

# Algorithmic and Combinatoric Aspects of Multiple Harmonic Sums

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# Outline

- 1 Motivation
- 2 Generating series
  - Ordinary G.S. of  $\{H_w(N), N \geq 0\}$
  - Noncommutative G.S. of  $\{P_w, w \in X^*\}$
- 3 Computing Asymptotic Expansion
  - Singular expansion
  - Asymptotic expansion

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# Multiple Harmonic Sums

- Generalized Harmonic Numbers

$$H_r(N) = \sum_{n=1}^N \frac{1}{n^r} \quad N \in \mathbb{N}, r \geq 0$$

Extended to compositions  $\underline{s} = (s_1, \dots, s_r)$

$$H_{\underline{s}}(N) = \sum_{N \geq n_1 > \dots > n_r > 0} \frac{1}{n_1^{s_1} \dots n_r^{s_r}}$$

- Appear in the study of probabilities (quadtrees [Flajolet et al., 93], maxima in hypercubes [Devroye et al., 05]), and also in quantum physics, knot theory...etc

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# Our goal

- Asymptotic behaviour of  $H_{\underline{s}}(N)$  ?
- Linked the behaviour of  $P_{\underline{s}}(z) = \sum_{N \geq 0} H_{\underline{s}}(N)z^N$ , as  $z \rightarrow 1$ .  
But

$$P_{\underline{s}}(z) = \frac{1}{1-z} \text{Li}_{\underline{s}}(z)$$

► Polylogarithm ?

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

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# Definition

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For  $w \in X^*$ , we put  $P_w(z) = \frac{Li_w(z)}{1-z}$ .

## Proposition

Let  $w \in X^*x_1$ . Then  $P_w(z)$  is the ordinary generating series of  $\{H_w(N), N \geq 0\}$  :

$$P_w(z) = \sum_{N \geq 0} H_w(N)z^N$$

# Noncommutative generating series

Let 
$$L(z) = \sum_{w \in X^*} Li_w(z)w \quad \text{and} \quad P(z) = \sum_{w \in X^*} P_w(z)w.$$

Theorem (Factorization theorem)

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

where  $\sigma$  is the morphism defined by  $\sigma(x_0) = -x_1, \sigma(x_1) = -x_0$ .

This is due to the fact that [Hoang et al.,99]

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



## Example

For example,

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

Then, we deduce the *singular expansion* of  $P_{2,1}$  around  $z = 1$ .

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# Main Theorem

## Theorem

Let  $\mathcal{C} = \mathbb{C} \left[ z, \frac{1}{z}, \frac{1}{1-z} \right]$  and  $g \in \mathcal{C}[(P_w)_{w \in X^* x_1}]$ . There exist  $a_j \in \mathbb{C}$ ,  $\alpha_j \in \mathbb{Z}$  and  $\beta_j \in \mathbb{N}$  such that

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

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

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

# Proof(1)

- First : reduction to the case  $f(z) = P_w(z)$ .  
 Factorization of  $P \Rightarrow P_w(z) = \sum_{finite} \lambda_u P_u(1 - z), u \in X^* x_1$ .
- For  $u \in X^* x_1 \cup \{x_0\}$ , we have

$$P_u(1 - z) = \sum_{n \geq 0} H_u(n)(1 - z)^n$$

$$P_{x_0}(z) = \frac{\log(1 - z)}{z}.$$

$\Rightarrow$  The first expansion follows.

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# Example

From

$$\begin{aligned}
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 &\quad - \frac{1}{2}\frac{z}{1-z}\log^2(1-z)P_1(1-z) + \frac{\zeta(3)}{1-z},
 \end{aligned}$$

we deduce

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

## Proof(2)

- Note that  $(1 - z)^\alpha \log^\beta(1 - z) = (-1)^\beta \beta! (1 - z)^{\alpha+1} P_{y_1^\beta}(z)$ .  
 But  $[z^n] P_{y_1^\beta}(z) = H_{y_1^\beta}(n) = H_{1,1,\dots,1}(n)$ .

### Proposition

$H_{y_1^k}$  is an algebraic combination of  $\{H_r\}_{1 \leq r \leq k}$ , which are algebraically independent.

- Expansion of  $H_r(n)$  computable by Euler-MacLaurin
- Then, action of  $1 - z$  over  $P_w$

$$[z^n](1 - z)P_w(z) = H_w(n) - H_w(n - 1),$$

$$[z^n] \frac{P_w(z)}{1 - z} = \sum_{k=0}^n H_w(k).$$

## Example

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

But

$$\begin{aligned}
 [z^N] \frac{\zeta(3)}{1-z} &= \zeta(3) \\
 [z^N] \log(1-z) &= -\frac{1}{N},
 \end{aligned}$$

## Example(2)

$$\begin{aligned}
 [z^N] \frac{\log^2(1-z)}{2} &= [z^N] \frac{2!(1-z)P_{y_1^2}(z)}{2} \\
 &= [z^N](1-z)P_{y_1^2}(z) \\
 &= H_{y_1^2}(N) - H_{y_1^2}(N-1)
 \end{aligned}$$

But

$$H_{y_1^2}(N) = \frac{1}{2}[H_1^2(N) - H_2(N)].$$

So, we finally find :

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

*Thank you for your attention*

# Polylogarithms and Euler-Zagier sums : definitions

- For  $k$  a positive integer,

$$\text{Li}_k(z) = \sum_{n>0} \frac{z^n}{n^k}.$$

- For  $\underline{s} = (s_1, \dots, s_r)$ , and for  $|z| < 1$  we define

$$\text{Li}_{\underline{s}}(z) = \sum_{n_1 > \dots > n_r > 0} \frac{z^{n_1}}{n_1^{s_1} \dots n_r^{s_r}}.$$

For  $s_1 > 1$ , by an Abel's theorem, we have :

$$\lim_{z \rightarrow 1} \text{Li}_{\underline{s}}(z) = \lim_{N \rightarrow +\infty} \text{H}_{\underline{s}}(N) = \zeta(\underline{s}).$$

# Encoding by words

Encoding for  $\underline{s}$  :

$$\underline{s} = (s_1, \dots, s_r) \longleftrightarrow w = x_0^{s_1-1} x_1 \cdots x_0^{s_r-1} x_1 \in X^*,$$

where  $X = \{x_0, x_1\}$ .

$$\text{Li}_{\underline{s}}(z) = \text{Li}_w(z),$$

and in the same way, we denote

$$H_{\underline{s}}(N) = H_w(N), \quad \text{and} \quad \zeta(\underline{s}) = \zeta(w).$$

We extend also the definition of  $\text{Li}_w$  by putting  $\text{Li}_{x_0}(z) = \log(z)$ .

▶ Back

# Lyndon words

- $X^*$  totally ordered by putting :  $x_0 < x_1$  .
- $l$  Lyndon word iff  $l = uv, v \neq \epsilon \Rightarrow l < v$

## Example

Set of Lyndon words over  $X$ , of length  $\leq 4$  :

$$\text{Lyn}(X) = \{x_0, x_1, x_0^2 x_1, x_0 x_1^2, x_0^3 x_1, x_0^2 x_1^2, x_0 x_1^3, \dots\}$$

▶ Back



## P.B.W. Basis [Reutenauer, 93]

- For  $l \in \text{Lyn}(X)$ ,  $l = uv$ ,  $u, v \in \text{Lyn}(X)$  and  $v$  as long as possible

$$\begin{cases} Q_l &= [Q_u, Q_v] = Q_u Q_v - Q_v Q_u \\ Q_x &= x \quad \text{if } x \in X, \end{cases}$$

- For  $l = xw \in \text{Lyn}(X)$ ,  $x \in X$ ,  
 $w = l_1^{\alpha_1} l_2^{\alpha_2} \dots l_k^{\alpha_k}$ ,  $l_1 > l_2 > \dots > l_k$ .

$$S_l = x \frac{S_{l_1}^{\sqcup \alpha_1} \sqcup \dots \sqcup S_{l_k}^{\sqcup \alpha_k}}{\alpha_1! \alpha_2! \dots \alpha_k!},$$

where  $\sqcup$  denotes the shuffle product on words.

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# Lyndon words, bracket forms and dual basis

$I$	$Q_I$	$S_I$
$x_0$	$x_0$	$x_0$
$x_1$	$x_1$	$x_1$
$x_0x_1$	$[x_0, x_1]$	$x_0x_1$
$x_0^2x_1$	$[x_0, [x_0, x_1]]$	$x_0^2x_1$
$x_0x_1^2$	$[[x_0, x_1], x_1]$	$x_0x_1^2$
$x_0^3x_1$	$[x_0, [x_0, [x_0, x_1]]]$	$x_0^3x_1$
$\vdots$	$\vdots$	$\vdots$
$x_0^3x_1^3$	$[x_0, [x_0, [[[x_0, x_1], x_1], x_1]]]$	$x_0^3x_1^3$
$x_0^2x_1x_0x_1^2$	$[x_0, [[x_0, x_1], [[x_0, x_1], x_1]]]$	$3x_0^3x_1^3 + x_0^2x_1x_0x_1^2$

▶ Back

## Going further

$$H_1(N) \sim \log N + \gamma - \sum_{k=1}^{+\infty} \frac{B_k}{k} \frac{1}{N^k},$$

$$H_r(N) \sim \zeta(r) - \frac{1}{(r-1)N^{r-1}} - \sum_{k=r}^{+\infty} \frac{B_{k-r+1}}{k-r+1} \binom{k-1}{r-1} \frac{1}{N^k}$$

And

$$H_{y_1^k} = \sum_{a_1+2a_2+\dots+ka_k=k} (-1)^{k-\sum a_i} \frac{H_1^{a_1} \dots H_k^{a_k}}{1^{a_1} a_1! \dots k^{a_k} a_k!}$$

# Outline

- 4 Combinatorics on words
  - Shuffle Algebras
  - Polylogarithms

# Shuffle products

The *shuffle* (resp. *stuffle*) of  $u = au'$  and  $v = bv' \in X^*$  (resp.  $u = y_i u'$  and  $v = y_j v' \in Y^*$ ) is defined by

$$\begin{aligned} \epsilon \sqcup u &= u \sqcup \epsilon = u \text{ and} \\ u \sqcup v &= a(u' \sqcup v) + b(u \sqcup v'), \end{aligned}$$

resp.  $\epsilon \sqcup u = u \sqcup \epsilon = u$  and

$$u \sqcup v = y_i(u' \sqcup v) + y_j(u \sqcup v') + y_{i+j}(u' \sqcup v').$$

For example,

- $x_0 x_1 \sqcup x_1 = x_1 x_0 x_1 + 2x_0 x_1^2$  and  $y_2 \sqcup y_1 = y_1 y_2 + y_2 y_1 + y_3$ ,
- $x_0 x_1 \sqcup x_0 x_1 = 2x_0 x_1 x_0 x_1 + 4x_0 x_1^2$  and  $y_2 y_1 \sqcup y_3 = y_2 y_1 y_3 + y_2 y_3 y_1 + y_3 y_2 y_1 + y_2 y_4 + y_5 y_1$ .

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# Justification of the stuffle product

$$\sum_{n=1}^N \frac{1}{n^{s_1}} \sum_{m=1}^N \frac{1}{m^{s_2}} = \sum_{N \geq n > m > 0} \frac{1}{n^{s_1} m^{s_2}} + \sum_{N \geq m > n > 0} \frac{1}{m^{s_2} n^{s_1}} + \sum_{N \geq n > 0} \frac{1}{n^{s_1 + s_2}}$$

$$\begin{aligned} H_{s_1}(N)H_{s_2}(N) &= H_{s_1, s_2}(N) + H_{s_2, s_1}(N) + H_{s_1 + s_2}(N) \\ y_{s_1} \sqcup y_{s_2} &= y_{s_1, s_2} + y_{s_2, s_1} + y_{s_1 + s_2} \end{aligned}$$

With the convention  $H_{\underline{s}} = H_w$ ,

Theorem (Hoang, 03)

Let  $\mathcal{H}_{\mathbb{C}} = (\text{span}_{\mathbb{C}}(H_w \mid w \in Y^*), \cdot)$ . Then  $\mathcal{H}_{\mathbb{C}} \simeq (\mathbb{C}\langle Y \rangle, \sqcup)$

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# Polylogarithms : properties (1)

$$\underline{s} = (s_1, \dots, s_r) \longleftrightarrow u = x_0^{s_1-1} x_1 \cdots x_0^{s_r-1} x_1 \in X^*$$

Putting  $\omega_0 = \frac{dz}{z}$  and  $\omega_1 = \frac{dz}{1-z}$ , we have

$$\text{Li}_{\underline{s}}(z) = \text{Li}_u(z) = \int_{0 \rightsquigarrow z} \omega_0^{s_1-1} \omega_1 \cdots \omega_0^{s_r-1} \omega_1.$$

$\Rightarrow$  Allows to extend the definition of  $\text{Li}_u$  over  $X^*$  with the definition

$$\text{Li}_{x_0}(z) = \log(z).$$

## Polylogarithms : properties (2)

Theorem (Hoang et al.,00)

*The  $\mathbb{C}$ -algebra of  $\{\text{Li}_w, w \in X^*\}$  is isomorphic to  $(\mathbb{C}\langle X \rangle, \sqcup)$ .*

### Examples

Since  $x_0x_1 \sqcup x_1 = x_1x_0x_1 + 2x_0x_1^2$ , we get :

$$\text{Li}_2 \text{Li}_1 = \text{Li}_{1,2} + 2 \text{Li}_{2,1}$$

From  $x_0x_1 \sqcup x_0x_1 = 2x_0x_1x_0x_1 + 4x_0x_1^2$ , we get :

$$\text{Li}_2^2 = 2 \text{Li}_{2,2} + 4 \text{Li}_{2,1}$$