

**Grothendieck-Teichmüller Lie theory
and multiple zeta values**

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Lecture 2B

Multiple zeta values

Outline

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A) Multiple zeta values (“double shuffle”)

Definition

Furusho's theorem: injection $\mathfrak{grt} \hookrightarrow \mathfrak{ds}$

B) $\text{Gal}(\overline{\mathbb{Q}}/\mathbb{Q})$ and the Deligne-Ihara Lie algebra DI_p

Definition

Ihara's theorem: injection $DI_p \hookrightarrow \mathfrak{grt} \otimes \mathbb{Q}_p$

C) Kashiwara-Vergne Lie algebra

The Kashiwara-Vergne problem (Alekseev-Torossian)

Schneps' theorem: injection $\mathfrak{grt} \hookrightarrow \mathfrak{kv}$

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Definitions, properties of MTM and motivic multizetas

The fundamental (free) Lie algebra \mathfrak{fr} of MTM

Brown's theorem: motivic multizetas generate MTM

Corollaries: $DI_p = \mathfrak{fr} \otimes \mathbb{Q}_p$ and $\mathfrak{fr} \hookrightarrow \mathfrak{grt} \hookrightarrow \mathfrak{ds}$.

Introduction to multiple zeta values

For each sequence (k_1, \dots, k_r) of strictly positive integers, $k_1 \geq 2$, the **multiple zeta value** is defined by the convergent series

$$\zeta(k_1, \dots, k_r) = \sum_{n_1 > \dots > n_r > 0} \frac{1}{n_1^{k_1} \dots n_r^{k_r}}.$$

These real numbers have been studied since Euler (1775).

We will see that they form a \mathbb{Q} -algebra, the *multizeta algebra* \mathcal{Z} .

Two multiplications of multizeta values

1. Shuffle multiplication

Straightforward integration yields

$$\zeta(k_1, \dots, k_r) = (-1)^r \int_0^1 \int_0^{t_1} \cdots \int_0^{t_{n-1}} \frac{dt_n}{t_n - \epsilon_n} \cdots \frac{dt_2}{t_2 - \epsilon_2} \frac{dt_1}{t_1 - \epsilon_1}$$

where

$$(\epsilon_1, \dots, \epsilon_n) = (\underbrace{0, \dots, 0}_{k_1-1}, 1, \underbrace{0, \dots, 0}_{k_2-1}, 1, \dots, \underbrace{0, \dots, 0}_{k_r-1}, 1).$$

The product of two simplices is a union of simplices, giving an expression for the product of two multizeta values as a sum of multizeta values. This is the **shuffle product**.

Example. We have

$$\zeta(2) = \int_0^1 \int_0^{t_1} \frac{dt_2}{1-t_2} \frac{dt_1}{t_1}$$

$$\zeta(2, 2) = \int_0^1 \int_0^{t_1} \int_0^{t_2} \int_0^{t_3} \frac{dt_4}{1-t_4} \frac{dt_3}{t_3} \frac{dt_2}{1-t_2} \frac{dt_1}{t_1}$$

$$\zeta(3, 1) = \int_0^1 \int_0^{t_1} \int_0^{t_2} \int_0^{t_3} \frac{dt_4}{1-t_4} \frac{dt_3}{1-t_3} \frac{dt_2}{t_2} \frac{dt_1}{t_1}$$

and

$$\zeta(2)^2 = 2\zeta(2, 2) + 4\zeta(3, 1).$$

Indeed we have

$$\begin{aligned} \zeta(2)^2 &= \int_0^1 \int_0^{t_1} \frac{dt_2}{1-t_2} \frac{dt_1}{t_1} \cdot \int_0^1 \int_0^{t_3} \frac{dt_4}{1-t_4} \frac{dt_3}{t_3} \\ &= \int_{0 < t_2 < t_1 < 1, 0 < t_4 < t_3 < 1} \frac{dt_2}{1-t_2} \frac{dt_1}{t_1} \frac{dt_4}{1-t_4} \frac{dt_3}{t_3} \end{aligned}$$

and the integration region can be broken up into six simplices:

$$\begin{cases} 0 < t_4 < t_3 < t_2 < t_1 < 1, & 0 < t_4 < t_2 < t_3 < t_1 < 1, \\ 0 < t_4 < t_2 < t_1 < t_3 < 1, & 0 < t_2 < t_4 < t_3 < t_1 < 1, \\ 0 < t_2 < t_4 < t_1 < t_3 < 1, & 0 < t_2 < t_1 < t_4 < t_3 < 1. \end{cases}$$

Bringing them all back to $0 < t_4 < t_3 < t_2 < t_1 < 1$ by variable change gives the result.

The x, y notation for shuffle

Definitions.

- For two words $u, v \in \mathbb{Q}\langle x, y \rangle$, the **shuffle product** $sh(u, v)$ is the set or formal sum of permutations of the letters of u and v where the letters of each word remain ordered.

Example. $sh(y, xy) = yxy + 2xyy$.

- A **convergent word** $w \in \mathbb{Q}\langle x, y \rangle$ is a word $w = xvy$.

The reason for this notation is that it gives a bijection

$$\{\text{tuples with } k_1 \geq 2\} \leftrightarrow \{\text{convergent words}\}$$

given by

$$(k_1, \dots, k_r) \leftrightarrow x^{k_1-1}y \dots x^{k_r-1}y.$$

As a notation, we use this to write

$$\zeta(k_1, \dots, k_r) = \zeta(x^{k_1-1}y \dots x^{k_r-1}y).$$

The usefulness is that the shuffle relation on ζ -values is simply:

$$\zeta(u)\zeta(v) = \zeta(sh(u, v)).$$

2. Stuffle multiplication

The product of two series over ordered indices can be expressed as a sum of series over ordered indices. This is the **stuffle product** of multizeta values.

Example. We have

$$\begin{aligned}\zeta(2)^2 &= \left(\sum_{n>0} \frac{1}{n^2} \right) \left(\sum_{m>0} \frac{1}{m^2} \right) \\ &= \sum_{n>m>0} \frac{1}{n^2 m^2} + \sum_{m>n>0} \frac{1}{n^2 m^2} + \sum_{n=m>0} \frac{1}{n^4} \\ &= 2\zeta(2, 2) + \zeta(4).\end{aligned}$$

Each of these two multiplication laws shows that the \mathbb{Q} -vector space \mathcal{Z} has a \mathbb{Q} -algebra structure.

The x, y notation for stuffle

We write

$$st((k_1, \dots, k_r), (l_1, \dots, l_s))$$

for the formal sum of sequences that come from this way of calculating the product of $\zeta(k_1, \dots, k_r)\zeta(l_1, \dots, l_s)$. For example

$$st((2), (2)) = (2, 2) + (2, 2) + (4).$$

A recursive formula for the stuffle is given by

$$st(1, (r_1, \dots, r_i)) = st((r_1, \dots, r_j), 1) = 1,$$

$$st((r_1, \dots, r_i), (s_1, \dots, s_j)) = (r_1, st((r_2, \dots, r_i), (s_1, \dots, s_j))) + (s_1, st((r_1, \dots, r_i), (s_2, \dots, s_j))) + (r_1 + s_1, st((r_2, \dots, r_i), (s_2, \dots, s_j)))$$

We can also express the sequences as convergent words, and write the stuffle product as $u * v$, for example $st((2), (2)) = (2, 2) + (2, 2) + (4)$ becomes

$$xy * xy = xyxy + xyxy + xxxy = 2xyxy + x^3y.$$

Finally, writing $y_i = x^{i-1}y$, we note that all convergent words in x, y can be written $y_{i_1} \cdots y_{i_r}$, and the stuffle can be written

$$\begin{aligned} & st(y_{i_1}, \dots, y_{i_r}, (y_{j_1}, \dots, y_{j_s})) = \\ & y_{i_1} \cdot st(y_{i_2}, \dots, y_{i_r}, (y_{j_1}, \dots, y_{j_s})) \\ & + y_{j_1} \cdot st(y_{i_1}, \dots, y_{i_r}, (y_{j_2}, \dots, y_{j_s})) \\ & + y_{i_1+j_1} \cdot st(y_{i_2}, \dots, y_{i_r}, (y_{j_2}, \dots, y_{j_s})). \end{aligned}$$

Formal multizeta values

For every convergent word $w \in x\mathbb{Q}\langle x, y \rangle y$, let $Z(w)$ denote a formal symbol associated to w .

The *formal multizeta value* \mathbb{Q} -algebra \mathcal{FZ} is generated by the symbols $Z(w)$ subject to the relations:

$$Z(u)Z(v) = Z(sh(u, v))$$

$$Z(u)Z(v) = Z(st(u, v))$$

$$Z(st(y, w) - sh(y, w)) = 0.$$

Notice that in the last relation, the term yw disappears, so it is a sum of convergent multizetas.

For a (formal) multizeta value $Z(k_1, \dots, k_r)$:

$$\mathbf{weight} \quad n = k_1 + \dots + k_r, \quad \mathbf{depth} = r.$$

The algebra $\mathcal{FZ} = \bigoplus_n \mathcal{FZ}_n$ is **weight-graded** (NOT KNOWN for \mathcal{Z}).

$$\left\{ \begin{array}{l} \mathcal{FZ}_0 = \mathbb{Q} \\ \mathcal{FZ}_1 = \{0\}, \\ \mathcal{FZ}_2 = \langle Z(2) \rangle \\ \mathcal{FZ}_3 = \langle Z(3) \rangle \\ \mathcal{FZ}_4 = \langle Z(4) \rangle \\ \mathcal{FZ}_5 = \langle Z(5), Z(2)Z(3) \rangle \\ \mathcal{FZ}_6 = \langle Z(2)^3, Z(3)^2 \rangle \\ \mathcal{FZ}_7 = \langle Z(7), Z(2)Z(5), Z(2)^2Z(3) \rangle \end{array} \right.$$

The double shuffle Lie algebra

It is useful to quotient by products in order to seek **ring generators** of \mathcal{FZ} .

Let \mathcal{I} be the ideal of \mathcal{FZ} generated by

$$\mathcal{FZ}_0, \mathcal{FZ}_2, \text{ and all products } \mathcal{FZ}_{>0}^2.$$

The vector space of **new formal multizeta values** (**ring generators**) is the quotient

$$\text{nfz} = \mathcal{FZ}/\mathcal{I}.$$

Duality

We have the following duality diagram ($\overline{Z}(w)$ denotes the symbolic dual of a word $w \in \mathbb{Q}\langle x, y \rangle$):

$$\begin{array}{ccc}
 \mathbb{Q}\langle \overline{Z}(w) \rangle & \xrightarrow{\text{duality}} & \mathbb{Q}\langle x, y \rangle \\
 \downarrow \text{double shuffle} & & \uparrow \\
 \mathcal{FZ} & \xrightarrow{\text{duality}} & \mathcal{U}\mathfrak{ds} \\
 \downarrow \text{mod products} & & \uparrow \text{Lie inclusion} \\
 \mathfrak{nfz} & \xrightarrow{\text{duality}} & \mathfrak{nfz}^* = \mathfrak{ds}
 \end{array}$$

The enveloping algebra $\mathcal{U}\mathfrak{ds}$ is the dual of \mathcal{FZ} .

Goncharov defined an explicit coproduct on $\mathbb{Q}(\overline{Z}(w))$. He did not show that it passes to \mathcal{FZ} or to a cobracket on \mathfrak{nfz} , but this result follows from a remarkable theorem due to G. Racinet: the vector space dual \mathfrak{ds} of \mathfrak{nfz} is a Lie algebra.

Double shuffle Lie algebra \mathfrak{ds}

For every $f \in \text{Lie}[x, y]$, define a derivation D_f of $\text{Lie}[x, y]$ by $D_f(x) = 0$, $D_f(y) = [y, f]$. Define the **Poisson Lie bracket** on $\text{Lie}[x, y]$ by

$$[D_f, D_g] = D_{\{f, g\}}, \quad \text{so} \quad \{f, g\} = [f, g] + D_f(g) - D_g(f).$$

The double shuffle Lie algebra \mathfrak{ds} can be defined as above by duality, or defined directly:

$$\mathfrak{ds} = \{f \in \text{Lie}[x, y] \mid \pi_y(f) + f_{\text{corr}} \text{ primitive for } \Delta_*\}$$

where

$$f_{\text{corr}} = \sum_{n \geq 1} \frac{(-1)^{n-1}}{n} (f | x^{n-1} y) y_1^n$$

and Δ_* is the coproduct defined on $\mathbb{Q}\langle y_i \rangle$ by

$$\Delta_*(y_i) = \sum_{k+l=i} y_k \otimes y_l.$$

Theorem 6. (Racinet) *The vector space \mathfrak{ds} is weight-graded and it is a Lie algebra under the Poisson bracket. Thus \mathfrak{nfz} is a Lie coalgebra, and it can be seen explicitly that Goncharov's cobracket is dual to the Poisson bracket.*

Why study the double shuffle Lie algebra?

The Lie algebra \mathfrak{ds} contains all the structural information for \mathcal{FZ} , and it is easier to study explicitly, because it is a Lie algebra of polynomials.

It is known (by using the Drinfeld associator) that for each odd weight $n \geq 3$, **there exists an element of depth 1 in \mathfrak{ds}_n** . The dimensions of \mathfrak{ds}_3 , \mathfrak{ds}_5 , \mathfrak{ds}_7 , \mathfrak{ds}_9 are equal to 1.

$$f_3 = [x, [x, y]] + [[x, y], y]$$

$$\begin{aligned} f_5 = & [x, [x, [x, [x, y]] + 2[x, [x, [[x, y], y]]] - \frac{3}{2}[[x, [x, y]], [x, y]] \\ & + 2[x, [[[x, y], y], y]] + \frac{1}{2}[[x, y], [[x, y], y]] \\ & + [[[[x, y], y], y], y] \end{aligned}$$

Depth 1 elements for \mathfrak{ds}_{11} , \mathfrak{ds}_{13} etc. can easily be calculated, but it is still hard to see how to make a “really good choice”. One obvious canonical-looking candidate is to let f_n be the element corresponding to $\zeta(n) \in \mathfrak{nfz}$ under the isomorphism inherited from $\mathbb{Q}\langle x, y \rangle \simeq \mathbb{Q}[\overline{Z}(w)]$ mapping a word w to its dual symbol $\overline{Z}(w)$. But this choice does not have any particularly wonderful number-theoretic properties.

Double shuffle Lie algebra \mathfrak{ds}

!!Major object of study in formal multizeta theory!!

Are there canonical depth 1 elements in each odd weight??

Do they generate??

Are they free ??

Some motivations for believing that the answers to these questions are all **yes** are given in the next sections.

Fundamental structure conjecture on multizeta values.

*Double shuffle relations generate **ALL** algebraic relations between multizeta values.*

Main Conjecture. *We have an isomorphism $\mathfrak{grt} \simeq \mathfrak{ds}$ given by $f(x, y) \mapsto f(x, -y)$.*

Motivations for the conjecture

The inspiration is the Drinfeld associator

$$\phi(x, y) = 1 + \sum_{w \in \mathbb{Q}\langle x, y \rangle} \zeta(w)w.$$

Theorem 7. (*Drinfeld*) Let $\bar{\phi}$ denote the power series $\phi(x, y)$ with coefficients reduced from \mathcal{Z} to nz . Then

- $\bar{\phi}(x, -y)$ satisfies the double shuffle relations;
- $\bar{\phi}(x, y)$ satisfies the defining pentagon relation of **grt**.

So real (reduced) ζ values satisfy the pentagon relation: it is natural to ask whether formal zeta values also do.

Calculations gave evidence for the conjecture by showing up to weight 19:

$$\begin{aligned} \mathbf{grt}_n &\simeq \mathbf{ds}_n \\ f(x, y) &\mapsto f(x, -y) \end{aligned}$$

About four years ago, a breakthrough:

Theorem 8 (Furusho, 2008) *The map $f(x, y) \mapsto f(x, -y)$ gives an injection*

$$\mathbf{grt} \hookrightarrow \mathfrak{ds}$$

Example of relations between double zeta values

Gangl-Kaneko-Zagier proved that there are $\dim S_k(\mathrm{SL}_2(\mathbb{Z}))$ independent linear relations between formal double zetas for every even weight $n \geq 12$. By definition, these relations do come from double shuffle.

For example:

$$28 \zeta(9, 3) + 150 \zeta(7, 5) + 168 \zeta(5, 7) = \frac{5197}{691} \zeta(12)$$

in weight 12.

But do these relations come from \mathbf{grt} ? It turns out that they do. In fact, they are related to the period-polynomial relations in \mathbf{grt} , which via $\mathbf{grt} \hookrightarrow \mathfrak{ds}$ are also valid in \mathfrak{ds} . We have:

Theorem 9. *Under the duality-isomorphism of $\mathcal{U}\mathfrak{ds}$ with \mathcal{FZ} , the period-polynomial relations in \mathbf{grt} give rise to period-polynomial relations in \mathfrak{ds} that are exactly dual to the GKZ relations between formal multiple zeta values.*

Proof of Furusho's injection $\text{grt} \hookrightarrow \mathfrak{ds}$

Furusho actually works with unipotent groups. His proof uses double polylogarithms and a relation they satisfy similar to stuffle. The proof we give is a simplified version that works directly in the Lie situation.

Main objects: (1) **Bar construction:** Let $V_{0,5}$ denote the dual of the braid Lie algebra $\text{Lie } P_5$. The duals of the generators x_{ij} are the five 1-forms

$$\omega_{12} = \frac{dx}{x}, \omega_{23} = \frac{dx}{1-x}, \omega_{34} = \frac{dy}{1-y}, \omega_{45} = \frac{dy}{y}, \omega_{24} = \frac{xdy + ydx}{1-xy}.$$

The space $V_{0,5}$ is called the “bar-construction”, and its elements are sums of words in the ω_{ij} , called “bar-symbols” and denoted $[\omega_{i_1, j_1} | \cdots | \omega_{i_n, j_n}]$. They are the elements that annihilate the kernel $\text{FreeLie}[x_{12}, x_{23}, x_{34}, x_{45}, x_{24}] \twoheadrightarrow \text{Lie } P_5$.

A defining property for elements of $V_{0,5}$ inside the algebra of all bar-words is that if I is an index set of pairs in $\{(12), (23), (34), (45), (24)\}$ and $v = \sum_I a_i [\omega_{i_1} | \cdots | \omega_{i_r}]$, then v lies in $V_{0,5}$ if and only if

$$v = \sum_I a_i [\omega_{i_1} | \cdots | \omega_{i_j} \wedge \omega_{i_{j+1}} | \omega_{i_r}] = 0 \quad (P)$$

for $j = 1, \dots, r - 1$.

Examples. In weight 1, there is no kernel, so all the ω_{ij} lie in $V_{0,5}$. In weight 2, we have $[x_{12}, x_{45}] = 0$ in $\text{Lie } P_5$, so the element $[\omega_{12}|\omega_{45}] + [\omega_{45}|\omega_{12}]$ lies in $V_{0,5}$. In weight 3, an example is given by $[\omega_{24}|\omega_{12}|\omega_{24}] + [\omega_{24}|\omega_{45}|\omega_{24}]$. Indeed for $j = 1$ and $j = 2$ we need (P) to hold, i.e.

$$\begin{cases} [\omega_{24} \wedge \omega_{12} + \omega_{24} \wedge \omega_{45}|\omega_{24}] = 0 \\ [\omega_{24}|\omega_{12} \wedge \omega_{24} + \omega_{45} \wedge \omega_{24}] = 0, \end{cases}$$

which both hold since

$$\begin{aligned} \omega_{24} \wedge \omega_{12} + \omega_{24} \wedge \omega_{45} &= \frac{xdy + ydx}{1 - xy} \wedge \frac{dx}{x} + \frac{xdy + ydx}{1 - xy} \wedge \frac{dy}{y} \\ &= \frac{xdy}{1 - xy} \wedge \frac{dx}{x} - \frac{ydx}{1 - xy} \wedge \frac{dy}{y} \\ &= \frac{dx dy}{1 - xy} - \frac{dx dy}{1 - xy} \\ &= 0. \end{aligned}$$

(2) **Chen iterated integrals:** The iterated integral of a word along a path $\gamma : (0, 1) \rightarrow M_{0,5}$ is defined by

$$\int_{0 < t_1 < \dots < t_n < 1} \omega_{i_1, j_1}(\gamma(t_1)) \cdots \omega_{i_n, j_n}(\gamma(t_n)).$$

The elements of $V_{0,5}$ are characterized in the vector space spanned by all words as being precisely those linear combinations having the property that an iterated integral over one these elements is independent of the homotopy class of the integration path γ .

(3) **Generalized stuffle:** Let $Sh^{\leq}(r, s)$ be the set of surjective maps $\sigma : \{1, \dots, r + s\} \rightarrow \{1, \dots, N\}$ such that $\sigma(1) < \dots < \sigma(r)$ and $\sigma(r + 1) < \dots < \sigma(r + s)$. For each $\sigma \in Sh^{\leq}(r, s)$, let

$$c^\sigma(\mathbf{a}, \mathbf{b}) = (c_1, \dots, c_N)$$

be defined by

$$c_i = \begin{cases} a_k + b_{l-r} & \text{if } \sigma^{-1}(i) = \{k, l\} \text{ with } k \leq r < l \\ a_k & \text{if } \sigma^{-1}(i) = \{k\} \text{ with } k \leq r \\ b_{k-r} & \text{if } \sigma^{-1}(i) = \{k\} \text{ with } k > r, \end{cases}$$

let

$$\sigma(\mathbf{a}, \mathbf{b}) = ((c_1, \dots, c_j), (c_{j+1}, \dots, c_N))$$

where $j = \min(\sigma(r), \sigma(r + s))$, and finally, let

$$\sigma(X, Y) = \begin{cases} (X, Y) & \text{if } \sigma^{-1}(N) = r + s \\ (Y, X) & \text{if } \sigma^{-1}(N) = r \\ XY & \text{if } \sigma^{-1}(N) = \{r, r + s\}. \end{cases}$$

Note that the $c^\sigma(\mathbf{a}, \mathbf{b})$ are nothing but the stuffle of \mathbf{a} and \mathbf{b} , and the $\sigma(\mathbf{a}, \mathbf{b})$ are the same sequences, but cut into two subsequences.

(4) Consider the single-polylogarithm functions

$$Li_{\mathbf{a}}(X) = \sum_{0 < m_1 < \dots < m_k} \frac{X^{m_k}}{m_1^{a_1} \dots m_k^{a_k}}.$$

They can be obtained as iterated integrals over bar symbols in $V_{0,5}$ in just the two 1-forms ω_{12}, ω_{23} .

Example. We have

$$\begin{aligned} Li_{(2)}(X) &= \sum_{m>0} \frac{X^m}{m^2} \\ &= \int_{0 < t_1 < t_2 < X} [\omega_{12} | \omega_{23}] \\ &= \int_{0 < t_1 < t_2 < X} [\omega_{12} | \omega_{23}] \\ &= \int_0^X \int_0^{t_2} \frac{dt_2}{t_2} \frac{dt_1}{1-t_1} \\ &= \sum_{i \geq 0} \frac{1}{(i+1)} \int_0^X \frac{dt_2}{t_2} t_2^{i+1} \\ &= \sum_{i \geq 0} \frac{1}{(i+1)} \int_0^X t_2^i dt_2 \\ &= \sum_{i \geq 0} \frac{1}{(i+1)^2} X^{i+1} \\ &= \sum_{m>0} \frac{X^m}{m^2}. \end{aligned}$$

Similarly, consider the double polylogarithms

$$Li_{\mathbf{a},\mathbf{b}}(X, Y) = \sum_{\substack{0 < m_1 < \dots < m_k \\ < n_1 < \dots < n_l}} \frac{X^{m_k} Y^{n_l}}{m_1^{a_1} \dots m_k^{a_k} n_1^{b_1} \dots n_l^{b_l}}.$$

As for the simple polylogs, these can be obtained as iterated integrals on $M_{0,5}$ of elements of $V_{0,5}$, denoted by $l_{\mathbf{a},\mathbf{b}}^{X,Y}$, along a path $\gamma : (0, 1) \rightarrow M_{0,5}$ from $(0, 0)$ to (X, Y) .

Example. $l_{(2,1)}^{X,Y} = [\omega_{24}|\omega_{12}|\omega_{24}] + [\omega_{24}|\omega_{45}|\omega_{24}]$.

Both the double polylogarithms and the corresponding bar-symbols satisfy a “lifted” version of the stuffle product:

$$\sum_{\sigma \in Sh^{\leq}(r,s)} Li_{\sigma(\mathbf{a},\mathbf{b})}(\sigma(X, Y)) = Li_{\mathbf{a}}(X) Li_{\mathbf{b}}(Y)$$

and

$$\sum_{\sigma \in Sh^{\leq}(r,s)} l_{\sigma(\mathbf{a},\mathbf{b})}^{\sigma(X,Y)} = l_{\mathbf{a}}^X l_{\mathbf{b}}^Y.$$

Remark. The generalized stuffle relations for polylogs are not mysterious. Polylogs are just generalizations of multiple zeta values, integrating over paths ending at arbitrary points. The multiple zeta values satisfy stuffle because of the way one multiplies their series expression, and the generalized stuffle for polylogs comes up exactly the same way.

Now we can prove Furusho's theorem. Let $i_{ijk} : \text{Lie}[x, y] \rightarrow \text{Lie } P_5$ be defined by $i_{ijk}(x) = x_{ij}$, $i_{ijk}(y) = x_{jk}$. Let $p_j : \text{Lie } P_5 \rightarrow \text{Lie}[x, y]$ be defined by $p_j(x_{ij}) = 0$ for all i . (In particular $p_3(x_{45}) = p_3(x_{12}) = x$, $p_3(x_{51}) = y$.) Then a long but straightforward lemma shows that

$$\left\{ \begin{array}{ll} l_{\mathbf{a}}^{XY} = l_{\mathbf{a}} \circ p_3 & \text{for all } (\mathbf{a}, \mathbf{b}) \\ l_{\mathbf{a}, \mathbf{b}}^{X, Y} \circ i_{123} = 0 & \text{for all } (\mathbf{a}, \mathbf{b}) \\ l_{\mathbf{a}, \mathbf{b}}^{Y, X} \circ i_{543} = 0 & \text{for all } (\mathbf{a}, \mathbf{b}) \\ l_{\mathbf{a}, \mathbf{b}}^{X, Y} \circ i_{451} = l_{\mathbf{ab}} & \text{for all } (\mathbf{a}, \mathbf{b}) \\ l_{\mathbf{a}, \mathbf{b}}^{Y, X} \circ i_{215} = l_{\mathbf{ab}} & \text{for all } (\mathbf{a}, \mathbf{b}) \\ l_{\mathbf{a}, \mathbf{b}}^{Y, X} \circ i_{432} = 0 & \text{for all } (\mathbf{a}, \mathbf{b}) \neq ((1, \dots, 1), (1 \dots, 1)) \end{array} \right.$$

Now, take two sequences \mathbf{a}, \mathbf{b} not both made of 1's. Assume $f \in \text{Lie}[x, y]$ satisfies the pentagon. Then we have

$$\begin{aligned} l_{\mathbf{a}}^{XY} (f(x_{45}, x_{51}) + f(x_{12}, x_{23})) &= l_{\mathbf{a}} \circ p_3 (f(x_{45}, x_{51}) + f(x_{12}, x_{23})) = \\ &= l_{\mathbf{a}} \circ p_3 (f(x_{45}, x_{51})) = l_{\mathbf{a}}(f), \end{aligned}$$

and

$$\begin{aligned} l_{\mathbf{a}, \mathbf{b}}^{X, Y} (f(x_{45}, x_{51}) + f(x_{12}, x_{23})) &= \\ l_{\mathbf{a}, \mathbf{b}}^{X, Y} \circ i_{451}(f) + l_{\mathbf{a}, \mathbf{b}}^{X, Y} \circ i_{123}(f) &= l_{\mathbf{ab}}(f), \end{aligned}$$

and finally

$$\begin{aligned} l_{\mathbf{a}, \mathbf{b}}^{Y, X} (f(x_{45}, x_{51}) + f(x_{12}, x_{23})) &= \\ l_{\mathbf{a}, \mathbf{b}}^{Y, X} (f(x_{43}, x_{32}) + f(x_{21}, x_{15}) + f(x_{54}, x_{43})) &= \\ = l_{\mathbf{a}, \mathbf{b}}^{Y, X} \circ i_{432}(f) + l_{\mathbf{a}, \mathbf{b}}^{Y, X} \circ i_{215}(f) + l_{\mathbf{a}, \mathbf{b}}^{Y, X} \circ i_{543}(f) &= \\ = l_{\mathbf{a}, \mathbf{b}}^{Y, X} \circ i_{215}(f) = l_{\mathbf{ab}}(f). \end{aligned}$$

Now using the stuffle-type relation for the symbols, we find that

$$\begin{aligned}
0 &= \sum_{\sigma \in Sh^{\leq}(r,s)} l_{\sigma(\mathbf{a},\mathbf{b})}^{\sigma(X,Y)} (f(x_{45}, x_{51}) + f(x_{12}, x_{23})) \\
&= \sum_{\sigma \in Sh^{\leq}(r,s)} l_{c^{\sigma}(\mathbf{a},\mathbf{b})}(f) \\
&= \sum_{\mathbf{c} \in st(\mathbf{a},\mathbf{b})} l_{\mathbf{c}}(f).
\end{aligned}$$

This shows that f satisfies stuffle when the sequences are not all 1's. A final proposition shows that such an f can be uniquely modified by the addition of a single term in y^n to satisfy the whole stuffle. QED

Note: Converse still open!