Iterated Integrals and Knizhnik–Zamolodchikov Equations

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Introduction

For three variables $0 \leq x \leq y \leq z \leq 1$, an iterated integral looks like

$$\int_0^1 \left(\int_0^z \left(\int_0^y f(x,y,z)dx \right) dy \right) dz, \text{or simply } \int_0^1 \int_0^z \int_0^y f(x,y,z)dxdydz.$$

The theory of iterated integrals was first invented by K. T. Chen in order to construct functions on the infinite-dimensional space of paths on a manifold and has since become an important tool in various branches of math and physics.

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Definition

Let M be a smooth manifold and ω_1, ..., ω_n be $\mathbb{C}$-valued 1-forms on M and let $\gamma : [0,1] \to M$ be a path. Write

$$\gamma^*\omega_i = f_i(t)dt,$$

for the pullback of the forms ω_i to the interval $[0,1]$. Define

$$\begin{aligned}\int_\gamma \omega_1 \ldots \omega_n &= \int_{0\leq t_1 \leq \ldots \leq t_n \leq 1} f_n(t_n)\cdots f_1(t_1)dt_1 \ldots dt_n \\ &= \int_0^1 \int_0^{t_n} \cdots \int_0^{t_2} f_n(t_n)f_{n-1}(t_{n-1})\ldots f_1(t_1)dt_1 dt_2 \ldots dt_n,\end{aligned}$$

which will be called the iterated integral of ω_1, ..., ω_n along γ. Moreover, define the iterated integral of empty product of 1-forms to be 1.

Proposition

Iterated integrals satisfy the following properties:
(a) If $\gamma^{-1}(t) = \gamma(1-t)$ denotes the reversal of the path γ, then

$$\int_{\gamma^{-1}} \omega_1 ... \omega_n = (-1)^n \int_{\gamma} \omega_n ... \omega_1 .$$

(b) If α, β are two paths, denote the path obtianed by first traversing β then α by $\alpha\beta$, then

$$\int_{\alpha\beta} \omega_1 \dots \omega_n = \sum_{i=0}^{n} \int_{\alpha} \omega_1 \dots \omega_i \int_{\beta} \omega_{i+1} \dots \omega_n .$$

Proposition

(c) The shuffle property:

$$\int_\gamma \omega_1 \dots \omega_r \int_\gamma \omega_{r+1} \dots \omega_{r+s} = \sum_{\sigma \in \mathrm{Shuff}(r,s)} \int_\gamma \omega_{\sigma(1)} \dots \omega_{\sigma(r+s)},$$

where $\mathrm{Shuff}(r,s)$ *is the set:*

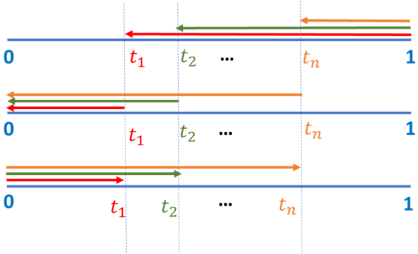
$$\mathrm{Shuff}(r,s) = \left\{ \begin{matrix} \textit{all permutations } \sigma \textit{ of } (r+s) \textit{ indices such that} \\ \sigma(1) < \dots < \sigma(r) \textit{ and } \sigma(r+1) < \dots < \sigma(r+s) \end{matrix} \right\}.$$

Proof: (a)

$$\int_{\gamma^{-1}} \omega_1 \ldots \omega_n = \int_1^0 \int_1^{t_1} \cdots \int_1^{t_{n-1}} f_1(t_1) f_2(t_2) \ldots f_n(t_n) dt_n dt_{n-1} \ldots dt_1$$

$$= \int_1^0 \int_{t_n}^0 \cdots \int_{t_2}^0 f_n(t_n) f_{n-1}(t_{n-1}) \ldots f_1(t_1) dt_1 dt_2 \ldots dt_n$$

$$= (-1)^n \int_\gamma \omega_n \ldots \omega_1.$$



(b) Let $0 < x < 1$, then

$$\begin{aligned}&\{(t_1, t_2, \ldots, t_n) \in \mathbb{R}^n : 0 \leq t_1 \leq t_2 \leq \cdots \leq t_n \leq 1\}\\ &= \bigcup_{k=0}^{n} \{(t_1, \ldots, t_k) \in \mathbb{R}^k : 0 \leq t_1 \leq \ldots \leq t_k \leq x\}\\ &\qquad \times \{(t_{k+1}, \ldots, t_n) \in \mathbb{R}^{n-k} : x \leq t_{k+1} \leq \ldots \leq t_{n-1} \leq_{t_n}\}.\end{aligned}$$

(c) On the R.H.S. of (5), all $(r + s)$ indices are ordered, but on the L.H.S. only the r indices and the s indices are ordered, so on the R.H.S. we need to count all permutations such that only the r indices and the s indices are ordered.

Schrödinger Equation for the Time-evolution Operator

State ket $\mathbb{R} \to \mathbb{C}^n, t \mapsto |v, t\rangle$.
Consider its time evolution $t_0 \mapsto t$ from initial condition: $|\alpha, t_0\rangle$.
Denote the state ket at t obtained from the initial condition by $|\alpha, t_0; t\rangle$.
Define the time-evolution operator $\mathcal{U}(t, t_0)$ by an equation which relates the two kets:

$$|\alpha, t_0; t\rangle = \mathcal{U}(t, t_0)|\alpha, t_0\rangle.$$

Proposition

The time-evolution operator satisfies the following properties:
(a) $\mathcal{U}^\dagger(t, t_0)\mathcal{U}(t, t_0) = 1$. *(conservation of probability)*
(b) $\mathcal{U}(t_2, t_0) = \mathcal{U}(t_2, t_1)\mathcal{U}(t_1, t_0)$, $(t_2 > t_1 > t_0)$. *(the compostion property)*

Define the infinitesimal time-evolution operator $\mathcal{U}(t_0 + dt, t_0)$:

$$\mathcal{U}(t_0 + dt, t_0) = 1 - \frac{iHdt}{\hbar}.$$

Applying the composition property to the time evolution operator at t_0, $t_1 = t$ and $t_2 = t + dt$ gives us the Schrödinger equation for the time-evolution operator

$$i\hbar \frac{\partial}{\partial t}\mathcal{U}(t, t_0) = H\mathcal{U}(t, t_0).$$

Now let us solve this equation. In general, the Hamiltonians are time-dependent and do not commute at differet times. Note that by the definition of the time-evolution operator,

$$\mathcal{U}(t_0, t_0) = 1,$$

write the differential equation by an integral equation

$$\mathcal{U}(t, t_0) = 1 - \frac{i}{\hbar} \int_{t_0}^{t} H(s)\mathcal{U}(s, t_0) ds,$$

then we can apply Picard's method to solve this equation by successive approximation: let $\mathcal{U}_0(t, t_0) = \mathcal{U}(t_0, t_0) = 1$ be the constant function and define for $n \geq 0$,

$$\mathcal{U}_{n+1}(t, t_0) = 1 - \frac{i}{\hbar} \int_{t_0}^{t} H(s)\mathcal{U}_n(s, t_0) ds,$$

then assuming $t_0 \leq t_1 \leq \ldots \leq t_n = t$,

$$\begin{aligned}
\mathcal{U}_1(t, t_0) &= 1 - \frac{i}{\hbar}\int_{t_0}^{t} H(t_1)\mathcal{U}_0(t, t_0)dt_1, \\
\mathcal{U}_2(t, t_0) &= 1 - \frac{i}{\hbar}\int_{t_0}^{t} H(t_2)\mathcal{U}_0(t, t_0)dt_1 \\
&\quad + \left(\frac{-i}{\hbar}\right)^2 \int_{t_0}^{t}\int_{t_0}^{t_2} H(t_2)H(t_1)\mathcal{U}_1(t, t_0)\mathcal{U}_2(t_1, t_0)dt_1\,dt, \\
&\ldots \\
\mathcal{U}_n(t, t_0) &= 1 + \sum_{n\geq 1}\left(\frac{-i}{\hbar}\right)^n \int_{t_0}^{t}\int_{t_0}^{t_{n-1}}\ldots\int_{t_0}^{t_2} H(t)\ldots H(t_2)H(t_1)\mathcal{U}_0(t, t_0)dt_1\,dt_2\ldots dt, \\
&= 1 + \sum_{n\geq 1}\left(\frac{-i}{\hbar}\right)^n \int_{t_0\leq t_1\leq t_2\leq\ldots\leq t} H(t)\ldots H(t_2)H(t_1)dt_1\,dt_2\ldots dt, \\
&\ldots
\end{aligned}$$

If $\lim_{n\to\infty}\mathcal{U}_n(t, t_0)$ exists, it gives the solution and is called the Dyson series.

Monodromy of the solution

Let M be a smooth manifold and $\hat{\mathcal{A}}$ a completed graded algebra over the complex numbers. Choose a set $\omega_1, \ldots, \omega_p$ of $\mathbb{C}$-valued closed differential 1-forms on X and a set $c_1, \ldots, c_p$ of homogeneous elements of $\hat{\mathcal{A}}$ of degree 1. Consider the closed 1-form

$$\omega = \sum_{i=1}^{p} \omega_j c_j$$

with values in $\hat{\mathcal{A}}$. The Knizhnik-Zamolodchikov equation is a particular case of the following very general equation

$$dI = \omega I,$$

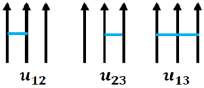
where $I : M \to A$ is the unknown function.

Given a local solution I of the equation and $a \in \hat{\mathcal{A}}$, we can extend a local solution at x_0 along a loop $\gamma : [0,1] \to M$ we arrive to another solution I_1, also defined in a neighbourhood of x_0. Let $I_1(x_0) = a_\gamma$. Suppose that a_0 is an invertible element of $\hat{\mathcal{A}}$. The fact that the local solutions form a free one-dimensional $\hat{\mathcal{A}}$-module implies thatthe two solutions I_0 and I_1 are proportional to each other: $I_1 = I_0 a_0^{-1} a_\gamma$. Therefore, we get a homomorphism $\pi_1(X) \to \hat{\mathcal{A}}^*$from the fundamental group of X into the multiplicative group of the units of $\hat{\mathcal{A}}$, called the monodromy representation. Analogous to the Dyson series, solving this equation iteratively gives

$$I(t) = 1 + \sum_{m=1}^{\infty} \int_{0 \le t_1 \le \ldots \le t_n \le 1} \omega(t_n) \cdots \omega(t_1)$$

The value $I(1)$ represents the monodromy of the solution over the loop γ. Each iterated integral $I_m(1)$ is a homotopy invariant (of “order m”) of γ.

Let $M = \mathbb{C}^3 \setminus \mathcal{H}$, where $\mathcal{H} = \{z_1 = z_3\} \cup \{z_1 = z_2\} \cup \{z_2 = z_3\}$. (The configuration space of 3 distinct points in $\mathbb{C}$). Note that a loop γ in this space can be identified with a pure braid on 3 strands. The horizontal chord diagrams on 3 strands $\mathcal{A}^h(3)$ is generated by



subject to the relations

$$[u_{jk}, u_{jl} + u_{kl}] = 0,$$

so we have

Proposition

$\mathcal{A}^h(3)$ is a direct product of the free algebra on two generators u_{12} and u_{23}, and the free commutative algebra on one generator $u = u_{12} + u_{23} + u_{13}$.

The KZ equation for 3 points is

$$dI = \frac{1}{2\pi i}\left(u_{12} d\log(z_2 - z_1) + u_{13} d\log(z_3 - z_1) + u_{23} d\log(z_3 - z_2)\right) I$$

which is a partial differential equation in 3 variables. Make the substituion

$$I = (z_3 - z_1)^{\frac{u}{2\pi i}} G,$$

this equation can be reduced to

$$dG = \frac{1}{2\pi i}\left(u_{12} d\log\left(\frac{z_2 - z_1}{z_3 - z_1}\right) + u_{23} d\log\left(1 - \frac{z_2 - z_1}{z_3 - z_1}\right)\right) G.$$

Denoting $\frac{z_2 - z_1}{z_3 - z_1}$ by z, we see that it satisfies the ODE (the reduced KZ equation),

$$\frac{dG}{dz} = \left(\frac{A}{z} + \frac{B}{z-1}\right) G,$$

where $A = \frac{u_{12}}{2\pi i}$, $B = \frac{u_{23}}{2\pi i}$.

Definition

Multiple polylogarithms are nested sum of the form

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

where $s_1,\dots,s_k$ and $z_1,\dots,z_k$ are complex numbers such that the sum converges. In particular, setting $z_j = 1$ gives us multiple zeta values

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

Iterated integrals on $\mathbb{C} \setminus \{0, 1\}$

The multiple polylogarithms (in one variable) can be defined via iterated integrals:
Let $X = \{x_0, x_1\}$ be an alphabet in two letters and $X^\times$ be the set of words in x_0, x_1 and the empty word e. Let $\mathbb{Q}\langle x_0, x_1\rangle$ be the vector space generated by the words in X, equipped with the shuffle product:

$$x_{i_1} \dots x_{i_r} \sqcup\!\sqcup\, x_{i_{r+1}} \dots x_{i_{r+s}} = \sum_{\sigma \in \mathrm{Shuff}(r,s)} x_{\sigma(1)} \cdots x_{\sigma(r+s)},$$

and where $e \sqcup\!\sqcup\, w = w \sqcup\!\sqcup\, e = w$ for all $w \in X^*$.

To every word $w \in X^*$, we associate a multivalued function $\mathrm{Li}_w(z)$ on $M = \mathbb{C} \setminus \{0, 1\}$ as follows:
Let $\omega_0 = \frac{dz}{z}$, $\omega_1 = \frac{dz}{z-1}$ be 1-forms defined on M, γ be a smooth path from 0 to z on M.
1) If w ends with x_1, write $w = x_0^{s_k-1}x_1 \ldots x_0^{s_1-1}x_1$ and let

$$\mathrm{Li}_w(z) = \int_\gamma \omega_1\omega_0^{s_k-1}\omega_1 \ldots \omega_0^{s_1-1} = \mathrm{Li}_{s_1,\ldots,s_k}(1, \ldots, 1, z_1)$$

Denote $\mathrm{Li}_{s_1,\ldots,s_k}(z_1, 1, \ldots, 1)$ by $\mathrm{Li}_{s_1,\ldots,s_k}(z)$. (multiple polylogarithm in one variable)
To see the equality, note that

$$\frac{d}{dz}\mathrm{Li}_{s_1,\ldots,s_k}(z) = \begin{cases} \frac{1}{z}\mathrm{Li}_{s_1-1,\ldots,s_k}(z), & \text{if} \quad s_1 > 1, \\ \frac{1}{1-z}\mathrm{Li}_{s_2,\ldots,s_k}(z), & \text{if} \quad s_1 = 1. \end{cases}$$

2) Set

$$\mathrm{Li}_{x_0^n}(z) = \frac{1}{n!}\log^n(z),$$

then any word can be composed by x_0^n and words which end with x_1 by the composition property of iterated integrals.
Consider the generating series

$$L(z) = \sum_{w \in X^*} w\mathrm{Li}_w(z),$$

it defines a multivalued function on M taking values in

$$\mathbb{C}[[X]] = \{\sum_{w \in X^*} S_w w : S_w \in \mathbb{C}\},$$

the ring of non-commutative formal power series in the words X^*, with the multiplication being the concatenation of words $(w_1 \cdot w_2 = w_1 w_2)$.

$L(z)$ satisfies the differential equation

$$\frac{d}{dz}L(z) = \left(\frac{x_0}{z} + \frac{x_1}{z-1}\right) L(z),$$

which is the one-dimensional Knizhnik–Zamolodchikov equation. Note that for words $w \neq x_0^n$,

$$\lim_{z \to 0} \mathrm{Li}_w(z) = 0,$$

we have

$$L(z) \sim \exp(x_0 \log z) \quad \text{as} \quad z \to 0.$$

Similarly, there exists another solution

$$L^1(z) \sim \exp(x_1 \log(1-z)) \quad \text{as} \quad z \to 1.$$

Define the Drinfel'd associator $\Phi(z)$ by an equation which relates the two solutions:

$$L(z) = L^1(z)\Phi(z),$$

we denote it by $\Phi(x_0, x_1)$.

Proposition

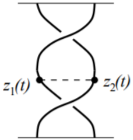
The coefficients of $\Phi(x_0, x_1)$ are multiple zeta values.

First, for all words $w \in x_0 X^* x_1$, $\mathrm{Li}_w(z)$ converges at the point $z = 1$, we have $\zeta(w) = \mathrm{Li}_w(1)$. Next, we can use the shuffle property $\zeta(w)\zeta(w') = \zeta(w ⧢ w')$to write any word by x_0, x_1 and $x_0 X^* x_1$:

$$
\begin{aligned}
&\zeta(x_0) = \zeta(x_1) = 0, \\
&\zeta(x_0 x_0) = \frac{1}{2}\zeta(x_0 ⧢ x_0) = \frac{1}{2}\zeta(x_0)\zeta(x_0) = 0, \\
&\zeta(x_0 x_1) = \zeta(2), \\
&\zeta(x_1 x_0) = \zeta(x_1 ⧢ x_0 - x_0 x_1) = \zeta(x_0)\zeta(x_1) - \zeta(x_0 x_1) = -\zeta(2), \\
&\zeta(x_1 x_1) = \frac{1}{2}\zeta(x_1 ⧢ x_1) = 0, \\
&\dots
\end{aligned}
$$

We have $\Phi(x_0, x_1) = 1 + \zeta(2)[x_0, x_1] + \zeta(3)([x_0, [x_0, x_1] - [x_0, x_1], x_1]) + \dots$

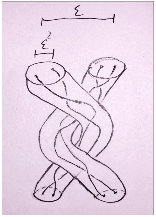
In the construction of the Kontsevich integral, $\mathbb{R}^3$ where the tangles are defined is represented as a product of complex plane $\mathbb{C}$ with coordinate z and real line $\mathbb{R}$ with coordinate t.



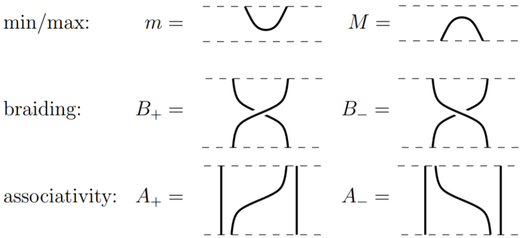
Intuitively, the Kontsevich integral counts the number of “twists” between strands in a tangle. For example, the number of twists between two strands in the above figure can be computed as

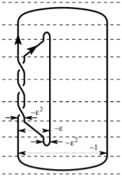
$$\frac{1}{2\pi i}\int_0^1 \frac{dz_1 - dz_2}{z_1 - z_2}.$$

Scales of symmetries: in the following figure, the twists of tubes produce an underlying twist for the twisting strands inside the tubes, if we call the twists of tube “first order” (ε), then the twists of strands are of second order (ε^2).



To construct the Kontsevich integral, cut the knot into several parts by some slices on t such that each part contains one of the three basic events:

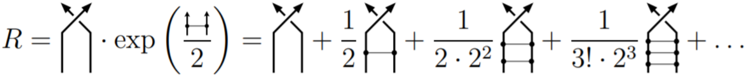




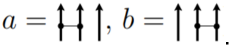
Now we can replace a knot by chord diagrams according to the followings rules:

$$
\begin{aligned}
& m, M \mapsto 1, \\
& B_+ \mapsto R, \quad B_- \mapsto R^{-1}, \\
& A_+ \mapsto \Phi, \quad A_- \mapsto \Phi^{-1}
\end{aligned}
\tag{1}
$$

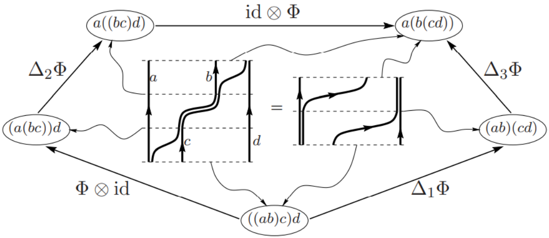
where

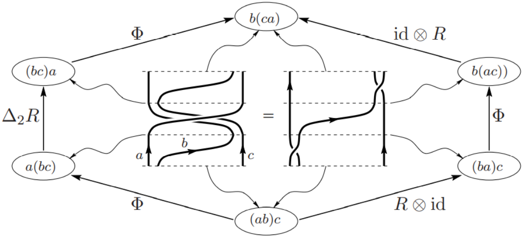


$$\Phi = 1 - \frac{\zeta(2)}{(2\pi i)^2}[a, b] - \frac{\zeta(3)}{(2\pi i)^3}([a, [a, b]] + [b, [a, b]) + \dots$$



Then compute the product of these diagrams from top to bottom.


$a((bc)d)$
$\mathrm{id} \otimes \Phi$
$a(b(cd))$
$\Delta_2\Phi$
$\Delta_3\Phi$
a
b
c
d
$=$
$(a(bc))d$
$(ab)(cd)$
$\Phi \otimes \mathrm{id}$
$\Delta_1\Phi$
$((ab)c)d$


$b(ca)$
Φ
$\mathrm{id} \otimes R$
$(bc)a$
$b(ac))$
$\Delta_2 R$
$=$
Φ
b
a
c
$a(bc)$
$(ba)c$
Φ
$R \otimes \mathrm{id}$
$(ab)c$