After having recalled some important results about combinatorics on words, like the existence of a basis for the shuffle algebras, we apply them to some special functions, the polylogarithms \( L_i(z) \) and to special numbers, the multiple harmonic sums \( H_n^s(N) \). In the "good" cases, both objects converge (respectively, as \( z \to 1 \) and as \( N \to +\infty \)) to the same limit, the polyzêta \( \zeta(s) \). For the divergent cases, using the technologies of noncommutative generating series, we establish, by techniques "à la Hopf", a theorem "à l'Abel", involving the generating series of polyzêtas. This theorem enables one to give an explicit form to generalized Euler constants associated with the divergent harmonic sums, and therefore, to get a very efficient algorithm to compute the asymptotic expansion of any \( H_n^s(N) \) as \( N \to +\infty \). Finally, we explore some applications of harmonic sums throughout the domain of discrete probabilities, for which our approach gives rise to exact computations, which can be then easily asymptotically evaluated.

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1. Introduction

For computation of discrete probabilities, we often need the asymptotic evaluation, in the scale of \( \{N^\alpha \ln^\beta(N), \alpha, \beta \in \mathbb{Z}\} \), of functions of an integer \( N \), as \( N \) becomes very large. For instance, harmonic numbers of order \( r \geq 1 \), \( H_r(N) \) (or generalized harmonic numbers) \( H_r(N) = \sum_{k=1}^{N} k^{-r} \) appear in the computation of complexities in the analysis of algorithms (Knuth, 1997; Flajolet and Sedgewick, 1996). Euler used his summation formula (also discovered afterwards, and independently, by MacLaurin) to
obtain
\[
\sum_{n=1}^{N} \frac{1}{n} = \log N + \gamma - \sum_{j=1}^{k-1} \frac{B_j}{j} \frac{1}{N^j} + O\left(\frac{1}{N^k}\right),
\]
(1)
\[
\sum_{n=1}^{N} \frac{1}{n^r} = \zeta(r) - \sum_{j=r-1}^{k-1} \frac{B_{j-r+1}}{j} \frac{1}{N^j} + O\left(\frac{1}{N^k}\right).
\]
(2)
where \(B_j\) are Bernoulli numbers and \(\gamma\) (resp. \(\zeta(r), r \geq 2\)) is called Euler–MacLaurin constant associated to the divergent harmonic number \(H_1(N)\) (resp. to the convergent harmonic number \(H_r(N), r \geq 2\) (Hardy, 2000).

Recently, the application of strategies of type divide and conquer to algorithms and hierarchical data structures on trees, led some authors to harmonic sums, associated to a composition \(s = (s_1, \ldots, s_r)\) (Flajolet and Vallée, 2000; Labelle and Laforest, 1995a)

\[
H_s(N) = \sum_{N \geq n_1 > \cdots > n_r > 0} \frac{1}{n_1^{s_1} \cdots n_r^{s_r}}
\]
(3)
which ordinary generating function, \(P_s\), is a polylogarithmic function:

\[
P_s(z) = \sum_{N \geq 1} H_s(N) z^N = \frac{\text{Li}_s(z)}{1 - z} \quad \text{with} \quad \text{Li}_s(z) = \sum_{n_1 > \cdots > n_r > 0} \frac{z^{n_1}}{n_1^{s_1} \cdots n_r^{s_r}}.
\]
(4)

We recall in Section 3 that the \(\mathbb{C}\)-algebra generated by polylogarithms \(\text{Li}_{s_1, \ldots, s_r}(z)\) and by logarithms \(\log^n(z), n \geq 1\), is isomorphic to the \(\mathbb{C}\)-shuffle algebra, over the two-letters alphabet \(X = \{x_0, x_1\}\) which is a free algebra and owns a basis, as recalled (Theorem 1) in Section 2, which sets up the background for the combinatorics on words. This point enables one to get algorithms for computing the monodromy (Hoang Ngoc Minh et al., 1998), the differential Galois group (Hoang Ngoc Minh, 2003a), functional equations of Kummer-type (Hoang Ngoc Minh et al., 1999) for these polylogarithms through their noncommutative generating series.

In Section 4, we now focus on the infinite alphabet \(Y = \{y_i\}_{i \geq 1}\). To each composition \((s_1, \ldots, s_r)\), we can associate a word \(w = y_{s_1} \cdots y_{s_r}\) over \(Y\). This way, polylogarithms, harmonic sums and their ordinary generating function can be indexed by words: \(H_w = H_{s_1, \ldots, s_r}, \text{Li}_w = \text{Li}_{s_1, \ldots, s_r}, P_w = P_{s_1, \ldots, s_r}\.

It is also proved that the \(\mathbb{C}\)-Hadamard algebra of ordinary generating functions \(P_w\) of harmonic sums is isomorphic to the \(\mathbb{C}\)-shuffle algebra, over \(Y\), leading so to the isomorphism between the \(\mathbb{C}\)-algebra of harmonic sums and the same \(\mathbb{C}\)-shuffle algebra, which is also free and owns a basis (Theorem 2).

Moreover, one important point linking \(\text{Li}_w(z)\) to \(H_w(N)\) is the fact that for \(w \in Y^* \setminus y_1 Y^*, \) the limits of \(\text{Li}_w(z), \) when \(z \to 1,\) and of \(H_w(N),\) when \(N \to \infty,\) exist, and by Abel Theorem, are equal, the common limit being the polyzêta

\[
\zeta(w) = \zeta(s_1, \ldots, s_r) = \sum_{n_1 > \cdots > n_r > 0} \frac{1}{n_1^{s_1} \cdots n_r^{s_r}}.
\]
(5)

In order to study the divergent cases, i.e. for \(w \in y_1 Y^*\), we consider the noncommutative generating series of polylogarithms, and of multiple harmonic sums \(A(z) = \sum_{w \in Y^*} \text{Li}_w(z) w\) and \(H(N) = \sum_{w \in Y^*} H_w(N) w,\) and we prove by techniques “à la Hopf" the following theorem “à l’Abel” (Theorem 6)

\[
\lim_{z \to 1} z^{-y_1 \text{Li}_y(z)} A(z) = \lim_{N \to \infty} \exp\left(\sum_{k \geq 1} H_{y_k}(N) \left(-\frac{y_1}{k}\right)^k\right) H(N) = S,
\]
(6)

\(S\) standing for the noncommutative generating series of convergent polyzêtas, factorised as an infinite product indexed by Lyndon words \(\mathcal{LYN}(Y) \setminus \{y_1\}.\) This enables one in particular to explicit the generalized Euler constants associated to divergent polyzêtas \(\{\zeta(w)\}_{w \in y_1 Y^*}\), and to get the asymptotic expansion of \(H_w(n).\) We show that these constants belong to the \(\mathbb{Q}\)-algebra generated by Euler constant \(\gamma\) and by convergent polyzêtas \(\{\zeta(w)\}_{w \in Y^* \setminus y_1 Y^*}.\) In fact, in order to get the asymptotic
behave of \( H_w(N) \), the structural properties of the generating series of \( \text{Li}_w, w \in X^* \), and more particularly its behaviour as \( z \to 1 \) had already given rise to another algorithm (Costermans et al., 2005a). And the existence of a basis for the shuffle algebra over \( Y \), joint to the isomorphism with the algebra of harmonic sums had also given rise to a third algorithm (Costermans et al., 2005b). We discuss each one of the three algorithms, compare them in terms of computing time, and conclude that the explicitation of generalized Euler constants improve significantly the two previous existing algorithms.

Section 5 is devoted to some applications, concerning various domains met throughout the area of discrete probabilities. In this section, we interpret some results found by different authors, Foata et al. (2001), Labelle and Laforest (1995a), Bai et al. (1998) and Ivanin (1976), in terms of harmonic sums, which enables us to use all combinatoric tools previously presented, either to get some asymptotical evaluation, either to get an exact expression (for instance the leading constant \( k_d \) – cf. Theorem 10 – involved in the asymptotical expansion of the variance of the number of maxima in a hypercube). The first example deals with the “hyperharmonic numbers”, that we rewrite as a difference of harmonic sums. The second example is interested in the parity of random multidimensional quadrees and we have a special look at some cases which make appear Euler transforms of harmonic sums. The third one exploits two formulas for the variance of the random number of maxima in a hypercube, and precises the algebraic nature (cf. Theorem 11) of the coefficients occurring in its asymptotic expansion.

2. Combinatorics on words

2.1. Hopf algebra

Considering a finite alphabet \( X = \{x_1, \ldots, x_k\} \) or an infinite alphabet \( Y = \{y_i, i \geq 0\} \), we denote the empty word by \( \epsilon \). The length of a word \( w = x_1 \ldots x_n \), i.e. the integer \( k \), is denoted by \( |w| \). If each letter of the alphabet is associated with an integer constant called weight, we call weight of a word the sum of the weights of its letters. For instance, the word \( w = y_1^3y_2y_3y_1 \) built over \( Y \) has for weight 8 and for length \( |w| = 5 \).

The set of words over \( X \) is denoted by \( X^* \). A noncommutative formal power series over \( X \), with coefficients in \( C \) is an application \( S : w \in X^* \mapsto \langle S|w\rangle \in C \). By abuse of notation, we will simply write \( S = \sum_{w \in X^*} \langle S|w\rangle w \). The set of formal power series over \( X \) with coefficients in \( C \) is denoted by \( C\langle X\rangle \).

**Definition 1.** Let \( y_i, y_j \in Y \) and \( u, v \in Y^* \). The shuffle (respectively, stuffle and minus-stuffle) product of \( u = y_iu' \) and \( v = y_jv' \) is the polynomial recursively defined by

\[
\begin{align*}
\epsilon \circ u &= u \circ \epsilon = u \quad \text{and} \quad u \circ v = y_i(u' \circ v) + y_j(u \circ v') \\
\epsilon \cdot u &= u \cdot \epsilon = u \quad \text{and} \quad u \cdot v = y_i(u' \cdot v) + y_j(u \cdot v') + y_{i+j}(u' \cdot v') \\
\epsilon \cdot u &= u \cdot \epsilon = u \quad \text{and} \quad u \cdot v = y_i(u' \cdot v) + y_j(u \cdot v') - y_{i+j}(u' \cdot v') .
\end{align*}
\]

**Remark 1.** Hoffman (2000) defines a family of “quasi-shuffle products” over \( C\langle Y\rangle \), \( Y \) being a locally finite set of generators, by

\[
\begin{align*}
\epsilon \cdot u &= u \cdot \epsilon = u \quad \text{and} \quad u \cdot v = y_i(u' \cdot v) + y_j(u \cdot v') + y_{i+j}(u' \cdot v') ,
\end{align*}
\]

where \( [\cdot, \cdot] \) is supposed to verify \([y_i, 0] = 0\), to be commutative, associative and also such that \([y_i, y_j]\) is either identically 0 or has for weight \( i + j \). The products \( \circ \) and \( \cdot \) can so naturally be seen as “quasi-shuffle products”.

The stuffle product \( \cdot \) enables one to define a linear application defined for \( w_1 \) and \( w_2 \in X^* \) by

\[
st : w_1 \otimes w_2 \in C\langle X \rangle \otimes C\langle X \rangle \to w_1 \cdot w_2 \in C\langle X \rangle ,
\]

extended to polynomials by linearity. Then, the linear application \( \mathbb{1} : k \in C \mapsto \mathbb{1}(k) = k \in C\langle X \rangle \) appears as a unity. So \( (C\langle X \rangle, st, 1) \) constitutes an associative and generated \( C \)-algebra. This algebra is known as shuffle algebra.

We define a coproduct by \( \Delta : w \in C\langle X \rangle \to \sum_{uv=w} u \otimes v \in C\langle X \rangle \otimes C\langle X \rangle . \) Then \( e : S \in C\langle X \rangle \mapsto e(S) = \langle S|\epsilon\rangle \in C \) appears as a counit for the coproduct \( \Delta \), and so \( (C\langle X \rangle, \Delta, e) \) becomes a (noncommutative) coalgebra.
For a word \( w = y_{s_1} \cdots y_{s_r} \), we can define the action of a composition \( I = (i_1, \ldots, i_l) \) of the integer \( r \) (i.e. a finite sequence of positive integers summing to \( r \)) by

\[
I[w] = y_{s_{i_1} + \cdots + s_{i_l}} y_{s_{i_l+1} + \cdots + s_{i_{l+1}}} \cdots y_{s_{i_r} + \cdots + s_{i_l+1} + \cdots + s_{i_r}}.
\]

**Example 1.** Let \( w = y_3^2 y_0^2 y_2 \) and \( I = (1, 2, 3, 1) \) a composition of \( 7 \) then \( I[w] = y_1 y_2 y_6 y_2 \).

Then, the bialgebra \((\mathcal{C}(X), \ast, 1, \Delta, e)\) becomes in fact an Hopf algebra, which antipode \( S \) is given by (Hoffman, 2000) \( S(w) = (-1)^{|w|} \sum_{i \in \text{Comp}(r)} I[y_{s_i} \cdots y_{s_r}] \), \( \text{Comp}(r) \) standing for the set of composition of \( r \).

**Remark 2.** The Hopf algebraic structure remains almost the same when replacing the stuffle product by shuffle or minus-stuffle products, except for the antipode. In the first case, this one is given by \( S(w) = (-1)^{|w|} \tilde{w} \), with \( y_{s_1} \cdots y_{s_r} = y_{s_r} \cdots y_{s_1} \) (mirror function). In the case of the minus-stuffle product, the antipode is the same as the one given for the stuffle product, but with the action of the composition \( I = (i_1, \ldots, i_l) \) corrected by a factor \((-1)^l\). More generally, for a quasi-stuffle \( \ast \), we shall define this action by

\[
I[w] = [y_{s_1}, \ldots, y_{s_{i_l}}] \cdots [y_{s_{i_l+1} + \cdots + s_{i_{l+1}}}, \ldots, y_{s_r}] .
\]

\[ \Box \]

2.2. Lyndon words and Radford theorem

By definition, a Lyndon word is a nonempty word \( l \in X^+ \) strictly smaller than any of its proper right factors (Reutenauer, 1993) (for lexicographical order), i.e. for all \( u, v \in X^+ \setminus \{\varepsilon\} \), \( l = uv \Rightarrow l < u \). The set of Lyndon words over \( X \) is denoted by \( \text{Lyn} X \).

**Theorem 1 (Radford, 1979).** Let \( C_1 = \mathbb{C} \oplus (X_0 \mathcal{C}(X) X_1) \) be the set of polynomials, called "convergent", over \( X \). Then, \((\mathcal{C}(X), \ast, \varepsilon) \simeq \mathbb{C}[\text{Lyn} X] = C_1[x_0, x_1] \).

**Theorem 2 (Malvenuto and Reutenauer, 1995).** Let \( C_2 = \mathbb{C} \oplus (Y \setminus Y_1 \mathcal{C}(Y)) \simeq C_1 \) be the set of polynomials, called "convergent" over \( Y \). Then, \((\mathcal{C}(Y), \ast, \varepsilon) \simeq (\mathcal{C}(Y), \ast) \simeq \mathbb{C}[\text{Lyn} Y] = C_2[y_1] \).

**Example 2.**

\[
\begin{align*}
x_1 x_0 x_1 x_0 x_1 + 2x_0 x_2 x_0 x_1 + 2x_0 x_1 x_0 x_2 & = \frac{1}{2} x_0 x_1 x_0 x_1 x_0 x_1 x_0 x_1 - 2x_0 x_1 x_0 x_1 x_0 x_1 x_0 x_1 \in \mathbb{C}[\text{Lyn} X] \\
& = x_0 x_1 x_0 x_1 x_0 x_1 x_0 x_1 + x_1 \in C_1[x_0, x_1],
\end{align*}
\]

\[
\begin{align*}
y_2 y_4 y_1 + y_2 y_1 y_2 y_4 + y_1 y_2 y_4 + y_2 y_5 + y_3 y_4 & = y_4 \ast y_2 \ast y_4 y_1 - y_4 y_2 \ast y_1 - y_6 \ast y_1 \in \mathbb{C}[\text{Lyn} Y] \\
& = y_2 y_4 \ast y_1 \in C_2[y_1].
\end{align*}
\]

2.3. Bracket forms and dual basis

The bracket form \( \tilde{S} \) of a Lyndon word \( l = uv \), with \( l, u, v \in \text{Lyn} X \) and the word \( v \) being as long as possible (factorisation – unique – called standard of a Lyndon word) is recursively defined by

\[
\begin{align*}
\tilde{S}_l & = [\tilde{S}_u, \tilde{S}_v] = \tilde{S}_v \tilde{S}_u - \tilde{S}_u \tilde{S}_v \\
\tilde{S}_x & = x \quad \text{for every letter } x \in X.
\end{align*}
\]

It is known that the set \( \mathcal{B}_1 = \{ \tilde{S}_l \mid l \in \text{Lyn} X \} \) is a basis for the free Lie algebra. Moreover, each word \( w \in X^* \) can be expressed, uniquely, as a decreasing (concatenation) product of Lyndon words:

\[
w = \ell_1^{\eta_1} \ell_2^{\eta_2} \cdots \ell_k^{\eta_k}, \quad l_1 > l_2 > \cdots > l_k, \ k \geq 0.
\]  
(7)

The Poincaré–Birkhoff–Witt basis \( \mathcal{B} = \{ \tilde{S}_w \mid w \in X^* \} \) can be obtained from (7) putting (Reutenauer, 1993) \( \tilde{S}_w = \tilde{S}_1^{\eta_1} \tilde{S}_2^{\eta_2} \cdots \tilde{S}_k^{\eta_k} \).
Its dual basis $\mathcal{B}^* = \{ \delta_w : w \in X^* \}$ can be then computed by

$$\delta_w = \frac{\epsilon_1^{a_1} \cdots \epsilon_l^{a_l} x^w}{a_1 x_1 \cdots a_l x_l}, \quad \delta_l = x \delta_w, \quad \forall l \in \mathcal{L} \text{yn} X,$$

where $l = xw$, $x \in X$, $w \in X^*$.

In Reutenauer (1993), it is proved that $\mathcal{B}$ and $\mathcal{B}^*$ are dual basis of $\mathbb{C}(X)$, i.e. $(\delta_u | \delta_v) = \delta_u, v$, for all words $u$, $v \in X^*$ with $\delta_u, v = 1$ if $u = v$, else 0.

3. Polylogarithms

3.1. Encoding by words

Let us consider the following two differential forms $\omega_0(z) = dz/z$ and $\omega_1(z) = dz/(1-z)$. The polylogarithm $Li_k(z)$ is defined for a composition $s = (s_1, \ldots, s_r)$ and for a complex $z$ such that $|z| < 1$ by

$$Li_k(z) = \sum_{n_1 > \cdots > n_r > 0} \frac{z^{n_1}}{n_1^{s_1} \cdots n_r^{s_r}}.$$

(8)

This expression corresponds to the iterated integral over $\omega_0$, $\omega_1$ and along the path $0 \rightarrow z$,

$$Li_s = \int_{0 \rightarrow z} \omega_0^{s_1-1} \omega_1 \cdots \omega_r^{s_r-1} w_1.$$

(9)

Let $X = \{x_0, x_1\}$. We shall by now identify any composition $s = (s_1, \ldots, s_r)$ with its encoding word $w = x_0^{s_1-1} x_1 \cdots x_r^{s_r-1}$ over $X^* x_1$, identification suggested by the previous formula. We obtain so a concatenation isomorphism from the $\mathbb{C}$-algebra of compositions into the subalgebra $\mathbb{C}(X) x_1 \subset \mathbb{C}(X)$. In that way, the polylogarithm $Li_k$ defined by the formula (8) can be also indexed by $w \in X^* x_1$.

To extend the definition of polylogarithms over $X^*$, we put $Li_{k_0}(z) = \log(z)$. By linearity, the definition of $Li_w$ is extended to polynomials on $\mathbb{C}(X)$. One of the most important facts concerning these polylogarithms is the following result, i.e. the isomorphism with a shuffle algebra, for the usual product $\oplus$.

**Theorem 3** (Hoang Ngoc Minh et al., 1998). The map $L : w \mapsto Li_w$ is an isomorphism from $(\mathbb{C}(X), \oplus)$ to $(\mathbb{C}[Li_w]_{w \in X^*}, \cdot)$.

3.2. Noncommutative generating series

The noncommutative generating series of polylogarithms, $L = \sum_{w \in X^*} Li_w \ w$, satisfies Drinfel’d differential equation (Drinfel’d, 1990) $dL = (x_0 \omega_0 + x_1 \omega_1) L$, with the initial condition $L(\varepsilon) = e^{x_0 \log \varepsilon} + O(\sqrt{\varepsilon})$, for $\varepsilon \rightarrow 0^+$. This enables one to prove that $L$ is the exponential of a Lie series. From the factorisation of a monoid by Lyndon words $l \in \mathcal{L} \text{yn} X$, we get the factorisation of the series $L$ (Hoang Ngoc Minh et al., 1998):

$$L(z) = e^{x_1 \log \frac{1}{1-z}} \left[ \prod_{l \in \mathcal{L} \text{yn} X \setminus \{x_0, x_1\}} e^{Li_l(z)} \right] e^{x_0 \log z}.$$

(10)

For all $l \in \mathcal{L} \text{yn} X \setminus \{x_0, x_1\}$, we have $S_l \in x_0 X^* x_1$. So, let us put

$$L_{\text{reg}} = \prod_{l \in \mathcal{L} \text{yn} X \setminus \{x_0, x_1\}} e^{Li_l} \text{ and } Z = L_{\text{reg}}(1).$$

(11)

Let $\sigma$ be the monoid endomorphism verifying $\sigma(x_0) = -x_1$, $\sigma(x_1) = -x_0$, we also get (Hoang Ngoc Minh et al., 1999)

$$L(z) = \sigma[L(1-z)]Z = e^{x_0 \log z} \sigma[L_{\text{reg}}(1-z)] e^{-x_1 \log(1-z)} Z.$$

(12)
**Definition 2 (Hoang Ngoc Minh et al., 2001).** Let \( \zeta_{\omega} : (\mathbb{C} \langle X \rangle, \omega) \to (\mathbb{C}, \cdot) \) be the algebra morphism (i.e. for \( u, v \in X^* \), \( \zeta_{\omega}(u \cdot v) = \zeta_{\omega}(u) \zeta_{\omega}(v) \)) verifying for all convergent word \( w \in X_0X^*X_1 \), \( \zeta_{\omega}(w) = \zeta(w) \), and such that \( \zeta_{\omega}(x_0) = \zeta_{\omega}(x_1) = 0 \).

Then, the noncommutative generating series \( Z_{\omega} = \sum_{w \in X^*} \zeta_{\omega}(w) \) \( w \) verifies \( Z_{\omega} = Z \) (Hoang Ngoc Minh et al., 2001). In consequence, \( Z_{\omega} \) is the unique Lie exponential verifying \( \langle Z_{\omega}^n|_{x_0} \rangle = \langle Z_{\omega}^n|_{x_1} \rangle = 0 \) and \( \langle Z_{\omega}|w\rangle = \zeta(w) \), for any \( w \in X_0X^*X_1 \).

**Remark 3.** Eq. (12) enables one to reach the expansion of any \( \text{Li}_w(z) \) around \( z = 1 \) (a singular expansion if \( w \in x_1X^*x_1 \)). For example,

\[
\text{Li}_{2,1}(1 - z) = -\text{Li}_3(z) + \log(z)\text{Li}_2(z) - \log^2(z)\text{Li}_1(z)/2 - \zeta(2)\text{Li}_1(z) + \zeta(3) = (-1 - \zeta(2))z + z \log(z) - z \log^2(z)/2 + \zeta(3) + O(|z|). \quad \square
\]

### 4. Special values

#### 4.1. Symmetric functions

Let \( \{t_i\}_{i \in \mathbb{N}^+} \) be an infinite set of variables, and let us define the (modified) symmetric functions \( \lambda_k^{(r)} \) and the sums of powers \( \psi_k^{(r)} \) by

\[
\lambda_k^{(r)}(t) = \sum_{n_1 \geq \ldots \geq n_k > 0} t_{n_1}^r \ldots t_{n_k}^r \quad \text{and} \quad \psi_k^{(r)}(t) = \sum_{n > 0} t_{n}^r.
\] (13)

**Remark 4.** In the case \( r = 1 \), we find the classical elementary symmetric functions \( \{\lambda_k^{(1)}\}_{k \geq 1} \) (MacDonald, 1995). \( \square \)

They are, respectively, coefficients of the following generating functions

\[
\lambda_k^{(r)}(t|z) = \sum_{k \geq 0} \lambda_k^{(r)}(t)z^k = \prod_{i \geq 1} (1 + t_i^r z) \quad \text{and}
\] (14)

\[
\psi_k^{(r)}(t|z) = \sum_{k \geq 0} \psi_k^{(r)}(t)z^{k-1} = \sum_{i \geq 1} \frac{t_i^r}{1 - t_i^r z}.
\] (15)

These generating functions satisfy a Newton identity \( d/dz \log \lambda_k^{(r)}(t|z) = \psi_k^{(r)}(t|z - 1) \).

We also recall the Waring formula (putting \( \lambda_0^{(r)} = 1 \)):

\[
\lambda_k^{(r)} = \frac{(-1)^k}{k!} \sum_{s_1 + \ldots + s_k = k} \binom{k}{s_1, \ldots, s_k} \left( -\frac{\psi_1^{(r)}}{1} \right)^{s_1} \ldots \left( -\frac{\psi_k^{(r)}}{k} \right)^{s_k}. \quad (16)
\]

#### 4.2. Quasi-symmetric functions

To the composition \( s = (s_1, \ldots, s_r) \), we now also associate the word \( w = y_{s_1} \ldots y_{s_r} \), defined over the alphabet \( Y = \{y_i, i \geq 0\} \).

The number of occurrences of letter \( y_i \) in the word \( w \in Y^* \) is denoted by \( |w|_i \).

Let \( w = y_{s_1} \ldots y_{s_r} \in Y^* \). The quasi-symmetric functions \( F_w \) and \( G_w \), of depth \( r = |w| \) and of degree (or weight) \( s_1 + \ldots + s_r \), are defined by

\[
F_w(t) = \sum_{n_1 \geq \ldots \geq n_r > 0} t_{n_1}^{s_1} \ldots t_{n_r}^{s_r} \quad \text{and} \quad G_w(t) = \sum_{n_1 \geq \ldots \geq n_r > 0} t_{n_1}^{s_1} \ldots t_{n_r}^{s_r}.
\] (17)
Remark 5. There exist explicit relations between the functions $G_w$ and $F_w$. For simplicity in the expression of the relations, we express them with multi-indexed notations rather than the word-indexed notation we just defined. Precisely, if $I = (i_1, \ldots, i_r)$ (resp. $J = (j_1, \ldots, j_p)$) is a composition of $n$ (resp. of $r$) then $J \circ I = (i_1 + \cdots + j_{i_1}, i_{j_1+1} + \cdots + j_{i_1+j_2}, \ldots, i_{j_{p-1}+1} + \cdots + i_r)$ is a composition of $n$. If $s = (s_1, \ldots, s_r)$ then we have (Hoffman, 2004) $G_s = \sum_{J \in \text{Comp}(r)} F_{J \circ s}$ and $F_s = \sum_{J \in \text{Comp}(r)} (-1)^{|J|-r} G_{J \circ s}$. The second formula, in which $|J|$ is the number of parts of $J$, being derived from the first one by Möbius inversion. For example, $G_{(1,2,1)} = F_{(1,2,1)} + F_{(1,3)} + F_{(1,3)} + F_{(4)}$, and $F_{(1,2,1)} = G_{(1,2,1)} - G_{(3,1)} - G_{(1,3)} + G_{(4)}$. More generally, for a composition of length $r$, the conversion from a form to the other one make appear $\text{Card}(\text{Comp}(r)) = 2^r - 1$ terms. □

In particular, $F_{y^r} = \lambda_k^{(r)}$ and $F_{y^r} = G_{y^r} = \psi_k^{(r)}$. As a consequence, integrating differential equation given by Newton identity shows that functions $F_{y^r}$ and $F_{y^r}$ are linked by the formula

\[
\sum_{k \geq 0} F_{y^r} z^k = \exp \left[ - \sum_{k \geq 1} F_{y^r} \frac{(-z)^k}{k} \right] \quad \text{(or } \sum_{k \geq 0} G_{y^r} z^k = \exp \left[ \sum_{k \geq 1} G_{y^r} \frac{z^k}{k} \right] \).
\]

By linearity, the definitions of $F_w$ and $G_w$ are extended to polynomials on $C(Y)$.

If $u$ (resp. $v$) is a word in $Y^*$, of length $r$ and of weight $q$ (resp. of length $s$ and of weight $p$), $F_u \omega^v_w$ and $G_u \omega^v_w$ are quasi-symmetric functions of depth $r + s$ and of weight $p + q$, and one has

\[
F_u \omega^v_w = F_u F_v \quad \text{and } G_u \omega^v_w = G_u G_v.
\]  

Since functions $F_w$, $w \in Y^*$ are linearly independent (Gessel, 1984), the remarkable identity (16) can be then seen as

\[
y^k_r = \frac{(-1)^k}{k!} \sum_{s_1 + \cdots + s_k = k \atop s_1, \ldots, s_k > 0} \frac{k!}{s_1! \cdots s_k!} \frac{(-y^r)^{s_1}}{1^s_1} \cdots \frac{(-y^r)^{s_k}}{k^s_k}.
\]  

4.3. Multiple harmonic sums

Definition 3. For any $w = y_{s_1} \ldots y_{s_r} \in Y^*$, let us define the maps $H_w$ and $H_w$ from $\mathbb{N}_+$ to $\mathbb{Q}$ by

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

We use the conventions $H_w(0) = H_w(0) = \infty$ for any nonempty word $w$ and $H_w = H_w \equiv 1$.

By linearity, the definitions of $H_w$ and $H_w$ are extended to polynomials on $C(Y)$.

For $N \geq 1$ and $w \in Y^*$, any $H_w(N)$ (resp. $H_w(N)$) can be obtained by specializing variables $\{t_i\}_{N \geq 1}$ at $t_i = 1/1$ and, for $i > N$, $t_i = 0$ in the quasi-symmetric function $F_w$ (resp. $G_w$) (Hoffman, 1997). In particular, the relations given in Remark 5 turn into

\[
H_s = \sum_{J \in \text{Comp}(r)} H_{J \circ s} \quad \text{and } H_s = \sum_{J \in \text{Comp}(r)} (-1)^{|J|-r} H_{J \circ s}.
\]

Moreover, from relations (19), we get

Proposition 1 (Hoffman, 1997). For $u, v \in Y^*$, $H_u \omega^v_w = H_u H_v$ and $H_u \omega^v_w = H_u H_v$.

Let $w = y_j \omega' \in Y^*$ such that $|w| = r$. One has

\[
H_w(N) = \sum_{l=r}^{N} \frac{H_{w'}(l-1)}{l} \quad \text{and } H_w(N) = \sum_{l=1}^{N} \frac{H_{w'}(l)}{l}.
\]

In consequence,

Theorem 4. For any $w = y_j \omega' \in Y^*$, $H_w(N)$ and $H_w(N)$ converge when $N \rightarrow +\infty$ if and only if $s > 1$. Therefore, if $s \geq 2$ then the limits $\lim_{N \rightarrow +\infty} H_w(N)$ and $\lim_{N \rightarrow +\infty} H_w(N)$ are denoted, respectively, by $\zeta(w)$ and by $\zeta(w)$. This justifies the fact that $w$ was said to be convergent in this case (otherwise, it is said to be divergent).
4.4. Noncommutative generating series over $Y$

**Proposition 2** (Hoang Ngoc Minh, 2003b). For $w \in X^*$, let $P_{w}(z) = (1 - z)^{-1}L_{w}(z)$. Thus, for $u, v \in Y^*$, $P_{u \circ v} = P_{u} \circ P_{v}$, where $\circ$ denotes the Hadamard product.

**Proof.** This comes from the fact that, for $u \in Y^*$, $P_{u}(z) = \sum_{N \geq 0} H_{u}(N)z^{N}$, so $P_{u}$ appears as the generating series of $\{H_{u}(N), N \geq 0\}$. The proposition follows then directly from **Proposition 1**, and from the definition of the Hadamard product. \(\Box\)

As consequences of **Theorem 3**, we also have

**Theorem 5** (Hoang Ngoc Minh, 2003b). The map $P : u \mapsto P_{u}$ is an isomorphism from polynomial algebra $(\mathbb{C}[Y], \cdot)$ to the Hadamard algebra $(\mathbb{C}[P_{u}], \circ)$. Therefore, the map $H : u \mapsto H_{u}$ (resp. $\overline{H} : u \mapsto \overline{H}_{u}$) is an isomorphism from $(\mathbb{C}(Y), \cdot)$ (resp. $(\mathbb{C}[Y], \circ)$) to the algebra $(\mathbb{C}[H_{w}], \cdot)$ (resp. $(\mathbb{C}[\overline{H}_{w}], \cdot)$).

The noncommutative generating series $P(z) = \sum_{w \in X^*} P_{w}(z) = (1 - z)^{-1}L(z)$, can be factorised, from the factorisation (10) of the series $L$, in

$$P(z) = e^{-(x_{1}+1) \log(1-z)_{\text{reg}}(z)e^{x_{0} \log z}}. \quad (23)$$

Let $\pi_{Y}$ the projector from $\mathbb{C}(X)$ to $\mathbb{C}(Y)$ erasing the monomials ending with $x_{0}$, i.e. for any word $w \in X^*$, $\pi_{Y}(w x_{0}) = 0$ and $\pi_{Y}(x_{0}^{s_{1}} - x_{1} \cdots x_{0}^{s_{k}} - x_{k}) = y_{s_{1}} \cdots y_{s_{k}}$. Then

$$A(z) = \pi_{Y} L(z) \sum_{k \in \mathbb{N}} \exp \left( y_{1} \log \frac{1}{1-z} \right) \pi_{Y} Z. \quad (24)$$

Since $P_{y_{1}^{k}}(z) = (1 - z)^{-1}L_{y_{1}^{k}}(z) = (-1)^{k}(1 - z)^{-1} \log^{k}(1 - z)/k!$, we get another expression for the factorisation of $P$, when projected onto $\mathbb{C}(Y)$:

**Lemma 1.** Let $\text{Mono}(z) = e^{-(x_{1}+1) \log(1-z)}$. Then

$$\pi_{Y} \text{Mono} = \sum_{k \in \mathbb{N}} P_{y_{1}^{k}} y_{1}^{k} \quad \text{and} \quad \pi_{Y} \text{Mono}^{-1} = \sum_{k \in \mathbb{N}} P_{y_{1}^{k}} (-y_{1})^{k}.$$

Looking now at the coefficient of $z^{N}$ in the Taylor expansion of $P_{y_{1}^{k}}$, which is, using a common notation, $[z^{N}]P_{y_{1}^{k}}(z) = H_{y_{1}^{k}}(N)$, we derive from Eq. (18) the following

**Lemma 2.** Let $\text{Const} = \sum_{k \in \mathbb{N}} H_{y_{1}^{k}} y_{1}^{k}$. Then

$$\text{Const} = \exp \left[ -\sum_{k \geq 1} H_{y_{k}} (-y_{1})^{k} / k \right] \quad \text{and} \quad \text{Const}^{-1} = \exp \left[ \sum_{k \geq 1} H_{y_{k}} (-y_{1})^{k} / k \right].$$

With the introduction of the series $\text{Mono}$, we can now sum up Eqs. (10) and (12) into

**Proposition 3.** $P(z) \sum_{z \rightarrow 0} e^{x_{0} \log z} \text{and} P(z) \sum_{z \rightarrow 1} \text{Mono}(z) Z$.

**Corollary 1.** Let $\Pi(z) = \pi_{Y} P(z) = \sum_{w \in Y^*} P_{w}(z) w$. Then $\Pi(z) \sum_{z \rightarrow 1} \pi_{Y} \text{Mono}(z) \pi_{Y} Z$.

Once again, looking at Taylor coefficients of $P_{w}$, we derive, as a direct consequence of **Lemma 1**, the following equivalent for the generating series $H(N) = \sum_{w \in Y^*} H_{w}(N) w$.

**Corollary 2.** $H(N) \sum_{N \rightarrow \infty} \text{Const}(N) \pi_{Y} Z$.

**Theorem 6** (Hoang Ngoc Minh, 2007).

$$\lim_{z \rightarrow 1} \exp \left( y_{1} \log(1-z) \right) A(z) = \lim_{N \rightarrow \infty} \exp \left( \sum_{k \geq 1} H_{y_{k}}(N) \frac{(-y_{1})^{k}}{k} \right) H(N) = \pi_{Y} Z,$$

where the limit shall be understood as a limit word by word.

This rewriting of Formula (24), and of **Corollary 2** provides a theorem “à l’Abel”, linking the behaviour of the series $A$ as $z$ tends to 1 with the asymptotic behaviour of multiple harmonic sums (seen as Taylor coefficients) as $N$ tends to $+\infty$. 

4.5. Generalized Euler constants

Since $Z$ is well known (and of course $\pi_\gamma Z$ also) and already studied, let us see now how to exploit Theorem 6 to get precise information about divergent harmonic sums.

Definition 4. We define, for any word $w \in Y^*$, the "generalized Euler constant", denoted by $\zeta_{\omega}(w)$, as the constant occurring in the asymptotic expansion of $H_w(n)$ in the scale of $\{n^\alpha \log^\beta(n), \alpha \in \mathbb{Z}, \beta \in \mathbb{Z}\}$.

Proposition 4. The map $\zeta_{\omega} : (\mathbb{C}(Y), \omega) \rightarrow (\mathbb{C}, \cdot)$ is an algebra morphism (i.e. verifies for all $u, v \in Y^*$, $\zeta_{\omega}(u \cdot v) = \zeta_{\omega}(u) \cdot \zeta_{\omega}(v)$), such that for a convergent word $w \in Y^* \setminus \gamma_1 Y^*$, $\zeta_{\omega}(w) = \zeta(w)$ and $\zeta_{\omega}(\gamma_1) = \gamma$.

Notation. For convenience, we will by now denote by $Z$ the $\mathbb{Q}$-algebra generated by $\{\zeta(w), w \in Y^* \setminus \gamma_1 Y^*\}$, and by $Z'$ the $\mathbb{Q}$-algebra generated by $Z$ and $\gamma$.

This proposition, consequence of the Proposition 1, provides sufficient conditions to compute all constants $\zeta_{\omega}(w), w \in Y^*$. Indeed, Theorem 2 enables one to write any word $w \in Y^*$ as a combination of (stuffle) powers of $\gamma_1$, with coefficients in the set of convergent words. Precisely, $w = \sum_{|w|} c_j(w) \omega_j \omega_1^{\omega_j}$, with $c_j(w)$ convergent polynomials (which is equivalent to $H_w = \sum_{j=0} H_j(w)H_1^j$).

Example 3. Let $w = y_1^2 y_2$, then

$$c_2(w) = 0, \quad c_2(w) = 2y_2, \quad c_1(w) = -y_2 y_1 - y_3, \quad c_0(w) = y_2 y_1 + y_3 y_1 + y_4/2,$$

and applying Proposition 4 leads to (using the reduction table of polyzêtas)

$$\zeta_{\omega}(w) = \zeta(c_0(w)) + \zeta(c_1(w)) \gamma + \zeta(c_2(w)) \gamma^2 = \frac{7 \gamma (2)}{10} - \frac{2 \gamma (3)}{3} \gamma + \frac{\gamma (2)}{2} \gamma^2.$$

Proposition 5. $\zeta_{\omega}(\gamma_1^k) = \sum_{s_1, \ldots, s_k, \geq 0} \frac{(-1)^k}{s_1! \ldots s_k!} (-\gamma)^s_1 \left(\frac{-\gamma (2)}{k} \right)^s_2 \ldots \left(\gamma (k) \right)^{s_k}$.

Proof. By Formula (20) and applying the (surjective) morphism $\zeta_{\omega}$, we get the expected result.

In consequence,

Theorem 7 (Hoang Ngoc Minh, 2003b). For $k > 0$, the constant $\zeta_{\omega}(\gamma_1^k)$ associated to divergent polyzêta $\zeta(\gamma_1^k)$ is a polynomial of degree $k$ in $\gamma$ with coefficients in $\mathbb{Q}[\gamma (2), \gamma (2l + 1)]_{0 < i \leq (k - 1)/2}$. Moreover, for $l = 0, \ldots, k$, the coefficient of $\gamma^l$ is of weight $k - l$.

Example 4. $\zeta_{\omega}(\gamma_1^2) = \frac{\gamma^2 - \gamma (2)}{2}, \quad \zeta_{\omega}(\gamma_1^3) = \frac{\gamma^3 - 3 \gamma (2) \gamma + 2 \gamma (3)}{6}$.

Let us consider the (exponential) partial Bell polynomials in the variables $\{t_i\}_{i \geq 1}, b_{n,k}(t_1, \ldots, t_{n-k+1})$, defined by the exponential generating series:

$$\sum_{n=0}^{\infty} \sum_{k=0}^{n} b_{n,k}(t_1, \ldots, t_{n-k+1}) \frac{y^n u^k}{n!} = \exp \left( u \sum_{l=1}^{\infty} \frac{t_l u^l}{l!} \right).$$

(25)

In particular, we have

Lemma 3. Let $t_m = (-1)^{m+1}(m - 1)! \zeta_{\omega}(m)$, for $m \geq 1$. Then

$$\exp \left[ - \sum_{k \geq 1} \zeta_{\omega}(k) \frac{(-y_1)^k}{k} \right] = 1 + \sum_{n \geq 1} \left[ \sum_{k=1}^{n} b_{n,k}(\gamma, -\gamma (2), 2 \gamma (3), \ldots) \right] \frac{y^n}{n!}.$$

Let us build the noncommutative generating series of $\zeta_{\omega}(w)$ and let us take the constant part of the two members of $H(N)_{n \to \infty} \text{Const}(N) \pi_\gamma Z$, we have
Theorem 8 (Hoang Ngoc Minh, 2007). Let 

\[ Z_{\omega} = \sum_{w \in Y^*} \xi_{\omega}(w) \] 

be the noncommutative generating series of the constants \( \xi_{\omega}(w) \). Then

\[ Z_{\omega} = \left[ 1 + \sum_{n \geq 1} \left( \sum_{k=1}^n b_{n,k}(\gamma, -\xi(2), 2\xi(3), \ldots) \right) \right] \pi_Y Z. \]

Identifying coefficients of \( y^k \) in each member leads to

Corollary 3. For all \( w \in Y^* \setminus y_1 Y^* \) and \( k \geq 0 \), we have

\[ \xi_{\omega}(y^k) = \frac{k}{\pi_X} \left( \sum_{i=0}^k \sum_{j=1}^i \binom{i}{j} b_{i,j}(\gamma, -\xi(2), 2\xi(3), \ldots) \right), \]

\( \pi_X w \) standing for the translation of \( w \) in alphabet \( X \).

Finally, using the expression of \( \xi_{\omega}(x_1^{k-1} \pi_X w) \) given in Hoang Ngoc Minh et al. (2001), i.e. for a word \( u \in X^* x_1^k, \xi_{\omega}(x_1^k u) = \xi(x_0(x_1^k \omega u)) \), we get the following

Corollary 4. For all \( w \in Y^* \setminus y_1 Y^* \) and \( k \geq 0 \), we have

\[ \xi_{\omega}(y^k) = \frac{k}{\pi_X} \left( \sum_{i=0}^k \sum_{j=1}^i \binom{i}{j} b_{i,j}(\gamma, -\xi(2), 2\xi(3), \ldots) \right), \]

with \( u \) defined as the suffix such that \( \pi_X w = x_0 u \).

Example 5. Consider the word \( y^2 y_2 \), corresponding, with the previous notations, to \( k = 2 \) and \( w = y_2 \), then \( \pi_X w = x_1 \), so \( u = x_1 \) and

\[ \xi(x_0((-x_1)^2 \omega u)) = 3\xi(x_0 x_1^2), \quad \xi(x_0((-x_1) \omega u)) = -2\xi(x_0 x_1^2), \quad \xi(x_0 u) = \xi(x_0 x_1). \]

So, \( \xi_{\omega}(y^2 y_2) = \xi_{\omega}(x_1^2 \pi_X y_2) + \xi_{\omega}(x_1 \pi_X y_2) b_{1,1}(\gamma, -\xi(2)) + \xi(2)(b_{2,1}(-\xi(2)) + b_{2,2}(\gamma))/2 \)

\[ = 3\xi(2, 1, 1) - 2\xi(2, 1) - 2\xi(2, 2) + \xi(2)(-\xi(2) + \gamma^2)/2, \]

and using the reduction table, we find \( \xi_{\omega}(y^2 y_2) = \xi(2) \gamma^2 - 2\xi(3) \gamma + 7\xi(2)/10 \), a result in agreement with Example 3.

Remark 6. We can in fact derive Proposition 5 from Corollary 3, in the special case \( w = \epsilon \), since all values \( \xi_{\omega}(x_1^{k-1}) \) are equal to zero, except when \( i = k \), giving rise to \( \xi_{\omega}(\epsilon) = 1 \), so \( \xi_{\omega}(y^k) = 1/k! \left( \sum_{j=1}^k b_{k,j}(\gamma, -\xi(2), 2\xi(3), \ldots, (-1)^{k-1}(k-1)!\xi(k)) \right) \).

In consequence,

Theorem 9 (Hoang Ngoc Minh, 2003b). For \( w \in Y^* \setminus y_1 Y^* \), \( k \geq 0 \), the constant \( \xi_{\omega}(y^k) \) associated to \( \xi(y^k \omega) \) is a polynomial of degree \( k \) in \( \gamma \) and with coefficients in \( \mathbb{Z} \). Moreover, for \( l = 0, \ldots, k \), the coefficient of \( y^l \) is of weight \( |w| + k - l \).

4.6. Asymptotic aspects of harmonic sums

In the previous section, we introduced the constant \( \xi_{\omega}(w) \) as the constant term involved in the asymptotic expansion, of \( H_w(n) \). Let us be more precise about the computation of this expansion.

A first path (see Costermans et al. (2005a)) to get this expansion is given by the property of \( L \) (relation (12)), that we interpret immediately on \( P \) by \( P(1-z) = (1-z)z^{-1}[\sigma P(z)]Z \). Then, for a given word \( w \), we can write \( P_w(z) \) as a \( \mathbb{C} \left[z, z^{-1}, (1-z)^{-1}\right] \)-linear combination of some \( P_u(1-z) \), that we can expand up to any order, getting so a singular expansion of \( P_w(z) \) around \( z = 1 \), in the scale of functions \( \{(1-z)^{\alpha} \log(1-z)^{\beta}, \alpha \in \mathbb{Z}, \beta \in \mathbb{N}\} \). According to singularity analysis principles, this expansion gives rise to an asymptotic expansion of its Taylor coefficient \( [z^n]P_w(z) \), i.e. \( H_w(n) \).
Example 6. Following Remark 3, we have

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

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

But \([z^N]\zeta(3)(1-z)^{-1} = \zeta(3),\) \([z^N]\log(1-z) = -N^{-1},\) \([z^N]\log^2(1-z) = \frac{2!(1-z)\gamma_1^2(z)}{2} = H_{\gamma_1}^2(N) - H_{\gamma_1}^2(N-1) \ldots .\]

We find finally, using Formula (20) which expresses \(H_{\gamma_1}\) as a polynomial combination of single-indexed harmonic sums (i.e. generalized harmonic numbers),

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

This approach is very efficient, but the main difficulty is to extract from Formula (12) the coefficients of a particular word \(w\), mostly when the weight of \(w\) grows. We will refer to this algorithm as Algo 1.

Another path to get the asymptotic expansion of \(H_w(n)\) is to start from the recursive Formula (22), and to expand the numerator. This gives rise to a recursive algorithm, which initialization is given by the Euler–Maclaurin summation formula giving the expansion of generalized harmonic numbers.

Example 7.

\[
H_{4,2}(N) = \zeta(4, 2) - \sum_{i=N+1}^{\infty} \frac{H_2(i-1)}{i^4}, \quad \text{but} \quad H_2(i-1) = \zeta(2) - \frac{1}{i} - \frac{1}{2} \frac{1}{i^2} + O\left(\frac{1}{i^3}\right),
\]

So,

\[
H_{4,2}(N) = \zeta(4, 2) - \zeta(2) \sum_{i=N+1}^{\infty} \frac{1}{i^4} + \sum_{i=N+1}^{\infty} \frac{1}{i^3} + \frac{1}{2} \sum_{i=N+1}^{\infty} \frac{1}{i^2} + \sum_{i=N+1}^{\infty} O\left(\frac{1}{i}\right).
\]

Expanding the sums in \(N\), we finally find

\[
H_{4,2}(N) = \zeta(4, 2) - \frac{1}{3} \frac{\zeta(2)}{N^3} + \frac{1}{2} \frac{\zeta(2)}{N^4} + \frac{1}{4} \frac{\zeta(2)}{N^5} - \frac{1}{3} \frac{\zeta(2)}{N^6} + \frac{2}{5} \frac{\zeta(2)}{N^7} + O\left(\frac{1}{N^8}\right).
\]

Unfortunately, these basic principles do not work for a divergent word, for example, \(w = y_1y_2\), since using Euler–Maclaurin summation formula can give the divergent part and the infinitesimal part, but not the \(N\)-free term (we are going to make this point precise). A possible solution to avoid this problem was given in Costermans et al. (2005b), and consisted in decomposing the divergent word thanks to Theorem 2. For instance, \(y_1y_2 = y_1 \omega y_2 - y_2y_1 - y_3\), so there are just the computations of the expansions for \(y_2y_1\) and \(y_3\) left, expansions for which the previous principles may be applied. The main problem here is the cost of the decomposition from Theorem 2, mostly when the length of the word \(w\) grows. We refer to this algorithm as Algo 2.

Following an idea suggested by B. Salvy, the authors were interested in seeing what happened when applying naively Euler–Maclaurin formula on the numerator, in Formula (22), without making difference between divergent and convergent words. To be more explicit, let us explain the case \(w = y_1y_2\): using the software Maple  

\[\text{2 In the following lines, to avoid some steps, unnecessary for the reader, we do not show the instructions for collecting, re-ordering, expanding, etc.}\]
> numer1 := asympt(eulermac(1/k^2, k = 1..n - 1, 2), n);
> numer1 := \(\frac{\pi^2}{6} - \frac{1}{n} + O\left(\frac{1}{n^2}\right)\)
> numer2 := asympt(eulermac(1/k^2, k = 1..n - 1, 3), n);
> numer2 := \(\frac{\pi^2}{6} - \frac{1}{n} - \frac{2}{n^2} + O\left(\frac{1}{n^2}\right)\)

> asympt(eulermac(numer1/n, n = 1..N, 2), N);
\[\frac{1}{6} \pi^2 \ln(N) - \frac{1}{6} \pi^2 + \frac{1}{6} \pi^2 \gamma + \frac{1}{2} \pi^2 + 1 \frac{1}{N} + O\left(\frac{1}{N^2}\right)\]
> asympt(eulermac(numer2/n, n = 1..N, 2), N);
\[\frac{1}{6} \pi^2 \ln(N) - \frac{1}{6} \pi^2 + \frac{1}{6} \pi^2 \gamma - \frac{1}{2} \pi^2 + 1 \frac{1}{2} \pi^2 + 1 \frac{1}{N} + O\left(\frac{1}{N^2}\right)\]

Here we can see that expanding further the numerator modifies the final constant term. In fact, we turned this idea into an efficient (and correct) algorithm by replacing the previous wrong \(N\)-free term \(-\pi^2/6 + \pi^2 \gamma / 6 - \zeta(3)/2\) by \(\zeta(2) - 2 \zeta(3)\). This new algorithm, that we will call Algo 3 appears as the fastest of our three methods.

Here are some examples of time for computing the expansion of \(H_w(N)\) up to \(O(N^{-3})\). For Algo 1, the series \(L\) and \(\sigma(L)Z\) are supposed to be constructed, and the computing time starts with the extraction of coefficient \(w\) in both series. The empty value on the third line means precisely that the construction of the series \(\sigma(L)Z\) cannot be computed in a "reasonable" time.

<table>
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<th>length</th>
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<th>Algo 2</th>
<th>Algo 3</th>
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<td>3</td>
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<td>-</td>
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5. Applications to discrete probabilities

5.1. Coupon collector’s problem

Foata et al. (2001) considered the coupon collector’s problem, in the case where the collector, supposed to be the eldest, has got a brotherhood, say \(r\) brothers. When he gets a coupon he has already, he gives it to his oldest brother, who keeps it or gives it to the oldest of the \(r - 1\) remaining brothers, and so on. Defining \(T\) the (random) number of chocolate bars he must buy to complete his collection made of \(m\) different coupons, and \(M_{ij}\) the number of empty places in the collection of the \(j\)-th brother at this time, Foata et al. (2001) show that \(E[M_{ij}] = \sum_{j=0}^{k} K_{m,ij}^{(k)}\), where for all \(m \geq 1\), \(K_{m,ij}^{(1)} = 1\) and \(K_{m,ij}^{(k)} = \sum_{j=2}^{m} K_{j}^{(k-1)} / j\).

Foata et al. (2001) remarked that these numbers \(K_{m,ij}^{(k)}\), called hyperharmonic numbers are variations of generalized harmonic numbers \(H_{ij}(m)\). Indeed, for \(k \geq 1\), \(K_{m,ij}^{(k)}\) can be written as \(K_{m,ij}^{(k)} = H_{ij}^{(k)}(m) - H_{ij}^{(k-1)}(m)\).

**Proof.** By induction on \(k\). It is obvious if \(k = 1\) (recall that \(H_{ij} \equiv 1\)). Then supposing it is true for \(k > 1\), and since \(K_{1,ij}^{(k)} = 0\), we just apply Formula (22)
\[K_{m,j}^{(k+1)} = \sum_{j=2}^{m} K_{j}^{(k)} / j = \sum_{j=1}^{m} H_{j}^{(k)} - H_{j}^{(k-1)} = H_{j}^{(k+1)}(m) - H_{j}^{(k)}(m). \]
\(\square\)
Consequently, $\mathbb{E}[M_1^{(k)}]$ may be further simplified in $\mathbb{E}[M_0^{(k)}] = H_{\gamma_1}(m)$. For instance, as $m$ tends to $+\infty$,

$$\mathbb{E}[M_1^{(2)}] = \frac{1}{2} \ln^2(m) + \gamma \ln(m) + \frac{\gamma^2 + \zeta(2)}{2} + \frac{\ln(m) + \gamma - 1}{m} + O \left( \frac{\ln(m)}{m^2} \right)$$

$$\mathbb{E}[M_1^{(3)}] = \frac{1}{6} \ln^3(m) + \frac{1}{2} \ln^2(m) \gamma + \left( \frac{\gamma^2 + \zeta(2)}{2} \right) \ln(m) + \frac{\gamma \zeta(2)}{2} \frac{\gamma^3}{6} + \frac{\zeta(3)}{3} + O \left( \frac{\ln^2(m)}{m} \right)$$

$$\mathbb{E}[M_1^{(4)}] = \frac{1}{24} \ln^4(m) + \frac{1}{6} \ln^3(m) \gamma + \left( \frac{\gamma^2 + \zeta(2)}{4} \right) \ln^2(m) + \frac{\gamma \zeta(2)}{2} \frac{\gamma^3}{6} + \frac{\zeta(3)}{3} \gamma + \frac{9}{40} \gamma \zeta(2)^2 + O \left( \frac{\ln^3(m)}{m} \right).$$

5.2. Root-subtrees in multidimensional quadrees

Following the notations suggested in Labelle and Laforest (1995b) and Labelle et al. (2006), given the hypercube $[0, 1]^d$, an initial point $X_1 = (t_1, \ldots, t_d)$ divides the hypercube in $2^d$ hyperoctants, and we index by the binary word $\epsilon_1 \ldots \epsilon_d \in \{0, 1\}^d$, the hyperoctant containing the vertex $(\epsilon_1, \ldots, \epsilon_d)$.

Let $S$ be a set of binary words encoding hyperoctants, we denote by $J_n[S]$ the probability that $n$ points i.i.d fall in this set. With the practical notations $t_i^{(0)} = t_i$ and $t_i^{(1)} = 1 - t_i$, probability $J_n[S]$ is given by the following multiple integral

$$J_n[S] = \int_0^1 \cdots \int_0^1 f_n(t_1, \ldots, t_d)^{n-1} dt_1 \ldots dt_d. \tag{26}$$

where $f_n(t_1, \ldots, t_d) = \sum_{\epsilon \in S} \prod_{i=1}^d t_i^{(\epsilon_i)}$.

**Example 8.** In dimension 2, let $X_1 = (t_1, t_2)$ and $S = \{01, 11\}$ (encoding the two quadrants “north”), or rather (identifying the binary encoding with its decimal equivalent) $S = \{1, 3\}$, then

$$J_n[S] = \int_0^1 \int_0^1 (t_1(1-t_2) + (1-t_1)(1-t_2))^{n-1} dt_1 dt_2.$$

One can remark that replacing a set $S$ with its complement replaces, in Formula (26), the expression $f_n(t_1, \ldots, t_d)$ by its 1’s complement. By consequence, $\overline{S}$ standing for the complement set of $S$, $J_n[S] = \sum_{k=1}^n (-1)^{k-1} \binom{n-1}{k-1} J_n[\overline{S}]$.

In the case where $S = \{1, 2, 3, 4, 5, 6, 7\}$, then $\overline{S} = \{0\}$, and

$$J_n[S] = \sum_{k=1}^n (-1)^{k-1} \frac{n}{k-1} \frac{1}{k^2} = -\frac{1}{n} \sum_{k=1}^n (-1)^k \binom{n}{k} \frac{1}{k^2}.$$

Here we are facing an Euler transform, and we can use some interesting (combinatoric) properties linking the operators $\nabla$ and $\Sigma$, defined by – cf. (Hoffman, 2005) –

$$\nabla : (a_n)_{n \geq 0} \mapsto \left( \sum_{k=0}^n (-1)^k \binom{n}{k} a_k \right)_{n \geq 0}, \quad \Sigma : (a_n)_{n \geq 0} \mapsto \left( \sum_{k=0}^n a_k \right)_{n \geq 0}.$$

Indeed, Hoffman (2005) showed that $\Sigma \nabla H_n = -H_{n+\delta}$, with $\delta$ uniquely associated to $w$ is constructed as follows : if $w = y_{s_1} \ldots y_{s_r}$ has for weight $\bar{n}$, then you can consider the partial sums
\{s_1, s_1 + s_2, \ldots, s_1 + \cdots + s_{r-1}\} as a (maybe empty) subset of \{1, \ldots, n - 1\}, for which you can take the complement set and construct from it the unique word \(w^n\) of weight \(n\). For example, \(y_2^r = y_1y_1, y_1^2 = y_2y_1^2\).

Coming back to \(S = \{1, 2, 3, 4, 5, 6, 7\}\), and since \(\Sigma \nabla = \nabla \Sigma^{-1}\), we have

\[
J_n[S] = -\frac{1}{n} \nabla \Sigma^{-1} H_{y_2} (n) = \frac{1}{n} H_{y_2} (n) = \frac{1}{n} H_{y_1} (n).
\]

Another example, still in dimension \(d = 3\). If \(S = \{2, 3, 4, 5, 6, 7\}\), then \(J_k[S] = k^{-2}\).

\[
J_n[S] = \sum_{k=1}^{n} (-1)^{k-1} \binom{n-1}{k-1} \frac{H_{y_1} (k)}{k^2} = -\frac{1}{n} \sum_{k=1}^{n} (-1)^{k} \binom{n}{k} \frac{H_{y_1} (k)}{k} = -\frac{1}{n} \nabla \Sigma^{-1} H_{y_1} (n)
\]

\[
= \frac{1}{n} H_{y_2} (n) = \frac{1}{n} H_{y_1} (n).
\]

A last example, with \(d = 3\), and \(S = \{3, 4, 5, 6, 7\}\), for which \(J_k[S] = H_{y_1} (k) / k^2\).

\[
J_n[S] = \sum_{k=1}^{n} (-1)^{k-1} \binom{n-1}{k-1} \frac{H_{y_1} (k)}{k^2} = -\frac{1}{n} \sum_{k=1}^{n} (-1)^{k} \binom{n}{k} \frac{H_{y_1} (k)}{k} = -\frac{1}{n} \nabla \Sigma^{-1} H_{y_1} (n)
\]

\[
= \frac{1}{n} H_{y_2} (n) = \frac{1}{n} H_{y_1} (n).
\]

### 5.3. Maxima in hypercubes

Let \(Q = \{q_1, \ldots, q_n\}\) be a set of independent and identically distributed random vectors in \(\mathbb{R}^d\). A point \(q_i = (q_{i1}, \ldots, q_{id})\) is said to be dominated by \(q_j = (q_{j1}, \ldots, q_{jd})\) if \(q_{ij} < q_{kj}\) for all \(k \in \{1, \ldots, d\}\) and a point \(q_i\) is called a maximum of \(Q\) if none of the other points dominates it. The number of maxima of \(Q\) is denoted by \(K_{n,d}\).

Recently, Bai et al. (2005) proposed a method for computing an asymptotic expansion of the variance and the study of \(\nabla \text{var}(K_{n,d})\) for random samples from \([0, 1]^d\) is precisely the goal of the present section. For that, we exploit the following result, first derived by Ivanin (1976):

\[
\mathbb{E}(K_{n,d}^2) = \sum_{1 \leq i_1 \leq \cdots \leq i_l \leq 1 \leq \cdots \leq 1 \leq d-l} \frac{1}{i_1 \cdots i_l d-l} + \sum_{1 \leq i_1 \leq \cdots \leq i_{d-1} \leq n} \binom{d}{i_1 \cdots i_{d-1} j_1 \cdots j_{d-1}}^n,
\]

where the sum \((*)\) is taken over indices verifying \(1 \leq i_1 \cdots \leq i_{j-1} \leq l, 1 \leq i_t \leq \cdots \leq i_{d-2} \leq l\) and \(l + 1 \leq j_1 \leq \cdots \leq j_{d-1} \leq n\). After having given an alternative derivation for this formula, Bai et al. deduce, by analytic and combinatoric considerations, as the main result of (Bai et al., 1998), the following equivalent\footnote{The value of the mean of \(K_{n,d}\) is known to be \(H_{y_2} (n)\) (Barndorff-Nielsen and Sobel, 1966).}

\[
\nabla \text{var}(K_{n,d}) \sim \left(\frac{1}{(d-1)!} + \kappa_d\right) \ln^{d-1}(n), \quad \text{with}\]

\[
\kappa_d = \sum_{t=1}^{d-2} \frac{1}{t!(d-1-t)!} \sum_{i_1 \geq 1} \frac{1}{i_1} \sum_{i_t=1}^{i_1 \cdots i_{d-2-t}} \frac{1}{i_t \cdots i_{d-2-t}}
\]

the sum \((***)\) being calculated over all indices verifying \(1 \leq i_1 \leq \cdots \leq i_{t-1} \leq l\) and \(1 \leq j_1 \leq \cdots \leq j_{d-2-t} \leq l\).
We first focus on the asymptotic equivalent of $\nabla \text{ar}(K_{n,d})$ from Formula (28), $\kappa_d$ being re-written, with our tools, in the following way

$$
\kappa_d = \frac{1}{(d-1)!} \sum_{t=1}^{d-2} \binom{d-1}{t} \sum_{l \geq 1} \frac{1}{\rho} H_{\frac{1}{\rho} y_1^{d-1} \omega y_1^{d-2}}(l).
$$

We need a last ad hoc notation.

**Definition 5.** Let $S$ be a subset of $Y$, and $\rho$ a positive integer, we define $S_\rho$, as the set of words containing only letters in $S$, and of weight equal to $\rho$.

**Example 9.** Let $S = \{y_1, y_2\}$ and $\rho = 4$ then $S_\rho = \{y_1^4, y_1 y_2 y_1, y_2^2 y_2, y_2 y_1^2, y_2\}$.

We recall that $|w|_2$ stands for the number of occurrences of the letter $y_2$ in $w$, and so we turn Eq. (29) into a closed form (Costermans and Hoang Ngoc Minh, 2007).

**Theorem 10.** $\kappa_d = \frac{1}{(d-1)!} \sum_{w \in \{y_1, y_2\}_{d-3}} (-1)^{|w|_2} \binom{2(d-2-|w|_2)}{d-2-|w|_2} \xi(y_2 w)$.

**Example 10.** For $d = 7$, we get

$$
6 k_7 = \left(\begin{array}{c}
10 \\
5 \end{array}\right) \xi(2, 1, 1, 1, 1) - \left(\begin{array}{c}
8 \\
4 \end{array}\right) \xi(2, 2, 1, 1) + \xi(2, 1, 2, 1) + \xi(2, 1, 1, 2) \\
+ \left(\begin{array}{c}
6 \\
3 \end{array}\right) \xi(2, 2, 2).
$$

For $d = 9$ and $d = 10$, using the reduction table, we get

$$
k_9 = -\frac{17}{1920} \xi(6, 2) + \frac{11}{160} \xi(3) \xi(5) + \frac{1}{320} \xi(2) \xi(3)^2 + \frac{1891}{89600} \xi(2)^4
$$

$$
k_{10} = \frac{529}{75600} \xi(2)^2 \xi(5) + \frac{33941}{635400} \xi(3) \xi(5) + \frac{17}{3360} \xi(2) \xi(7) + \frac{4354560}{4354560} \xi(3)^3.
$$

Now, interested in the whole expansion of the variance, we can turn Expression (27) into $E(K_{n,d}^2) = H_{d-1}(n) + \sum_{1 \leq r \leq d-1} \binom{d}{r} \sum_{l=1}^{n-1} \frac{1}{r} H_{d-1}(l) H_{d-1}(l) H_{d-1}(n; l + 1)$, the notation $H_{w}(n; l + 1)$ being the same as in **Definition 3**, but where all indices involved in the summation are bounded lowerly by $l + 1$. From this point, we get the following

**Theorem 11** (Costermans and Hoang Ngoc Minh, 2007). For all $d \geq 2$, there exist an integer $K > 0$, some integers $(\alpha_i)_{1 \leq i \leq K}$ and some words $w_i \in Y^*$ such that $\nabla \text{ar}(K_{n,d}) = \sum_{i=1}^{K} \alpha_i H_{w_i}(n)$.

By consequence, there exist algorithmically computable coefficients $\alpha_i$, $\beta_{j,k} \in Z'$ such that, for any dimension $d$ and any order $M$,

$$
\nabla \text{ar}(K_{n,d}) = \sum_{l=0}^{2d-2} \alpha_l \ln^l(n) + \sum_{j=1}^{M} \frac{1}{n^j} \sum_{k=0}^{2d-2} \beta_{j,k} \ln^k(n) + o \left( \frac{1}{n^M} \right).
$$
Example 11.

\[ \begin{align*}
\mathbb{V} & \text{ar}(K_{3,1}) = -H_{y_1}^2 + 2H_{y_1y_2} - 4H_{y_1y_2y_3} + 2H_{y_2y_3} + H_{y_3}^2, \\
\mathbb{V} & \text{ar}(K_{4,1}) = H_{y_1}^2 + 6H_{y_1y_2} - 14H_{y_1y_2y_3} + 6H_{y_1y_2y_3} + 2H_{y_2y_3}^2 + 4H_{y_3} - 2H_{y_1y_2y_3} - 2H_{y_2y_3}, \\
\text{So, } \mathbb{V} & \text{ar}(K_{n,3}) = \left( \frac{1}{2} + \kappa_3 \right) \ln^2(n) + \left( 10\xi(3) + 2\xi(2)\gamma + \gamma \right) \ln(n) + \frac{1}{2}\gamma^2 \\
& \quad - 10\xi(3)\gamma + \frac{83}{10} \xi(2)^2 + \xi(2)\gamma^2 + \frac{1}{2} \xi(2) + o(1), \\
\mathbb{V} & \text{ar}(K_{n,4}) = \left( \frac{1}{3!} + \kappa_4 \right) \ln^3(n) + \left( -\frac{53}{5} \xi(2)^2 + 6\xi(3)\gamma + \frac{1}{2} \gamma \right) \ln^2(n) \\
& \quad + \left( 97\xi(5) - \frac{106}{5} \xi(2)^2 \gamma + 16\xi(2)\xi(3) + 6\xi(3)\gamma^2 + \frac{1}{2} \xi(2) + \frac{1}{2} \gamma^2 \right) \ln(n) + \frac{1}{3} \xi(3) - \frac{53}{5} \xi(2)^2 \gamma^2 - \frac{3719}{70} \xi(2)^3 + \frac{1}{6} \gamma^3 + \frac{1}{2} \xi(2) \gamma \\
& \quad + 16\xi(2)\xi(3)\gamma - 3\xi(3)^2 + 2\xi(3)^3 + 97\xi(5)\gamma + o(1), \\
\mathbb{V} & \text{ar}(K_{n,5}) = \left( \frac{1}{4!} + \kappa_5 \right) \ln^4(n) + \left( -\frac{98}{3} \xi(5) + \frac{33}{10} \xi(2)^2 \gamma - \frac{13}{3} \xi(2) \xi(3) \right) \ln^3(n) \\
& \quad + \left( \frac{10123}{140} \xi(2)^3 + \frac{47}{2} \xi(3)^2 + \frac{99}{20} \xi(2)^2 \gamma^2 + \frac{1}{4} \gamma^2 + \frac{1}{4} \xi(2) \right) \ln^2(n) + \left( -\frac{1}{6} \gamma^3 + \frac{33}{10} \xi(2)^2 \gamma^3 \\
& \quad + \frac{1}{2} \xi(2) \gamma - 950\xi(7) - 13\xi(2)\xi(3)\gamma^2 + 47\xi(3)^2 \gamma + \frac{1}{3} \xi(3) \\
& \quad - \frac{317}{5} \xi(3)^2 \gamma^2 + \frac{10123}{70} \xi(2)^3 \gamma - 98\xi(5)\gamma^2 - 222\xi(2) \xi(5) \right) \ln(n) \\
& \quad - \frac{13}{3} \xi(2)\xi(3)\gamma^3 + \frac{47}{2} \xi(3)^2 \gamma^2 - \frac{317}{5} \xi(3) \xi(2)^2 \gamma - \frac{98}{3} \xi(5) \gamma^3 \\
& \quad + \left( \frac{33}{40} \xi(2)^2 \gamma^4 + \frac{32}{3} \xi(3)^2 \xi(5) \right) + \left( \frac{10123}{140} \xi(2)^3 \gamma^2 - 222\xi(2) \xi(5) \right) \gamma \\
& \quad + \frac{1}{24} \gamma^4 - 950\xi(7) \gamma + 50\xi(6,2) + \frac{1}{4} \xi(2)^2 \gamma^2 + \frac{1}{3} \xi(3) \gamma \\
& \quad + \frac{95}{6} \xi(2)^2 + \frac{13473}{350} \xi(2)^4 + o(1). 
\end{align*} \]

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References


