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

Christian Costermans and Hoang Ngoc Minh

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 occuring 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 la $\mathbb{Q}$-algèbre engendré par les polyzêtas convergents et par la constante d'Euler γ.

1. Introduction

Let $Q = \{q_1, \ldots, q_n\}$ be a set of independent and identically distributed random vectors in $\mathbb{R}^d$. A point $q_i = (q_{i_1}, \ldots, q_{i_d})$ is said to be dominated by $q_j = (q_{j_1}, \ldots, q_{j_d})$ if $q_{i_k} < q_{j_k}$ for all $k \in [1, .., d]$ 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 $\mathbb{V}ar(K_{n,d})$ 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**] :

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

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

$$(2) \qquad \mu_{n,d} = \mathbb{E}(K_{n,d}) = \sum_{1 \le i_1 \le \ldots \le i_{d-1} \le n} \frac{1}{i_1 \ldots i_{d-1}}.$$

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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

$$\mathbb{V}ar(K_{n,d}) \sim \left(\frac{1}{(d-1)!}+\kappa_d\right)\ln^{d-1}(n), \tag{3}$$

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

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

These two formulas (1) and (4) give rise to harmonic sums $\mathrm{A}_{\mathbf{s}}(N)$, closely related to $\mathrm{H}_{\mathbf{s}}(N)$ and defined for a composition $\mathbf{s}=(s_1,\ldots,s_r)$ by

$$\mathrm{A}_{\mathbf{s}}(N)=\sum_{N\geq n_1\geq\ldots\geq n_r>0}\frac{1}{n_1^{s_1}\ldots n_r^{s_r}} \quad\text{and}\quad \mathrm{H}_{\mathbf{s}}(N)=\sum_{N\geq n_1>\ldots>n_r>0}\frac{1}{n_1^{s_1}\ldots n_r^{s_r}}. \tag{5}$$

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

$$\mathrm{A}_{\mathbf{s}}(N)=\sum_{J\in\mathrm{Comp}(r)}\mathrm{H}_{J\circ\mathbf{s}}(N) \quad\text{and}\quad \mathrm{H}_{\mathbf{s}}(N)=\sum_{J\in\mathrm{Comp}(r)}(-1)^{l(J)-r}\mathrm{A}_{J\circ\mathbf{s}}(N), \tag{6}$$

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

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

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)

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

where $\mathbf{s}=(2,s_2,\ldots,s_r)$ and $|\mathbf{s}|_2$ stands for the number of occurences 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 $\mathbb{V}ar(K_{n,d})$ via the asymptotic expansion of $\mathrm{H}_{\mathbf{s}}(N)$ (*c.f.* Theorem 9) :

$$\mathbb{V}ar(K_{n,d})=\sum_{i=0}^{2d-2}\alpha_i\ln^i(n)+\sum_{j=1}^{M}\frac{1}{n^j}\sum_{k=0}^{2d-2}\beta_{j,k}\ln^k(n)+\mathrm{o}\left(\frac{1}{n^M}\right), \tag{9}$$

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**]

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

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

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

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

leading to the asymptotic expansion of the harmonic sum $\mathrm{H}_r(N)=\sum_{n=1}^N n^{-r}$. We now are interested on *multiple* harmonic sums $\mathrm{H}_{\mathbf{s}}$ and their derivated $\mathrm{A}_{\mathbf{s}}$. We have already proposed in [**5**] a recursive method, widely based on the Euler-MacLaurin formula and based on the algebraic structure of $\mathrm{H}_{\mathbf{s}}$, 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 :

$$\mathrm{P}_{\mathbf{s}}(z)=\sum_{n\geq 0}\mathrm{H}_{\mathbf{s}}(n)z^n=\frac{\mathrm{Li}_{\mathbf{s}}(z)}{1-z},\quad\text{where}\quad \mathrm{Li}_{\mathbf{s}}(z)=\sum_{n_1>\ldots>n_r>0}\frac{z^{n_1}}{n_1^{s_1}\ldots n_r^{s_r}}. \tag{13}$$

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

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

They are respectively coefficients of the following generating functions

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

These generating functions satisfy a Newton identity

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

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

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

To the composition $\mathbf{s}=(s_1,\ldots,s_r)$, we associate the word $w=y_{s_1}\ldots y_{s_r}$ 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 occurences 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) $s_1+\ldots+s_r$, is defined by

$$\mathrm{F}_w(\underline{t})=\sum_{n_1>\ldots>n_r>0}t_{n_1}^{s_1}\ldots t_{n_r}^{s_r}\quad\text{and}\quad\mathrm{G}_w(\underline{t})=\sum_{n_1\geq\ldots\geq n_r>0}t_{n_1}^{s_1}\ldots t_{n_r}^{s_r}. \tag{18}$$

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

$$\sum_{k\geq 0}\mathrm{F}_{y_1^k}z^k=\exp\Big[-\sum_{k\geq 1}\mathrm{F}_{y_k}\frac{(-z)^k}{k}\Big]\quad\Big(\text{or}\quad\sum_{k\geq 0}\mathrm{G}_{y_1^k}z^k=\exp\Big[\sum_{k\geq 1}\mathrm{G}_{y_k}\frac{z^k}{k}\Big]\Big). \tag{19}$$

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

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*

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

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

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

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

EXAMPLE 1. $y_1 \shuffle y_2 = y_1y_2 + y_2y_1$, $y_1 \stuffle y_2 = y_1y_2 + y_2y_1 + y_3$ *and* $y_1 \minusstuffle y_2 = y_1y_2 + y_2y_1 - y_3$.

PROPOSITION 1. *The operation $\minusstuffle$ is commutative and associative.*

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

In the same way, we show that $w_1 \minusstuffle (w_2 \minusstuffle w_3) = (w_1 \minusstuffle w_2) \minusstuffle w_3$ by induction on $|w_1| + |w_2| + |w_3|$. Once again, the hypothesis is proved by (20) when $|w_1| + |w_2| + |w_3| \le 1$. Then, the calculation of $y_iw_1 \minusstuffle (y_jw_2 \minusstuffle y_kw_3)$ gives

$$\begin{aligned}
&y_i(w_1 \minusstuffle y_j(w_2 \minusstuffle y_kw_3)) + y_j(y_iw_1 \minusstuffle (w_2 \minusstuffle y_kw_3)) - y_{i+j}(w_1 \minusstuffle (w_2 \minusstuffle y_kw_3))\\
&+y_i(w_1 \minusstuffle y_k(y_jw_2 \minusstuffle w_3)) + y_k(y_iw_1 \minusstuffle (y_jw_2 \minusstuffle w_3)) - y_{i+k}(w_1 \minusstuffle (y_jw_2 \minusstuffle w_3))\\
&-y_i(w_1 \minusstuffle y_{j+k}(w_2 \minusstuffle w_3)) - y_{j+k}(y_iw_1 \minusstuffle (w_2 \minusstuffle w_3)) + y_{i+j+k}(w_1 \minusstuffle (w_2 \minusstuffle w_3))
\end{aligned}$$

On the other hand, the calculation of $(y_iw_1 \minusstuffle y_jw_2) \minusstuffle y_kw_3$ gives

$$\begin{aligned}
&y_i((w_1 \minusstuffle y_jw_2) \minusstuffle y_kw_3) + y_k(y_i(w_1 \minusstuffle y_jw_2) \minusstuffle w_3) - y_{i+k}((w_1 \minusstuffle y_jw_2) \minusstuffle w_3)\\
&+y_j((y_iw_1 \minusstuffle w_2) \minusstuffle y_kw_3) + y_k(y_j(y_iw_1 \minusstuffle w_2) \minusstuffle w_3) - y_{j+k}((y_iw_1 \minusstuffle w_2) \minusstuffle w_3)\\
&-y_{i+j}((w_1 \minusstuffle w_2) \minusstuffle y_kw_3) - y_k(y_{i+j}(w_1 \minusstuffle w_2) \minusstuffle w_3) + y_{i+j+k}((w_1 \minusstuffle w_2) \minusstuffle w_3)
\end{aligned}$$

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

$$\begin{aligned}
&y_i(w_1 \minusstuffle y_j(w_2 \minusstuffle y_kw_3)) + y_i(w_1 \minusstuffle y_k(y_jw_2 \minusstuffle w_3)) + y_k(y_iw_1 \minusstuffle (y_jw_2 \minusstuffle w_3))\\
&-y_i(w_1 \minusstuffle y_{j+k}(w_2 \minusstuffle w_3)) - y_i((w_1 \minusstuffle y_jw_2) \minusstuffle y_kw_3) - y_k(y_i(w_1 \minusstuffle y_jw_2) \minusstuffle w_3)\\
&-y_k(y_j(y_iw_1 \minusstuffle w_2) \minusstuffle w_3) + y_k(y_{i+j}(w_1 \minusstuffle w_2) \minusstuffle w_3),
\end{aligned}$$

which can be further simplified using (20) in

$$\begin{aligned}
&y_i(w_1 \minusstuffle (y_jw_2 \minusstuffle y_kw_3)) + y_k(y_iw_1 \minusstuffle (y_jw_2 \minusstuffle w_3))\\
&-y_i((w_1 \minusstuffle y_jw_2) \minusstuffle y_kw_3) - y_k((y_iw_1 \minusstuffle y_jw_2) \minusstuffle w_3),
\end{aligned}$$

expression reduced to zero by the induction hypothesis. □

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

$$\mathrm{F}_{u \stuffle v} = \mathrm{F}_u\, \mathrm{F}_v \quad \text{and} \quad \mathrm{G}_{u \minusstuffle v} = \mathrm{G}_u\, \mathrm{G}_v.$$

The remarkable identity (17) can be then seen as

$$y_1^k = \frac{(-1)^k}{k!} \sum_{\substack{s_1,\ldots,s_k>0\\ s_1+\ldots+ks_k=k}} \binom{k}{s_1,\ldots,s_k} \frac{(-y_1)^{\stuffle s_1}}{1^{s_1}} \stuffle \ldots \stuffle \frac{(-y_k)^{\stuffle s_k}}{k^{s_k}} \tag{20}$$

$$= \frac{1}{k!} \sum_{\substack{s_1,\ldots,s_k>0\\ s_1+\ldots+ks_k=k}} \binom{k}{s_1,\ldots,s_k} \frac{y_1^{\minusstuffle s_1}}{1^{s_1}} \minusstuffle \ldots \minusstuffle \frac{y_k^{\minusstuffle s_k}}{k^{s_k}} \tag{21}$$

$$= \frac{y_1^{\shuffle k}}{k!}. \tag{22}$$

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*

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

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

We put also $\mathrm{H}_w(0) = \mathrm{A}_w(0) = 0$.

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 $\mathrm{H}_w(N)$ (resp. $\mathrm{A}_w(N)$) 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 $u, v \in Y^*, \mathrm{H}_{u \,⧢\!\!\!-\, v} = \mathrm{H}_u\, \mathrm{H}_v$ and $\mathrm{A}_{u \,\sqcup\!\!\sqcup\, v} = \mathrm{A}_u\, \mathrm{A}_v$.*

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

$$\mathrm{H}_w(N) = \sum_{l=r}^{N} \frac{\mathrm{H}_{w'}(l-1)}{l^s} \quad \text{and} \quad \mathrm{A}_w(N) = \sum_{l=1}^{N} \frac{\mathrm{A}_{w'}(l)}{l^s}. \tag{23}$$

In consequence,

Theorem 1. *For any $w = y_s w' \in Y^*$, $\mathrm{H}_w(N)$ and $\mathrm{A}_w(N)$ converge when $N \to +\infty$ if and only if $s > 1$. Therefore, if $s \geq 2$ then the limits $\lim_{N \to +\infty} \mathrm{H}_w(N)$ and $\lim_{N \to +\infty} \mathrm{A}_w(N)$ 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 $\mathrm{H}_w(N) \geq \mathrm{H}_{w'}(r-1) \sum_{l=r}^{N} l^{-s}$ shows the divergence of $\mathrm{H}_w(N)$ 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 $\mathrm{H}_{w'}(l)$, we need the following result : for any $w \in Y^*$, there exist a constant K and in integer α such that, for any $l > 1$, $\mathrm{H}_w(l) \leq K \ln^\alpha l$. 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 $\mathrm{H}_w(N)$ comes directly.

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

Let us consider the following two differential forms $\omega_0(z) = dz/z$ and $\omega_1(z) = dz/(1-z)$. The polylogarithm $\mathrm{Li}_{\mathbf{s}}(z)$ is defined for a composition $\mathbf{s} = (s_1, \ldots, s_r)$ 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 $0 \rightsquigarrow z$,

$$\mathrm{Li}_{\mathbf{s}} = \int_{0 \rightsquigarrow z} \omega_0^{s_1 - 1} \omega_1 \ldots \omega_0^{s_r - 1} w_1. \tag{24}$$

Let $X = \{x_0, x_1\}$. We shall also identify any composition $\mathbf{s} = (s_1, \ldots, s_r)$ with its encoding word $w = x_0^{s_1 - 1} x_1 \cdots x_0^{s_r - 1} x_1$ 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 $\mathrm{Li}_{\mathbf{s}}(z)$ 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 $\mathrm{Li}_{x_0}(z) = \log(z)$. 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 $\mathrm{Li} : w \mapsto \mathrm{Li}_w$ is an isomorphism from $(\mathbb{C}\langle X \rangle, \sqcup\!\!\sqcup)$ to $(\mathbb{C}\{\mathrm{Li}_w\}_{w \in X^*}, .)$.*

The polyzêtas are well defined only for the convergent words in $\{\epsilon\} \cup x_0 X^* x_1$, and linearly extended to $\mathrm{C}_1 = \mathbb{Q} \oplus x_0 \mathbb{Q}\langle X \rangle x_1$. Let $\mathrm{C}_2 = \mathbb{Q} \oplus (Y \setminus y_1 \mathbb{Q}\langle Y \rangle) \simeq \mathrm{C}_1$. By the Radford theorem [**17**], one has

$$(\mathbb{Q}\langle X \rangle, \sqcup\!\!\sqcup) \simeq \mathbb{Q}[\mathcal{L}ynX] = \mathrm{C}_1[x_0, x_1], \tag{25}$$

$$(\mathbb{Q}\langle Y \rangle, \sqcup\!\!\sqcup) \simeq (\mathbb{Q}\langle Y \rangle, ⧢\!\!\!-) \simeq \mathbb{Q}[\mathcal{L}ynY] = \mathrm{C}_2[y_1], \tag{26}$$

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

By Theorem 2, we have

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

By Proposition 2, one has

PROPOSITION 4 ([**14**]). *For* $u, v \in Y^* \setminus y_1 Y^*, \zeta(u \uplus v) = \zeta(u)\,\zeta(v)$ *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 equiped 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* $\mathrm{P}_w(z) = (1-z)^{-1}\mathrm{Li}_w(z)$. *Thus for* $u, v \in Y^*, \mathrm{P}_{u \uplus v} = \mathrm{P}_u \odot \mathrm{P}_v$, *where* $\odot$ *denotes the Hadamard product.*

As consequences of Theorem 2, we also have

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

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 $\mathrm{H}_w(N)$ for convergent words lies on the formula (23) and by induction on the length of w. Details are given in [**5**].

EXAMPLE 2.

$$\mathrm{H}_{4,2}(N) = \zeta(4,2) - \sum_{i=N+1}^{\infty} \frac{\mathrm{H}_2(i-1)}{i^4},$$

But $\mathrm{H}_2(i-1) = \zeta(2) - \frac{1}{i} - \frac{1}{2}\frac{1}{i^2} + \mathrm{O}\left(\frac{1}{i^3}\right)$ *so*

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

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

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

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 $\zeta(v), v \in \mathrm{C}_2$, such that $\mathrm{H}_w(N) \underset{N\to\infty}{\widetilde{}} q_w(\gamma)$ [**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

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

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

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

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

Considering this Taylor expansion, the recursive algorithm to get the expansion of $\mathrm{H}_w(N)$ can be summered in these two points :

- If $w = y_1 w'$ then compute Taylor expansion of w. Indeed, thanks to Formula (27),
$$\mathrm{H}_w = \sum_{k=0}^{|w|} \mathrm{H}_{c_k(w)} \frac{\mathrm{H}_1^k}{k!},$$
so we just need the expansion of $\mathrm{H}_{c_k(w)}(N)$
- If $w = y_s w'$ then compute the asymptotic expansion of $\mathrm{H}_{w'}(n-1)$ 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 $w \in Y^*$,*
$$\mathrm{H}_w(N) \sim \sum_{i=0}^{+\infty} b_i N^{\eta_i} \log^{\kappa_i}(N), \quad \textit{for} \quad N \to +\infty.$$

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 $\mathrm{H}_{y_1^2 y_2}(N)$ 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, $\mathrm{L} = \sum_{w \in X^*} \mathrm{Li}_w \; w$, satisfies Drinfel'd differential equation [**6, 7**]

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

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

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

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

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

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

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

Example 5. *This gives an alternative derivation of the asymptotic expansion of any $\mathrm{H}_w(N)$. Indeed, let us see the example of $w = y_2 y_1$,*
$$\begin{aligned}\mathrm{Li}_{2,1}(z) &= -\mathrm{Li}_3(1-z) + \log(1-z)\,\mathrm{Li}_2(1-z) - \frac{1}{2}\log^2(1-z)\,\mathrm{Li}_1(1-z) - \zeta(2)\,\mathrm{Li}_1(1-z) + \zeta(3) \\ &= -(1-z) + (1-z)\log(1-z) - \frac{1}{2}(1-z)\log^2(1-z) - \zeta(2)(1-z) + \zeta(3) + \mathrm{O}\left(|1-z|\right).\end{aligned}$$

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

and so, since $[z^N]\log^2(1-z)=[z^N]2!(1-z)\mathrm{P}_{1,1}(z)=2\left(\mathrm{H}_{1,1}(N)-\mathrm{H}_{1,1}(N-1)\right)$, *and using Identity* 20, *we get*

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

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

(32) $$\mathrm{L}(z)\widetilde{_{z\to0}}\exp(x_0\log z)\quad\text{and}\quad \mathrm{L}(z)\widetilde{_{z\to1}}\exp\left(x_1\log\frac{1}{1-z}\right)Z,$$

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) $$\Lambda(z)=\pi_Y\mathrm{L}(z)\widetilde{_{z\to1}}\exp\left(y_1\log\frac{1}{1-z}\right)\pi_Y Z.$$

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

(34) $$\mathrm{P}(z)=e^{-(x_1+1)\log(1-z)}\mathrm{L}_{\mathrm{reg}}(z)e^{x_0\log z}.$$

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

$$\mathrm{Mono}=\sum_{k\ge0}\mathrm{P}_{y_1^k}\,y_1^k\quad\textit{and}\quad\mathrm{Mono}^{-1}=\sum_{k\ge0}\mathrm{P}_{y_1^k}\,(-y_1)^k.$$

Since the coefficient of z^N in the Taylor expansion of $\mathrm{P}_{y_1^k}$ is $\mathrm{H}_{y_1^k}(N)$ then

LEMMA 2. *Let* $\mathrm{Const}=\sum_{k\ge0}\mathrm{H}_{y_1^k}\,y_1^k$. *Then*

$$\mathrm{Const}=\exp\left[-\sum_{k\ge1}\mathrm{H}_{y_k}\frac{(-y_1)^k}{k}\right]\quad\textit{and}\quad\mathrm{Const}^{-1}=\exp\left[\sum_{k\ge1}\mathrm{H}_{y_k}\frac{(-y_1)^k}{k}\right].$$

DEFINITION 3 ([**12**]). *Let* $\zeta_{ш}:(\mathbb{C}\langle X\rangle,ш)\to(\mathbb{C},.)$ *be the algebra morphism (*i.e. *for any* $u,v\in X^*,\zeta_{ш}(u\,ш\,v)=\zeta_{ш}(u)\zeta_{ш}(v)$*) verifying for any convergent word* $w\in x_0X^*x_1,\zeta_{ш}(w)=\zeta(w)$*, and such that* $\zeta_{ш}(x_0)=\zeta_{ш}(x_1)=0$.

Then, the noncommutative generating series $Z_{ш}=\sum_{w\in X^*}\zeta_{ш}(w)\,w$ verifies $Z_{ш}=Z$ [**12**]. In consequence, $Z_{ш}$ is the unique Lie exponential verifying $\langle Z_{ш}|x_0\rangle=\langle Z_{ш}|x_1\rangle=0$ and $\langle Z_{ш}|w\rangle=\zeta(w)$, for any $w\in x_0X^*x_1$.

PROPOSITION 7. $\mathrm{P}(z)\widetilde{_{z\to0}}e^{x_0\log z}$ *and* $\mathrm{P}(z)\widetilde{_{z\to1}}\mathrm{Mono}(z)Z$.

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

COROLLARY 1. *Let* $\Pi(z)=\pi_Y\mathrm{P}(z)=\sum_{w\in Y^*}\mathrm{P}_w(z)\,w$. *Then* $\Pi(z)\widetilde{_{z\to1}}\mathrm{Mono}(z)\pi_Y Z$.

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

COROLLARY 2. $\mathrm{H}(N)\widetilde{_{N\to\infty}}\mathrm{Const}(N)\pi_Y Z$.

THEOREM 4.

$$\lim_{z\to 1}\exp\Big(-y_1\log\frac{1}{1-z}\Big)\Lambda(z)=\lim_{N\to\infty}\exp\Big(\sum_{k\geq 1}\mathrm{H}_{y_k}(N)\frac{(-y_1)^k}{k}\Big)\mathrm{H}(N)=\pi_Y Z,$$

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. □

3.3. Generalized Euler constants associated to divergent polyzêtas.

DEFINITION 4. *Let* $\zeta_{\sqcup\!\sqcup} : (\mathbb{C}\langle Y\rangle, \sqcup\!\sqcup) \to (\mathbb{C}, .)$ *the algebra morphism (*i.e. *for any convergent word* $u, v \in Y^*, \zeta_{\sqcup\!\sqcup}(u \sqcup\!\sqcup v) = \zeta_{\sqcup\!\sqcup}(u)\zeta_{\sqcup\!\sqcup}(v)$*) verifying for any* $w \in Y^* \setminus y_1Y^*$, $\zeta_{\sqcup\!\sqcup}(w) = \zeta(w)$ *and such that* $\zeta_{\sqcup\!\sqcup}(y_1) = \gamma$.

PROPOSITION 8.

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

PROOF. By (20) and applying the (surjective) morphism $\zeta_{\sqcup\!\sqcup}$, we get the expected result. □

In consequence,

THEOREM 5 ([**13**]). *For* $k > 0$*, the constant* $\zeta_{\sqcup\!\sqcup}(y_1^k)$ *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* $l = 0, .., k$*, the coefficient of* γ^l *is of weight* $k - l$*.*

EXAMPLE 6.

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

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

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

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

n \ k	0	1	2	3	4	5
0	1					
1	0	t_1				
2	0	t_2	t_1^2			
3	0	t_3	$3t_1t_2$	t_1^3		
4	0	t_4	$3t_2^2+4t_1t_3$	$6t_1^2t_2$	t_1^4	
5	0	t_5	$10t_2t_3+5t_1t_4$	$10t_1^2t_3+15t_1t_2^2$	$10t_1^3t_2$	t_1^5

In particular, we have

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

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

Let us build the noncommutative generating series of $\zeta_{⧢}(w)$ and let us take the constant part of the two members of $\mathrm{H}(N) \underset{N\to\infty}{\sim} \mathrm{Const}(N)\pi_Y Z$, we have

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

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

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

Corollary 3. *For all* $w \in Y^*\setminus y_1Y^*$ *and* $k\geq 0$*, we have*

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

Example 8.

$$\begin{aligned}\zeta_{⧢}(y_1^2y_2) &= \zeta_{⧢}(y_1^2y_2)+\zeta_{⧢}(y_1y_2)b_{1,1}(\gamma)+\frac{\zeta(2)}{2!}\big(b_{2,1}(-\zeta(2))+b_{2,2}(\gamma)\big)\\ &= 3\zeta(2,1,1)-2\zeta(2,1)\gamma+\frac{\zeta(2)}{2}\left(-\zeta(2)+\gamma^2\right),\end{aligned}$$

and using the reduction table, we find

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

a result in agreement with Example 4.

In consequence,

Theorem 7 ([**13**]). *For* $w\in Y^*\backslash y_1Y^*, k\geq 0$*, the constant* $\zeta_{⧢}(y_1^k w)$ *associated to* $\zeta(y_1^k w)$ *is a polynomial of degree* k *in* γ *and with coefficients in* $\mathcal{Z}$*. Moreover, for* $l=0,..,k$*, the coefficient of* γ^l *is of weight* $|w|+k-l$*.*

4. Applications to maxima in hypercubes

Definition 5. *Let* $w = y_{s_1}\ldots y_{s_r}\in Y^*$*. For* $N\geq k\geq 1$*, the harmonic sum* $\mathrm{A}_w(N;k)$ *is defined as*

$$\mathrm{A}_w(N;k) = \sum_{N\geq n_1\geq\ldots\geq n_r\geq k}\frac{1}{n_1^{s_1}\ldots n_r^{s_r}}.$$

For convenience, we use the notation $\mathrm{A}_w(N)$ instead of $\mathrm{A}_w(N;1)$ (see Definition 2).

Proposition 9. *For any* $u,v\in Y^*, \mathrm{A}_{u ⧢ v}(N;k) = \mathrm{A}_u(N;k)\mathrm{A}_v(N;k)$*.*

In all the sequel, $|w|_2$ denotes the number of occurences 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:

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

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* $S_\rho = \{y_1^4, y_1y_2y_1, y_1^2y_2, y_2y_1^2, y_2^2\}$*.*

Theorem 8.

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

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

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

See Appendix A for more examples

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

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

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

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

Proposition 10. *For any integers $n\ge l$, $\mathrm{A}_{y_1^d}(n;l) = \displaystyle\sum_{\substack{k_1+\ldots+dk_d=d\\ k_1,\ldots,k_d>0}}\frac{\mathrm{A}_1^{k_1}(n;l)\ldots\mathrm{A}_d^{k_d}(n;l)}{1^{k_1}k_1!\ldots d^{k_d}k_d!}$*

Since $\mathrm{A}_r(n;l+1)=\mathrm{A}_r(n)-\mathrm{A}_r(l)$, for any integer r [1], this enables to turn the summand into a polynomial involving only some $\mathrm{A}_w(n)$ and $\mathrm{A}_w(l)$.

- 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 $\dfrac{A_w(l)}{l}$ left, but by Formula (23), they simply reduce to $A_{y_1w}(n-1)$.

$$\begin{aligned}\mathbb{V}ar(K_{n,3}) &= \mathbb{E}(K_{n,3}^2) - \mu_{n,3}^2\\ &= \mathrm{A}_{1,1}(n) + 3\,{\mathrm{A}_1}^2(n)\mathrm{A}_{1,1}(n-1) - 12\mathrm{A}_1(n)\mathrm{A}_{1,1,1}(n-1)\\ &+ 6\mathrm{A}_1(n)\mathrm{A}_{1,2}(n-1) + 18\,\mathrm{A}_{1,1,1,1}(n-1) - 12\,\mathrm{A}_{1,1,2}(n-1)\\ &- 12\mathrm{A}_{1,2,1}(n-1) + 6\mathrm{A}_{1,3}(n-1) + 3\mathrm{A}_2(n)\mathrm{A}_{1,1}(n-1) - \mathrm{A}_{1,1}^2(n).\end{aligned}$$

We can now compute the asymptotic expansion of $\mathbb{V}ar(K_{n,d})$.

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,*

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

This is a direct consequence of Proposition 6.

Example 11.

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

See Appendix B for more examples

[1] while 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

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

Appendix B: Asymptotic expansions of $\mathbb{V}ar(K_{n,d})$

$$
\begin{aligned}
\mathbb{V}ar(K_{n,4}) \;=\;& \left(\frac{1}{3!}+\kappa_4\right)\ln^3(n)+\left(-\frac{53}{5}\,\zeta(2)^2+6\,\zeta(3)\,\gamma+\frac{1}{2}\,\gamma\right)\ln^2(n)\\
+\;& \left(97\,\zeta(5)-\frac{106}{5}\,\zeta(2)^2\,\gamma+16\,\zeta(2)\,\zeta(3)+6\,\zeta(3)\,\gamma^2+\frac{1}{2}\,\zeta(2)+\frac{1}{2}\,\gamma^2\right)\ln(n)\\
+\;& \frac{1}{3}\,\zeta(3)-\frac{53}{5}\,\zeta(2)^2\,\gamma^2-\frac{3719}{70}\,\zeta(2)^3+\frac{1}{6}\,\gamma^3+\frac{1}{2}\,\zeta(2)\,\gamma\\
+\;& 16\,\zeta(2)\,\zeta(3)\,\gamma-3\,\zeta(3)^2+2\,\zeta(3)\,\gamma^3+97\,\zeta(5)\,\gamma+\mathrm{o}(1)
\end{aligned}
$$

$$
\begin{aligned}
\mathbb{V}ar(K_{n,5}) \;=\;& \left(\frac{1}{4!}+\kappa_5\right)\ln^4(n)+\left(\frac{1}{6}\,\gamma-\frac{98}{3}\,\zeta(5)+\frac{33}{10}\,\zeta(2)^2\,\gamma-\frac{13}{3}\,\zeta(2)\,\zeta(3)\right)\ln^3(n)\\
+\;& \left(\frac{10123}{140}\,\zeta(2)^3+\frac{47}{2}\,\zeta(3)^2+\frac{99}{20}\,\zeta(2)^2\,\gamma^2+\frac{1}{4}\,\gamma^2+\frac{1}{4}\,\zeta(2)-13\,\zeta(2)\,\zeta(3)\,\gamma\right.\\
-\;& \left.98\,\zeta(5)\,\gamma\right)\ln^2(n)+\left(\frac{1}{6}\,\gamma^3+\frac{33}{10}\,\zeta(2)^2\,\gamma^3+\frac{1}{2}\,\zeta(2)\,\gamma-950\,\zeta(7)\right.\\
-\;& 13\,\zeta(2)\,\zeta(3)\,\gamma^2+47\,\zeta(3)^2\,\gamma+\frac{1}{3}\,\zeta(3)-\frac{317}{5}\,\zeta(3)\,\zeta(2)^2+\frac{10123}{70}\,\zeta(2)^3\,\gamma\\
-\;& \left.98\,\zeta(5)\,\gamma^2-222\,\zeta(2)\,\zeta(5)\right)\ln(n)-\frac{13}{3}\,\zeta(2)\,\zeta(3)\,\gamma^3+\frac{47}{2}\,\zeta(3)^2\,\gamma^2\\
-\;& \frac{317}{5}\,\zeta(3)\,\zeta(2)^2\,\gamma-\frac{98}{3}\,\zeta(5)\,\gamma^3+\frac{33}{40}\,\zeta(2)^2\,\gamma^4+\frac{32}{3}\,\zeta(3)\,\zeta(5)+\frac{10123}{140}\,\zeta(2)^3\,\gamma^2\\
-\;& 222\,\zeta(2)\,\zeta(5)\,\gamma+\frac{1}{24}\,\gamma^4-950\,\zeta(7)\,\gamma+50\,\zeta(6,2)+\frac{1}{4}\,\zeta(2)\,\gamma^2+\frac{1}{3}\,\zeta(3)\,\gamma\\
+\;& \frac{9}{40}\,\zeta(2)^2+\frac{95}{6}\,\zeta(2)\,\zeta(3)^2+\frac{134739}{350}\,\zeta(2)^4+\mathrm{o}(1)
\end{aligned}
$$

$$
\begin{aligned}
\mathbb{V}ar(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.\\
-\;& \left.\frac{22711}{2520}\,\zeta(2)^3\right)\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.\\
+\;& \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\\
+\;& \left.\frac{25}{2}\,\zeta(5)\,\gamma^2\right)\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.\\
+\;& \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\\
+\;& \left.\frac{381}{2}\,\zeta(2)\,\zeta(5)\,\gamma\right)\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.\\
-\;& \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\\
-\;& \left.684\,\zeta(3)\,\zeta(5)\,\gamma+\frac{19209}{8}\,\zeta(2)\,\zeta(7)+\frac{1}{24}\,\gamma^4\right)\ln(n)+\frac{127}{2}\,\zeta(2)\,\zeta(5)\,\gamma^3\\
+\;& \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+\mathrm{o}(1).
\end{aligned}
$$

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UNIVERSITÉ LILLE 2, 1 PLACE DÉLIOT, 59024 LILLE
E-mail address: ccostermans@univ-lille2.fr

UNIVERSITÉ LILLE 2, 1 PLACE DÉLIOT, 59024 LILLE
E-mail address: hoang@univ-lille2.fr