1 \ldots x_0^{s_r-1} x_1 \) over the finite alphabet \( X = \{x_0, x_1\} \). In the same way, \( s \) can be canonically associated to the word \( v = y_{s_1} \ldots y_{s_r} \) over the infinite alphabet \( Y = \{y_i\}_{i \geq 1} \). Moreover, in both alphabets, the empty multi-index will correspond to the empty word \( \epsilon \). We shall henceforth identify the multi-index \( s \) with its encoding by the word \( u \) (resp. \( v \)). We denote by \( X^* \) (resp. \( Y^* \)) the free monoid generated by \( X \) (resp. \( Y \)), which is the set of words over \( X \) (resp. \( Y \)). Noting \( C\langle X \rangle \) (resp. \( C\langle Y \rangle \)) the algebra of noncommutative polynomials with coefficients in \( C \), we obtain so a concatenation isomorphism from the \( C \)-algebra of multi-indexes into the algebra \( C\langle X \rangle \) (resp. \( C\langle Y \rangle \)). The coefficient of \( w \in X^* \) in a polynomial \( S \in C\langle X \rangle \) is denoted by \( \langle S | w \rangle \) or \( S_w \). The duality between polynomials is defined as follows
\[
\langle S | p \rangle = \sum_{w \in X^*} S_w p_w, \quad p \in C\langle X \rangle. \tag{8}
\]

The set of Lie monomials is defined by induction: the letters in \( X \) are Lie monomials and the Lie bracket \([a, b] = ab - ba\) of two Lie monomials \( a \) and \( b \) is a Lie monomial. A Lie polynomial is a \( C \)-linear combination of Lie monomials. The set of Lie polynomials is called the free Lie algebra.

2.2 Shuffle products

Let \( a, b \in X \) (resp. \( y_i, y_j \in Y \)) and \( u, v \in X^* \) (resp. \( Y^* \)). The shuffle (resp. stuffle) of \( u = au' \) and \( v = bv' \) (resp. \( u = y_iu' \) and \( v = y_jv' \)) is the polynomial recursively defined by
\[
\epsilon \shuffle u = u \cdot \epsilon = u \quad \text{and} \quad u \cdot v = a(u' \shuffle v) + b(u \shuffle v'),
\]
\[
\text{(resp. } \epsilon \shuffle u = u \cdot \epsilon = u \quad \text{and} \quad u \cdot v = y_i(u' \shuffle v) + y_j(u \shuffle v') + y_{i+j}(u' \shuffle v')). \tag{9}
\]

Example 2.
\[
x_0 x_1 \shuffle x_1 = x_1 x_0 x_1 + 2x_0 x_1^2
\]
\[
y_2 \shuffle y_1 = y_1 y_2 + y_2 y_1 + y_3. \tag{11}
\]

This product is extended to \( C\langle X \rangle \) (resp. \( C\langle Y \rangle \)) by linearity. With this product, \( C\langle X \rangle \) (resp. \( C\langle Y \rangle \)) is a commutative and associative \( C \)-algebra.
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2.3 Lyndon words and Radford’s theorem

By definition, a Lyndon word is a non empty word \( l \in X^* \) (resp. \( Y^* \)) which is lower than any of its proper right factors [14] (for the lexicographical ordering) i.e. for all \( u, v \in X^* \setminus \{\varepsilon\} \) (resp. \( Y^* \setminus \{\varepsilon\} \)), \( l = uv \Rightarrow l < v \). The set of Lyndon words of \( X \) (resp. \( Y \)) is denoted by \( \text{Lyn}(X) \) (resp. \( \text{Lyn}(Y) \)).

**Example 3.** For \( X = \{x_{0}, x_{1}\} \) with the order \( x_{0} < x_{1} \) the Lyndon words of length \( \leq 5 \) on \( X^* \) are (in lexicographical increasing order)

\[
\begin{align*}
\{x_{0}, x_{3}, x_{0}x_{1}, x_{0}x_{1}x_{3}, x_{0}x_{1}x_{3}, x_{0}x_{1}x_{3}, x_{3}, x_{0}x_{1}x_{3}, x_{0}x_{1}x_{3}, x_{0}x_{1}x_{3}, x_{1}, x_{0}x_{1}x_{3}, x_{0}x_{1}x_{3}, x_{0}x_{1}x_{3}, x_{0}x_{1}x_{3}, x_{0}x_{1}x_{3}, x_{0}x_{1}x_{3}, x_{0}x_{1}x_{3}\}.
\end{align*}
\]

For \( Y = \{y_{i}, i \geq 1\} \), with the order \( y_{i} < y_{j} \) when \( i > j \), here are the corresponding Lyndon words over \( Y \)

\[
\{y_{5}, y_{4}y_{1}, y_{3}, y_{3}y_{2}, y_{3}y_{1}, y_{3}y_{1}^{2}, y_{2}, y_{2}y_{1}, y_{2}y_{1}^{2}, y_{2}y_{1}^{3}, y_{1}\}.
\]

**Theorem 1 (Radford, [13, 14]).** Let

\[
C_{1} = C \oplus (C(X) \setminus x_{0}C(X)x_{1}) \quad \text{and} \quad C_{2} = C \oplus (C(Y) \setminus y_{1}C(Y))
\]

be the sets of convergent polynomials over \( X \) and \( Y \) respectively. Then,

\[
(C(X), \omega) \simeq (C[\text{Lyn}(X)], \omega) = (C_{1}[x_{0}, x_{1}], \omega),
\]

\[
(C(Y), \omega) \simeq (C[\text{Lyn}(Y)], \omega) = (C_{2}[y_{1}], \omega).
\]

**Example 4.**

\[
y_{2}y_{4}y_{1} + y_{2}y_{1}y_{4} + y_{1}y_{2}y_{4} + y_{2}y_{5} + y_{3}y_{4} = y_{4}y_{2}y_{1}y_{1} - y_{4}y_{2}y_{1}y_{1} - y_{6}y_{1}y_{1} \in C[\text{Lyn}(Y)]
\]

\[
y_{2}y_{4}y_{1}y_{1} \in C_{2}[y_{1}]
\]

2.4 Bracket forms and the dual basis

The **bracket form** \( Q_{l} \) of a Lyndon word \( l = uv \), with \( l, u, v \in \text{Lyn}(X) \) and the word \( v \) being as long as possible, is defined recursively by

\[
\left\{ \begin{array}{c}
Q_{l} = [Q_{u}, Q_{v}] \\
Q_{x} = x \quad \text{for each letter} \ x \in X,
\end{array} \right.
\]

It is classical that the set \( B_{1} = \{Q_{l} : l \in \text{Lyn}(X)\} \), ordered lexicographically, is a basis for the free Lie algebra. Moreover, each word \( w \in X^* \) can be expressed uniquely as a decreasing product of Lyndon words:

\[
w = l_{1}^{a_{1}}l_{2}^{a_{2}} \ldots l_{k}^{a_{k}}, \quad l_{1} > l_{2} > \cdots > l_{k}, \quad k \geq 0.
\]
The Poincaré–Birkhoff–Witt basis $B = \{Q_w; w \in X^*\}$ and its dual basis $B^* = \{S_w; w \in X^*\}$ are obtained from (12) by setting [14]

\[
\begin{align*}
Q_w & = Q_{i_1}^{a_1} Q_{i_2}^{a_2} \ldots Q_{i_k}^{a_k}, \\
S_w & = S_{i_1}^{\alpha_1} \ldots S_{i_k}^{\alpha_k}, \\
S_l & = x S_w, \quad \forall \ l \in \text{Lyn}(X), \text{ where } l = x w, x \in X, w \in X^*.
\end{align*}
\]

In [14], it is proved that $B$ and $B^*$ are dual bases of $\mathbb{C}<X>$ i.e. $(Q_u|S_v) = \delta_u^v$, for all words $u, v \in X^*$ with $\delta_u^v = 1$ if $u = v$, otherwise 0.

**Lemma 1.** For all $w \in x_0 X^* x_1$, one has $S_w \in x_0 \mathbb{Z}(X):x_1$.

**Proof.** The Lyndon words involved in the decomposition (12) of a word $w \in X^* x_1$ (resp. $w \in x_0 X^* x_1$) all belong to $X^* x_1$ (resp. $x_0 X^* x_1$). \hfill \Box

### 2.5 Polylogarithms

Let $C = \mathbb{C}[z, 1/z, 1/(z - 1)]$ and let $\omega_0$ and $\omega_1$ be the two following differential forms

\[
\omega_0(z) = \frac{dz}{z} \quad \text{and} \quad \omega_1(z) = \frac{dz}{1 - z}.
\]

One verifies the polylogarithm $\text{Li}_k(z)$, defined by Formula (6), is also the following *iterated integral* with respect to $\omega_0$ and $\omega_1$

\[
\text{Li}_k(z) = \int_{0 \rightarrow z} \omega_0^{s_1-1} \omega_1 \cdots \omega_0^{s_r-1} \omega_1.
\]

Thanks to the bijection from $Y^*$ to $X^* x_1$ previously explained, we can index the polylogarithms by the words of $X^* x_1$, or indistinctly by the words of $Y^*$.

We can extend (14) over $X^*$ by putting

\[
\text{Li}_k(z) = 1, \quad \text{Li}_{x_0}(z) = \log z, \quad \text{Li}_{x_1}(z) = \int_{0 \rightarrow z} \omega_1(t) \text{Li}_w(t), \quad \text{for } x_i \in X, w \in X^*.
\]

Therefore, $\text{Li}_w$ verifies the following identity [4]

\[
\forall u, v \in X^*, \quad \text{Li}_{u \uplus v} = \text{Li}_u \cdot \text{Li}_v.
\]

The extended definition enables to construct the noncommutative generating series [4]

\[
L = \sum_{w \in X^*} \text{Li}_w \cdot w
\]

as being the unique solution of the *Drinfel’d equation*, i.e. the differential equation [4]

\[
dL = [x_0 \omega_0 + x_1 \omega_1]L,
\]

satisfying the boundary condition

\[
L(\varepsilon) = e^{x_0 \log \varepsilon} + o(\sqrt{\varepsilon}), \quad \text{when} \quad \varepsilon \to 0^+.
\]

**Proposition 1 ([5]).** Let $\sigma$ be the monoid morphism defined over $X^*$ by $\sigma(x_0) = -x_1$ and $\sigma(x_1) = -x_0$.

Then,

\[
L(1 - z) = [\sigma L(z)] \prod_{l \in \text{Lyn}(X) \setminus \{x_0, x_1\}} e^{\zeta(S_l) Q_l}.
\]

**Example 5 ([5]).**

\[
\text{Li}_{x_0 x_1^2}(1 - z) = -\text{Li}_{x_0 x_1^2}(z) + \text{Li}_{x_0}(z) \text{Li}_{x_0 x_1}(z) - \frac{1}{2} \text{Li}_{x_0}^2(z) \text{Li}_{x_1}(z) + \zeta(3), \quad \text{i.e.}
\]

\[
\text{Li}_{2,1}(1 - z) = -\text{Li}_x(z) + \log(z) \text{Li}_x(z) + \frac{1}{2} \log^2(z) \log(1 - z) + \zeta(3).
\]
2.6 Harmonic sums

**Definition 1.** Let \( w = y_1 \ldots y_s \in Y^* \). For \( N \geq r \geq 1 \), the harmonic sum \( H_w(N) \) is defined as

\[
H_w(N) = \sum_{N \geq n_1 > \ldots > n_r > 0} \frac{1}{n_1^{s_1} \ldots n_r^{s_r}}.
\]

For \( 0 \leq N < r \), \( H_w(N) = 0 \) and, for the empty word \( e \), we put \( H_e(N) = 1 \), for any \( N \geq 0 \).

Let \( w = y_1 \ldots y_s \in Y^* \). If \( s_1 > 1 \) then, by an Abel’s theorem,

\[
\lim_{N \to \infty} H_w(N) = \lim_{z \to 1} \text{Li}_w(z) = \sum_{n_1 > \ldots > n_r > 0} \frac{1}{n_1^{s_1} \ldots n_r^{s_r}}.
\]

That is nothing but the polyzêta (or MZV [16]) \( \zeta(w) \) and the word \( w \in Y^* \setminus y_1 Y^* \) is said to be convergent. A polynomial of \( \mathbb{C}(Y) \) is said to be convergent when it is a linear combination of convergent words. The double shuffle algebra of polyzêtas is already pointed out and extensively studied in [3].

For \( w = y_s w' \), we have

\[
\zeta(w) = \sum_{l \geq 1} \frac{H_{w'}(l - 1)}{\Gamma(l)}, \quad (20)
\]

\[
H_{w}(N + 1) - H_{w}(N) = (N + 1)^{-s} H_{w'}(N) \quad (21)
\]

and, for any \( u, v \in Y^* [9] \)

\[
H_{u \shuffle v}(N) = H_{u}(N)H_{v}(N). \quad (22)
\]

3 Generating series

3.1 Definition and first properties

**Definition 2 ([8]).** Let \( w \in Y^* \) and let \( P_w(z) \) be the ordinary generating series of \( \{H_w(N)\}_{N \geq 0} \)

\[
P_w(z) = \sum_{N \geq 0} H_w(N) z^N.
\]

**Proposition 2 ([8]).** Extended by linearity, the map \( P : u \mapsto P_u \) is an isomorphism from \((\mathbb{C}(Y), \shuffle)\) to the Hadamard algebra of \((\{P_w\}_w \in Y^*, \cdot)\). Therefore, the map \( H : u \mapsto H_u = \{H_w(N)\}_{N \geq 0} \) is an isomorphism from \((\mathbb{C}(Y), \shuffle)\) to the algebra of \((\{H_w\}_w \in Y^*, \cdot)\).

**Proof.** The definition of the Hadamard product \( \sum_{n=0}^{\infty} a_n z^n \odot \sum_{n=0}^{\infty} b_n z^n = \sum_{n=0}^{\infty} a_n b_n z^n \), and the formula (22) gives \( P \) as an algebra morphism. Since the functions \( \{\text{Li}_w\}_w \in X^* \) are linearly independent over \( \mathbb{C} \) [4], \( P \) is the expected isomorphism.

**Proposition 3 ([8]).** For every word \( w \in Y^* \) and for \( z \in \mathbb{C} \) satisfying \( |z| < 1 \), one has \( \text{Li}_w(z) = (1 - z)P_w(z) \).

**Proof.** For \( w = y_sw' \), since \( P_w(z) = \sum_{N \geq 0} H_w(N) z^N \) and by using (21),

\[
(1 - z)P_w(z) = H_w(0) + \sum_{N \geq 1} \frac{H_{w'}(N - 1)}{N^s} z^N = \text{Li}_w(z).
\]

A direct consequence of this proposition and Identity (16) is

**Corollary 1.** For all \( u, v \in X^* \), for all \( z \in \mathbb{C} \) satisfying \( |z| < 1 \), \( P_u(z)P_v(z) = (1 - z)^{-1} P_{u \shuffle v}(z) \).

**Example 6.** Since \( x_1 \shuffle x_0 x_1 = x_1 x_0 x_1 + 2x_0 x_1^2 \) then we get

\[
P_{1,2}(z) = (1 - z)P_1(z)P_2(z) - 2P_{2,1}(z).
\]
Proposition 3 allows to extend the definition of $P_w$ over $X^*$ as we have already extended the definition of $L_{wu}$ over $X^*$. Moreover,

**Definition 3 ([8]).** Let $P$ be the noncommutative generating series of \{\(P_w\)\}_{w \in X^*}:

$$P = \sum_{w \in X^*} P_w w.$$

**Proposition 4 ([8]).** Let $\sigma$ be the monoid morphism defined over $X^*$ by $\sigma(x_0) = -x_1$ and $\sigma(x_1) = -x_0$. Then

$$P(1-z) = \frac{1-z}{z}[\sigma P(z)] \prod_{l \in \text{sym}(X) \setminus \{x_0, x_1\}} e^{c(S_l)Q_l}.$$

**Proof.** It follows immediately from Proposition 1. \hfill \Box

**Example 7.**

$$P_{2,1}(1-z) = \frac{1-z}{z} \left( -P_3(z) + \log(z)P_2(z) - \log^2(z)P_1(z) + \frac{\zeta(3)}{1-z} \right)$$

Thus,

$$P_{2,1}(z) = -\frac{z}{1-z} P_3(1-z) + \frac{z \log(1-z)}{1-z} P_2(1-z) - \frac{z}{2} \log^2(1-z) P_1(1-z) + \frac{\zeta(3)}{1-z}.$$

By Formula (22) and Proposition 2, for $w \in Y^*$, there exist a finite set $I$ and $(c_i)_{i \in I} \in \mathbb{C}^I$ such that the three following identities are equivalent

$$w = \sum_{i \in I} c_i y_i^{|w|_i}, \quad (23)$$

$$P_w = \sum_{i \in I} P_{c_i} \otimes P_{y_i}, \quad (24)$$

$$H_w = \sum_{i \in I} H_{c_i} H_{y_i}, \quad (25)$$

In particular, for $w = y_1^k$, we have,

**Lemma 2.** Let $M = (m_{i,j})_{1 \leq i,j \leq k}$ be the matrix defined by $m_{i,j} = \delta_{i,j+1}$ (Kronecker symbol). Let $c_{i,j}$ the matrix of size $k \times k$, whose coefficients are all zero, except the one equal to 1 at line $i$ and column $j$. Let

$$A = \begin{pmatrix} y_1 & 0 & \ldots & 0 \\ -\frac{y_1}{2} & \ddots & \ddots & \vdots \\ \vdots & \ddots & \ddots & 0 \\ (-1)^{k-1}y_k \\ k & \end{pmatrix} \quad \text{and} \quad B = \begin{pmatrix} H_{y_1} \\ -H_{y_2} \\ \vdots \\ (-1)^{k-2}H_{y_k} \\ k \end{pmatrix}.$$

Then

$$A^{k-1} \left[ M^\ell A^{(\ell)} M^\ell + \sum_{i=1}^\ell e_{i,i} \right] A = B^{k-1} \left[ M^\ell B^{(\ell)} M^\ell + \sum_{i=1}^\ell e_{i,i} \right] A.$$

**Proof.** The formula $y_1^k = (-1)^{k-1}k^{-1} \sum_{i=0}^{k-1} (-1)^i y_i^{\ell} y_{y_k-i} [6]$ can be written matricially as follows

$$\begin{pmatrix} y_1 \\ y_2^k \\ \vdots \\ y_k^{1} \\ y_1^k \end{pmatrix} = A \otimes y_1 \quad \begin{pmatrix} \epsilon \\ y_1 \\ \vdots \\ y_1^{k-1} \end{pmatrix} = A \otimes \begin{pmatrix} \epsilon & 0 & \ldots & 0 \\ 0 & y_1 & \ldots & 0 \\ \vdots & \ddots & \ddots & \vdots \\ 0 & \ldots & \ldots & y_1^{k-1} \end{pmatrix} \otimes \begin{pmatrix} \epsilon \\ \epsilon \\ \vdots \\ \epsilon \end{pmatrix}.$$

Here all powers and products are carried out with the shuffle product. Successively, we get the expected result. \hfill \Box
The word \( y_i \) appears then as a computablestuffle product ofwords of length 1. Hence,

**Proposition 5.** \( H_{y_i} \) is a combination of \( \{ H_{y_r} \}_{1 \leq r < k} \) which are algebraically independent.

**Proof.** The \( \{ H_{y_r} \}_{1 \leq r < k} \) are algebraically independent according to Proposition 2, as image by theisomorphism H of the Lyndon words \( \{ y_r \}_{1 \leq r < k} \). By Lemma 2, we get the expected result. \( \square \)

**Example 8.** Since

\[
y_1^2 = \frac{y_1 \cdot y_1 - y_2}{2} \quad \text{and} \quad \frac{y_1}{3} = \frac{2(y_1 + y_1 y_2) + (y_1 y_1 y_1 - y_2) y_1}{6}
\]

then we have

\[
H_{y_1^2} = \frac{H_{y_1}^2 - H_{y_2}}{2} \quad \text{and} \quad \frac{H_{y_1}}{2} = \frac{2(H_{y_2} - H_{y_1}H_{y_2}) + (H_{y_1}^2 - H_{y_2})H_{y_1}}{6}.
\]

Identities (23-25) give rise to two interpretations: (24) enables to decompose \( P_w \) in a basis of singular functions \( (1 - z)^a \log^b(1 - z) \) while (25) enables to compute an asymptotic expansion of its Taylor coefficients in terms of \( N^a \log^b N \) (or equivalently in terms of \( N^a H_{y_r}(N) \)). Before stating a theorem linking these two interpretations, we are interested in the action of \( C \) on Taylor coefficients; reciprocally, we are interested in the effects of changing Taylor coefficients on a function in \( C([P_w]_{w \in Y^*}] \).

### 3.2 Operations on the generating functions \( P_w \)

For \( f(z) = \sum_{n \geq 0} a_n z^n \), we will henceforth denote \([z^n]f(z) = a_n\) its \( n\)-th Taylor coefficient. Since multiplying or dividing by \( z \) acts very simply on \([z^n]f(z)\), we only have to study the effect of multiplying or dividing by \( 1 - z \).

\[
[z^n](1 - z)P_w(z) = H_w(n) - H_w(n - 1). \tag{26}
\]

\[
[z^n]P_w(z) \quad \text{at} \quad \frac{1}{1 - z} = \sum_{k=0}^{n} H_w(k). \tag{27}
\]

\[
\begin{cases}
(n + 1)H_w(n) - H_{w_{s-1}}w'(n) & \text{if } w = y_s w', \text{ with } s \neq 1 \\
(n + 1)H_w(n) - \sum_{j=1}^{n} H_{w'}(j - 1) & \text{if } w = y_1 y_1.
\end{cases} \tag{28}
\]

and, more generally,

**Proposition 6.**

\[
[z^n](1 - z)^k P_w(z) = \sum_{j=0}^{k} \binom{k}{j} (-1)^j H_w(n - j) \quad \text{and} \quad \frac{[z^n] P_w(z)}{(1 - z)^k} = \sum_{n \geq j_1 \geq \cdots \geq j_k \geq 0} H_w(j_k).
\]

### 3.3 Operations on Taylor coefficients of \( P_w \)

We are now to find how multiplying or dividing \( H_w(N) \) by \( N \) acts on \( P_w \).

#### 3.3.1 A particular case : \( w = \epsilon \)

The simple case \( w = \epsilon \), corresponding to \( H_\epsilon(N) = 1 \), can be studied and treated by the following

**Proposition 7.** For any \( q \in \mathbb{Z} \), one has

\[
y^q = \begin{cases}
[z^n](1 - z)P_{-q}(z) & \text{if } q < 0, \\
[z^n](1 - z)^{-1} & \text{if } q = 0, \\
[z^n] \frac{z}{1 - z} N_q \left( \frac{1}{1 - z} \right) & \text{if } q > 0,
\end{cases}
\]

where \( N_q \) is defined by the following recurrence

\[
N_0(X) = 1, \quad \text{and} \quad N_q(X) = X \sum_{j=0}^{q-1} (-1)^{q-1-j} \binom{q}{j} N_j(X).
\]
Example 9.
\[ n = [z^n] \left( \frac{z}{(1-z)^2} \right) = [z^n] \left( \frac{1}{(1-z)^2} - \frac{1}{1-z} \right), \]
\[ n^2 = [z^n] \left( \frac{2z}{(1-z)^3} - \frac{z}{(1-z)^2} \right) = [z^n] \left( \frac{2}{(1-z)^3} - \frac{3}{(1-z)^2} + \frac{1}{1-z} \right). \]

3.3.2 How to divide by \( n^k \)?

Let \( w = y_s \cdots y_1 \) and \( w' = y_s \cdots y_n \) be the suffix of \( w \), of length \( n - 1 \). The expression \( n^{-k}H_w(n) \), \( k \) positive integer, can be identified as follows
\[ n^{-k}H_w(n) = n^{-k}H_w(n-1) + n^{-s_1-k}H_{w'}(n-1) \quad \text{(29)} \]
\[ = [z^n]L_{y_k w+y_{1+k} w'}(z) \quad \text{(30)} \]
\[ = [z^n][(1-z)P_{y_k w+y_{1+k} w'}(z)]. \quad \text{(31)} \]

3.3.3 How to multiply by \( n^k \)?

In order to study the effect of multiplying by \( n^k \), \( k \) positive integer, we denote by \( \theta = z \partial/\partial z \) the Euler operator. Then for any integer \( k \),
\[ n^kH_w(n) = [z^n]\theta^kP_w(z). \quad \text{(32)} \]

So, we just have to compute \( \theta^kP_w(z) \). As in [7], let us introduce

**Definition 4.** For any word \( w = x_{i_j} \cdots x_{i_k} \) and for any composition \( \mathbf{r} = (r_1, \ldots, r_k) \), let \( \tau_r(w) \) be defined by \( \tau_r(w) = \tau_{r_1}(x_{i_1}) \cdots \tau_{r_k}(x_{i_k}) \) with,
\[ \tau_0(x_0) = x_0, \quad \tau_r(x_1) = x_1, \]
and, for \( r \in \mathbb{N}^* \), \( \tau_r(x_0) = \theta^r x_0 = 0 \) and \( \tau_r(x_1) = \theta^r \frac{z x_1}{1-z} = \frac{r! x_1}{(1-z)^{r+1}}. \)

We define the degree of \( \mathbf{r} \) by \( \deg(\mathbf{r}) = k \) and its weight by \( \text{wt}(\mathbf{r}) = k + r_1 + \cdots + r_k \).

By applying successively the operator \( \theta \) to \( L \), we get

**Lemma 3.** \( \theta^kL = A_kL \), where \( A_k \) is defined by
\[ A_k(z) = \sum_{\text{deg}(\mathbf{r})=l} \sum_{w \in X^{\text{deg}(\mathbf{r})}} \prod_{i=1}^l \left( \sum_{j=1}^{r_i} r_i + j - 1 \right) \tau_r(w). \]

**Proof.** This is a consequence of the recurrence relation verified by \( A_k \), which is \( A_0(z) = 1 \), and, for all \( l \in \mathbb{N}, A_{l+1}(z) = [\tau_0(x_0) + \tau_0(x_1)]A_l(z) + \theta A_l(z). \)

This lemma enables to extract the expression of \( \theta^kL_{x^0} \), for any word \( w \in X^* \).

**Example 10.**
\[ A_0(z) = 1, \]
\[ A_1(z) = x_0 + \frac{z}{1-z} x_1, \]
\[ A_2(z) = x_0^2 + \frac{z}{1-z} x_0 x_1 + \frac{z^2}{(1-z)^2} x_1^2 + \frac{1}{(1-z)^2} x_1. \]

So, for \( w = x_0^2 x_1 \),
\[ \theta L_{x_0^2 x_1} = \left( x_0 + \frac{z}{1-z} x_1 \right) L(z) \bigg|_{x_0^2 x_1} \]
\[ = L_{x_0 x_1}, \]
\[ \theta^2 L_{x_0^2 x_1} = \left( x_0^2 + \frac{z}{1-z} x_0 x_1 + \frac{z^2}{(1-z)^2} x_1^2 + \frac{1}{(1-z)^2} x_1 \right) L(z) \bigg|_{x_0^2 x_1} \]
\[ = L_{x_1}. \]
Lemma 4. Let \( \perp \) be the linear operator of \( \mathbb{Z}[X] \) defined by \( \perp X^n = (n+1)X^{n+1} + nX^n \) and \( \{B_l\}_{l \in \mathbb{N}} \in \mathbb{Z}[X] \) defined by \( B_0(X) = 1 \) and \( B_{l+1}(X) = \perp B_l(X) \). Then
\[
\theta^l (1 - z)^{-1} = (1 - z)^{-1} B_l(z(1 - z)^{-1}).
\]

Note that the head term of \( B_l, l \geq 1 \), is \( l!X^l \) and its trail term is \( X \).

Example 11. \( B_0(X) = 1, B_1(X) = X, B_2(X) = 2X^2 + X, B_3(X) = 6X^3 + 6X^2 + X \).

Proposition 8. With the notations of Lemma 4,
\[
\theta^k P(z) = \sum_{j=1}^{k} \sum_{w \in X^{\deg(r)}} \sum_{r \in X^{\deg(r)}} \left( \sum_{i=1}^{\deg(r)} \binom{k}{j} r_i + j - 1 \right) \binom{j}{r_i} P(z).
\]

Using Leibniz formula, one has
\[
\theta^k P_w(z) = \sum_{j=0}^{k} \binom{k}{j} \theta^{k-j} P(z) \frac{1}{1-z}.
\]

Equation (33)

Thanks to Lemma 3, we can extract the coefficient \( \theta^l P_w \) of \( w \) in \( \theta^l L \) : this can be written as \( C \)-linear combination of \( \Li_w \), with \( |v| \leq |w| - l \) (where \( |u| \) denotes the length of a word \( u \in X^* \)). We deduce so the expression of \( \theta^k P_w \).

Example 12. For \( w = x_0^2x_1 \) and \( k = 2 \),
\[
\theta^2 P_{x_0^2x_1}(z) = \sum_{j=0}^{2} \binom{2}{j} B_j \left( \frac{z}{1-z} \right) \frac{1}{1-z} \theta^{2-j} P_{x_0x_1}(z)
\]
\[
= \frac{1}{1-z} \Li_{x_1}(z) + \frac{2z}{1-z} \Li_{x_0x_1}(z) + \left( \frac{2}{1-z} \right)^2 \frac{z}{1-z} \Li_{x_0x_1}(z)
\]
\[
= P_{x_1}(z) + \frac{2z}{1-z} P_{x_0x_1}(z) + \frac{2z^2}{1-z} \Li_{x_0x_1}(z).
\]

So,
\[
n^2 \Li_3(n) = \left[ n^2 \right] \left( P_1(z) + \frac{2z}{1-z} P_2(z) + \frac{2z^2}{1-z} P_3(z) \right).
\]

4 The main theorem

Throughout the section, we will write
\[
f_n \sim \sum_{i=0}^{\infty} g_i(n) \quad \text{for} \quad n \rightarrow +\infty,
\]

for a scale of functions \( (g_i)_{i \in \mathbb{N}} \) i.e. verifying \( g_{i+1}(n) = O(g_i(n)) \), for all \( i \) to express that
\[
f_n = \sum_{i=0}^{I} g_i(n) + O(g_{I+1}(n)), \quad \text{for any} \quad I \geq 0.
\]

In the same way, given a scale of functions \( (h_i)_{i \in \mathbb{N}} \) around \( z = 1 \) (i.e. verifying \( h_{i+1}(1 - z) = O(h_i(1 - z)) \), when \( z \rightarrow 1 \)) we will write
\[
g(z) \sim \sum_{i=0}^{\infty} h_i(1 - z) \quad \text{for} \quad z \rightarrow 1,
\]

to mean
\[
g(z) = \sum_{i=0}^{I} h_i(1 - z) + O(h_{I+1}(1 - z)) \quad \text{for all} \quad I \geq 0.
\]
For \( w = y_1^k \), we know the expression of \( [z^n]P_{y_1^k}(z) = H_{y_1^k}(N) \) is given by Lemma 2. From the second form of Euler-MacLaurin formula, involving the Bernoulli numbers \( \{B_k\}_{k \geq 0} \), we get the following asymptotic expansions

\[
H_{y_1}(N) \sim \log N + \gamma - \sum_{k=1}^{+\infty} \frac{B_k}{k} \frac{1}{N^k},
\]

\[
H_{y_2}(N) \sim \zeta(r) - \frac{1}{(r-1)N^{r-1}} - \sum_{k=r}^{+\infty} \frac{B_{k-r+1}}{k-r+1} \left( \frac{k-1}{N^k} \right), \quad \text{for } r > 1.
\]

Thus, we can deduce the asymptotic expansions of \( H_{y_1^k}(N) \), for \( N \to +\infty \), from the asymptotic expansions of \( \{H_{y_2}(N)\}_{1 \leq r < k} \):

**Example 13.** From Example 8, we can deduce then

\[
H_{y_1^k}(N) = \frac{1}{2} (\log(N) + \gamma)^2 - \frac{1}{2} \zeta(2) + \frac{1}{2} \log(N) + \gamma + 1 - \frac{1}{12N^2} + O\left(\frac{1}{N^2}\right),
\]

\[
H_{y_3}(N) = \frac{1}{6} \log^3(N) + \frac{1}{2} \gamma \log^2(N) + \frac{1}{2} (\gamma^2 - \zeta(2)) \log(N) - \frac{1}{2} \zeta(2) \gamma + \frac{1}{3} \zeta(3) + \frac{1}{6} \gamma^3 + \frac{1}{4} \log^2(N)
\]

\[
+ \frac{1}{2} (\gamma + 1) \log(N) - \frac{1}{4} (2\gamma + \gamma^2 - \zeta(2)) \log(N) - \frac{1}{24N^2} - \frac{1}{8 + \frac{1}{12}} \log(N) + O\left(\frac{1}{N^2}\right).
\]

Let us see in the general case how to reach the Taylor expansion of \( g \in C([P_w]_{w \in Y^*}) \).

**Theorem 2.** Let \( g \in C([P_w]_{w \in Y^*}) \). There exist \( a_j \in \mathbb{C}, \alpha_j \in \mathbb{Z} \) and \( \beta_j \in \mathbb{N} \) such that

\[
g(z) \sim \sum_{j=0}^{+\infty} a_j (1-z)^{\alpha_j} \log^{\beta_j}(1-z), \quad \text{for } z \to 1.
\]

Therefore, there exist \( b_i \in \mathbb{C}, \eta_i \in \mathbb{Z} \) and \( \kappa_i \in \mathbb{N} \) such that

\[
[z^n]g(z) \sim \sum_{i=0}^{+\infty} b_i n^{\eta_i} \log^{\kappa_i}(n), \quad \text{for } n \to \infty.
\]

**Proof.** Considering Corollary 1, we only have firstly to obtain the asymptotic expansion for the case \( g(z) = P_w(z) \). Indeed, we get then the expansions of \( f(z)g(z) \), for \( f \in C \) by remarking that \( z = 1 - (1-z) \) and that \( z^{-1} = \sum_{n \geq 0} (1-z)^n \).

The first expansion can be derived from Proposition 4 which links the behaviour of \( P_w \) around \( z = 1 \) to the behaviour of some algebraic combination of functions \( \{P_w\}_{w \in X^*} \) around \( z = 0 \). Moreover, by Radford theorem 1, we can assume that each word \( u \) involved in this combination is a Lyndon word and so belongs to \( x_0 X^* x_1 \cup \{x_0, x_1\} \). But, remind that, in this case, we have \( P_u(z) = \sum_{n \geq 0} H_u(n) z^n \) and that \( P_{x_0}(z) = (1-z)^{-1} \log(z) \). So, the expected first expansion follows.

From

\[
(1-z)^{\alpha} \log(1-z)^{\beta} = (-1)^{\beta} (1-z)^{\alpha+1} P_{y_1^\beta}(z),
\]

we derive the second expansion by computing the Taylor coefficient \( [z^n](1-z)^{\alpha} \log(1-z)^{\beta} \). Since we have already explained how the multiplication by \( (1-z)^{\alpha} \) acts on the Taylor coefficients, we just have then to compute \( [z^n]P_{y_1^\beta} = H_{y_1^\beta}(n) \). For this, we use Lemma 2 which completes our proof.

Unfortunately, in the general case, knowing even the complete expansion of \( [z^n]g(z) \) only enables to get an asymptotic expansion of \( g(z) \), as \( z \to 1 \) up to order 0 (i.e. the *singular part* of the expansion). Indeed, Taylor coefficients of all functions \( (1-z)^k, k \geq 0 \) eventually vanish as in the following identity:

\[
\frac{1}{n} = [z^n] Li_1(z) = [z^n][Li_1(z) + (1-z)^2], \quad \text{as soon as } n > 2.
\]

In fact, to obtain this singular part, it is sufficient to know the asymptotic expansion of \( [z^n]g(z) \) up to order \( 2 - \epsilon, \epsilon > 0 \) [15].
Remark 1. In the case of a finite sum $\sum_{i \in I} b_i n^{Y_i} H_i^{(n)}(n)$, we are able to construct the unique function $f \in C([-|P_w|, \infty])$ such that,

$$\forall n \in \mathbb{N}, \quad [z^n] f(z) = \sum_{i \in I} b_i n^{Y_i} H_i^{(n)}(n),$$

as illustrated in Examples 9 and 12.

Remark 2. Note that the proof of Theorem 2 gives an effective construction of the asymptotic expansion of Taylor coefficients. In particular, applied to $g(z) = P_w(z)$ directly, it enables to find an asymptotic expansion of $H_w(N)$, as shown in the corollary below. Another algorithm, based on Euler Mac-Laurin formula, is available in [11].

Corollary 2. Let $\mathcal{Z}$ be the $\mathbb{Q}$-algebra generated by convergent polyzetas and let $\mathcal{Z}'$ be the $\mathbb{Q}[\gamma]$-algebra generated by $\mathcal{Z}$. Then there exist algorithmically computable coefficients $b_i \in \mathcal{Z}'$, $\kappa_i \in \mathbb{N}$ and $\eta_i \in \mathbb{Z}$ such that, for any $w \in Y^*$,

$$H_w(N) \sim \sum_{i=0}^{+\infty} b_i N^{\kappa_i} \log^{\eta_i}(N), \quad \text{for } N \to +\infty.$$

Example 14. From Example 7 we get, for $z \to 1$

$$P_{2,1}(z) = \frac{\zeta(3)}{1-z} + \log(1-z) - 1 - \frac{\log^2(1-z)}{2} + (1-z) \left( -\frac{\log^2(1-z)}{4} + \frac{\log(1-z)}{4} \right) + O(|1-z|).$$

But

$$[z^N] P_{2,1}(z) = \left[ z^N \right] \left( \frac{\zeta(3)}{1-z} + \log(1-z) - 1 - \frac{\log^2(1-z)}{2} + (1-z) \left( -\frac{\log^2(1-z)}{4} + \frac{\log(1-z)}{4} \right) + O(|1-z|) \right).$$

We find finally, using Example 13:

$$[z^N] P_{2,1}(z) = H_{2,1}(N) = \zeta(3) - \frac{\log(N) + 1 + \gamma}{N} + \frac{\log(N)}{2 N^2} + O\left(\frac{1}{N^2}\right).$$

Otherwise, by Example 6,

$$P_{1,2}(z) = (1-z)P_1(z)P_2(z) - 2P_{2,1}(z)$$

$$= (1-z) \frac{\log(1-z)}{1-z} - \frac{z}{1-z} \left( -P_2(1-z) + \log(1-z)P_1(1-z) + \zeta(2) \right) - 2P_{2,1}(z),$$

calculated thanks to Proposition 4. So,

$$[z^N] P_{1,2}(z) = H_{1,2}(N) = \zeta(2) \gamma - 2\zeta(3) + \zeta(2) \log(N) + \zeta(2) \frac{2}{2N} + O\left(\frac{1}{N^2}\right).$$

Corollary 3 ([8]). For any $w \in Y^*$, the $N$-free term in the asymptotic expansion of $H_w(N)$, when $N \to +\infty$, is a polynomial $q_w$ in $\mathcal{Z}[\gamma]$. This term is an element in $\mathcal{Z}$, if and only if $w$ is a convergent word.

Example 15. $q_{y_1y_2} = \zeta(2) \gamma - 2\zeta(3)$ and $q_{y_2y_1} = \zeta(3) = \zeta(2,1)$.

Question. For any convergent word $w$, are $\zeta(w)$ and $\gamma$ algebraically independent?
Example 16. For $s = (1, 1, 1)$,

$$A_{1,1,1}(N) = H_{1,1,1}(N) + H_{1,2}(N) + H_{2,1}(N) + H_3(N),$$

$$= \frac{1}{6} \log^3(N) + \frac{1}{2} \gamma \log^2(N) + \frac{1}{2} \left[ \gamma^2 + \gamma \zeta(2) \right] \log(N) - \frac{1}{2} \zeta(2) \gamma + \frac{1}{3} \zeta(3) + \frac{1}{6} \gamma^3 + \frac{1}{4} \frac{\log^2(N)}{N}$$

$$+ \frac{1}{2} \left( \gamma - 1 \right) \frac{\log(N)}{N} + \frac{1}{4} \left[ \gamma^2 - 2 \gamma + \zeta(2) \right] \frac{1}{N} - \frac{1}{24} \frac{\log^2(N)}{N^2} + \frac{1}{24} \left( 9 - 2 \gamma \right) \frac{\log(N)}{N^2} + O \left( \frac{1}{N^2} \right).$$

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References


