Eighth lecture: April 25, 2011

9 The structure of the shuffle and harmonic algebras

We shall see that the shuffle and harmonic algebras are polynomial algebras in the Lyndon words.

Consider the lexicographic order on X^* with $x_0 < x_1$ and denote by $\mathcal{L}$ the set of Lyndon words (see §3). We have seen that x_0 is the only Lyndon word which is not in $\mathfrak{H}^1_{ш}$, while x_0 and x_1 are the only Lyndon words which are not in $\mathfrak{H}^0_{ш}$.

For instance, there are $1 + 2 + 2^2 + 2^3 = 15$ words of weight ≤ 3, and 5 among them are Lyndon words:

$$x_0 < x_0^2 x_1 < x_0 x_1 < x_0 x_1^2 < x_1.$$

We introduce 5 variables

$$T_{10},\ T_{21},\ T_{11},\ T_{12},\ T_{01},$$

where T_{ij} corresponds to $x_0^i x_1^j$.

9.1 Shuffle

The structure of the commutative algebra $\mathfrak{H}_{ш}$ is given by *Radford Theorem.*

Theorem 33. *The three shuffle algebras are (commutative) polynomial algebras*

$$\mathfrak{H}_{ш} = K[\mathcal{L}]_{ш}, \quad \mathfrak{H}^1_{ш} = K\big[\mathcal{L} \setminus \{x_0\}\big]_{ш} \quad \textit{and} \quad \mathfrak{H}^0_{ш} = K\big[\mathcal{L} \setminus \{x_0, x_1\}\big]_{ш}.$$

We write the 10 non-Lyndon words of weight ≤ 3 as polynomials in these

Lyndon words as follows:

$$e = e,$$

$$x_0^2 = \frac{1}{2} x_0 ш x_0 = \frac{1}{2} T_{10}^2,$$

$$x_0^3 = \frac{1}{3} x_0 ш x_0 ш x_0 = \frac{1}{3} T_{10}^3,$$

$$x_0 x_1 x_0 = x_0 ш x_0 x_1 - 2 x_0^2 x_1 = T_{10} T_{11} - 2 T_{21},$$

$$x_1 x_0 = x_0 ш x_1 - x_0 x_1 = T_{10} T_{01} - T_{11},$$

$$x_1 x_0^2 = \frac{1}{2} x_0 ш x_0 ш x_1 - x_0 ш x_0 x_1 + x_0^2 x_1 = \frac{1}{2} T_{10}^2 T_{01} - T_{10} T_{11} + T_{21},$$

$$x_1 x_0 x_1 = x_0 x_1 ш x_1 - 2 x_0 x_1^2 = T_{11} T_{01} - 2 T_{12},$$

$$x_1^2 = \frac{1}{2} x_1 ш x_1 = \frac{1}{2} T_{01}^2,$$

$$x_1^2 x_0 = \frac{1}{2} x_0 ш x_1 ш x_1 - x_0 x_1 ш x_1 + x_0 x_1^2 = \frac{1}{2} T_{10} T_{01}^2 - T_{11} T_{01} + T_{12},$$

$$x_1^3 = \frac{1}{3} x_1 ш x_1 ш x_1 = \frac{1}{3} T_{01}^3.$$

Corollary 34. *We have*

$$\mathfrak{H}_ш = \mathfrak{H}_ш^1 [x_0]_ш = \mathfrak{H}_ш^0 [x_0, x_1]_ш \quad \textit{and} \quad \mathfrak{H}_ш^1 = \mathfrak{H}_ш^0 [x_1]_ш.$$

9.2 Harmonic algebra

Hoffman's Theorem gives the structure of the harmonic algebra $\mathfrak{H}_\star$:

Theorem 35. *The harmonic algebras are polynomial algebras on Lyndon words:*

$$\mathfrak{H}_\star = K[\mathcal{L}]_\star, \quad \mathfrak{H}_\star^0 = K\big[\mathcal{L} \setminus \{x_0, x_1\}\big]_\star \quad \textit{and} \quad \mathfrak{H}_\star^1 = K\big[\mathcal{L} \setminus \{x_0, x_1\}\big]_\star.$$

For instance, the 10 non-Lyndon words of weight ≤ 3 are polynomials in the

5 Lyndon words as follows:

$$e = e,$$

$$x_0^2 = x_0 \star x_0 = T_{10}^2,$$

$$x_0^3 = x_0 \star x_0 \star x_0 = T_{10}^3,$$

$$x_0x_1x_0 = x_0 \star x_0x_1 = T_{10}T_{11},$$

$$x_1x_0 = x_0 \star x_1 = T_{10}T_{01},$$

$$x_1x_0^2 = x_0 \star x_0 \star x_1 = T_{10}^2T_{01},$$

$$x_1x_0x_1 = x_0x_1 \star x_1 - x_0^2x_1 - x_0x_1^2 = T_{11}T_{01} - T_{21} - T_{12},$$

$$x_1^2 = \frac{1}{2}x_1 \star x_1 - \frac{1}{2}x_0x_1 = \frac{1}{2}T_{01}^2 - \frac{1}{2}T_{11},$$

$$x_1^2x_0 = \frac{1}{2}x_0 \star x_1 \star x_1 - \frac{1}{2}x_0 \star x_0x_1 = \frac{1}{2}T_{10}T_{01}^2 - \frac{1}{2}T_{10}T_{11},$$

$$x_1^3 = \frac{1}{6}x_1 \star x_1 \star x_1 - \frac{1}{2}x_0x_1 \star x_1 + \frac{1}{3}x_0^2x_1 = \frac{1}{6}T_{01}^3 - \frac{1}{2}T_{11}T_{01} + \frac{1}{3}T_{21}.$$

In the same way as Corollary 34 follows from Theorem 33, we deduce from Theorem 35:

Corollary 36. *We have*

$$\mathfrak{H}_\star = \mathfrak{H}_\star^1[x_0]_\star = \mathfrak{H}_\star^0[x_0, x_1]_\star \quad \textit{and} \quad \mathfrak{H}_\star^1 = \mathfrak{H}_\star^0[x_1]_\star.$$

Remark. Consider the diagram

$$\begin{array}{ccc} \mathfrak{H}_ш & \longrightarrow & K[\mathcal{L}]_ш \\ \Big\downarrow f & & \Big\downarrow g \\ \mathfrak{H}_\star & \longrightarrow & K[\mathcal{L}]_\star \end{array}$$

The horizontal maps are just the identitication of $\mathfrak{H}_ш$ with $K[\mathcal{L}]_ш$ and of $\mathfrak{H}_\star$ with $K[\mathcal{L}]_\star$. The vertical map f is the identity map on $\mathfrak{H}$, since the algebras $\mathfrak{H}_ш$ and $\mathfrak{H}_\star$ have the same underlying set $\mathfrak{H}$ (only the law differs). But the map g which makes the diagram commute is not a morphism of algebras: it maps each Lyndon word on itself, but consider, for instance, the image of the word x_0^2, as a polynomial in $K[\mathcal{L}]_ш$,

$$x_0^2 = (1/2)x_0 ш x_0 = (1/2)x_0^{ш 2},$$

but as a polynomial in $K[\mathcal{L}]_\star$,

$$x_0^2 = x_0 \star x_0 = x_0^{\star 2},$$

hence $g(T_{10}^2) = 2T_{10}^2$.

10 Regularized double shuffle relations

10.1 Hoffman standard relations

The relation $\zeta(2,1) = \zeta(3)$ is the easiest example of a whole class of linear relations among MZV.

For any word $w \in X^*$, each of $x_1 \star x_0 w x_1$ and $x_1 ш x_0 w x_1$ is the sum of $x_1 x_0 w x_1$ with other words in $x_0 X^* x_1$ (i.e. convergent words):

$$x_1 ш w - x_1 w \in \mathfrak{H}^0, \quad x_1 \star w - x_1 w \in \mathfrak{H}^0,$$

Hence

$$x_1 ш w - x_1 \star w \in \mathfrak{H}^0.$$

It turns out that these elements $x_1 ш w - x_1 \star w$ are in the kernel of $\widehat{\zeta} : \mathfrak{H}^0 \to \mathbf{R}$.

Proposition 37. *For $w \in \mathfrak{H}^0$,*

$$\widehat{\zeta}(x_1 \star w - x_1 ш w) = 0.$$

Since $x_1 ш e = x_1 \star e = e$, these relations are can be written in an equivalent way

$$\widehat{\zeta}(x_1 \star y_{\underline{s}} - x_1 ш y_{\underline{s}}) = 0 \quad \text{whenever } s_1 \geq 2.$$

They are called *Hoffman standard relations* between multiple zeta values.

Example. *Writing*

$$x_1 \star (x_0^{s-1} x_1) = y_1 \star y_s = y_1 y_s + y_s y_1 + y_{s+1}$$

and

$$x_1 ш (x_0^{s-1} x_1) = x_1 x_0^{s-1} x_1 + x_0 (x_1 ш x_0^{s-2} x_1) = \sum_{\nu=1}^{s} y_\nu y_{s+1-\nu} + y_s y_1,$$

we deduce

$$x_1 \star (x_0^{s-1} x_1) - x_1 ш (x_0^{s-1} x_1) = x_0^s x_1 - \sum_{\nu=1}^{s} x_0^{\nu-1} x_1 x_0^{s-\nu} x_1,$$

hence

$$\zeta(p) = \sum_{\substack{s+s'=p \\ s \geq 2,\ s' \geq 1}} \zeta(s, s').$$

Remark. *As we have seen, the word*

$$x_1 \star x_1 - x_1 ш x_1 = x_0 x_1$$

is convergent, but

$$\widehat{\zeta}(x_1 \star x_1 - x_1 ш x_1) = \zeta(2) \neq 0.$$

On the other hand a word like

$$x_1^2 \star x_0x_1 - x_1^2 \shuffle x_0x_1 = x_1x_0^2x_1 + x_0^2x_1^2 - x_1x_0x_1^2 - 2x_0x_1^3$$

is not convergent; also the "convergent part" of this word in the concatenation algebra $\mathfrak{H}$*, namely* $x_0^2x_1^2 - 2x_0x_1^3 = y_3y_1 - 2y_2y_1^2$*, does not belong to the kernel of* $\widehat{\zeta}$*:*

$$\zeta(3,1) = \frac{1}{4}\zeta(4), \quad \zeta(2,1,1) = \zeta(4).$$

We shall see (theorem 40*) that the convergent part in the shuffle algebra* $\mathfrak{H}_{\shuffle}$ *of a word of the form* $w \shuffle w_0 - w \star w_0$ *for* $w \in \mathfrak{H}^1$ *and* $w_0 \in \mathfrak{H}^0$ *is always in the kernel of* $\widehat{\zeta}$*.*

Hoffman's operator $d_1 : \mathfrak{H} \to \mathfrak{H}$ is defined by

$$\delta(w) = x_1 \star w - x_1 \shuffle w.$$

For $w \in \mathfrak{H}^0$, we have $d_1(w) \in \mathfrak{H}^0$ and the Hoffman standard relations (37) mean that it satisfies $d_1(\mathfrak{H}^0) \subset \ker \widehat{\zeta}$.

10.2 Ihara–Kaneko

There are further similar linear relations between MZV arising from *regularized double shuffle relations*

Recall Corollaries 34 and 36 of Radford and Hoffman concerning the structures of the algebras $\mathfrak{H}_{\shuffle}$ and $\mathfrak{H}_{\star}$ respectively (we take here for ground field K the field $\mathbf{R}$ of real numbers). From

$$\mathfrak{H}^1_{\shuffle} = \mathfrak{H}^0_{\shuffle}[x_1]_{\shuffle} \quad \text{and} \quad \mathfrak{H}^1_{\star} = \mathfrak{H}^0_{\star}[x_1]_{\star}$$

we deduce that there are two uniquely determined algebra morphisms

$$\widehat{Z}_{\shuffle} : \mathfrak{H}^1_{\star} \longrightarrow \mathbf{R}[X] \quad \text{and} \quad \widehat{Z}_{\star} : \mathfrak{H}^1_{\shuffle} \longrightarrow \mathbf{R}[T]$$

which extend $\widehat{\zeta}$ and map x_1 to X and T respectively: for $a_i \in \mathfrak{H}^0$,

$$\widehat{Z}_{\shuffle}\left(\sum_i a_i \shuffle x_1^{\shuffle i}\right) = \sum_i \widehat{\zeta}(a_i)X^i \quad \text{and} \quad \widehat{Z}_{\star}\left(\sum_i a_i \star x_1^{\star i}\right) = \sum_i \widehat{\zeta}(a_i)T^i.$$

Proposition 38. *There is a* $\mathbf{R}$*-linear isomorphism* $\varrho : \mathbf{R}[T] \to \mathbf{R}[X]$ *which makes commutative the following diagram:*

$$\begin{array}{ccc} & & \mathbf{R}[X] \\ & \widehat{Z}_{\shuffle} \nearrow & \\ \mathfrak{H}^1 & & \uparrow \varrho \\ & \searrow & \\ & \widehat{Z}_{\star} & \\ & & \mathbf{R}[T] \end{array}$$

The kernel of $\widehat{\zeta}$ is a subset of $\mathfrak{H}^0$ which is an ideal of the algebra $\mathfrak{H}^0_{ш}$ and also of the algebra $\mathfrak{H}^0_\star$. One can deduce from the existence of a bijective map ϱ as in proposition 38 that $\ker\widehat{\zeta}$ generates the same ideal in both algebras $\mathfrak{H}^1_{ш}$ and $\mathfrak{H}^1_\star$.

Explicit formulae for ϱ and its inverse ϱ^{-1} are given by means of the generating series

$$\sum_{\ell\geq 0}\varrho(T^\ell)\frac{t^\ell}{\ell!}=\exp\left(Xt+\sum_{n=2}^{\infty}(-1)^n\frac{\zeta(n)}{n}t^n\right). \tag{39}$$

and

$$\sum_{\ell\geq 0}\varrho^{-1}(X^\ell)\frac{t^\ell}{\ell!}=\exp\left(Tt-\sum_{n=2}^{\infty}(-1)^n\frac{\zeta(n)}{n}t^n\right).$$

For instance

$$\varrho(T^0)=1,\quad \varrho(T)=X,\quad \varrho(T^2)=X^2+\zeta(2),\quad \varrho(T^3)=X^3+3\zeta(2)X-2\zeta(3),$$

$$\varrho(T^4)=X^4+6\zeta(2)X^2-8\zeta(3)X+\frac{27}{2}\zeta(4).$$

It is instructive to compare the right hand side in (39) with the formula giving the expansion of the logarithm of Euler Gamma function:

$$\Gamma(1+t)=\exp\left(-\gamma t+\sum_{n=2}^{\infty}(-1)^n\frac{\zeta(n)}{n}t^n\right).$$

Also, ϱ may be seen as the differential operator of infinite order

$$\exp\left(\sum_{n=2}^{\infty}(-1)^n\frac{\zeta(n)}{n}\left(\frac{\partial}{\partial T}\right)^n\right)$$

(consider the image of e^{tT}).

10.3 Shuffle regularization of the divergent multiple zeta values, following Ihara and Kaneko

Recall that $\mathfrak{H}_{ш} = \mathfrak{H}^0[x_0,x_1]_{ш}$. Denote by $\mathrm{reg}_{ш}$ the $\mathbf{Q}$-linear map $\mathfrak{H}\to\mathfrak{H}^0$ which maps $w\in\mathfrak{H}$ onto its constant term when w is written as a polynomial in x_0,x_1 in the shuffle algebra $\mathfrak{H}^0[x_0,x_1]_{ш}$. Then $\mathrm{reg}_{ш}$ is a morphism of algebras $\mathfrak{H}_{ш}\to\mathfrak{H}^0_{ш}$. Clearly for $w\in\mathfrak{H}^0$ we have

$$\mathrm{reg}_{ш}(w)=w.$$

Here are the *regularized double shuffle relations* of Ihara and Kaneko.

Theorem 40. *For $w\in\mathfrak{H}^1$ and $w_0\in\mathfrak{H}^0$,*

$$\mathrm{reg}_{ш}(w ш w_0 - w\star w_0)\in\ker\widehat{\zeta}.$$

Define a *shuffle regularized extension of* $\widehat{\zeta} : \mathfrak{H}^0 \to \mathbf{R}$ as the map $\widehat{\zeta}_{ш} : \mathfrak{H} \to \mathbf{R}$ defined by

$$\widehat{\zeta}_{ш} = \widehat{\zeta} \circ \mathrm{reg}_{ш}.$$

Hence $\widehat{\zeta}_{ш}$ is nothing else than the composite of $\widehat{Z}_{ш}$ with the specialization map $\mathbf{R}[X] \to \mathbf{R}$ which sends X to 0.

With this definition of $\widehat{\zeta}_{ш}$ Theorem 40 can be written

$$\widehat{\zeta}_{ш}(w ш w_0 - w \star w_0) = 0$$

for any $w \in \mathfrak{H}^1$ and $w_0 \in \mathfrak{H}^0$.

Define a map $D_{ш} : \mathfrak{H} \longrightarrow \mathfrak{H}$ by $D_{ш}(e) = 0$ and

$$D_{ш}(x_{\epsilon_1} x_{\epsilon_2} \cdots x_{\epsilon_p}) = \begin{cases} 0 & \text{if } \epsilon_1 = 0, \\ x_{\epsilon_2} \cdots x_{\epsilon_p} & \text{if } \epsilon_1 = 1. \end{cases}$$

For instance, for $m \geq 0$ and for $w_0 \in \mathfrak{H}^0$,

$$D_{ш}^i(x_1^m w_0) = \begin{cases} x_1^{m-i} w_0 & \text{for } 0 \leq i \leq m, \\ 0 & \text{for } i > m. \end{cases}$$

One checks that $D_{ш}$ is a derivation on the algebra $\mathfrak{H}_{ш}$. Its kernel contains x_0^m and $\mathfrak{H}_{ш}^0$. There is a Taylor expansion for the elements of $\mathfrak{H}_{ш}^1$:

$$u = \sum_{i \geq 0} \frac{1}{i!} \mathrm{reg}_{ш}(D_{ш}^i u) ш y_1^{ш i}, \quad \text{hence} \quad \widehat{Z}_{ш}(u) = \sum_{i \geq 0} \frac{1}{i!} \mathrm{reg}_{ш}(D_{ш}^i(u) X^i,$$

and

$$\mathrm{reg}_{ш}(u) = \sum_{i \geq 0} \frac{(-1)^i}{i!} y_1^{ш i} ш D_{ш}^i u.$$

For $w_0 \in \mathfrak{H}^0$ with $w_0 = x_0 w$ (with $w \in \mathfrak{H}^1$) and for $m \geq 0$, we have

$$\mathrm{reg}_{ш}(y_1^m w_0) = (-1)^m x_0 (w ш y_1^m).$$

10.4 Harmonic regularization of the divergent multiple zeta values

There is also a *harmonic regularized extension of* $\widehat{\zeta}$ by means of the star product. Recall that, according to Hoffman's Corollary 36, $\mathfrak{H}_\star = \mathfrak{H}_\star^0[x_0, x_1]_\star$. Denote by $\mathrm{reg}_\star$ the $\mathbf{Q}$-linear map $\mathfrak{H} \to \mathfrak{H}^0$ which maps $w \in \mathfrak{H}$ onto its constant term when w is written as a polynomial in x_0, x_1 in the harmonic algebra $\mathfrak{H}_\star^0[x_0, x_1]_\star$. Then $\mathrm{reg}_\star$ is a morphism of algebras $\mathfrak{H}_\star \to \mathfrak{H}_\star^0$. Clearly for $w \in \mathfrak{H}^0$ we have

$$\mathrm{reg}_\star(w) = w.$$

The map $D_\star : \mathfrak{H}^1 \longrightarrow \mathfrak{H}^1$ defined by $D_\star(e) = 0$ and

$$D_\star(y_{s_1} y_{s_2} \cdots y_{s_k}) = \begin{cases} 0 & \text{if } s_1 = 1, \\ y_{s_2} \cdots y_{s_k} & \text{if } s_1 \geq 2, \end{cases}$$

is a derivation on the algebra $\mathfrak{H}^1_\star$ with kernel $\mathfrak{H}^0_\star$; there is a Taylor expansion for the elements of $\mathfrak{H}^1_\star$:

$$u = \sum_{i \geq 0} \frac{1}{i!} y_1^{\star i} \star \operatorname{reg}_\star(D_\star^i u), \quad \text{hence} \quad \widehat{Z}_\star(u) = \sum_{i \geq 0} \frac{1}{i!} \operatorname{reg}_\star(D_\star^i u) T^i,$$

and

$$\operatorname{reg}_\star(u) = \sum_{i \geq 0} \frac{(-1)^i}{i!} y_1^{\star i} \star (D_\star^i u).$$

For $w_0 \in \mathfrak{H}^0$ and for $m \geq 0$, we have

$$\operatorname{reg}_\star(y_1^m w_0) = \sum_{i=0}^{m} \frac{(-1)^i}{i!} (y_1^{m-i} w_0) \star y_1^i.$$