Multiple Polylogarithms and Multiple Zeta Values: Some Results and Conjectures

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Polylogarithms

$$\mathrm{Li}_1(x) = \log(1-x)^{-1} = \sum_{n=1}^{\infty} \frac{x^n}{n}, \quad |x| < 1.$$

$$\mathrm{Li}_s(x) = \int_0^x t^{-1}\mathrm{Li}_{s-1}(t)\,dt, \quad 1 < s \in \mathbf{Z}$$
$$= \sum_{n=1}^{\infty} \frac{x^n}{n^s}, \quad |x| \le 1.$$

$$\mathrm{Li}_s(1) = \sum_{n=1}^{\infty} \frac{1}{n^s} = \zeta(s).$$

The Dilogarithm

$$\mathrm{Li}_2(x) = \int_0^x t^{-1}\log(1-t)^{-1}\,dt = \sum_{n=1}^{\infty} \frac{x^n}{n^2}, \quad |x| \le 1.$$

- arises in the multiple integration of rational forms, eg.

$$\int_0^x \int_0^y \frac{a\,ds\,dt}{1-ast} = \mathrm{Li}_2(axy)$$

- QED, scattering of light
- connection with the Gaussian hypergeometric function:

$$\mathrm{Li}_2(x) = \lim_{\varepsilon\to 0+} \varepsilon^{-2}[{}_2F_1(\varepsilon,\varepsilon;1;x) - 1]$$

Inverting Pascal Matrices

Let a be real and let $P(a)$ be the matrix whose (m,n) entry is $\binom{m}{n}a^{m-n}$.

$$P(a) := \begin{bmatrix} 1 & & & \\ a & 1 & & \\ a^2 & 2a & 1 & \\ a^3 & 3a^2 & 3a & 1 \ddots \\ & \cdots & & \end{bmatrix}$$

Then $I = P(0)$ is the identity matrix and

$$P(a)P(b) = P(a+b).$$

Theorem 1 (Aggarwalla and Lamoureaux) *Let $\lambda \ne 1$. The inverse of $I - \lambda P(a)$ has (m,n) entry*

$$\begin{cases} 1/(1-\lambda), & \text{if } m = n; \\ \binom{m}{n}a^{m-n}\mathrm{Li}_{m-n}(\lambda), & \text{if } m \ne n. \end{cases}$$

Multiple Polylogarithms

For positive integer k, let

$$s_1, \ldots, s_k \in \mathbf{Z}^+,$$
$$z_1, \ldots, z_k \in \mathbf{C},$$

$|z_j| \le 1$ for $1 \le j \le k$.

$$\mathrm{Li}_{s_1,\ldots,s_k}(z_1,\ldots,z_k) := \sum_{n_1>\cdots>n_k>0} \prod_{j=1}^{k} z_j^{n_j} n_j^{-s_j},$$

$$\zeta(s_1, s_2, \ldots, s_k) := \mathrm{Li}_{s_1,s_2,\ldots,s_k}(1,1,\ldots,1).$$

$$k=1: \quad \begin{cases} \mathrm{Li}_s(z) = \sum_{n=1}^{\infty} z^n n^{-s}, \\ \zeta(s) = \mathrm{Li}_s(1). \end{cases}$$

$$k=2: \quad \zeta(s,t) = \sum_{n=1}^{\infty} n^{-s} \sum_{j=1}^{n-1} j^{-t}$$

Multiple Zeta Functions

These are obtained when each $z_j = 1$ in the multiple polylogarithm.

$$\zeta(s_1, \ldots, s_k) := \sum_{n_1>\cdots>n_k>0} \prod_{j=1}^{k} n_j^{-s_j}.$$

Their study goes back to Euler ($k=2$):

$$2\zeta(m,1) = m\zeta(m+1) - \sum_{j=1}^{m-2} \zeta(m-j)\zeta(j+1),$$

where $2 \le m \in \mathbf{Z}$.

One can also study $\zeta(s_1, \ldots, s_k)$ with complex arguments $s_1, \ldots, s_k \in \mathbf{C}$.

It can be shown that the multiple series is absolutely convergent if

$$\sum_{j=1}^{m} \Re(s_j) > m, \qquad m = 1, 2, \ldots, k.$$

It is then natural to inquire about

- analytic continuation,
- trivial zeros,
- values at the non-positive integers.

An extremely difficult problem is to classify all relations that exist between values of multiple zeta functions ("multiple zeta values") at *positive integer* arguments.

Define the *depth* of a multiple polylogarithm or multiple zeta function to be the number k of nested summations.

When can a nested sum of depth k be expressed (say polynomially with rational coefficients) in terms of sums with depth less than k?

Settling this question in complete generality is currently a hopeless prospect.

eg. Is $\zeta(5,3)/\zeta(5)\zeta(3)$ irrational?

Reductions at Arbitrary Depth

One of the earliest nontrivial successes at arbitrary depth was Broadhurst's settling of Zagier's conjecture

$$\zeta(\underbrace{3,1,3,1,\ldots,3,1}_{2n \text{ arguments}}) \stackrel{?}{=} 4^{-n}\zeta(\underbrace{4,4,\ldots,4}_{n \text{ arguments}}) = \frac{2\pi^{4n}}{(4n+2)!}$$

for $0 < n \in \mathbf{Z}$.

Abbreviate the first two members by $\zeta(\{3,1\}^n)$ and $4^{-n}\zeta(\{4\}^n)$.

More generally, for real x with $0 \le x \le 1$, let

$$\zeta_x(s_1,\ldots,s_k) := \mathrm{Li}_{s_1,\ldots,s_k}(x,1,\ldots,1) = \sum_{n_1 > \cdots > n_k > 0} x^{n_1} \prod_{j=1}^{k} n_j^{-s_j}.$$

Then (*Trans. Amer. Math. Soc.* **353** (2001), no. 3, 907–941):

Theorem 2

$$\sum_{n=0}^{\infty} \zeta_x(\{3,1\}^n) t^{4n} = {}_2F_1(z,-z;1;x)\,{}_2F_1(iz,-iz;1;x),$$

where $z = (1+i)t/2$.

When $x = 1$, Theorem 2 reduces to

$$\sum_{n=0}^{\infty} \zeta(\{3,1\}^n) t^{4n} = \frac{1}{\Gamma(1+z)\Gamma(1-z)} \cdot \frac{1}{\Gamma(1+iz)\Gamma(1-iz)} = \frac{\sin(\pi z)}{\pi z} \cdot \frac{\sinh(\pi z)}{\pi z} = \sum_{n=0}^{\infty} \frac{2(\pi t)^{4n}}{(4n+2)!}.$$

Factoring Solutions to Differential Equations

Theorem 3 *Let f and g be suitably differentiable functions of a single variable, and let t be a free parameter. Define $D_f = f(x)d/dx$, $D_g = g(x)d/dx$ and suppose that*

$$(D_f D_g + t)u = 0 \qquad (1)$$

$$(D_f D_g - t)v = 0. \qquad (2)$$

Then

$$(D_f^2 D_g^2 + 4t^2)uv = 0. \qquad (3)$$

Moreover, if u_1 and u_2 are linearly independent solutions to (1) *and if v_1 and v_2 are linearly independent solutions to* (2) *then $\{u_1v_1, u_1v_2, u_2v_1, u_2v_2\}$ are linearly independent solutions to* (3).

Proof Sketch. Verify that $uD_g^2 v + vD_g^2 u = 0$, and then calculate

$$\begin{aligned} D_f^2 D_g^2(uv) &= 2D_f^2(D_g u)(D_g v) \\ &= 2t[v(D_f D_g u) - u(D_f D_g v)] \\ &= -4t^2 uv. \end{aligned}$$

Linear independence follows from the following modified Wronskian determinate identity:

$$\begin{vmatrix} u_1v_1 & u_2v_1 & u_1v_2 & u_2v_2 \\ D_g u_1v_1 & D_g u_2v_1 & D_g u_1v_2 & D_g u_2v_2 \\ D_g^2 u_1v_1 & D_g^2 u_2v_1 & D_g^2 u_1v_2 & D_g^2 u_2v_2 \\ D_f D_g^2 u_1v_1 & D_f D_g^2 u_2v_1 & D_f D_g^2 u_1v_2 & D_f D_g^2 u_2v_2 \end{vmatrix} = 8t \begin{vmatrix} u_1 & u_2 \\ D_g u_1 & D_g u_2 \end{vmatrix}^2 \begin{vmatrix} v_1 & v_2 \\ D_g v_1 & D_g v_2 \end{vmatrix}^2.$$

This identity follows by direct computation using the differential equations for u and v.

□

Applications

For $0 \leq x \leq 1$ and complex $z = (1+i)t/2$, let

$$\begin{aligned}
\psi(z) &:= \Gamma'(z)/\Gamma(z),\\
Y_1(x,z) &:= {}_2F_1(z,-z;1;x),\\
Y_2(x,z) &:= (1-x){}_2F_1(1+z,1-z;2;1-x),\\
G(z) &:= \tfrac{1}{4}\{\psi(1+iz)+\psi(1-iz)-\psi(1+z)\\
&\qquad -\psi(1-z)\}.
\end{aligned}$$

Then (*Trans. AMS*)

$$\sum_{n=0}^{\infty} t^{4n}\zeta_x(\{3,1\}^n) = Y_1(x,z)Y_1(x,iz),$$

and (*Compositio Mathematica*, to appear)

$$z^2\sum_{n=0}^{\infty} t^{4n}\zeta_x(3,\{1,3\}^n) = G(z)Y_1(x,z)Y_1(x,iz) - \frac{Y_1(x,iz)Y_2(x,z)}{4Y_1(1,z)} + \frac{Y_1(x,z)Y_2(x,iz)}{4Y_1(1,iz)}$$

define entire functions of z.

Entirety in z turns out to be a simple consequence of the identity

$$\frac{(1+\alpha)_n}{n!}\,{}_2F_1\left(\begin{matrix}-n,1+\alpha+\beta+n\\1+\alpha\end{matrix}\,\middle|\,\frac{1-y}{2}\right) = \frac{(-1)^n(1+\beta)_n}{n!}\,{}_2F_1\left(\begin{matrix}-n,1+\alpha+\beta+n\\1+\beta\end{matrix}\,\middle|\,\frac{1+y}{2}\right)$$

for the Jacobi polynomials.

Here,

$$(a)_n := \frac{\Gamma(a+n)}{\Gamma(a)} = \prod_{j=1}^{n}(a+j-1)$$

is the rising factorial (Pochammer symbol).

Thus the apparent singularities in the generating functions are all removable.

Specialize $x=1$. It follows that for all positive integers n,

$$\zeta(\{3,1\}^n) = 4^{-n}\zeta(\{4\}^n) = \frac{2\pi^{4n}}{(4n+2)!},$$

$$\begin{aligned}
\zeta(3,\{1,3\}^n) &= 4^{-n}\sum_{k=0}^{n}\zeta(4k+3)\zeta(\{4\}^{n-k})\\
&= \sum_{k=0}^{n}\frac{2\pi^{4k}}{(4k+2)!}\left(-\frac{1}{4}\right)^{n-k}\zeta(4n-4k+3),
\end{aligned}$$

$$\begin{aligned}
\zeta(2,\{1,3\}^n) &= 4^{-n}\sum_{k=0}^{n}(-1)^k\zeta(\{4\}^{n-k})\Big\{(4k+1)\\
&\quad\times\zeta(4k+2) - 4\sum_{j=1}^{k}\zeta(4j-1)\zeta(4k-4j+3)\Big\}.
\end{aligned}$$

More Applications

Let $s=(1+x)/2$ and $z=(1+i)t/2$,

$$\zeta_x(\{\overline{1},1\}^n) := \mathrm{Li}_{1,\ldots,1}(-x,1,\{-1,1\}^{n-1}),$$

$$\zeta_x(\overline{1},\{1,\overline{1}\}^n) := \mathrm{Li}_{1,\ldots,1}(-x,\{1,-1\}^n),$$

$$\begin{aligned}
U(s,z) &:= {}_2F_1(z,-z;1;s)\\
&\quad - z(1-s){}_2F_1(1+z,1-z;2;1-s),
\end{aligned}$$

$$A(z) := \frac{\sqrt{\pi}}{\Gamma(1+z/2)\Gamma(1/2-z/2)}.$$

Then (*Compositio Mathematica*, to appear):

$$\sum_{n=0}^{\infty}\left[t^{2n}\zeta_x(\{\overline{1},1\}^n) + t^{2n+1}\zeta_x(\overline{1},\{1,\overline{1}\}^n)\right] = \frac{U(s,-z)U(s,iz)}{A(-z)A(iz)}$$

defines an entire function of z.

Entirety in z is again a simple consequence of the identity

$$\frac{(1+\alpha)_n}{n!}\,{}_2F_1\left(\begin{matrix}-n, 1+\alpha+\beta+n\\ 1+\alpha\end{matrix}\,\middle|\,\frac{1-y}{2}\right)$$
$$=\frac{(-1)^n(1+\beta)_n}{n!}\,{}_2F_1\left(\begin{matrix}-n, 1+\alpha+\beta+n\\ 1+\beta\end{matrix}\,\middle|\,\frac{1+y}{2}\right)$$

for the Jacobi polynomials.

Thus the apparent singularities in the generating functions are again all removable.

Again, specialize $x=1$. It follows that for all complex t,

$$\sum_{n=0}^{\infty}\left[t^{2n}\zeta(\{\overline{1},1\}^n)+t^{2n+1}\zeta(\overline{1},\{1,\overline{1}\}^n)\right]$$
$$=A\left(\frac{t}{1-i}\right)A\left(\frac{t}{1+i}\right)$$

and if $z=(1+i)t/2$, then

$$1+\sum_{n=0}^{\infty}\left[t^{2n+1}\zeta(\overline{1},\{\overline{1},1\}^n)+t^{2n+2}\zeta(\overline{1},\overline{1},\{1,\overline{1}\}^n)\right]$$
$$=\tfrac{1}{2}(1+i)zA(z)A(-iz)$$
$$\times\left\{\pi\,\mathrm{csc}(\pi z)-i\pi\,\mathrm{csch}(\pi z)+4G(z)\right\}.$$

From these generating series identities, explicit formulæ for the alternating Euler sums

$$\zeta(\{\overline{1},1\}^n),\ \zeta(\overline{1},\{1,\overline{1}\}^n),$$

and

$$\zeta(\overline{1},\{\overline{1},1\}^n),\ \zeta(\overline{1},\overline{1},\{1,\overline{1}\}^n)$$

can be obtained.

- Analytic Continuation: T. Arakawa, M. Kaneko, S. Akiyama, S. Egami, Y. Tanigawa, H. Ishikawa
- Partial fractions: Euler and Nielsen, Y. Ohno
- Special functions: J. & D. Borwein, D. Broadhurst, D. Bowman
- Series transformations: Subbarao, Ramanujan
- Linear algebra: D. Bailey, R. Girgensohn
- Contour integration: P. Flajolet & B. Salvy
- Harmonic algebra: M. Hoffman, K. Ihara
- Lyndon Bases: D. Broadhurst, M. Bigotte
- Combinatorics: H. Minh, P. Lisoněk
- Tate Motives: T. Terasoma, A. Goncharov
- Knot Theory: T. Le, J. Murakami, T. Takamuki

The Simplex Integral

There is a representation, due to Kontsevich, for multiple zeta values in terms of a simplex integral.

If $s_1,\ldots,s_k$ are positive integers, then

$$\zeta(s_1,\ldots,s_k)=\int\prod_{j=1}^{k}\left(\prod_{r=1}^{s_j-1}\frac{dt_r^{(j)}}{t_r^{(j)}}\right)\frac{dt_{s_j}^{(j)}}{1-t_{s_j}^{(j)}},$$

where the integral is over the simplex

$$1>t_1^{(1)}>\cdots>t_{s_1}^{(1)}>\cdots>t_1^{(k)}>\cdots>t_{s_k}^{(k)}>0,$$

and is abbreviated by

$$\int_0^1\prod_{j=1}^{k}a^{s_j-1}b,\qquad a=dt/t,\quad b=dt/(1-t).$$

eg.

$$
\begin{aligned}
\zeta(2,1) &= \sum_{n>m>0} n^{-2}m^{-1} \\
&= \sum_{k=1}^{\infty}\sum_{j=1}^{\infty}(k+j)^{-2}k^{-1} \\
&= \sum_{k=1}^{\infty} k^{-1}\sum_{j=1}^{\infty}(k+j)^{-1}\int_0^1 t^{k+j-1}\,dt \\
&= \sum_{k=1}^{\infty} k^{-1}\int_0^1 t^{-1}\sum_{j=1}^{\infty}\int_0^t u^{k+j-1}\,du\,dt \\
&= \int_0^1 t^{-1}\int_0^t (1-u)^{-1}\sum_{k=1}^{\infty} k^{-1}u^k\,du\,dt \\
&= \int_0^1 t^{-1}\int_0^t (1-u)^{-1}\sum_{k=1}^{\infty}\int_0^u v^{k-1}\,dv\,du\,dt \\
&= \int_0^1 t^{-1}\int_0^t (1-u)^{-1}\int_0^u (1-v)^{-1}\,dv\,du\,dt \\
&= \int\limits_{1>t>u>v>0} \frac{dt}{t}\cdot\frac{du}{1-u}\cdot\frac{dv}{1-v} \\
&= \int_0^1 ab^2.
\end{aligned}
$$

Duality

Let s_j and r_j be non-negative integers ($1 \le j \le k$), and let

$$m = \sum_{j=1}^{k}(s_j + 2 + r_j).$$

Then

$$
\begin{aligned}
&\zeta(s_1+2,\{1\}^{r_1},\ldots,s_k+2,\{1\}^{r_k}) \\
&= \int_0^1 \prod_{j=1}^{k} a^{s_j+1}b^{r_j+1} \\
&= \int\limits_{1>t_1>\cdots>t_m>0} \prod_{j=1}^{m} f_j(t_j)\,dt_j \\
&= \int\limits_{1>u_m>\cdots>u_1>0} \prod_{j=1}^{m} f_j(u_j)\,du_j, \quad u_j = 1-t_j \\
&= \int_0^1 \prod_{j=k}^{1} a^{r_j+1}b^{s_j+1} \\
&= \zeta(r_k+2\{1\}^{s_k},\ldots,r_1+2,\{1\}^{s_1}),
\end{aligned}
$$

originally conjectured by Hoffman.

This is the only known non-trivial instance of an equivalence between two multiple zeta values.

A related integral representation enabled Y. Ohno to prove the following beautiful generalization of the duality identity. Let

$$S(p;m) := \sum_{c_1+\cdots+c_n=m} \zeta(p_1+c_1,\ldots,p_n+c_n),$$

where the sum is over all non-negative integers $c_1,\ldots,c_n$ which sum to m.

As in the duality identity, define the dual argument lists

$$p := (s_1+2,\{1\}^{r_1},\ldots,s_k+2,\{1\}^{r_k})$$

and

$$p' := (r_k+2,\{1\}^{s_k},\ldots,r_1+2,\{1\}^{s_1}).$$

Then $S(p;m) = S(p';m)$.

When $m = 0$, Ohno's result reduces to duality.

Another interesting specialization is obtained by taking $p = (k+1)$ and $m = n-k-1$.

One then deduces Granville's theorem, originally conjectured independently by Courtney Moen and Michael Schmidt:

$$\sum_{s_1+\cdots+s_k=n} \zeta(s_1,\ldots,s_k) = \zeta(n),$$

where the sum is over all positive integers $s_1,\ldots,s_k$ which sum to n and $s_1 > 1$.

The MacMahon Integral

Major Percy MacMahon's Omega operator discards terms with non-positive exponents from formal Laurent series in $\lambda_1, \dots, \lambda_k$. Thus, if $0 \le x_1, \dots, x_k \le 1$, then

$$\begin{aligned}
&\mathrm{Li}_{s_1,\dots,s_k}(x_1,\dots,x_k)\\
&= \sum_{n_1>\cdots>n_k>0} \prod_{j=1}^k x_j^{n_j} n_j^{-s_j}\\
&= \Omega \prod_{j=1}^k \sum_{n_j>0} n_j^{-s_j}\big(x_j\lambda_j\lambda_{j-1}^{-1}\big)^{n_j}, \qquad \lambda_0 := 1\\
&= \Omega \prod_{j=1}^k \mathrm{Li}_{s_j}(y_j), \qquad y_j := x_j\lambda_j\lambda_{j-1}^{-1}\\
&= \Omega \prod_{j=1}^k \int\limits_{1>u_1^{(j)}>\cdots>u_{s_j}^{(j)}>0} \left(\prod_{r=1}^{s_j-1} \frac{du_r^{(j)}}{u_r^{(j)}}\right) \frac{y_j\, du_{s_j}^{(j)}}{1-y_j u_{s_j}^{(j)}}.
\end{aligned}$$

Thus, we have

$$\begin{aligned}
&\mathrm{Li}_{s_1,\dots,s_k}(x_1,\dots,x_k)\\
&= \Omega \prod_{j=1}^k \int\limits_{1>u_1^{(j)}>\cdots>u_{s_j}^{(j)}>0} \left(\prod_{r=1}^{s_j-1} \frac{du_r^{(j)}}{u_r^{(j)}}\right)\\
&\qquad \times \sum_{m_j=1}^\infty \left(x_j\lambda_j\lambda_{j-1}^{-1}\right)^{m_j} \left(u_{s_j}^{(j)}\right)^{m_j-1} du_{s_j}^{(j)}\\
&= \int_{\Delta(\vec{s})} \left\{\prod_{j=1}^k \left(\prod_{r=1}^{s_j-1} \frac{du_r^{(j)}}{u_r^{(j)}}\right)\right\}\\
&\qquad \times \sum_{m_1>\cdots>m_k>0} \prod_{j=1}^k \left(x_j u_{s_j}^{(j)}\right)^{m_j} \frac{du_{s_j}^{(j)}}{u_{s_j}^{(j)}},
\end{aligned}$$

where $\Delta(\vec{s})$ denotes the set of all integration variables satisfying

$$1 > u_1^{(j)} > u_2^{(j)} > \cdots > u_{s_j}^{(j)} > 0$$

for $j = 1, 2, \dots, k$.

Since $0 \le y_j < 1$ for each $j = 1, 2, \dots, k$ implies

$$\begin{aligned}
&\sum_{m_1>\cdots>m_k>0} \prod_{j=1}^k y_j^{m_j}\\
&= \sum_{n_1=1}^\infty \cdots \sum_{n_k=1}^\infty y_1^{n_1+\cdots+n_k} y_2^{n_2+\cdots+n_k} \cdots y_k^{n_k}\\
&= \frac{y_1}{1-y_1} \cdot \frac{y_1y_2}{1-y_1y_2} \cdots \frac{y_1y_2\cdots y_k}{1-y_1y_2\cdots y_k},
\end{aligned}$$

it follows that

$$\begin{aligned}
&\mathrm{Li}_{s_1,\dots,s_k}(x_1,\dots,x_k)\\
&\qquad = \int_{\Delta(\vec{s})} \prod_{j=1}^k \left\{\tau\left(\prod_{m=1}^j x_m u_{s_m}^{(m)}\right) \prod_{r=1}^{s_j} \frac{du_r^{(j)}}{u_r^{(j)}}\right\},
\end{aligned}$$

where $\tau(x) := x/(1-x)$.

Shuffles

The simplex integral representation leads to a shuffle multiplication rule satisfied by multiple zeta values.

Suppose that $x, y \in \mathbf{R}$ and $f_j : [y, x] \to \mathbf{R}$ are integrable functions for $j = 1, 2, \dots, n$.

It is customary to make the abbreviation

$$\int_y^x \prod_{j=1}^n \alpha_j := \int\limits_{x>t_1>t_2>\cdots>t_n>y} \prod_{j=1}^n f_j(t_j)\, dt_j,$$

where $\alpha_j := f_j(t_j)\, dt_j$.

<u>Convention</u>: the integral is equal to 1 if $n = 0$ regardless of the values of x and y.

Let σ be a permutation of $\{1, 2, \ldots, m+n\}$ such that $\sigma^{-1}(j) < \sigma^{-1}(k)$ for all $1 \le j < k \le m$ and $m+1 \le j < k \le m+n$.

Denote the set of all $\binom{m+n}{n}$ such permutations σ by Shuff(m,n).

Then

$$\Big(\int_y^x \prod_{j=1}^m \alpha_j\Big)\Big(\int_y^x \prod_{j=m+1}^{m+n} \alpha_j\Big) = \sum_{\sigma\in \mathrm{Shuff}(m,n)} \int_y^x \prod_{j=1}^{m+n} \alpha_{\sigma(j)},$$

and so define the shuffle product $\sqcup\!\sqcup$ by

$$\Big(\prod_{j=1}^m \alpha_j\Big) \sqcup\!\sqcup \Big(\prod_{j=m+1}^{m+n} \alpha_j\Big) := \sum_{\sigma\in \mathrm{Shuff}(m,n)} \prod_{j=1}^{m+n} \alpha_{\sigma(j)}.$$

The Shuffle Algebra

Let A be a finite set and let A^* denote the free monoid generated by A.

Regard A as an alphabet and the elements of A^* as words formed by concatenating any finite number of letters (repetitions permitted) from the alphabet A.

By linearly extending the concatenation product to the set $\mathbf{Q}\langle A\rangle$ of rational linear combinations of elements of A^*, we obtain a non-commutative polynomial ring with indeterminates the elements of A and with multiplicative identity 1 denoting the empty word.

The shuffle product is alternatively defined first on words by the recursion

$$\begin{cases} 1 \sqcup\!\sqcup w = w \sqcup\!\sqcup 1 = w, \\ au \sqcup\!\sqcup bv = a(u \sqcup\!\sqcup bv) + b(au \sqcup\!\sqcup v), \end{cases}$$

($\forall a, b \in A$ and $\forall u, v, w \in A^*$) and then extended linearly to $\mathbf{Q}\langle A\rangle$.

eg.

$$\begin{aligned}(ab - 2b) \sqcup\!\sqcup c &= ab \sqcup\!\sqcup c - 2b \sqcup\!\sqcup c \\ &= abc + acb + cab - 2bc - 2cb\end{aligned}$$

One checks that the shuffle product so defined is associative and commutative, and thus $\mathbf{Q}\langle A\rangle$ equipped with the shuffle product becomes a commutative $\mathbf{Q}$-algebra, denoted $\mathrm{Sh}_{\mathbf{Q}}[A]$.

In what follows, if A is an alphabet and $u, v \in A^*$, we'll denote by $\{u \sqcup\!\sqcup v\}$ the multi-set of words appearing (with multiplicity) in the expansion of $u \sqcup\!\sqcup v$.

For example, suppose $A = \{a, b\}$. Since $ab \sqcup\!\sqcup ab = 4aabb + 2abab$, we have

$$\{ab \sqcup\!\sqcup ab\} = \{abab, abab, aabb, aabb, aabb, aabb\},$$

which, as a multi-set, *properly* contains $\{abab, aabb\}$.

Theorem 4 *(Euro. J. Comb., to appear) Let r be a positive integer, let A be an alphabet, and let $a_1, a_2, \ldots \in A$ be such that $a_{r+m} = a_m$ for all positive integers m. Fix a positive integer n, and define multi-sets $S_0 = S_{2n} = \{a_1 a_2 \cdots a_{2nr}\}$, and*

$$S_k = \{a_1 a_2 \cdots a_{kr} \sqcup\!\sqcup a_1 a_2 \cdots a_{(2n-k)r}\},$$

for $k = 1, 2, \ldots, 2n-1$. Then $S_{k-1} \subseteq S_k$ for $k = 1, 2, \ldots, n$, and $S_{k+1} \subseteq S_k$ for $k = n, n+1, \ldots, 2n-1$.

Corollary 1 *Let n be a non-negative integer, and let $\{a,b\}$ be an alphabet. Then*

$$\sum_{k=-n}^{n}(-1)^k\left[(ab)^{n+k} ⧢ (ab)^{n-k}\right]=(4a^2b^2)^n.$$

Corollary 2 *Let n be a non-negative integer. Then*

$$\sum_{k=-n}^{n}(-1)^k\zeta(\{2\}^{n+k})\zeta(\{2\}^{n-k})=4^n\zeta(\{3,1\}^n).$$

Proof of Corollary 1. We prove the trivially equivalent convolution formula

$$\sum_{k=0}^{2n}(-1)^{n+k}[(ab)^k ⧢ (ab)^{2n-k}]=(4a^2b^2)^n. \quad (4)$$

In Theorem 4, let $A=\{a,b\}$ and $r=2$. In view of the multi-set inclusions indicated by Theorem 4, there must be

$$\sum_{k=0}^{2n}(-1)^{n+k}|S_k|=\sum_{k=0}^{2n}(-1)^{n+k}\binom{4n}{2k}=4^n$$

terms on each side of (4), counting multiplicity. Furthermore, the word $(a^2b^2)^n$ occurs 4^n times in S_n, since each a and each b can take two positions. Since $(a^2b^2)^n$ cannot occur in S_k for $k\neq n$, (4) follows immediately. □

One can similarly prove an intriguing shuffle factorization due to Broadhurst.

Let $i^2=-1$. Then in the formal power series ring $(\mathrm{Sh}_{\mathbf{Q}}[c,b])[[z]]$, we have the identity

$$A\left(\frac{z}{1-i}\right) ⧢ A\left(\frac{z}{1+i}\right)=M(z)$$

where

$$\begin{aligned}A(z)&=\sum_{n=0}^{\infty}(cbz^2)^n(1+cz)\\&=1+cz+cbz^2+cbcz^3+cbcbz^4+\cdots\end{aligned}$$

and

$$\begin{aligned}M(z)&=\sum_{n=0}^{\infty}(c^2b^2z^4)^n(1+cz+c^2z^2+c^2bz^3)\\&=1+cz+c^2z^2+c^2bz^3+c^2b^2z^4+\cdots\end{aligned}$$

Other shuffle convolution formulæ can be established in a similar manner.

For example, if $\{a,b\}$ is an alphabet and n is a positive integer, then

$$2\sum_{k=-n}^{n}(-1)^k[(ab)^{n+k} ⧢ (ba)^{n-k}] = (4abba)^n+(4baab)^n.$$

With a little more work, one can also establish a shuffle convolution formula for

$$\sum_{k=-n}^{n}(-1)^k[(a^2b)^{n+k} ⧢ (a^2b)^{n-k}], \qquad 1\le n\in\mathbf{Z},$$

and as a consequence, a corresponding identity for

$$\zeta(\{5,1\}^n):=\zeta(\underbrace{5,1,\ldots,5,1}_{2n\text{ arguments}}), \qquad 1\le n\in\mathbf{Z}.$$

In principle, it should be possible to extend this approach to $\zeta(\{2p+1,1\}^n)$ for any positive integers n and p, but the shuffle convolution formulæ become prohibitively complicated as p increases.

Let n be a positive integer. Observe that in $(a^4b^2)^n$, every occurrence of a^4 after the first is separated on both sides by b^2, and hence there are $2n-1$ ways in which a single transposition of a letter b with an adjacent letter a can be performed. If we let $\left[\begin{matrix}2n-1\\k\end{matrix}\right]$ denote the sum of the $\binom{2n-1}{k}$ words obtained from $(a^4b^2)^n$ by making k such transpositions, then we have the following result.

Theorem 5 *Let n be a positive integer. Then*

$$\sum_{k=-n}^{n}(-1)^k[(a^2b)^{n-k} ⧢ (a^2b)^{n+k}] = 3^n\sum_{k=1}^{2n}2^k\left[\begin{matrix}2n-1\\2n-k\end{matrix}\right].$$

Example. When $n=2$, the right hand side of Theorem 5 is equal to

$$\begin{aligned}&18a^3ba^2ba^2bab+144a^4b^2a^4b^2\\&+36(a^3baba^3bab+a^3ba^2ba^3b^2+a^4baba^2bab)\\&+72(a^4b^2a^3bab+a^4baba^3b^2+a^3baba^4b^2).\end{aligned}$$

Definition 6 (EJC 5(1) 1998, #R38) *For integers $m \ge n \ge 0$ let*

$$S_{m,n}$$

denote the set of words occurring in the shuffle product

$$(ab)^n \sqcup\!\sqcup (ab)^{m-n}$$

in which the subword a^2 appears exactly n times.

Let

$$T_{m,n}$$

be the <u>sum</u> *of the $\binom{m}{2n}$ distinct words in $S_{m,n}$.*

For all other pairs (m,n) define $T_{m,n} := 0$.

eg. $S_{3,1} = \{a^2b^2ab, a^2bab^2, aba^2b^2\}$, $T_{3,1} = a^2b^2ab + a^2bab^2 + aba^2b^2$. Each word in $S_{3,1}$ occurs 4 times in $(ab) \sqcup\!\sqcup (ab)^2$.

Theorem 7 (JCTA 97 (2001) (1), 43–61) *Let x and y be commuting indeterminates, and let m be a non-negative integer. In the commutative polynomial ring $(\mathsf{Sh}_{\mathbf{Q}}[a,b])[x,y]$ we have the shuffle convolution formula*

$$\sum_{k=0}^{m} x^k y^{m-k}\left[(ab)^k \sqcup\!\sqcup (ab)^{m-k}\right] = \sum_{n=0}^{\lfloor m/2 \rfloor} (4xy)^n (x+y)^{m-2n}\, T_{m,n}.$$

Corollary 3 *Let m be a non-negative integer. Then*

$$\sum_{k=-m}^{m} (-1)^k \left[(ab)^{m+k} \sqcup\!\sqcup (ab)^{m-k}\right] = (4a^2b^2)^m.$$

Corollary 4 *Let m be a non-negative integer. Then*

$$\sum_{k=-m}^{m} (-1)^k \zeta(\{2\}^{m+k})\zeta(\{2\}^{m-k}) = 4^m \zeta(\{3,1\}^m).$$

Let $S_{m,n}$ be as in Definition 6. Note that each word in $S_{m,n}$ has a unique representation

$$(ab)^{m_0} \prod_{k=1}^{n} (a^2b)(ab)^{m_{2k-1}} b (ab)^{m_{2k}}, \qquad (5)$$

in which $m_0, m_1, \ldots, m_{2n}$ are non-negative integers with sum $m-2n$.

Conversely, every ordered $(2n+1)$-tuple of non-negative integers with sum $m-2n$ gives rise to a unique word in $S_{m,n}$ via (5).

Let $C_{2n+1}(m-2n)$ denote the set of ordered non-negative integer compositions of $m-2n$ with $2n+1$ parts. Then we have a bijective correspondence $\varphi : C_{2n+1}(m-2n) \to S_{m,n}$.

Now define

$$Z(\vec{s}) := \int_0^1 \varphi(\vec{s}), \qquad \vec{s} \in C_{2n+1}(m-2n),$$

where we identify the abstract letters a and b with the differential 1-forms dt/t and $dt/(1-t)$, respectively.

Thus, if $\vec{s} = (m_0, m_1, \ldots, m_{2n})$, then (following Broadhurst)

$$\begin{aligned} Z(\vec{s}) &= \int_0^1 (ab)^{m_0} \prod_{k=1}^{n} (a^2b)(ab)^{m_{2k-1}} b (ab)^{m_{2k}} \\ &= \zeta(\{2\}^{m_0}, 3, \{2\}^{m_1}, 1, \{2\}^{m_2}, 3, \{2\}^{m_3}, 1, \\ &\qquad \ldots, 3, \{2\}^{m_{2n-1}}, 1, \{2\}^{m_{2n}}). \end{aligned}$$

The argument list consists of m_j consecutive twos inserted after the jth element of the string $\{3,1\}^n$ for $j = 0, 1, \ldots, 2n$.

It turns out that

$$\sum_{\vec{s} \in C_{2n+1}(m-2n)} Z(\vec{s}) = \frac{2\pi^{2m}}{(2m+2)!}\binom{m+1}{2n+1},$$

for all non-negative integers m and n with $m \ge 2n$.

Theorem 8 *Let m and n be non-negative integers with $m \geq 2n$. Then*

$$\sum_{\vec{s} \in C_{2n+1}(m-2n)} Z(\vec{s}) = \frac{2\pi^{2m}}{(2m+2)!}\binom{m+1}{2n+1}.$$

Corollary 5 *Let n be a non-negative integer. Then*

$$\zeta(\{3,1\}^n) = \frac{2\pi^{4n}}{(4n+2)!}.$$

Proof. Put $m = 2n$ in Theorem 8, and note that $Z(\{0\}^{2n+1}) = \zeta(\{3,1\}^n)$.

A more compelling formulation of Theorem 8 can be given as follows.

Again, let $\vec{s} = (m_0, m_1, \ldots, m_{2n})$ and put (following Broadhurst again)

$$\mathcal{C}(\vec{s}) := Z(\vec{s}) + \sum_{j=1}^{2n} Z(m_j, m_{j+1}, \ldots, m_{2n}, m_0, \ldots, m_{j-1}).$$

In other words, sum over all cyclic permutations of the argument list $\vec{s}$. Then

$$\begin{aligned} \sum_{\vec{s} \in C_{2n+1}(m-2n)} \mathcal{C}(\vec{s}) &= Z(m) \times |C_{2n+1}(m-2n)| \\ &= \frac{\pi^{2m}}{(2m+1)!}\binom{m}{2n} \end{aligned}$$

is an equivalent formulation.

Theorem 9 *Let m and n be non-negative integers with $m \geq 2n$. Then*

$$\begin{aligned} \sum_{\vec{s} \in C_{2n+1}(m-2n)} \mathcal{C}(\vec{s}) &= Z(m) \times |C_{2n+1}(m-2n)| \\ &= \frac{\pi^{2m}}{(2m+1)!}\binom{m}{2n}. \end{aligned}$$

Corollary 6 *If n is a non-negative integer, then*

$$\mathcal{C}(1, \{0\}^{2n}) = Z(2n+1).$$

Broadhurst's cyclic insertion conjecture can be restated as the assertion that

$$\mathcal{C}(\vec{s}) = Z(m), \qquad \forall \vec{s} \in C_{2n+1}(m-2n)$$

and integers $m \geq 2n \geq 0$.

Theorem 9 reduces the problem to proving that $\mathcal{C}(\vec{s})$ is invariant for $\vec{s} \in C_{2n+1}(m-2n)$.

Conjecture: The invariance can be proved using only the shuffle property of multiple zeta values plus the known values $\zeta(\{2n\}^k)$.

Theorem 8 *Let m and n be non-negative integers with $m \geq 2n$. Then*

$$\sum_{\vec{s} \in C_{2n+1}(m-2n)} Z(\vec{s}) = \frac{2\pi^{2m}}{(2m+2)!}\binom{m+1}{2n+1}.$$

Proof. It suffices to prove that with $a = dt/t$, $b = dt/(1-t)$, we have

$$\int_0^1 T_{m,n} = \frac{2\pi^{2m}}{(2m+2)!}\binom{m+1}{2n+1}.$$

Let

$$J(z) := \sum_{k=0}^{\infty} z^{2k} \int_0^1 (ab)^k = \sum_{k=0}^{\infty} z^{2k} \zeta(\{2\}^k).$$

Then [BBB]

$$J(z) = \begin{cases} \dfrac{\sinh(\pi z)}{\pi z}, & \text{if } z \neq 0, \\ 1, & \text{if } z = 0. \end{cases}$$

We have

$$J(z\cos\theta)J(z\sin\theta)$$

$$= \frac{\sinh(\pi z\cos\theta)}{\pi z\cos\theta}\cdot\frac{\sinh(\pi z\sin\theta)}{\pi z\sin\theta}$$

$$= \frac{\cosh \pi z(\cos\theta+\sin\theta) - \cosh\pi z(\cos\theta-\sin\theta)}{2\pi^2 z^2\sin\theta\cos\theta}$$

$$= \frac{\cosh\pi z\sqrt{1+\sin 2\theta}-\cosh \pi z\sqrt{1-\sin 2\theta}}{\pi^2z^2\sin 2\theta}$$

$$=\sum_{m=1}^\infty \frac{(\pi z)^{2m}\{(1+\sin2\theta)^m-(1-\sin2\theta)^m\}}{(2m)!\,\pi^2z^2\sin 2\theta}$$

$$=\sum_{m=0}^\infty\frac{2(\pi z)^{2m}}{(2m+2)!}\sum_{n=0}^{\lfloor m/2\rfloor}\binom{m+1}{2n+1}(\sin 2\theta)^{2n}.$$

Now recall Theorem 7:

$$\sum_{k=0}^{m} x^k y^{m-k}\left[(ab)^k \sqcup\!\sqcup (ab)^{m-k}\right] = \sum_{n=0}^{\lfloor m/2\rfloor}(4xy)^n(x+y)^{m-2n}\,T_{m,n}.$$

Putting $x = z^2\cos^2\theta$ and $y = z^2\sin^2\theta$ yields

$$J(z\cos\theta)J(z\sin\theta)$$

$$= \left[\sum_{k=0}^\infty (z\cos\theta)^{2k}\int_0^1 (ab)^k\right]\left[\sum_{j=0}^\infty (z\sin\theta)^{2j}\int_0^1 (ab)^j\right]$$

$$= \sum_{m=0}^\infty\sum_{n=0}^{m}(z\cos\theta)^{2n}(z\sin\theta)^{2m-2n} \times\int_0^1 (ab)^n \sqcup\!\sqcup (ab)^{m-n}$$

$$= \sum_{m=0}^\infty\sum_{n=0}^{\lfloor m/2\rfloor}(4z^4\sin^2\theta\cos^2\theta)^n \times (z^2\cos^2\theta+z^2\sin^2\theta)^{m-2n}\int_0^1 T_{m,n}$$

$$= \sum_{m=0}^\infty z^{2m}\sum_{n=0}^{\lfloor m/2\rfloor}(\sin 2\theta)^{2n}\int_0^1 T_{m,n}.$$

Conjecture 10

$$Z(a_1,b_1,a_2,b_2,a_3)+Z(a_2,b_1,a_3,b_2,a_1) + Z(a_3,b_1,a_1,b_2,a_2)$$

$$= Z(a_1,b_2,a_2,b_1,a_3)+Z(a_2,b_2,a_3,b_1,a_1) + Z(a_3,b_2,a_1,b_2,a_2)$$

Conjecture 11 *Let $q_1 = q_2 = t^3$, and for $n \ge 1$,*

$$n(n+1)^2 q_{n+2} = n(2n+1)q_{n+1} + (n^3 + (-1)^{n+1}t^3)q_n.$$

Then

$$\lim_{n\to\infty} q_n = t^3\prod_{n=1}^\infty\left(1+\frac{t^3}{8n^3}\right).$$

Equivalently, for all positive integers n,

$$\mathrm{Li}_{\{2,1\}^n}(\{-1,1\}^n) \stackrel{?}{=} 8^{-n}\mathrm{Li}_{\{2,1\}^n}(\{1,1\}^n)$$
$$\iff \zeta(\{\overline{2},1\}^n) \stackrel{?}{=} 8^{-n}\zeta(\{2,1\}^n) = 8^{-n}\zeta(\{3\}^n).$$