# Structure and Asymptotic Expansion of Multiple Harmonic Sums

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# Outline

# Multiple Harmonic Sums (M.H.S.)

- Generalized Harmonic Numbers

$$\mathrm{H}_r(N) = \sum_{n=1}^{N} \frac{1}{n^r} \qquad N \in \mathbb{N}, r \geq 0$$

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

$$\mathrm{H}_{\underline{\mathbf{s}}}(N) = \sum_{N \geq n_1 > \ldots > n_r > 0} \frac{1}{n_1^{s_1} \ldots n_r^{s_r}}$$

- Appear in the study of probabilities (quadtrees [Flajolet et al., 93]), in quantum physics [Blümlein, 99], in knot theory...etc

# Our results

- Description of the algebra of Multiple Harmonic Sums (M.H.S), *isomorphic* to a *shuffle algebra*.
- Algorithm to compute the Asymptotic Expansion (A.E.) of $\mathrm{H}_{\underline{\mathbf{s}}}(N)$, as $N \to +\infty$, i.e. a polynomial $p \in \mathbb{R}[X, Y]$ verifying

$$\mathrm{H}_{\underline{\mathbf{s}}}(N) = p\left(\log N, \frac{1}{N}\right) + \mathrm{O}\left(\frac{1}{N^q}\right).$$

# Symbolic encoding

We adopt the following encoding :

$$\underline{\mathbf{s}} = (s_1, \ldots, s_r) \longleftrightarrow w = y_{s_1} \cdots y_{s_r} \in Y^*,$$

$$\text{where } Y = \{y_i | i \in \mathbb{N} \setminus \{0\}\}.$$

We now denote $\mathrm{H}_{\underline{\mathbf{s}}}(N) = \mathrm{H}_w(N)$ and, for $s_1 > 1$,

$$\lim_{N \to +\infty} \mathrm{H}_{\underline{\mathbf{s}}}(N) = \zeta(\underline{\mathbf{s}}) = \zeta(w) \quad (MZV).$$

# Outline

# Harmonic product

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

$$\Rightarrow \mathrm{H}_{y_{s_1}}(N)\mathrm{H}_{y_{s_2}}(N)=\mathrm{H}_{y_{s_1}y_{s_2}}(N)+\mathrm{H}_{y_{s_2}y_{s_1}}(N)+\mathrm{H}_{y_{s_1+s_2}}(N)$$

The commutative *harmonic* product of two words is defined by

$$\begin{aligned}\epsilon \uplus u &= u,\\ (y_i u)\uplus(y_j v) &= y_i(u\uplus v)+y_j(u\uplus v)+y_{i+j}(u\uplus v).\end{aligned}$$

## Theorem (Hoffman, 97)

*For any* $u,v\in Y^*$, $H_{u\uplus v}(N)=H_u(N)\,H_v(N)$.

# Isomorphism theorem

## Example

$$\begin{aligned} y_2 y_5 \uplus y_4 &= y_2(y_5 \uplus y_4) + y_4(y_2 y_5 \uplus \epsilon) + y_6(y_5 \uplus \epsilon) \\ &= y_2(y_5 y_4 + y_4 y_5 + y_9) + y_4 y_2 y_5 + y_6 y_5 \\ &= y_2 y_5 y_4 + y_2 y_4 y_5 + y_4 y_2 y_5 + y_2 y_9 + y_6 y_5. \end{aligned}$$

So,

$$\mathrm{H}_{2,5}(N)\mathrm{H}_4(N) = \mathrm{H}_{2,5,4}(N)+\mathrm{H}_{2,4,5}(N)+\mathrm{H}_{4,2,5}(N)+\mathrm{H}_{2,9}(N)+\mathrm{H}_{6,5}(N).$$

Denoting $\mathcal{H}_{\mathbb{R}} = (\text{ Span } \{H_w\}_{w \in Y^*}, .)$, we have a better result :

## Theorem

$$\mathcal{H}_{\mathbb{R}} \simeq (\mathbb{R}\langle Y \rangle), \uplus ).$$

# Radford theorem

## Theorem (Radford, Hoffman, 97)

$$(\mathbb{R}\langle Y\rangle, \,\text{⧢}\,) \simeq (\mathbb{R}[Lyn(Y)], \,\text{⧢}\,)$$

Any word can be decomposed, *uniquely*, as a product of Lyndon words. Lyndon word?

*Remark :* The process is constructive. Construction?

## Corollary

$$\mathcal{H}_{\mathbb{R}} \simeq \mathbb{R}[\mathrm{H}_l, l \in Lyn(Y)].$$

# Examples

## Example

$$y_1 y_4 y_2 = y_1 \uplus y_4 y_2 - y_4 y_1 y_2 - y_4 y_2 y_1 - y_4 y_3 - y_5 y_2.$$

$$\iff \quad \mathrm{H}_{1,4,2} = \mathrm{H}_1 \mathrm{H}_{4,2} - \mathrm{H}_{4,1,2} - \mathrm{H}_{4,2,1} - \mathrm{H}_{4,3} - \mathrm{H}_{5,2}.$$

## Corollary

*The Harmonic Sums* $\{\mathrm{H}_w, w \in Y^*\}$ *are* $\mathbb{R}$*-linearly independent.*

# Outline

# Recursive definition of $\mathrm{H}_w$

For $w = y_{s_1} \ldots y_{s_r} = y_{s_1} w'$,

$$\begin{aligned}
\mathrm{H}_w(N) &= \sum_{N \geq n_1 > \ldots > n_r > 0} \frac{1}{n_1^{s_1} \ldots n_r^{s_r}} \\
&= \sum_{n_1 = r}^{N} \frac{1}{n_1^{s_1}} \sum_{n_1 - 1 \geq n_2 > \ldots > n_r > 0} \frac{1}{n_2^{s_2} \ldots n_r^{s_r}} \\
&= \sum_{i = r}^{N} \frac{1}{i^{s_1}} \mathrm{H}_{w'}(i-1).
\end{aligned}$$

# Principle of the algorithm

- If $w = y_r, r \geq 1$ the asymptotic expansion of $\mathrm{H}_r(N)$ is known (Euler-MacLaurin).

Example

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

- If $w = y_r w'$, we use the recursive definition under the form

$$\mathrm{H}_w(N) = \zeta(w) - \sum_{i=N+1}^{+\infty} \frac{1}{i^{s_1}} \mathrm{H}_{w'}(i-1)$$

and we replace $\mathrm{H}_{w'}(i-1)$ by its A.E.

# Example for $w = y_4 y_2$

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

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

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

# Example for $w = y_4 y_2$ (2)

So, expanding the remainder in $N$,

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

*Remark* : we got an A.E. up to order 6 by computing an A.E. of the numerator up to order 3.

# Case of a divergent word $w = y_1 y_4$

- Problem : $\zeta(1,4)$ diverges ! Indeed, $\mathrm{H}_w(N)$ converges when $N \to \infty$ iff $w = y_{s_1} w'$ with $s_1 > 1$.
- Solution: Radford decomposition.
  Since $y_1 y_4 = y_1 \uplus y_4 - y_4 y_1 - y_5$, we have

$$
\begin{aligned}
\mathrm{H}_{1,4}(N) &= \mathrm{H}_1(N)\mathrm{H}_4(N) - \mathrm{H}_{4,1}(N) - \mathrm{H}_5(N) \\
&= \frac{\pi^4}{90} \ln(N) + \frac{\pi^4}{90}\gamma - \zeta(4,1) - \zeta(5) + \frac{\pi^4}{180}\frac{1}{N} \\
&- \frac{\pi^4}{1080}\frac{1}{N^2} + \frac{1}{9}\frac{1}{N^3} + \left(\frac{\pi^4}{10800} - \frac{1}{24}\right)\frac{1}{N^4} + \mathrm{O}\left(\frac{1}{N^5}\right)
\end{aligned}
$$

- Conclusion : need to store a table of A.E. for M.H.S. indexed by Lyndon words.

*Thank you for your attention*

# Lyndon words

- $Y$ ordered by $y_i < y_j$ if $i > j \Rightarrow$ lexicographical order over $Y^*$
- $l \in Y^*$ Lyndon word $\Leftrightarrow$ $l$ strictly smaller than any of its proper right factors.
  We denote by $Lyn(Y)$ the set of Lyndon words over $Y$.
- Example : $w = y_1 y_4 y_2 \notin Lyn(Y)$ since $w > y_2$.
  But $u = y_4 y_2 y_1 \in Lyn(Y)$.

Back

# Construction

## Theorem

*Any nonempty word $w \in Y^*$ may be written uniquely as a decreasing product of Lyndon words :*

$$w = l_1^{\alpha_1} l_2^{\alpha_2} \dots l_n^{\alpha_n}, \quad l_i \in Lyn(Y), \quad l_1 > l_2 > \dots > l_n.$$

## Lemma

*Let $w = l_1^{\alpha_1} l_2^{\alpha_2} \dots l_n^{\alpha_n} \in Y^*$. Then, putting*

$$Q_w = \frac{l_1^{\sqcup\!\sqcup\, \alpha_1} \sqcup\!\sqcup\, l_2^{\sqcup\!\sqcup\, \alpha_2} \dots \sqcup\!\sqcup\, l_n^{\sqcup\!\sqcup\, \alpha_n}}{\alpha_1! \alpha_2! \dots \alpha_n!},$$

*we have $Q_w = w + R_w$, where $R_w$ only contains words smaller than $w$.* Back