

Variance for the Number of Maxima in Hypercubes and Generalized Euler's γ constants

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ABSTRACT. In this work, we obtain some results *à l'Abel* dealing with noncommutative generating series of polylogarithms and multiple harmonic sums, by using techniques *la Hopf*. In particular, this enables to explicit generalized Euler constants associated to divergent polyzêtas. As application, we present a combinatorial approach of the variance for the number of maxima in hypercubes. This leads to an explicit expression, in terms of convergent polyzêtas, of the dominant term in the asymptotic expansion of this variance. Moreover, we get an algorithm to compute this expansion, and show that all coefficients occurring belong to the \mathbb{Q} -algebra generated convergent polyzêtas and by Euler's γ constant.

Dans ce travail, nous obtenons des résultats *à l'Abel* concernant les séries génératrices non commutatives de polylogarithmes et sommes harmoniques multiples, en utilisant des techniques *à la Hopf*. En particulier, ceci nous permet d'expliciter les constantes d'Euler généralisées associées à des polyzêtas divergents. Comme application, nous présentons une approche combinatoire de la variance du nombre de maxima dans un hypercube. Celle-ci amène à une expression explicite, en termes de polyzêtas, du terme dominant du développement asymptotique de cette variance. De plus, nous obtenons un algorithme pour calculer ce développement, et montrons que tous les coefficients intervenant appartiennent à l'algèbre \mathbb{Q} -engendré par les polyzêtas convergents et par la constante d'Euler γ .

1. Introduction

Let $Q = \{q_1, \dots, q_n\}$ be a set of independent and identically distributed random vectors in \mathbb{R}^d . A point $q_i = (q_{i_1}, \dots, q_{i_d})$ is said to be dominated by $q_j = (q_{j_1}, \dots, q_{j_d})$ if $q_{i_k} < q_{j_k}$ for all $k \in [1, \dots, d]$ 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, in [2], Bai et al. proposed a method for computing an asymptotic expansion of the variance and the study of $\text{Var}(K_{n,d})$ 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 [16] :

$$(1) \quad \mathbb{E}(K_{n,d}^2) = \mu_{n,d} + \sum_{1 \leq t \leq d-1} \binom{d}{t} \sum_{l=1}^{n-1} \frac{1}{l} \sum_{(*)} \frac{1}{i_1 \dots i_{d-2} j_1 \dots j_{d-1}},$$

where the sum $(*)$ is taken over indices verifying $1 \leq i_1 \dots \leq i_{t-1} \leq l, 1 \leq i_t \leq \dots \leq i_{d-2} \leq l$ and $l+1 \leq j_1 \leq \dots \leq j_{d-1} \leq n$. In Formula (1), $\mu_{n,d}$ stands for the mean of $K_{n,d}$, first calculated by Barndorff-Nielsen and Sobel [3]

$$(2) \quad \mu_{n,d} = \mathbb{E}(K_{n,d}) = \sum_{1 \leq i_1 \leq \dots \leq i_{d-1} \leq n} \frac{1}{i_1 \dots i_{d-1}}.$$

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After having given an alternative derivation for this formula, Bai et al. deduce, by analytic and combinatoric considerations, as the main result of [1], the following equivalent

$$(3) \quad \text{Var}(K_{n,d}) \sim \left(\frac{1}{(d-1)!} + \kappa_d \right) \ln^{d-1}(n),$$

$$(4) \quad \text{with } \kappa_d = \sum_{t=1}^{d-2} \frac{1}{t!(d-1-t)!} \sum_{l \geq 1} \frac{1}{l^2} \sum_{i_1 \dots i_{t-1} j_1 \dots j_{d-2-t}}^{(**)} \frac{1}{n^{s_1} \dots n^{s_r}}$$

the sum $(**)$ being calculated over all indices verifying $1 \leq i_1 \leq \dots \leq i_{t-1} \leq l$ and $1 \leq j_1 \leq \dots \leq j_{d-2-t} \leq l$.

These two formulas (1) and (4) give rise to harmonic sums $A_{\mathbf{s}}(N)$, closely related to $H_{\mathbf{s}}(N)$ and defined for a composition $\mathbf{s} = (s_1, \dots, s_r)$ by

$$(5) \quad A_{\mathbf{s}}(N) = \sum_{N \geq n_1 \geq \dots \geq n_r > 0} \frac{1}{n_1^{s_1} \dots n_r^{s_r}} \quad \text{and} \quad H_{\mathbf{s}}(N) = \sum_{N \geq n_1 > \dots > n_r > 0} \frac{1}{n_1^{s_1} \dots n_r^{s_r}}.$$

There exist explicit relations between the $A_{\mathbf{s}}(N)$ and $H_{\mathbf{s}}(N)$. Precisely, let $\text{Comp}(n)$ be the *set of compositions* of n . If $I = (i_1, \dots, i_r)$ (resp. $J = (j_1, \dots, j_p)$) is a composition of n (resp. of r) then $J \circ I = (i_1 + \dots + i_{j_1}, i_{j_1+1} + \dots + i_{j_1+j_2}, \dots, i_{k-j_p+1} + \dots + i_k)$ is a composition of n . By Möbius inversion, one has [15]

$$(6) \quad A_{\mathbf{s}}(N) = \sum_{J \in \text{Comp}(r)} H_{J \circ \mathbf{s}}(N) \quad \text{and} \quad H_{\mathbf{s}}(N) = \sum_{J \in \text{Comp}(r)} (-1)^{l(J)-r} A_{J \circ \mathbf{s}}(N),$$

where $l(J)$ is the number of parts of J . Therefore, from the algebraic and combinatoric properties of $A_{\mathbf{s}}$ (or equivalently, of $H_{\mathbf{s}}$) and their limit $\underline{\zeta}(\mathbf{s})$ (or equivalently, $\zeta(\mathbf{s})$)

$$(7) \quad \underline{\zeta}(\mathbf{s}) = \sum_{n_1 \geq \dots \geq n_r > 0} \frac{1}{n_1^{s_1} \dots n_r^{s_r}} \quad \text{and} \quad \zeta(\mathbf{s}) = \sum_{n_1 > \dots > n_r > 0} \frac{1}{n_1^{s_1} \dots n_r^{s_r}}, \quad \text{for } s_1 > 1,$$

we will deduce two main results, first the explicit value of κ_d in terms of convergent $\underline{\zeta}(\mathbf{s})$ of weight $d-1$ (c.f. Theorem 8)

$$(8) \quad \kappa_d = \frac{1}{(d-1)!} \sum_{\substack{(2, s_2, \dots, s_r) \\ s_i \in \{1, 2\}, 2 \leq i \leq r \leq d-2}} (-1)^{|\mathbf{s}|_2+1} \binom{2(d-1-|\mathbf{s}|_2)}{d-1-|\mathbf{s}|_2} \underline{\zeta}(\mathbf{s}),$$

where $\mathbf{s} = (2, s_2, \dots, s_r)$ and $|\mathbf{s}|_2$ stands for the number of occurrences of 2 in \mathbf{s} (for example $|(2, 1, 2, 2, 1)|_2 = 3$). We then give an algorithm to compute the asymptotic expansion of $\text{Var}(K_{n,d})$ via the asymptotic expansion of $H_{\mathbf{s}}(N)$ (c.f. Theorem 9) :

$$(9) \quad \text{Var}(K_{n,d}) = \sum_{i=0}^{2d-2} \alpha_i \ln^i(n) + \sum_{j=1}^M \frac{1}{n^j} \sum_{k=0}^{2d-2} \beta_{j,k} \ln^k(n) + o\left(\frac{1}{n^M}\right),$$

where $\alpha_i, \beta_{j,k}$ belong the \mathbb{Q} -algebra generated by Euler's γ constant and by convergent polyzêtas.

For an analytic function f verifying $\int_1^\infty |f^{(2k)}(t)| dt < \infty, k \in \mathbb{N}_+$, the Euler-Mac Laurin summation formula asserts that there exist a constant C_f , called Euler-MacLaurin constant associated to $\sum_{n \geq 1} f_n$, such that [8]

$$(10) \quad \sum_{n=1}^N f(n) = C_f + \int_1^N f(x) dx + \frac{f(N)}{2} + \sum_{j=1}^k \frac{B_{2j}}{(2j)!} f^{(2j-1)}(N) + O\left(\int_N^\infty |f^{(2k)}(t)| dt\right),$$

where the $\{B_k\}_{k \geq 0}$ are the Bernoulli numbers. One of the most common application of this formula consists in taking $f(x) = x^{-r}, r \in \mathbb{N}_+$, which leads to

$$(11) \quad \sum_{n=1}^N \frac{1}{n} = \log N + \gamma - \sum_{j=1}^{k-1} \frac{B_j}{j} \frac{1}{N^j} + O\left(\frac{1}{N^k}\right),$$

$$(12) \quad \sum_{n=1}^N \frac{1}{n^r} = \zeta(r) - \sum_{j=r-1}^{k-1} \frac{B_{j-r+1}}{j} \binom{j}{r-1} \frac{1}{N^j} + O\left(\frac{1}{N^k}\right),$$

leading to the asymptotic expansion of the harmonic sum $H_r(N) = \sum_{n=1}^N n^{-r}$. We now are interested on *multiple* harmonic sums $H_{\mathbf{s}}$ and their derivated $A_{\mathbf{s}}$. We have already proposed in [5] a recursive method, widely based on the Euler-MacLaurin formula and based on the algebraic structure of $H_{\mathbf{s}}$, to get this asymptotic expansion. An other algorithm is also proposed in [4] and based on the asymptotic behaviour at the singularity $z = 1$ of the following ordinary generating series of the multiple harmonic sums :

$$(13) \quad P_{\mathbf{s}}(z) = \sum_{n \geq 0} H_{\mathbf{s}}(n) z^n = \frac{\text{Li}_{\mathbf{s}}(z)}{1-z}, \quad \text{where} \quad \text{Li}_{\mathbf{s}}(z) = \sum_{n_1 > \dots > n_r > 0} \frac{z^{n_1}}{n_1^{s_1} \dots n_r^{s_r}}.$$

In this paper, in continuation of [4, 5], we establish a theorem *à l'Abel* (c.f. Theorem 4) concerning the noncommutative generating series of multiple sums and of polylogarithms by use of techniques *à la Hopf*. In particular, this enables to obtain, once again, the asymptotic expansion of multiple harmonic sums (c.f. Corollary 2) and to explicit the *generalized* Euler's γ constants associated to divergent polyzêtas (c.f. Theorem 6) as the N -free term in their asymptotic expansion. As applications of these expansions and these constants, we evaluate the variance for the number of maxima in hypercubes.

2. The constant problem, algorithmic determination

2.1. Algebraic combinatoric aspects. Let $\{t_i\}_{i \in \mathbb{N}_+}$ be an infinite set of variables. The elementary symmetric functions λ_k and the sums of powers ψ_k are defined by

$$(14) \quad \lambda_k(\underline{t}) = \sum_{n_1 > \dots > n_k > 0} t_{n_1} \dots t_{n_k} \quad \text{and} \quad \psi_k(\underline{t}) = \sum_{n > 0} t_n^k.$$

They are respectively coefficients of the following generating functions

$$(15) \quad \lambda(\underline{t}|z) = \sum_{k > 0} \lambda_k(\underline{t}) z^k = \prod_{i \geq 1} (1 + t_i z) \quad \text{and} \quad \psi(\underline{t}|z) = \sum_{k > 0} \psi_k(\underline{t}) z^{k-1} = \sum_{i \geq 1} \frac{t_i}{1 - t_i z}.$$

These generating functions satisfy a Newton identity

$$(16) \quad d/dz \log \lambda(\underline{t}|z) = \psi(\underline{t} - z).$$

The fundamental theorem from symmetric functions theory asserts that the $\{\lambda_k\}_{k \geq 0}$ are linearly independent, and remarkable identities give (putting $\lambda_0 = 1$) :

$$(17) \quad \lambda_k = \frac{(-1)^k}{k!} \sum_{\substack{s_1, \dots, s_k > 0 \\ s_1 + \dots + s_k = k}} \binom{k}{s_1, \dots, s_k} \left(-\frac{\psi_1}{1}\right)^{s_1} \dots \left(-\frac{\psi_k}{k}\right)^{s_k}$$

To the composition $\mathbf{s} = (s_1, \dots, s_r)$, we associate the word $w = y_{s_1} \dots y_{s_r}$ defined over the alphabet $Y = \{y_i, i \in \mathbb{N}_+\}$. Its *length* is r , also denoted by $|w|$ and its *weight* is $\sum_{i=1}^r s_i$. The set of words over Y is denoted by Y^* . The empty word is usually denoted by ϵ ($|\epsilon| = 0$).

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

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

$$(18) \quad F_w(\underline{t}) = \sum_{n_1 > \dots > n_r > 0} t_{n_1}^{s_1} \dots t_{n_r}^{s_r} \quad \text{and} \quad G_w(\underline{t}) = \sum_{n_1 \geq \dots \geq n_r > 0} t_{n_1}^{s_1} \dots t_{n_r}^{s_r}.$$

In particular, $F_{y_1^k} = \lambda_k$ and $F_{y_k} = G_{y_k} = \psi_k$. As a consequence, the functions $\{F_{y_1^k}\}_{k \geq 0}$ are linearly independent and integrating differential equation (16) shows that functions $F_{y_1^k}$ and F_{y_k} are linked by the formula

$$(19) \quad \sum_{k \geq 0} F_{y_1^k} z^k = \exp \left[- \sum_{k \geq 1} F_{y_k} \frac{(-z)^k}{k} \right] \quad \left(\text{or} \quad \sum_{k \geq 0} G_{y_1^k} z^k = \exp \left[\sum_{k \geq 1} G_{y_k} \frac{z^k}{k} \right] \right).$$

By linearity, the definitions of F_w and G_w are extended to polynomials on $\mathbb{Q}(Y)$.

DEFINITION 1. Let $y_i, y_j \in Y$ and $u, v \in Y^*$. The shuffle product of $u = y_i u'$ and $v = y_j v'$ is the polynomial recursively defined by

$$\epsilon \sqcup u = u \sqcup \epsilon = u \quad \text{and} \quad u \sqcup v = y_i(u' \sqcup v) + y_j(u \sqcup v').$$

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In the same way, the minus-stuffle of u and v is the polynomial recursively defined by

$$\epsilon \sqcup u = u \sqcup \epsilon = u \quad \text{and} \quad u \sqcup v = y_i(u' \sqcup v) + y_j(u \sqcup v') - y_{i+j}(u' \sqcup v').$$

EXAMPLE 1. $y_1 \sqcup y_2 = y_1 y_2 + y_2 y_1$, $y_1 \sqcup y_2 = y_1 y_2 + y_2 y_1 + y_3$ and $y_1 \sqcup y_2 = y_1 y_2 + y_2 y_1 - y_3$.

PROPOSITION 1. The operation \sqcup is commutative and associative.

PROOF. To show that $w_1 \sqcup w_2 = w_2 \sqcup w_1$, we proceed by induction on $|w_1| + |w_2|$. The induction hypothesis is proved by (20) when $|w_1| + |w_2| \leq 1$ and the induction step is proved by (20).

In the same way, we show that $w_1 \sqcup (w_2 \sqcup w_3) = (w_1 \sqcup w_2) \sqcup w_3$ by induction on $|w_1| + |w_2| + |w_3|$. Once again, the hypothesis is proved by (20) when $|w_1| + |w_2| + |w_3| \leq 1$. Then, the calculation of $y_i w_1 \sqcup (y_j w_2 \sqcup y_k w_3)$ gives

$$\begin{aligned} & y_i(w_1 \sqcup y_j(w_2 \sqcup y_k w_3)) + y_j(y_i w_1 \sqcup (w_2 \sqcup y_k w_3)) - y_{i+j}(w_1 \sqcup (w_2 \sqcup y_k w_3)) \\ & + y_i(w_1 \sqcup y_k(y_j w_2 \sqcup w_3)) + y_k(y_i w_1 \sqcup (y_j w_2 \sqcup w_3)) - y_{i+k}(w_1 \sqcup (y_j w_2 \sqcup w_3)) \\ & - y_i(w_1 \sqcup y_{j+k}(w_2 \sqcup w_3)) - y_{j+k}(y_i w_1 \sqcup (w_2 \sqcup w_3)) + y_{i+j+k}(w_1 \sqcup (w_2 \sqcup w_3)) \end{aligned}$$

On the other hand, the calculation of $(y_i w_1 \sqcup y_j w_2) \sqcup y_k w_3$ gives

$$\begin{aligned} & y_i((w_1 \sqcup y_j w_2) \sqcup y_k w_3) + y_k(y_i(w_1 \sqcup y_j w_2) \sqcup w_3) - y_{i+k}((w_1 \sqcup y_j w_2) \sqcup w_3) \\ & + y_j((y_i w_1 \sqcup w_2) \sqcup y_k w_3) + y_k(y_j(y_i w_1 \sqcup w_2) \sqcup w_3) - y_{j+k}((y_i w_1 \sqcup w_2) \sqcup w_3) \\ & - y_{i+j}((w_1 \sqcup w_2) \sqcup y_k w_3) - y_k(y_{i+j}(w_1 \sqcup w_2) \sqcup w_3) + y_{i+j+k}((w_1 \sqcup w_2) \sqcup w_3) \end{aligned}$$

Subtracting both expressions and using the induction hypothesis lead us to :

$$\begin{aligned} & y_i(w_1 \sqcup y_j(w_2 \sqcup y_k w_3)) + y_i(w_1 \sqcup y_k(y_j w_2 \sqcup w_3)) + y_k(y_i w_1 \sqcup (y_j w_2 \sqcup w_3)) \\ & - y_i(w_1 \sqcup y_{j+k}(w_2 \sqcup w_3)) - y_i((w_1 \sqcup y_j w_2) \sqcup y_k w_3) - y_k(y_i(w_1 \sqcup y_j w_2) \sqcup w_3) \\ & - y_k(y_j(y_i w_1 \sqcup w_2) \sqcup w_3) + y_k(y_{i+j}(w_1 \sqcup w_2) \sqcup w_3), \end{aligned}$$

which can be further simplified using (20) in

$$\begin{aligned} & y_i(w_1 \sqcup (y_j w_2 \sqcup y_k w_3)) + y_k(y_i w_1 \sqcup (y_j w_2 \sqcup w_3)) \\ & - y_i((w_1 \sqcup y_j w_2) \sqcup y_k w_3) - y_k((y_i w_1 \sqcup y_j w_2) \sqcup w_3), \end{aligned}$$

expression reduced to zero by the induction hypothesis. \square

If u (resp. v) is a word in Y^* , of length r and of weight p (resp. of length s and of weight q), $F_{u \sqcup v}$ and $G_{u \sqcup v}$ are quasi-symmetric functions of depth $r + s$ and of weight $p + q$, and one has

$$F_{u \sqcup v} = F_u F_v \quad \text{and} \quad G_{u \sqcup v} = G_u G_v.$$

The remarkable identity (17) can be then seen as

$$(20) \quad y_1^k = \frac{(-1)^k}{k!} \sum_{\substack{s_1, \dots, s_k > 0 \\ s_1 + \dots + k s_k = k}} \binom{k}{s_1, \dots, s_k} \frac{(-y_1)^{\sqcup s_1}}{1^{s_1}} \sqcup \dots \sqcup \frac{(-y_k)^{\sqcup s_k}}{k^{s_k}}$$

$$(21) \quad = \frac{1}{k!} \sum_{\substack{s_1, \dots, s_k > 0 \\ s_1 + \dots + k s_k = k}} \binom{k}{s_1, \dots, s_k} \frac{y_1^{\sqcup s_1}}{1^{s_1}} \sqcup \dots \sqcup \frac{y_k^{\sqcup s_k}}{k^{s_k}}$$

$$(22) \quad = \frac{y_1^{\sqcup k}}{k!}.$$

DEFINITION 2. For any $w \in Y^*$, let us define the maps H_w and A_w from \mathbb{N}_+ to \mathbb{Q} as follows

$$H_w(N) = \begin{cases} 1 & \text{if } w = \epsilon, \\ \sum_{N \geq n_1 > \dots > n_r > 0} \frac{1}{n_1^{s_1} \dots n_r^{s_r}} & \text{if } w = y_{s_1} \dots y_{s_r}. \end{cases}$$

$$A_w(N) = \begin{cases} 1 & \text{if } w = \epsilon, \\ \sum_{N \geq n_1 \geq \dots \geq n_r > 0} \frac{1}{n_1^{s_1} \dots n_r^{s_r}} & \text{if } w = y_{s_1} \dots y_{s_r}. \end{cases}$$

We put also $H_w(0) = A_w(0) = 0$.

By linearity, the definitions of H_w and A_w are extended to polynomials on $\mathbb{Q}\langle Y \rangle$.

For $N \geq 1$ and $w \in Y^*$, any $H_w(N)$ (resp. $A_w(N)$) can be obtained by specializing variables $\{t_i\}_{N \geq i \geq 1}$ at $t_i = 1/i$ and, for $i > N$, $t_i = 0$ in the quasi-symmetric function F_w (resp. G_w) [14]. Therefore,

PROPOSITION 2 ([14]). For $u, v \in Y^*$, $H_{u \sqcup v} = H_u H_v$ and $A_{u \sqcup v} = A_u A_v$.

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

$$(23) \quad H_w(N) = \sum_{l=r}^N \frac{H_{w'}(l-1)}{l^s} \quad \text{and} \quad A_w(N) = \sum_{l=1}^N \frac{A_{w'}(l)}{l^s}.$$

In consequence,

THEOREM 1. For any $w = y_s w' \in Y^*$, $H_w(N)$ and $A_w(N)$ 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 $\lim_{N \rightarrow +\infty} A_w(N)$ are denoted respectively by $\zeta(w)$ and by $\underline{\zeta}(w)$. In this case, w is said to be convergent (otherwise, it is said to be divergent).

PROOF. The immediate minorization $H_w(N) \geq H_{w'}(r-1) \sum_{l=r}^N l^{-s}$ shows the divergence of $H_w(N)$ when $s = 1$, i.e. $w \in y_1 Y^*$. To show the convergence when $w \in Y^* \setminus y_1 Y^*$ by dominating correctly $H_{w'}(l)$, we need the following result : for any $w \in Y^*$, there exist a constant K and in integer α such that, for any $l > 1$, $H_w(l) \leq K \ln^\alpha l$. This result can be shown by Formula (23), and by induction on the length of w . Using a last time Formula (23), the convergence of $H_w(N)$ comes directly.

The same proof can be done for $A_w(N)$. From Formula (6), the $\underline{\zeta}(w)$ can be expressed as linear combination of convergent polyzêtas (and *vice versa*). \square

Let us consider the following two differential forms $\omega_0(z) = dz/z$ and $\omega_1(z) = dz/(1-z)$. The polylogarithm $\text{Li}_{\mathbf{s}}(z)$ is defined for a composition $\mathbf{s} = (s_1, \dots, s_r)$ and for a complex z such that $|z| < 1$ by Formula (13) corresponds to the iterated integral over ω_0, ω_1 and along the integration path $0 \rightsquigarrow z$,

$$(24) \quad \text{Li}_{\mathbf{s}} = \int_{0 \rightsquigarrow z} \omega_0^{s_1-1} \omega_1 \dots \omega_0^{s_r-1} \omega_1.$$

Let $X = \{x_0, x_1\}$. We shall also identify any composition $\mathbf{s} = (s_1, \dots, s_r)$ with its encoding word $w = x_0^{s_1-1} x_1 \dots x_0^{s_r-1} x_1$ over $X^* x_1$. We obtain so a concatenation isomorphism from the \mathbb{Q} -algebra of compositions into the subalgebra $\mathbb{Q}\langle X \rangle x_1 \subset \mathbb{Q}\langle X \rangle$. In that way, the polylogarithm $\text{Li}_{\mathbf{s}}(z)$ defined by the formula (13) can be also indexed by $w \in X^* x_1$. To extend the definition of polylogarithms over X^* , we put $\text{Li}_{x_0}(z) = \log(z)$. By linearity, the definition of Li_w is extended to polynomials on $\mathbb{Q}\langle X \rangle$.

Introducing the analogous shuffle product over X^* as in the definition 1, we get

THEOREM 2 ([10]). The map $\text{Li} : w \mapsto \text{Li}_w$ is an isomorphism from $(\mathbb{C}\langle X \rangle, \sqcup)$ to $(\mathbb{C}\{\text{Li}_w\}_{w \in X^*}, \cdot)$.

The polyzêtas are well defined only for the convergent words in $\{\epsilon\} \cup x_0 X^* x_1$, and linearly extended to $C_1 = \mathbb{Q} \oplus x_0 \mathbb{Q}\langle X \rangle x_1$. Let $C_2 = \mathbb{Q} \oplus (Y \setminus y_1 \mathbb{Q}\langle Y \rangle) \simeq C_1$. By the Radford theorem [17], one has

$$(25) \quad (\mathbb{Q}\langle X \rangle, \sqcup) \simeq \mathbb{Q}[\mathcal{Lyn}X] = C_1[x_0, x_1],$$

$$(26) \quad (\mathbb{Q}\langle Y \rangle, \sqcup) \simeq (\mathbb{Q}\langle Y \rangle, \sqcup) \simeq \mathbb{Q}[\mathcal{Lyn}Y] = C_2[y_1],$$

where $\mathcal{Lyn}X$ and $\mathcal{Lyn}Y$ are the sets of Lyndon words over X and Y respectively.

By Theorem 2, we have

PROPOSITION 3 ([9]). For $u, v \in X^*$, $\text{Li}_{u \sqcup v} = \text{Li}_u \text{Li}_v$. Thus, for $u, v \in x_0 X^* x_1$, $\zeta(u \sqcup v) = \zeta(u)\zeta(v)$.

By Proposition 2, one has

PROPOSITION 4 ([14]). For $u, v \in Y^* \setminus y_1 Y^*$, $\zeta(u \sqcup v) = \zeta(u) \zeta(v)$ and $\underline{\zeta}(u \sqcup v) = \underline{\zeta}(u) \underline{\zeta}(v)$.

Let \mathcal{Z} be the \mathbb{Q} -algebra generated by convergent polyzêtas $\{\zeta(w)\}_{w \in x_0 X^* x_1}$. This algebra is equipped two products (c.f. propositions 3 and 4) and is already studied in [9] and it is conjectured to be free algebra. In the same way, let \mathcal{Z}' be the $\mathbb{Q}[\gamma]$ -algebra generated by \mathcal{Z} . It is also conjectured that γ is transcendental over \mathcal{Z} [9].

PROPOSITION 5 ([13]). For $w \in X^*$, let $P_w(z) = (1-z)^{-1} \text{Li}_w(z)$. Thus for $u, v \in Y^*$, $P_{u \sqcup v} = P_u \odot P_v$, where \odot denotes the Hadamard product.

As consequences of Theorem 2, we also have

THEOREM 3 ([13]). The map $P : u \mapsto P_u$ is an isomorphism from polynomial algebra $(\mathbb{C}\langle Y \rangle, \sqcup)$ over the Hadamard algebra $(\mathbb{C}\{P_w\}_{w \in Y^*}, \odot)$. Moreover, the map $H : u \mapsto H_u = \{H_u(N)\}_{N \geq 0}$ (resp. $A : u \mapsto A_u = \{A_u(N)\}_{N \geq 0}$) is an isomorphism from $(\mathbb{C}\langle Y \rangle, \sqcup)$ (resp. $(\mathbb{C}\langle Y \rangle, \sqcup)$) over the algebra $(\mathbb{C}\{H_w\}_{w \in Y^*}, \cdot)$ (resp. $(\mathbb{C}\{A_w\}_{w \in Y^*}, \cdot)$).

3. Explicit determination of Euler's γ constants

3.1. Some remarks on asymptotic expansion of multiple harmonic sums. The determination of the asymptotic expansion of $H_w(N)$ for convergent words lies on the formula (23) and by induction on the length of w . Details are given in [5].

EXAMPLE 2.

$$H_{4,2}(N) = \zeta(4, 2) - \sum_{i=N+1}^{\infty} \frac{H_2(i-1)}{i^4},$$

But $H_2(i-1) = \zeta(2) - \frac{1}{i} - \frac{1}{2} \frac{1}{i^2} + O\left(\frac{1}{i^3}\right)$ so

$$H_{4,2}(N) = \zeta(4, 2) - \zeta(2) \sum_{i=N+1}^{\infty} \frac{1}{i^4} + \sum_{i=N+1}^{\infty} \frac{1}{i^5} + \frac{1}{2} \sum_{i=N+1}^{\infty} \frac{1}{i^6} + \sum_{i=N+1}^{\infty} O\left(\frac{1}{i^7}\right)$$

Finally, using again Euler-MacLaurin formula, for (simple) harmonic sums, we get

$$H_{4,2}(N) = \zeta(4, 2) - \frac{1}{3} \frac{\zeta(2)}{N^3} + \frac{\frac{1}{2} \zeta(2) + \frac{1}{4}}{N^4} - \frac{\frac{1}{3} \zeta(2) + \frac{2}{5}}{N^5} + O\left(\frac{1}{N^6}\right)$$

Unfortunately, it is easy to see that this consideration does not enable to get the asymptotic expansion for a divergent word. More precisely, you can get the right divergent terms in the scale of $\{\ln^\alpha(N), \alpha \in \mathbb{N}_+\}$ and the right infinitesimal terms in the scale $\{\ln^\alpha(N)N^{-\beta}, \alpha \in \mathbb{N}, \beta \in \mathbb{N}_+\}$, but you can not reach the N -free term. By (26), for any $w \in Y^*$, there exists a polynomial q_w on γ with coefficients which are combination on $\zeta(v), v \in C_2$, such that $H_w(N) \underset{N \rightarrow \infty}{\sim} q_w(\gamma)$ [13].

If we now consider the derivation D verifying $Dw = 0$ for a convergent word w and $D(y_1 w) = w$, for any word w , then for any $w \in Y^*$, we get the Taylor expansion of w as follows

$$(27) \quad w = \sum_{k=0}^{|w|} c_k(w) \sqcup \frac{y_1^{\sqcup k}}{k!}, \quad \text{with} \quad c_k(w) = \sum_{i=0}^{|w|-k} \frac{(-y_1)^i D^i}{i!} D^k(w),$$

where all products and powers are carried out with the stuffle product \sqcup , and all $c_k(w)$ being convergent polynomials.

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

$$\begin{aligned} c_2(w) &= \frac{y_1^{\sqcup 0}}{0!} \sqcup y_2 = y_2 \\ c_1(w) &= y_1 y_2 - y_1 \sqcup y_2 = -y_2 y_1 - y_3 \\ c_0(w) &= y_1^2 y_2 - y_1 \sqcup y_1 y_2 + \frac{y_1^{\sqcup 2}}{2!} \sqcup y_2 = y_2 y_1^2 + y_3 y_1 + \frac{1}{2} y_4 \end{aligned}$$

Considering this Taylor expansion, the recursive algorithm to get the expansion of $H_w(N)$ can be summed in these two points :

- If $w = y_1 w'$ then compute Taylor expansion of w . Indeed, thanks to Formula (27),

$$H_w = \sum_{k=0}^{|w|} H_{c_k(w)} \frac{H_1^k}{k!},$$

so we just need the expansion of $H_{c_k(w)}(N)$

- If $w = y_s w'$ then compute the asymptotic expansion of $H_{w'}(n-1)$ and then use Euler-MacLaurin summation formula.

PROPOSITION 6 ([4, 5]). *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 $w \in Y^*$,*

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

With the previous notations, we can conclude that the N -free term is given by

$$\sum_{k=0}^{|w|} \zeta(c_k(w)) \frac{\gamma^k}{k!}.$$

EXAMPLE 4. *For $w = y_1^2 y_2$, the N -free term occuring in the asymptotic expansion of $H_{y_1^2 y_2}(N)$ is*

$$\begin{aligned} \sum_{k=0}^2 \zeta(c_k(w)) \frac{\gamma^k}{k!} &= \zeta(2) \frac{\gamma^2}{2!} + (-\zeta(2, 1) - \zeta(3))\gamma + (\zeta(2, 1, 1) + \zeta(3, 1) + \frac{1}{2}\zeta(4)) \\ &= \frac{\zeta(2)}{2}\gamma^2 - 2\zeta(3)\gamma + \frac{7}{10}\zeta(2)^2. \end{aligned}$$

In the next section, we give an explicite determination of such polynomial.

3.2. Results à l'Abel for noncommutative generating series. Let $\mathcal{C} = \mathbb{C}[z, \frac{1}{z}, \frac{1}{1-z}]$. The noncommutative generating series of polylogarithms, $L = \sum_{w \in X^*} \text{Li}_w w$, satisfies Drinfel'd differential equation [6, 7]

$$(28) \quad dL = (x_0 \omega_0 + x_1 \omega_1)L \quad \text{with the condition } L(\varepsilon) = e^{x_0 \log \varepsilon} + O(\sqrt{\varepsilon}) \quad \text{for } \varepsilon \rightarrow 0^+.$$

This enables to prove that L is the exponential of a Lie series [10]. From the factorization of monoid by Lyndon words $l \in \mathcal{Lyn}X$, we get the factorization of the series L [10] :

$$(29) \quad L(z) = e^{x_1 \log \frac{1}{1-z}} \left[\prod_{l \in \mathcal{Lyn}X \setminus \{x_0, x_1\}} e^{\text{Li}_{S_l}(z)[l]} \right] e^{x_0 \log z}.$$

For all $l \in \mathcal{Lyn}X \setminus \{x_0, x_1\}$, we have $S_l \in x_0 X^* x_1$. So, let us put [10]

$$(30) \quad L_{\text{reg}} = \prod_{l \in \mathcal{Lyn}X \setminus \{x_0, x_1\}} e^{\text{Li}_{S_l}[l]} \quad \text{and} \quad Z = L_{\text{reg}}(1).$$

Let σ be the monoid endomorphism verifying $\sigma(x_0) = -x_1, \sigma(x_1) = -x_0$, we also get [11]

$$(31) \quad L(z) = \sigma[L(1-z)]Z = e^{x_0 \log z} \sigma[L_{\text{reg}}(1-z)] e^{-x_1 \log(1-z)} Z.$$

EXAMPLE 5. *This gives an alternative derivation of the asymptotic expansion of any $H_w(N)$. Indeed, let us see the example of $w = y_2 y_1$,*

$$\begin{aligned} \text{Li}_{2,1}(z) &= -\text{Li}_3(1-z) + \log(1-z) \text{Li}_2(1-z) - \frac{1}{2} \log^2(1-z) \text{Li}_1(1-z) - \zeta(2) \text{Li}_1(1-z) + \zeta(3) \\ &= -(1-z) + (1-z) \log(1-z) - \frac{1}{2} (1-z) \log^2(1-z) - \zeta(2)(1-z) + \zeta(3) + O(|1-z|). \end{aligned}$$

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

and so, since $[z^N] \log^2(1-z) = [z^N] 2!(1-z)P_{1,1}(z) = 2(H_{1,1}(N) - H_{1,1}(N-1))$, and using Identity 20, we get

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

In consequence, from (29) and (31), we get respectively

$$(32) \quad L(z) \underset{z \rightarrow 0}{\sim} \exp(x_0 \log z) \quad \text{and} \quad L(z) \underset{z \rightarrow 1}{\sim} \exp\left(x_1 \log \frac{1}{1-z}\right) Z,$$

where the equivalency shall be understood as an equivalence word by word. Let π_Y a projector from $\mathbb{C}\langle\langle X \rangle\rangle$ to $\mathbb{C}\langle\langle Y \rangle\rangle$ erasing the monomials ending with the letter x_0 . Then

$$(33) \quad \Lambda(z) = \pi_Y L(z) \underset{z \rightarrow 1}{\sim} \exp\left(y_1 \log \frac{1}{1-z}\right) \pi_Y Z.$$

In consequence, defining $P(z) = \sum_{w \in X^*} P_w(z) w = \frac{L(z)}{1-z}$, noncommutative generating series defined over \mathcal{C} , we get, by (29)

$$(34) \quad P(z) = e^{-(x_1+1) \log(1-z)} L_{\text{reg}}(z) e^{x_0 \log z}.$$

LEMMA 1. Let $\text{Mono}(z) = e^{-(x_1+1) \log(1-z)}$. Then

$$\text{Mono} = \sum_{k \geq 0} P_{y_1^k} y_1^k \quad \text{and} \quad \text{Mono}^{-1} = \sum_{k \geq 0} P_{y_1^k} (-y_1)^k.$$

Since the coefficient of z^N in the Taylor expansion of $P_{y_1^k}$ is $H_{y_1^k}(N)$ then

LEMMA 2. Let $\text{Const} = \sum_{k \geq 0} H_{y_1^k} y_1^k$. Then

$$\text{Const} = \exp\left[-\sum_{k \geq 1} H_{y_k} \frac{(-y_1)^k}{k}\right] \quad \text{and} \quad \text{Const}^{-1} = \exp\left[\sum_{k \geq 1} H_{y_k} \frac{(-y_1)^k}{k}\right].$$

DEFINITION 3 ([12]). Let $\zeta_{\sqcup} : (\mathbb{C}\langle\langle X \rangle\rangle, \sqcup) \rightarrow (\mathbb{C}, \cdot)$ be the algebra morphism (i.e. for any $u, v \in X^*$, $\zeta_{\sqcup}(u \sqcup v) = \zeta_{\sqcup}(u)\zeta_{\sqcup}(v)$) verifying for any convergent word $w \in x_0 X^* x_1$, $\zeta_{\sqcup}(w) = \zeta(w)$, and such that $\zeta_{\sqcup}(x_0) = \zeta_{\sqcup}(x_1) = 0$.

Then, the noncommutative generating series $Z_{\sqcup} = \sum_{w \in X^*} \zeta_{\sqcup}(w) w$ verifies $Z_{\sqcup} = Z$ [12]. In consequence, Z_{\sqcup} is the unique Lie exponential verifying $\langle Z_{\sqcup} | x_0 \rangle = \langle Z_{\sqcup} | x_1 \rangle = 0$ and $\langle Z_{\sqcup} | w \rangle = \zeta(w)$, for any $w \in x_0 X^* x_1$.

PROPOSITION 7. $P(z) \underset{z \rightarrow 0}{\sim} e^{x_0 \log z}$ and $P(z) \underset{z \rightarrow 1}{\sim} \text{Mono}(z)Z$.

PROOF. From $P(z) = e^{-(x_1+1) \log(1-z)} L_{\text{reg}}(z) e^{x_0 \log z}$, we can deduce the behaviour of $P(z)$ around 0. From Formula (31), we get the behaviour of $P(z)$ around 1. \square

COROLLARY 1. Let $\Pi(z) = \pi_Y P(z) = \sum_{w \in Y^*} P_w(z) w$. Then $\Pi(z) \underset{z \rightarrow 1}{\sim} \text{Mono}(z) \pi_Y Z$.

From this, we extract, taking care of Lemma 1, Taylor coefficients of P_w , and we get

COROLLARY 2. $H(N) \underset{N \rightarrow \infty}{\sim} \text{Const}(N) \pi_Y Z$.

THEOREM 4.

$$\lim_{z \rightarrow 1} \exp\left(-y_1 \log \frac{1}{1-z}\right) \Lambda(z) = \lim_{N \rightarrow \infty} \exp\left(\sum_{k \geq 1} H_{y_k}(N) \frac{(-y_1)^k}{k}\right) H(N) = \pi_Y Z,$$

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

PROOF. This is a consequence of Formula (33), of Lemma 2 and of Corollary 2. \square

3.3. Generalized Euler constants associated to divergent polyzêtas.

DEFINITION 4. Let $\zeta_{\sqcup} : (\mathbb{C}\langle Y \rangle, \sqcup) \rightarrow (\mathbb{C}, \cdot)$ the algebra morphism (i.e. for any convergent word $u, v \in Y^*$, $\zeta_{\sqcup}(u \sqcup v) = \zeta_{\sqcup}(u)\zeta_{\sqcup}(v)$) verifying for any $w \in Y^* \setminus y_1 Y^*$, $\zeta_{\sqcup}(w) = \zeta(w)$ and such that $\zeta_{\sqcup}(y_1) = \gamma$.

PROPOSITION 8.

$$\zeta_{\sqcup}(y_1^k) = \sum_{\substack{s_1, \dots, s_k > 0 \\ s_1 + \dots + k s_k = k}} \frac{(-1)^k}{s_1! \dots s_k!} (-\gamma)^{s_1} \left(-\frac{\zeta(2)}{2}\right)^{s_2} \dots \left(-\frac{\zeta(k)}{k}\right)^{s_k}.$$

PROOF. By (20) and applying the (surjective) morphism ζ_{\sqcup} , we get the expected result. \square

In consequence,

THEOREM 5 ([13]). For $k > 0$, the constant $\zeta_{\sqcup}(y_1^k)$ associated to divergent polyzêta $\zeta(y_1^k)$ is a polynomial of degree k in γ with coefficients in $\mathbb{Q}[\zeta(2), \zeta(2i+1)]_{0 < i \leq (k-1)/2}$. Moreover, for $l = 0, \dots, k$, the coefficient of γ^l is of weight $k-l$.

EXAMPLE 6.

$$\begin{aligned} \zeta_{\sqcup}(y_1^2) &= \frac{\gamma^2 - \zeta(2)}{2}, \\ \zeta_{\sqcup}(y_1^3) &= \frac{\gamma^3 - 3\zeta(2)\gamma + 2\zeta(3)}{6}, \\ \zeta_{\sqcup}(y_1^4) &= \frac{80\zeta(3)\gamma - 60\zeta(2)\gamma^2 + 6\zeta(2)^2 + 10\gamma^4}{240}, \\ \zeta_{\sqcup}(y_1^5) &= \frac{-20\zeta(2)\zeta(3) + 20\zeta(3)\gamma^2 - 10\zeta(2)\gamma^3 + \gamma^5 + 3\zeta^2(2)\gamma + 24\zeta(5)}{120}. \end{aligned}$$

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

$$(35) \quad \sum_{n=0}^{\infty} \sum_{k=0}^n b_{n,k}(t_1, \dots, t_{n-k+1}) \frac{v^n u^k}{n!} = \exp\left(u \sum_{l=1}^{\infty} t_l \frac{v^l}{l!}\right).$$

EXAMPLE 7 (Polynomials $b_{n,k}$ for $n \leq 5$).

$n \backslash k$	0	1	2	3	4	5
0	1					
1	0	t_1				
2	0	t_2	t_1^2			
3	0	t_3	$3t_1 t_2$	t_1^3		
4	0	t_4	$3t_2^2 + 4t_1 t_3$	$6t_1^2 t_2$	t_1^4	
5	0	t_5	$10t_2 t_3 + 5t_1 t_4$	$10t_1^3 t_2 + 15t_1 t_2^2$	$10t_1^3 t_2$	t_1^5

In particular, we have

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

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

Let us build the noncommutative generating series of $\zeta_{\sqcup}(w)$ and let us take the constant part of the two members of $\mathbf{H}(N) \xrightarrow{N \rightarrow \infty} \mathbf{Const}(N) \pi_Y Z$, we have

THEOREM 6. Let $Z_{\sqcup} = \sum_{w \in Y^*} \zeta_{\sqcup}(w) w$ be the noncommutative generating series of the constants $\zeta_{\sqcup}(w)$. Then

$$Z_{\sqcup} = \left[1 + \sum_{n \geq 1} \left(\sum_{k=1}^n b_{n,k}(\gamma, -\zeta(2), 2\zeta(3), \dots) \right) \frac{y_1^n}{n!} \right] \pi_Y Z.$$

Identifying coefficients of $y_1^k w$ in each member leads to

COROLLARY 3. For all $w \in Y^* \setminus y_1 Y^*$ and $k \geq 0$, we have

$$\zeta_{\sqcup}(y_1^k w) = \sum_{i=0}^k \frac{\zeta_{\sqcup}(y_1^{k-i} w)}{i!} \left[\sum_{j=1}^i b_{i,j}(\gamma, -\zeta(2), 2\zeta(3), \dots) \right].$$

EXAMPLE 8.

$$\begin{aligned} \zeta_{\sqcup}(y_1^2 y_2) &= \zeta_{\sqcup}(y_1^2 y_2) + \zeta_{\sqcup}(y_1 y_2) b_{1,1}(\gamma) + \frac{\zeta(2)}{2!} (b_{2,1}(-\zeta(2)) + b_{2,2}(\gamma)) \\ &= 3\zeta(2, 1, 1) - 2\zeta(2, 1)\gamma + \frac{\zeta(2)}{2} (-\zeta(2) + \gamma^2), \end{aligned}$$

and using the reduction table, we find

$$\zeta_{\sqcup}(y_1^2 y_2) = \frac{\zeta(2)}{2} \gamma^2 - 2\zeta(3)\gamma + \frac{7}{10} \zeta(2)^2,$$

a result in agreement with Example 4.

In consequence,

THEOREM 7 ([13]). For $w \in Y^* \setminus y_1 Y^*$, $k \geq 0$, the constant $\zeta_{\sqcup}(y_1^k w)$ associated to $\zeta(y_1^k w)$ is a polynomial of degree k in γ and with coefficients in \mathcal{Z} . Moreover, for $l = 0, \dots, k$, the coefficient of γ^l is of weight $|w| + k - l$.

4. Applications to maxima in hypercubes

DEFINITION 5. Let $w = y_{s_1} \dots y_{s_r} \in Y^*$. For $N \geq k \geq 1$, the harmonic sum $A_w(N; k)$ is defined as

$$A_w(N; k) = \sum_{N \geq n_1 \geq \dots \geq n_r \geq k} \frac{1}{n_1^{s_1} \dots n_r^{s_r}}.$$

For convenience, we use the notation $A_w(N)$ instead of $A_w(N; 1)$ (see Definition 2).

PROPOSITION 9. For any $u, v \in Y^*$, $A_{u \sqcup v}(N; k) = A_u(N; k) A_v(N; k)$.

In all the sequel, $|w|_2$ denotes the number of occurrences of the letter y_2 in w and we focus on the asymptotic equivalent of $\mathbb{V}ar(K_{n,d})$ from Formula (3), κ_d given by Formula (4). This one can be re-written, with our tools, in the following way:

$$\kappa_d = \frac{1}{(d-1)!} \sum_{t=1}^{d-2} \binom{d-1}{t} \sum_{l \geq 1} \frac{1}{l^2} A_{y_1^{t-1} \sqcup y_1^{d-2-t}}(l)$$

We need a last *ad hoc* notation.

DEFINITION 6. Let S be a subset of Y , and ρ a positive integer, we define S_ρ as the set of words containing only letters in S , and of weight equal to ρ .

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

THEOREM 8.

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

EXAMPLE 10. For $d = 7$, we get

$$6! \kappa_7 = \binom{10}{5} \zeta(2, 1, 1, 1, 1) - \binom{8}{4} \left(\zeta(2, 2, 1, 1) + \zeta(2, 1, 2, 1) + \zeta(2, 1, 1, 2) \right) + \binom{6}{3} \zeta(2, 2, 2).$$

See Appendix A for more examples

The last step consists in reducing into polyzêta, and then use the reduction table.

$$\begin{aligned} \kappa_{11} &= \frac{209}{302400} \zeta(5) \zeta(2) \zeta(3) + \frac{2893}{6048000} \zeta(2)^2 \zeta(3)^2 + \frac{3311}{460800} \zeta(3) \zeta(7) \\ &\quad - \frac{517}{921600} \zeta(8, 2) + \frac{39457}{9676800} \zeta(5)^2 + \frac{426341}{221760000} \zeta(2)^5 \end{aligned}$$

Let us come back to Expression (1), that we can interpret, in terms of harmonic sums,

$$\mathbb{E}(K_{n,d}^2) = A_{y_1^{d-1}}(n) + \sum_{1 \leq t \leq d-1} \binom{d}{t} \sum_{l=1}^{n-1} \frac{1}{l} A_{y_1^{t-1}}(l) A_{y_1^{d-t-1}}(l) A_{y_1^{d-1}}(n; l+1),$$

PROPOSITION 10. For any integers $n \geq l$, $A_{y_1^d}(n; l) = \sum_{\substack{k_1 + \dots + k_d = d \\ k_1, \dots, k_d > 0}} \frac{A_1^{k_1}(n; l) \dots A_d^{k_d}(n; l)}{1^{k_1} k_1! \dots d^{k_d} k_d!}$

Since $A_r(n; l+1) = A_r(n) - A_r(l)$, for any integer r ¹, this enables to turn the summand into a polynomial involving only some $A_w(n)$ and $A_w(l)$.

- Thanks to Proposition 9, we are able to turn each polynomial (in harmonic sums) into a linear combination of harmonic sums.
- Finally, there are only sums over l of type $\frac{A_w(l)}{l}$ left, but by Formula (23), they simply reduce to $A_{y_1 w}(n-1)$.

$$\begin{aligned} \text{Var}(K_{n,3}) &= \mathbb{E}(K_{n,3}^2) - \mu_{n,3}^2 \\ &= A_{1,1}(n) + 3 A_1^2(n) A_{1,1}(n-1) - 12 A_1(n) A_{1,1,1}(n-1) \\ &\quad + 6 A_1(n) A_{1,2}(n-1) + 18 A_{1,1,1,1}(n-1) - 12 A_{1,1,2}(n-1) \\ &\quad - 12 A_{1,2,1}(n-1) + 6 A_{1,3}(n-1) + 3 A_2(n) A_{1,1}(n-1) - A_{1,1}^2(n). \end{aligned}$$

We can now compute the asymptotic expansion of $\text{Var}(K_{n,d})$.

THEOREM 9. There exist algorithmically computable coefficients $\alpha_i, \beta_{j,k} \in \mathcal{Z}'$ such that, for any dimension d and any order M ,

$$\text{Var}(K_{n,d}) = \sum_{i=0}^{2d-2} \alpha_i \ln^i(n) + \sum_{j=1}^M \frac{1}{n^j} \sum_{k=0}^{2d-2} \beta_{j,k} \ln^k(n) + o\left(\frac{1}{n^M}\right).$$

This is a direct consequence of Proposition 6.

EXAMPLE 11.

$$\begin{aligned} \text{Var}(K_{n,3}) &= \left(\frac{1}{2} + \kappa_3\right) \ln^2(n) + (-10\zeta(3) + 2\zeta(2)\gamma + \gamma) \ln(n) + \frac{1}{2} \gamma^2 \\ &\quad - 10\zeta(3)\gamma + \frac{83}{10} \zeta(2)^2 + \zeta(2)\gamma^2 + \frac{1}{2} \zeta(2) + o(1) \end{aligned}$$

See Appendix B for more examples

¹while this is absolutely false if you replace r by a word of length greater or equal than 2.

Appendix A: values of constants κ_d

$$\begin{aligned}
\kappa_2 &= 0 \\
\kappa_3 &= \zeta(2) \\
\kappa_4 &= 2\zeta(3) \\
\kappa_5 &= \frac{33}{40}\zeta(2)^2 \\
\kappa_6 &= \frac{5}{4}\zeta(5) + \frac{1}{6}\zeta(2)\zeta(3) \\
\kappa_7 &= \frac{1451}{7560}\zeta(2)^3 + \frac{7}{72}\zeta(3)^2 \\
\kappa_8 &= \frac{1729}{5760}\zeta(7) + \frac{181}{3600}\zeta(3)\zeta(2)^2 + \frac{13}{360}\zeta(2)\zeta(5) \\
\kappa_9 &= -\frac{17}{1920}\zeta(6,2) + \frac{11}{160}\zeta(3)\zeta(5) + \frac{1}{320}\zeta(2)\zeta(3)^2 + \frac{1891}{89600}\zeta(2)^4 \\
\kappa_{10} &= \frac{529}{75600}\zeta(2)^2\zeta(5) + \frac{33941}{6350400}\zeta(2)^3\zeta(3) + \frac{17}{3360}\zeta(2)\zeta(7) \\
&\quad + \frac{199271}{4354560}\zeta(9) + \frac{11}{12960}\zeta(3)^3 \\
\kappa_{11} &= \frac{209}{302400}\zeta(5)\zeta(2)\zeta(3) + \frac{2893}{6048000}\zeta(2)^2\zeta(3)^2 + \frac{3311}{460800}\zeta(3)\zeta(7) - \frac{517}{921600}\zeta(8,2) \\
&\quad + \frac{39457}{9676800}\zeta(5)^2 + \frac{426341}{221760000}\zeta(2)^5 \\
\kappa_{12} &= -\frac{13}{100800}\zeta(3)\zeta(6,2) + \frac{877}{302400}\zeta(2)\zeta(9) + \frac{299}{604800}\zeta(5)\zeta(3)^2 + \frac{13}{907200}\zeta(2)\zeta(3)^3 \\
&\quad + \frac{7949}{6048000}\zeta(2)^2\zeta(7) + \frac{1081}{1411200}\zeta(5)\zeta(2)^3 + \frac{172157}{423360000}\zeta(2)^4\zeta(3) \\
&\quad - \frac{586337}{232243200}\zeta(11) - \frac{13}{100800}\zeta(8,2,1) \\
\kappa_{13} &= \frac{169}{3456000}\zeta(5)\zeta(3)\zeta(2)^2 - \frac{1703}{43545600}\zeta(7)\zeta(2)\zeta(3) + \frac{9061}{8294400}\zeta(3)\zeta(9) \\
&\quad + \frac{471809}{348364800}\zeta(5)\zeta(7) - \frac{13}{604800}\zeta(2)^2\zeta(6,2) - \frac{13}{215040}\zeta(2)\zeta(8,2) \\
&\quad + \frac{4667}{381024000}\zeta(2)^3\zeta(3)^2 + \frac{11947}{174182400}\zeta(10,2) - \frac{13}{483840}\zeta(8,2,1,1) \\
&\quad + \frac{13}{2903040}\zeta(3)^4 - \frac{2873}{87091200}\zeta(2)\zeta(5)^2 + \frac{11884374679}{152562009600000}\zeta(2)^6.
\end{aligned}$$

Appendix B: Asymptotic expansions of $\text{Var}(K_{n,d})$

$$\begin{aligned}
\text{Var}(K_{n,4}) &= \left(\frac{1}{3!} + \kappa_4\right) \ln^3(n) + \left(-\frac{53}{5} \zeta(2)^2 + 6 \zeta(3) \gamma + \frac{1}{2} \gamma\right) \ln^2(n) \\
&+ \left(97 \zeta(5) - \frac{106}{5} \zeta(2)^2 \gamma + 16 \zeta(2) \zeta(3) + 6 \zeta(3) \gamma^2 + \frac{1}{2} \zeta(2) + \frac{1}{2} \gamma^2\right) \ln(n) \\
&+ \frac{1}{3} \zeta(3) - \frac{53}{5} \zeta(2)^2 \gamma^2 - \frac{3719}{70} \zeta(2)^3 + \frac{1}{6} \gamma^3 + \frac{1}{2} \zeta(2) \gamma \\
&+ 16 \zeta(2) \zeta(3) \gamma - 3 \zeta(3)^2 + 2 \zeta(3) \gamma^3 + 97 \zeta(5) \gamma + o(1) \\
\text{Var}(K_{n,5}) &= \left(\frac{1}{4!} + \kappa_5\right) \ln^4(n) + \left(\frac{1}{6} \gamma - \frac{98}{3} \zeta(5) + \frac{33}{10} \zeta(2)^2 \gamma - \frac{13}{3} \zeta(2) \zeta(3)\right) \ln^3(n) \\
&+ \left(\frac{10123}{140} \zeta(2)^3 + \frac{47}{2} \zeta(3)^2 + \frac{99}{20} \zeta(2)^2 \gamma^2 + \frac{1}{4} \gamma^2 + \frac{1}{4} \zeta(2) - 13 \zeta(2) \zeta(3) \gamma\right. \\
&- 98 \zeta(5) \gamma \left.) \ln^2(n) + \left(\frac{1}{6} \gamma^3 + \frac{33}{10} \zeta(2)^2 \gamma^3 + \frac{1}{2} \zeta(2) \gamma - 950 \zeta(7)\right. \right. \\
&- 13 \zeta(2) \zeta(3) \gamma^2 + 47 \zeta(3)^2 \gamma + \frac{1}{3} \zeta(3) - \frac{317}{5} \zeta(3) \zeta(2)^2 + \frac{10123}{70} \zeta(2)^3 \gamma \\
&- 98 \zeta(5) \gamma^2 - 222 \zeta(2) \zeta(5) \left.) \ln(n) - \frac{13}{3} \zeta(2) \zeta(3) \gamma^3 + \frac{47}{2} \zeta(3)^2 \gamma^2\right. \\
&- \frac{317}{5} \zeta(3) \zeta(2)^2 \gamma - \frac{98}{3} \zeta(5) \gamma^3 + \frac{33}{40} \zeta(2)^2 \gamma^4 + \frac{32}{3} \zeta(3) \zeta(5) + \frac{10123}{140} \zeta(2)^3 \gamma^2 \\
&- 222 \zeta(2) \zeta(5) \gamma + \frac{1}{24} \gamma^4 - 950 \zeta(7) \gamma + 50 \zeta(6, 2) + \frac{1}{4} \zeta(2) \gamma^2 + \frac{1}{3} \zeta(3) \gamma \\
&+ \frac{9}{40} \zeta(2)^2 + \frac{95}{6} \zeta(2) \zeta(3)^2 + \frac{134739}{350} \zeta(2)^4 + o(1) \\
\text{Var}(K_{n,6}) &= \left(\frac{1}{5!} + \kappa_6\right) \ln^5(n) + \left(\frac{1}{24} \gamma + \frac{25}{4} \zeta(5) \gamma + \frac{5}{6} \zeta(2) \zeta(3) \gamma - \frac{25}{6} \zeta(3)^2\right. \\
&- \frac{22711}{2520} \zeta(2)^3 \left.) \ln^4(n) + \left(\frac{1}{12} \gamma^2 + \frac{1231}{30} \zeta(3) \zeta(2)^2 - \frac{50}{3} \zeta(3)^2 \gamma\right. \right. \\
&+ \frac{8729}{24} \zeta(7) + \frac{127}{2} \zeta(2) \zeta(5) + \frac{1}{12} \zeta(2) + \frac{5}{3} \zeta(2) \zeta(3) \gamma^2 - \frac{22711}{630} \zeta(2)^3 \gamma \\
&+ \frac{25}{2} \zeta(5) \gamma^2 \left.) \ln^3(n) + \left(-55 \zeta(6, 2) - \frac{241}{6} \zeta(2) \zeta(3)^2 + \frac{1231}{10} \zeta(3) \zeta(2)^2 \gamma\right. \right. \\
&+ \frac{1}{12} \gamma^3 + \frac{1}{4} \zeta(2) \gamma + \frac{8729}{8} \zeta(7) \gamma - \frac{2331589}{4200} \zeta(2)^4 + \frac{1}{6} \zeta(3) + \frac{25}{2} \zeta(5) \gamma^3 \\
&+ \frac{5}{3} \zeta(2) \zeta(3) \gamma^3 - 342 \zeta(3) \zeta(5) - 25 \zeta(3)^2 \gamma^2 - \frac{22711}{420} \zeta(2)^3 \gamma^2 \\
&+ \frac{381}{2} \zeta(2) \zeta(5) \gamma \left.) \ln^2(n) + \left(\frac{8729}{8} \zeta(7) \gamma^2 - \frac{2331589}{2100} \zeta(2)^4 \gamma + \frac{381}{2} \zeta(2) \zeta(5) \gamma^2\right. \right. \\
&- \frac{241}{3} \zeta(2) \zeta(3)^2 \gamma + \frac{1231}{10} \zeta(3) \zeta(2)^2 \gamma^2 - 19 \zeta(3)^3 + \frac{1}{4} \zeta(2) \gamma^2 + \frac{9}{40} \zeta(2)^2 \\
&- \frac{50}{3} \zeta(3)^2 \gamma^3 - 110 \zeta(6, 2) \gamma + \frac{25}{4} \zeta(5) \gamma^4 + \frac{1}{3} \zeta(3) \gamma + \frac{21919}{20} \zeta(2)^2 \zeta(5) \\
&- \frac{22711}{630} \zeta(2)^3 \gamma^3 + \frac{135593}{315} \zeta(2)^3 \zeta(3) + \frac{182179}{18} \zeta(9) + \frac{5}{6} \zeta(2) \zeta(3) \gamma^4 \\
&- 684 \zeta(3) \zeta(5) \gamma + \frac{19209}{8} \zeta(2) \zeta(7) + \frac{1}{24} \gamma^4 \left.) \ln(n) + \frac{127}{2} \zeta(2) \zeta(5) \gamma^3\right. \\
&+ \frac{1231}{30} \zeta(3) \zeta(2)^2 \gamma^3 - \frac{241}{6} \zeta(2) \zeta(3)^2 \gamma^2 - 342 \zeta(3) \zeta(5) \gamma^2 + \frac{1}{6} \zeta(2) \zeta(3) \gamma^5 \\
&+ \frac{1}{6} \zeta(2) \zeta(3) + \frac{182179}{18} \zeta(9) \gamma + \frac{9}{40} \zeta(2)^2 \gamma - 19 \zeta(3)^3 \gamma + \frac{1}{6} \zeta(3) \gamma^2 \\
&- \frac{2331589}{4200} \zeta(2)^4 \gamma^2 + \frac{1}{5} \zeta(5) - 55 \zeta(6, 2) \gamma^2 - 325 \zeta(8, 2) + \frac{135593}{315} \zeta(2)^3 \zeta(3) \gamma \\
&- 55 \zeta(2) \zeta(6, 2) + \frac{1}{12} \zeta(2) \gamma^3 + \frac{8729}{24} \zeta(7) \gamma^3 - \frac{22711}{2520} \zeta(2)^3 \gamma^4 - \frac{25}{6} \zeta(3)^2 \gamma^4 + \frac{1}{120} \gamma^5 \\
&- 945 \zeta(5)^2 - \frac{6237237}{2200} \zeta(2)^5 + \frac{767}{30} \zeta(2)^2 \zeta(3)^2 - \frac{9031}{12} \zeta(3) \zeta(7) - 392 \zeta(5) \zeta(2) \zeta(3) \\
&+ \frac{5}{4} \zeta(5) \gamma^5 + \frac{21919}{20} \zeta(2)^2 \zeta(5) \gamma + \frac{19209}{8} \zeta(2) \zeta(7) \gamma + o(1).
\end{aligned}$$

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