Baker-Campbell-Hausdorff formula revisited

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2020.09.18-09.20

The 3rd Conference on Operad Theory and Related Topics

Jilin/Online

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Outline

1. Mould Calculus
   - Mould Algebra
   - Comoulds and Mould Expansions
   - Symmetrality and Alternality

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1. Mould Calculus
   - Mould Algebra
   - Comoulds and Mould Expansions
   - Symmetrality and Alternality
2. Baker-Campbell-Hausdorff Formulas
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Outline

Letters and Words

- $\mathbb{N} := \{0, 1, 2, 3, \cdots\} := \{0\} \cup \mathbb{N}^*$
- $\mathcal{N}$: alphabet (the elements: "letters") , e.g.
  $\mathcal{N} = \Omega := \{x, y\}$, a two-letter alphabet
- $\underline{\mathcal{N}}$ the corresponding set of "words" (or "strings"):

$$\underline{\mathcal{N}} := \{\underline{n} = n_1 \cdots n_r \mid r \in \mathbb{N},\ n_1, \ldots, n_r \in \mathcal{N}\}.$$

  e.g. $\underline{\Omega} = \{x^{p_1} y^{q_1} \cdots x^{p_r} y^{q_r} \mid p_i, q_i \in \mathbb{N}\}$
- The concatenation law
  $(a_1 \cdots a_r, b_1 \cdots b_s) \in \underline{\mathcal{N}} \times \underline{\mathcal{N}} \mapsto a_1 \cdots a_r\, b_1 \cdots b_s \in \underline{\mathcal{N}}$
- monoid structure, with the empty word $\varnothing$ as unit.

Mould

- A $\mathbf{k}$-valued mould on $\mathcal{N}$ is a function on $\underline{\mathcal{N}}$:

$$\begin{aligned} M : \underline{\mathcal{N}} &\rightarrow \mathbf{k} \\ \underline{n} &\mapsto M^{\underline{n}} \end{aligned}$$

- The set of all moulds is denoted by $\mathbf{k}^{\underline{\mathcal{N}}}$.
- e.g. $\mathbf{k} := \mathbf{Q}$, $I_x, I_y \in \mathbf{Q}^{\underline{\Omega}}$ are defined by

$$I_x^{\underline{\omega}} := \begin{cases} 1 & \text{if } \underline{\omega} \text{ is the one-letter word } x \\ 0 & \text{else,} \end{cases}$$

$$I_y^{\underline{\omega}} := \begin{cases} 1 & \text{if } \underline{\omega} \text{ is the one-letter word } y \\ 0 & \text{else.} \end{cases}$$

Mould Multiplication

- for any two moulds $M, N \in \mathbf{k}^{\underline{\mathcal{N}}}$, the mould multiplication is $(M \times N)^{\underline{n}} := \sum_{(\underline{a},\underline{b}) \text{ such that } \underline{n}=\underline{a}\,\underline{b}} M^{\underline{a}} N^{\underline{b}} \quad \text{for } \underline{n} \in \underline{\mathcal{N}},$
- For instance,

$$(M \times N)^{n_1 n_2} = M^{\varnothing} N^{n_1 n_2} + M^{n_1} N^{n_2} + M^{n_1 n_2} N^{\varnothing}.$$

- $\mathbf{k}^{\underline{\mathcal{N}}}$ *is an associative* $\mathbf{k}$*-algebra*, noncommutative if $\mathcal{N}$ has more than one element, whose unit is the mould $\mathbb{1}$ defined by $\mathbb{1}^{\varnothing} = 1$ and $\mathbb{1}^{\underline{n}} = 0$ for $\underline{n} \neq \varnothing$

Two important moulds: Exp and Log

- a mould M has order $\geq p$ if $M^{\underline{n}} = 0$ for each word $\underline{n}$ of length $< p$.
- If ord $M \geq p$ and ord $N \geq q$, then $\operatorname{ord}(M \times N) \geq p + q$. In particular, if $M^{\varnothing} = 0$, then ord $M^{\times k} \geq k$ for each $k \in \mathbb{N}^*$,
- hence the following moulds are well-defined
  $\mathrm{e}^M := \sum_{k\in\mathbb{N}} \frac{1}{k!} M^{\times k}$
  $\log(\mathbb{1} + M) := \sum_{k\in\mathbb{N}^*} \frac{(-1)^{k-1}}{k} M^{\times k}$
  (because, for each $\underline{n} \in \underline{\mathcal{N}}$, only finitely many terms contribute to $(\mathrm{e}^M)^{\underline{n}}$ or $(\log(\mathbb{1} + M))^{\underline{n}}$).

Two important moulds: Exp and Log

We thus get mutually inverse bijections

$$\{\, M \in \mathbf{k}^{\underline{\mathcal{N}}} \mid M^{\varnothing} = 0 \,\} \quad \underset{\log}{\overset{\exp}{\rightleftarrows}} \quad \{\, M \in \mathbf{k}^{\underline{\mathcal{N}}} \mid M^{\varnothing} = 1 \,\}.$$

Exp and Log

- Example: $S_\Omega := \mathrm{e}^{I_x} \times \mathrm{e}^{I_y}$
-

$$S_\Omega^{\underline{\omega}} = \begin{cases} \dfrac{1}{p!q!} & \text{if } \underline{\omega} \text{ is of the form } x^p y^q \text{ with } p, q \in \mathbb{N} \\ 0 & \text{else,} \end{cases}$$

Outline

Complete Filtered Associative Algebra $\mathcal{A}$

- To deal with infinite expansions, we need complete filtered associative algebra, *i.e.* there is an order function $\operatorname{ord}\colon \mathcal{A} \to \mathbb{N} \cup \{\infty\}$ compatible with sum and product,[1] such that every family $(X_i)_{i\in I}$ of $\mathcal{A}$ is formally summable provided, for each $p \in \mathbb{N}$, all the X_i's have order $\geq p$ except finitely many of them.
- For the talk,

$$\mathcal{A} = A[[t]]$$

for the associative algebra A with the order function relative to powers of t,

[1] here $\operatorname{ord}(X+Y) \geq \min\{\operatorname{ord} X, \operatorname{ord} Y\}$ and $\operatorname{ord}(XY) \geq \operatorname{ord} X + \operatorname{ord} Y$ for any $X, Y \in \mathcal{A}$, and $\operatorname{ord} X = \infty$ iff $X = 0$.

Associative Comould

- Suppose that we are given a family $(B_n)_{n\in\mathcal{N}}$ in $\mathcal{A}$ such that all the B_n's have order ≥ 1 and, for each $p \in \mathbb{N}$, only finitely many of them are not of order $\geq p$.
- We call associative comould generated by $(B_n)_{n\in\mathcal{N}}$ the family $(B_{\underline{n}})_{\underline{n}\in\underline{\mathcal{N}}}$ defined by $B_{\varnothing} := 1_{\mathcal{A}}$ and

$$B_{n_1\cdots n_r} := B_{n_1}\cdots B_{n_r} \quad \text{for all } r \geq 1 \text{ and } n_1,\ldots,n_r \in \mathcal{N}.$$

- For $\Omega = \{x, y\}$, $B_x := tX$, $B_y := tY \in A[[t]]$; $B_{x^p y^q} = t^{p+q} X^p Y^q \in A[[t]]$

Mould-Comould Expansion

- The formula

$$M \in \mathbf{k}^{\underline{\mathcal{N}}} \mapsto MB := \sum_{\underline{n} \in \underline{\mathcal{N}}} M^{\underline{n}} B_{\underline{n}} \in \mathcal{A}$$

  defines a morphism of associative algebras (Associative mould expansion)
- Moreover,

$$M^{\varnothing} = 0 \;\Rightarrow\; (\mathrm{e}^{M})B = \mathrm{e}^{MB},$$

$$M^{\varnothing} = 1 \;\Rightarrow\; (\log M)B = \log(MB)$$

  by

$$(M \times N)B = (MB)(NB)$$

An Example

- Given $X, Y \in A$, an associative algebra, and $\mathcal{A} = A[[t]]$
- $\mathbf{k} = \mathbf{Q}$, $\mathcal{N} = \Omega := \{x, y\}$
- the associative comould generated by

$$B_x := tX, \qquad B_y := tY.$$

- $tX = I_x B,\ tY = I_y B$ with $I_x, I_y \in \mathbf{Q}^{\underline{\Omega}}$ defined by

$$I_x^{\underline{\omega}} := \begin{cases} 1 & \text{if } \underline{\omega} \text{ is the one-letter word } x \\ 0 & \text{else,} \end{cases}$$

- $\mathrm{e}^{tX} = \mathrm{e}^{I_x} B$, $\mathrm{e}^{tY} = \mathrm{e}^{I_y} B$, and

$$\mathrm{e}^{tX}\mathrm{e}^{tY} = S_\Omega B,\ S_\Omega := \mathrm{e}^{I_x} \times \mathrm{e}^{I_y}$$

An Example

- $$S_{\Omega}^{\underline{\omega}} = \begin{cases} \frac{1}{p!q!} & \text{if } \underline{\omega} \text{ is of the form } x^p y^q \text{ with } p, q \in \mathbb{N} \\ 0 & \text{else,} \end{cases}$$

- we get another way of writing $\mathrm{e}^{tX}\mathrm{e}^{tY} = \sum \frac{t^{p+q}}{p!q!} X^p Y^q$.

- $$\log(\mathrm{e}^{tX}\mathrm{e}^{tY}) = T_{\Omega} B$$

  with $T_{\Omega} := \log S_{\Omega}$.

Lie Comoulds

- Lie algebra structure on $\mathcal{A}$ induced by the commutators $\operatorname{ad}_A B = [A, B]$
- We call Lie comould generated by $(B_n)_{n\in\mathcal{N}}$ the family $(B_{[\underline{n}]})_{\underline{n}\in\underline{\mathcal{N}}}$ of $\mathcal{A}$ defined by $B_{[\varnothing]} := 0$ and

$$B_{[n_1\cdots n_r]} := \operatorname{ad}_{B_{n_1}} \cdots \operatorname{ad}_{B_{n_{r-1}}} B_{n_r} = [B_{n_1}, [\cdots [B_{n_{r-1}}, B_{n_r}] \cdots]].$$

- Lie mould expansion associated with a mould $M \in \mathbf{k}^{\underline{\mathcal{N}}}$ by the formula

$$M[B] := \sum_{\underline{n}\in\underline{\mathcal{N}}\setminus\{\varnothing\}} \frac{1}{r(\underline{n})} M^{\underline{n}} B_{[\underline{n}]} \in \mathcal{A},$$

where $r(\underline{n})$ denotes the length of a word $\underline{n}$.

Lie Comoulds

- Division by $r(\underline{n})$ is just a convenient normalization choice.
- we will prove the BCH theorem by showing how to pass from

$$\log(\mathrm{e}^{tX}\mathrm{e}^{tY}) = T_\Omega B = (\log S_\Omega)B$$

to a Lie mould expansion.

Outline

Shuffling

- the shuffling of two words $\underline{a} = \omega_1 \cdots \omega_\ell$ and $\underline{b} = \omega_{\ell+1} \cdots \omega_r$ is the set of all the words $\underline{n}$ which can be obtained by interdigitating the letters of $\underline{a}$ and those of $\underline{b}$ while preserving their internal order in $\underline{a}$ and $\underline{b}$,
- *i.e.* the words which can be written $\underline{n} = \omega_{\tau(1)} \cdots \omega_{\tau(r)}$ with a permutation τ such that[2] $\tau^{-1}(1) < \cdots < \tau^{-1}(\ell)$ and $\tau^{-1}(\ell+1) < \cdots < \tau^{-1}(r)$.

[2]Indeed, $\tau^{-1}(i)$ is the position in $\underline{n}$ of ω_i, the i-th letter of $\underline{a}\,\underline{b}$.

Shuffling

- the shuffling coefficient $\mathrm{sh}\binom{\underline{a},\underline{b}}{\underline{n}}$ is just the number of such permutations τ,
- we set $\mathrm{sh}\binom{\underline{a},\underline{b}}{\underline{n}} := 0$ whenever $\underline{n}$ does not belong to the shuffling of $\underline{a}$ and $\underline{b}$.
- For instance, if n, m, p, q are four distinct elements of $\mathcal{N}$,

$$\mathrm{sh}\begin{pmatrix} nmp, mq \\ nmqpm \end{pmatrix} = 0, \qquad \mathrm{sh}\begin{pmatrix} nmp, mq \\ mnqmp \end{pmatrix} = 1, \qquad \mathrm{sh}\begin{pmatrix} nmp, mq \\ nmmqp \end{pmatrix} = 2.$$

- We also define, for arbitrary words $\underline{n}$ and $\underline{a}$, $\mathrm{sh}\binom{\underline{a},\varnothing}{\underline{n}} = \mathrm{sh}\binom{\varnothing,\underline{a}}{\underline{n}} = 1$ if $\underline{a} = \underline{n}$, 0 else.

Alternal and Symmetral Moulds

- A mould $M \in \mathbf{k}^{\underline{\mathcal{N}}}$ is said to be alternal if $M^{\varnothing} = 0$ and

$$\sum_{\underline{n} \in \underline{\mathcal{N}}} \mathrm{sh}\binom{\underline{a},\ \underline{b}}{\underline{n}} M^{\underline{n}} = 0 \quad \text{for any two nonempty words } \underline{a},\ \underline{b}.$$

- A mould $M \in \mathbf{k}^{\underline{\mathcal{N}}}$ is said to be symmetral if $M^{\varnothing} = 1$ and

$$\sum_{\underline{n} \in \underline{\mathcal{N}}} \mathrm{sh}\binom{\underline{a},\ \underline{b}}{\underline{n}} M^{\underline{n}} = M^{\underline{a}} M^{\underline{b}} \quad \text{for any two words } \underline{a},\ \underline{b}.$$

Alternal and Symmetral Moulds: Examples

- any mould M whose support is contained in the set of one-letter words (*i.e.* $r(\underline{n}) \neq 1 \Rightarrow M^{\underline{n}} = 0$) is alternal.
- For instance, the moulds I_x and I_y are alternal.
- An elementary example of symmetral mould is E defined by $E^{\underline{n}} := \frac{1}{r(\underline{n})!}$. Indeed, since the total number of words obtained by shuffling of any $\underline{a}, \underline{b} \in \underline{\mathcal{N}}$ (counted with multiplicity) is $\binom{r(\underline{a}\,\underline{b})}{r(\underline{a})}$,

$$\sum_{\underline{n} \in \underline{\mathcal{N}}} \mathrm{sh}\begin{pmatrix} \underline{a}, \underline{b} \\ \underline{n} \end{pmatrix} E^{\underline{n}} = \frac{r(\underline{a}\,\underline{b})!}{r(\underline{a})!\,r(\underline{b})!} \cdot \frac{1}{r(\underline{a}\,\underline{b})!} = E^{\underline{a}} E^{\underline{b}}.$$

- the moulds e^{I_x}, e^{I_y} and S_Ω are symmetral, and that T_Ω is alternal.

Alternal v.s. Symmetral

we are interested in the shuffling coefficients because of the following classical relation between the Lie comould and the associative comould:

Theorem (Écalle)

$$B_{[\underline{n}]} = \sum_{(\underline{a},\underline{b})\in\underline{\mathcal{N}}\times\underline{\mathcal{N}}} (-1)^{r(\underline{b})} r(\underline{a}) \, \mathrm{sh}\binom{\underline{a},\ \underline{b}}{\underline{n}} \, B_{\underline{\widetilde{b}}\,\underline{a}} \quad \textit{for all } \underline{n} \in \underline{\mathcal{N}},$$

where, for an arbitrary word $\underline{b} = b_1 \cdots b_s$, *we denote by* $\widetilde{\underline{b}}$ *the reversed word:* $\widetilde{\underline{b}} = b_s \cdots b_1$

Alternal v.s. Symmetral

An immediate and useful consequence is

Theorem (Écalle)

If M is an alternal mould, then $M[B] = MB$, i.e.

$$\sum_{\underline{n}\in\underline{\mathcal{N}}\setminus\{\varnothing\}} \frac{1}{r(\underline{n})} M^{\underline{n}} B_{[\underline{n}]} = \sum_{\underline{n}\in\underline{\mathcal{N}}} M^{\underline{n}} B_{\underline{n}}.$$

- Note that by definition, $MB \in \mathcal{A}$, however now $MB \in Lie(\mathcal{A})$ due to the fact that M is alternal.
- The above theorem is a highly nontrivial fact for alternal mould which makes the mould calculus a powerful tool in many situations.

Alternal v.s. Symmetral

PROOF:

$M[B] = \sum_{\underline{n} \neq \varnothing} \sum_{\underline{a}, \underline{b}} (-1)^{r(\underline{b})} \frac{r(\underline{a})}{r(\underline{n})} \operatorname{sh}\left(\frac{\underline{a}, \underline{b}}{\underline{n}}\right) M^{\underline{n}} B_{\widetilde{\underline{b}}\,\underline{a}}$. Now,

$\operatorname{sh}\left(\frac{\underline{a}, \underline{b}}{\underline{n}}\right) \neq 0 \Rightarrow r(\underline{n}) = r(\underline{a}) + r(\underline{b})$, hence

$$M[B] = \sum_{r(\underline{a})+r(\underline{b}) \geq 1} (-1)^{r(\underline{b})} \frac{r(\underline{a})}{r(\underline{a})+r(\underline{b})} \left(\sum_{\underline{n} \in \underline{\mathcal{N}}} \operatorname{sh}\binom{\underline{a}, \underline{b}}{\underline{n}} M^{\underline{n}} \right) B_{\widetilde{\underline{b}}\,\underline{a}}$$

$$= \sum_{\underline{a} \neq \varnothing} M^{\underline{a}} B_{\underline{a}} = MB$$

(the internal sum is $M^{\underline{a}}$ when $\underline{b} = \varnothing$ and it does not contribute when $\underline{a}$ or $\underline{b} \neq \varnothing$ because of alternality, nor when $\underline{a} = \varnothing$ because of the factor $r(\underline{a})$).

Alternal v.s. Symmetral

- *Any mould expansion associated with an alternal mould thus belongs to the (closure of the) Lie subalgebra of $\mathcal{A}$ generated by the B_n's*, since it can be rewritten as a Lie mould expansion, involving only commutators of the B_n's.
- it is related to the classical Dynkin-Specht-Wever projection lemma in the context of free Lie algebras
- the concepts of symmetrality and alternality are related to certain combinatorial Hopf algebras, as emphasized by F. Menous in his work on the renormalization theory in perturbative quantum field theory

Alternal v.s. Symmetral

- The product of two symmetral moulds is symmetral.
- The logarithm of a symmetral mould is alternal.
- The exponential of an alternal mould is symmetral.

Alternal v.s. Symmetral

- The mould I defined by

$$I^{\underline{n}} = \begin{cases} 1 & \text{if } r(\underline{n}) = 1 \\ 0 & \text{else,} \end{cases}$$

  is alternal (being supported in one-letter words).
- The symmetral mould E is e^{I}.

Alternal v.s. Symmetral

- the set of all symmetral moulds is a group for mould multiplication,
- the set of all alternal moulds is a Lie algebra for mould commutator,
- $M,\ N$ alternal $\Rightarrow\ [M,N][B] = \big[M[B], N[B]\big]$.
- Let us also mention a manifestation of the antipode of the Hopf algebra related to moulds:

$$M \text{ alternal } \Rightarrow\ S(M) = -M,$$

$$M \text{ symmetral } \Rightarrow\ S(M) = \text{multiplicative inverse of } M,$$

where $S(M)^{n_1\cdots n_r} := (-1)^r M^{n_r\cdots n_1}$.

Hopf-algebraic aspects of mould calculus

- Denote by $\mathbf{k}\underline{\mathcal{N}}$ the linear span of the set of words, *i.e.* the $\mathbf{k}$-vector space consisting of all formal sums $c = \sum c_{\underline{n}}\, \underline{n}$ with finitely many nonzero coefficients $c_{\underline{n}} \in \mathbf{k}$.
- The set of moulds can be identified with the set of linear forms on $\mathbf{k}\underline{\mathcal{N}}$, any $M \in \mathbf{k}^{\underline{\mathcal{N}}}$ being identified with the linear form $c \mapsto \sum M^{\underline{n}} c_{\underline{n}}$ (in other words, we extend the function $M\colon \underline{\mathcal{N}} \to \mathbf{k}$ to $\mathbf{k}\underline{\mathcal{N}}$ by linearity).
- Now, $\mathbf{k}\underline{\mathcal{N}}$ is a Hopf algebra

Hopf-algebraic aspects of mould calculus

- if we define multiplication by extending

$$(\underline{a}, \underline{b}) \mapsto \underline{a} ⧢ \underline{b} := \sum \mathrm{sh}\left({\underline{a}, \underline{b} \atop \underline{n}} \right) \underline{n}$$

  by bilinearity ("shuffling product" of two words),
- comultiplication by extending

$$\underline{n} \mapsto \sum_{\underline{n} = \underline{a}\,\underline{b}} \underline{a} \otimes \underline{b}$$

  by linearity,
- and antipode by extending $n_1 \cdots n_r \mapsto (-1)^r n_r \cdots n_1$ by linearity
- the unit is $\varnothing$ and the counit is $c \mapsto c_\varnothing$

Hopf-algebraic aspects of mould calculus

- The associative algebra structure of $\mathbf{k}^{\underline{\mathcal{N}}}$ is then dual to the coalgebra structure of $\mathbf{k}\,\underline{\mathcal{N}}$
- the set of symmetral moulds identifies itself with the group of characters of $\mathbf{k}\,\underline{\mathcal{N}}$, since a mould M is symmetral if and only if $M(\varnothing) = 1$ and $M(c \sqcup\!\sqcup c') = M(c)M(c')$ for all c, c',
- the set of alternal moulds identifies itself with the Lie algebra of infinitesimal characters of $\mathbf{k}\,\underline{\mathcal{N}}$, since a mould M is alternal if and only if $M(c \sqcup\!\sqcup c') = M(c)c'_{\varnothing} + c_{\varnothing}M(c')$.

Outline

BCH Theorem

Let A be an associative algebra. We now use mould calculus to prove

Theorem (BCH Theorem)

Suppose $X, Y \in A$. Let $\Psi = \mathrm{e}^{tX}\mathrm{e}^{tY} \in \mathcal{A} = A[[t]]$. Then

$$\log \Psi \in \mathrm{Lie}(X, Y)[[t]],$$

where $\mathrm{Lie}(X, Y)$ is the Lie subalgebra of A generated by X and Y.

BCH Theorem: Proof

- Half of the work has already been done in our main Example!
- With the two-letter alphabet $\Omega = \{x, y\}$, $B_x = tX$ and $B_y = tY$, we have $\log \Psi = T_\Omega B$ with $T_\Omega = \log S_\Omega$, $S_\Omega = \mathrm{e}^{I_x} \times \mathrm{e}^{I_y}$.
- The mould S_Ω is symmetral: I_x and I_y are alternal (they are supported in the set of one-letter words) hence e^{I_x} and e^{I_y} are symmetral and so is their product.
- It follows that T_Ω is alternal.
- then

$$\log \Psi = T_\Omega B = T_\Omega [B].$$

In particular, being expressed as a Lie mould expansion, $\log \Psi$ lies in $\mathrm{Lie}(X, Y)[[t]]$.

Outline

Dynkin's Formula

Theorem (Dynkin)

In the above situation,

$$\log \Psi = \sum \frac{(-1)^{k-1}}{k} \frac{t^\sigma}{\sigma} \frac{[X^{p_1} Y^{q_1} \cdots X^{p_k} Y^{q_k}]}{p_1! q_1! \cdots p_k! q_k!}$$

with summation over all $k \in \mathbb{N}^*$ *and* $(p_1, q_1), \cdots, (p_k, q_k) \in \mathbb{N} \times \mathbb{N} \setminus \{(0,0)\}$, *where* $\sigma := p_1 + q_1 + \cdots + p_k + q_k$ *and* $[X^{p_1} Y^{q_1} \cdots X^{p_k} Y^{q_k}] := \mathrm{ad}_X^{p_1} \mathrm{ad}_Y^{q_1} \cdots \mathrm{ad}_X^{p_k} \mathrm{ad}_Y^{q_k - 1} Y$ *if* $q_k \geq 1$ *and* $\mathrm{ad}_X^{p_1} \mathrm{ad}_Y^{q_1} \cdots \mathrm{ad}_X^{p_k - 1} X$ *if* $q_k = 0$.

Dynkin's Formula: Proof

With the same notation as before, by definition,

$$T_{\underline{\Omega}}^{\underline{\omega}} = \sum_{k\geq 1} \frac{(-1)^{k-1}}{k} \sum_{\substack{\underline{\omega}^1,\ldots,\underline{\omega}^k \in \underline{\Omega}\setminus\{\varnothing\} \\ \underline{\omega}=\underline{\omega}^1\cdots\underline{\omega}^k}} S_{\underline{\Omega}}^{\underline{\omega}^1} \cdots S_{\underline{\Omega}}^{\underline{\omega}^k} \quad \text{for each word } \underline{\omega},$$

so

$$\log \Psi = \sum_{k\geq 1} \frac{(-1)^{k-1}}{k} \sum_{\underline{\omega}^1,\ldots,\underline{\omega}^k \in \underline{\Omega}\setminus\{\varnothing\}} \frac{1}{r(\underline{\omega}^1)+\cdots+r(\underline{\omega}^k)} S_{\underline{\Omega}}^{\underline{\omega}^1} \cdots S_{\underline{\Omega}}^{\underline{\omega}^k} B_{[\underline{\omega}^1\cdots\underline{\omega}^k]}.$$

This exactly gives us the Dynkin formula!

Outline

Kimura's Formula(2017)

Theorem (Kimura, 2017)

Let $X, Y \in A$ as in BCH Theorem. Then $\Psi = \mathrm{e}^{tX}\mathrm{e}^{tY}$ can be written

$$\Psi = 1_{\mathcal{A}} + \sum_{r=1}^{\infty} \sum_{n_1,\ldots,n_r=1}^{\infty} \frac{1}{n_r(n_r+n_{r-1})\cdots(n_r+\cdots+n_1)} D_{n_1}\cdots D_{n_r}$$

$$\text{with } D_n := \frac{t^n}{(n-1)!}\,\mathrm{ad}_X^{n-1}(X+Y) \quad \text{for each } n \geq 1.$$

Kimura's Formula(2017):Proof

Lemma

$\Psi = \mathrm{e}^{tX}\mathrm{e}^{tY}$ *is the unique element of* $\mathcal{A} = A[[t]]$ *such that*

$$\Psi_{|t=0} = 1_{\mathcal{A}}, \qquad t\partial_t\Psi = D\Psi, \qquad \textit{where } D := t\,\mathrm{e}^{tX}(X+Y)\,\mathrm{e}^{-tX}.$$

Kimura's Formula(2017):Proof

Let $\mathcal{N} := \mathbb{N}^*$ and consider the associative comould associated with the family $(D_n)_{n\in\mathcal{N}}$ defined above. We have

$$D = \sum_{n\in\mathcal{N}} D_n = ID,$$

where D in the LHS is the element of $A[[t]]$ defined in the lemma, while the RHS is the mould expansion associated with the mould I.

Kimura's Formula(2017):Proof

Lemma

For any mould $S \in \mathbf{Q}^{\underline{\mathcal{N}}}$,

$$t\partial_t(SD) = (\nabla S)D,$$

where ∇S *is the mould defined by*

$$(\nabla S)^{n_1\cdots n_r} := (n_1 + \cdots + n_r)S^{n_1\cdots n_r} \quad \textit{for each word } n_1\cdots n_r \in \underline{\mathcal{N}}.$$

Kimura's Formula(2017):Proof

- These lemmas inspire us to look for a solution to $t\partial_t\Psi = D\Psi$ in the form of a mould expansion:
- $\Psi = SD$ *will be solution if* $S \in \mathbf{Q}^{\underline{\mathcal{N}}}$ *is solution to the mould equation*

$$S^{\varnothing} = 1, \qquad \nabla S = I \times S$$

(indeed: we have $(\nabla S)D = t\partial_t\Psi$ on the one hand, and $(I \times S)D = (ID)(SD) = D\Psi$ on the other hand, and $S^{\varnothing} = 1$ ensures $\operatorname{ord}(\Psi - 1_{\mathcal{A}}) \geq 1$ because $\operatorname{ord} D_{\underline{n}} \geq 1$ for all nonempty word $\underline{n}$).

Kimura's Formula(2017):Proof

- Now the second part of mould equation is equivalent to

$$(n_1+\cdots+n_r)S^{n_1\cdots n_r} = S^{n_2\cdots n_r} \quad \text{for each nonempty word } n_1\cdots n_r \in \underline{\mathcal{N}}$$

- thus the mould equation has a unique solution: the mould $S_{\mathcal{N}} \in \mathbf{Q}^{\underline{\mathcal{N}}}$ defined by

$$S_{\mathcal{N}}^{n_1\cdots n_r} := \frac{1}{n_r(n_r+n_{r-1})\cdots(n_r+\cdots+n_1)} \quad \text{for each } n_1\cdots n_r \in \underline{\mathcal{N}}.$$

- In conclusion, $S_{\mathcal{N}}$ is a solution to the mould equation, thus $S_{\mathcal{N}}D$ is a solution to $t\partial_t\Psi = D\Psi$, thus

$$S_{\mathcal{N}}D = \Psi = \mathrm{e}^{tX}\mathrm{e}^{tY}$$

and Kimura's formula is proved.

Outline

$S_{\mathcal{N}}$ is symmetral

The mould $S_{\mathcal{N}} \in \mathbf{Q}^{\underline{\mathcal{N}}}$ that we have just constructed happens to be a very common and useful object of mould calculus. It is well-known

Lemma

The mould $S_{\mathcal{N}}$ defined by the formula

$$S_{\mathcal{N}}^{n_1 \cdots n_r} := \frac{1}{n_r(n_r + n_{r-1}) \cdots (n_r + \cdots + n_1)} \quad \text{for each } n_1 \cdots n_r \in \underline{\mathcal{N}}.$$

is symmetral.

a new formula for $\log \Psi$

From this, the Lie character is manifest—the new formula thus contains the BCH theorem:

Corollary

Let $T_{\mathcal{N}} := \log S_{\mathcal{N}} \in \mathbf{Q}^{\underline{\mathcal{N}}}$*. Then, with the notation of Kimura's Theorem, we have* $\log \Psi = T_{\mathcal{N}}[D]$*, i.e.*

$$\log(\mathrm{e}^{tX}\mathrm{e}^{tY}) = \sum_{r\geq 1} \sum_{n_1,\ldots,n_r=1}^{\infty} \frac{1}{r}\, T_{\mathcal{N}}^{n_1\cdots n_r}\,[D_{n_1},[\cdots[D_{n_{r-1}},D_{n_r}]\cdots]] \in \mathrm{Lie}(X,$$

BCH Formula

From the definition $T_{\mathcal{N}} = \sum_{k=1}^{\infty} \frac{(-1)^{k-1}}{k} (S_{\mathcal{N}} - \mathbb{1})^{\times k}$, we can write down the coefficients for words of small length:

$$
\begin{aligned}
T^{n_1} &= S^{n_1} = \frac{1}{n_1} \\
T^{n_1 n_2} &= S^{n_1 n_2} - \frac{1}{2} S^{n_1} S^{n_2} = \frac{n_1 - n_2}{2 n_1 n_2 (n_1 + n_2)} \\
T^{n_1 n_2 n_3} &= S^{n_1 n_2 n_3} - \frac{1}{2} S^{n_1 n_2} S^{n_3} - \frac{1}{2} S^{n_1} S^{n_2 n_3} + \frac{1}{3} S^{n_1} S^{n_2} S^{n_3} \\
T^{n_1 n_2 n_3 n_4} &= S^{n_1 n_2 n_3 n_4} - \frac{1}{2} S^{n_1} S^{n_2 n_3 n_4} - \frac{1}{2} S^{n_1 n_2} S^{n_3 n_4} - \frac{1}{2} S^{n_1 n_2 n_3} S^{n_4} \\
&\quad + \frac{1}{3} S^{n_1} S^{n_2} S^{n_3 n_4} + \frac{1}{3} S^{n_1} S^{n_2 n_3} S^{n_4} + \frac{1}{3} S^{n_1 n_2} S^{n_3} S^{n_4} - \frac{1}{4} S^{n_1} S^{n_2} S^{n
\end{aligned}
$$

BCH recovered from Lie Mould Expansion $\log\Psi = T_{\mathcal{N}}[D]$

$$\log\Psi = \sum_{n_1=1}^{\infty} T^{n_1} D_{n_1} + \sum_{n_1,n_2=1}^{\infty} \frac{1}{2} T^{n_1 n_2}[D_{n_1}, D_{n_2}]$$
$$+ \sum_{n_1,n_2,n_3=1}^{\infty} \frac{1}{3} T^{n_1 n_2 n_3}[D_{n_1}, [D_{n_2}, D_{n_3}]]$$
$$+ \sum_{n_1,n_2,n_3,n_4=1}^{\infty} \frac{1}{4} T^{n_1 n_2 n_3 n_4}[D_{n_1}, [D_{n_2}, [D_{n_3}, D_{n_4}]]] + \cdots$$

BCH recovered from Lie Mould Expansion $\log \Psi = T_{\mathcal{N}}[D]$

$$
\begin{aligned}
& t(X+Y) + \frac{t^2}{2}[X,Y] + \frac{t^3}{3!}[X,[X,Y]] + \frac{t^4}{4!}[X,[X,[X,Y]]] \\
& \quad + \frac{t^5}{5!}[X,[X,[X,[X,Y]]]] + \cdots \\
& - \frac{t^3}{12}([(X+Y),[X,Y]]) - \frac{t^4}{24}([(X+Y),[X,[X,Y]]]) \\
& \quad - \frac{t^5}{120}[[X,Y],[X,[X,Y]]] - \frac{t^5}{80}[(X+Y),[X,[X,[X,Y]]]] + \cdots \\
& + \frac{t^5}{720}[(X+Y),[(X+Y),[X,[X,Y]]]] - \frac{t^5}{240}[[X,Y],[(X+Y),[X,Y]]] \\
& + \frac{t^5}{720}[(X+Y),[(X+Y),[(X+Y),[X,Y]]]] + \cdots
\end{aligned}
$$

BCH recovered from Lie Mould Expansion $\log \Psi = T_{\mathcal{N}}[D]$

$$
\begin{aligned}
& t(X+Y) + \frac{t^2}{2}[X,Y] + \frac{t^3}{12}([X,[X,Y]] + [Y,[Y,X]]) \\
& - \frac{t^4}{24}[Y,[X,[X,Y]]] - \frac{t^5}{720}[X,[X,[X,[X,Y]]]] \\
& - \frac{t^5}{720}[Y,[Y,[Y,[Y,X]]]] + \frac{t^5}{360}[X,[Y,[Y,[Y,X]]]] \\
& + \frac{t^5}{360}[Y,[X,[X,[X,Y]]]] + \frac{t^5}{120}[Y,[X,[Y,[X,Y]]]] \\
& + \frac{t^5}{120}[X,[Y,[X,[Y,X]]]] + \cdots .
\end{aligned}
$$

Outline

Merits

One of the merits of the mould calculus approach is that the formulas are easily generalized to the case of

$$\Psi = \mathrm{e}^{tX_1} \cdots \mathrm{e}^{tX_N} \in A[[t]],$$

where A is our associative algebra and $X_1, \ldots, X_N \in A$ for some $N \geq 2$.

The First Generalization: Dynkin

Theorem

Let $\mathbb{N}^N_* := \{\, p \in \mathbb{N}^N \mid p_1 + \cdots + p_N \geq 1 \,\}$. *We have*

$$\log \Psi = \sum \frac{(-1)^{k-1}}{k} \frac{t^\sigma}{\sigma} \frac{\left[X_1^{p_1^1} \cdots X_N^{p_N^1} \cdots X_1^{p_1^k} \cdots X_N^{p_N^k}\right]}{p_1^1! \cdots p_N^1! \cdots p_1^k! \cdots p_N^k!}$$

with summation over all $k \in \mathbb{N}^*$ *and* $p^1, \cdots, p^k \in \mathbb{N}^N_*$, *where* $\sigma := \sum_{i=1}^{k} \sum_{j=1}^{N} p_j^i$ *and the bracket denote nested commutators as before.*

The Second Generalization: Kimura

Theorem

In the above situation, $\Psi = \mathrm{e}^{tX_1} \cdots \mathrm{e}^{tX_N}$ *can also be written*

$$\Psi = 1_{\mathcal{A}} + \sum_{r=1}^{\infty} \sum_{n_1,\dots,n_r=1}^{\infty} \frac{1}{n_r(n_r+n_{r-1})\cdots(n_r+\cdots+n_1)} \mathfrak{D}_{n_1} \cdots \mathfrak{D}_{n_r} \tag{1}$$

$$\textit{with } \mathfrak{D}_n := t^n \sum_{j=1}^{N} \sum_{\substack{m_1,\dots,m_{j-1}\in\mathbb{N} \\ m_1+\cdots+m_{j-1}=n-1}} \frac{\mathrm{ad}_{X_1}^{m_1} \cdots \mathrm{ad}_{X_{j-1}}^{m_{j-1}}}{m_1! \cdots m_{j-1}!} X_j; \quad \forall n \geq 1. \tag{2}$$

The Second Generalization: Kimura

Note that formula (1) involves exactly the same rational coefficients as in the case $N = 2$. The only difference in the formula is that the D_n's have been generalized to the $\mathfrak{D}_n$'s which are defined in (2) and read

$$\mathfrak{D}_n := t(X_1 + \cdots + X_N) \text{ for } n = 1$$

when $n > 1$,

$$\mathfrak{D}_n := t^n \frac{\mathrm{ad}_{X_1}^{n-1}}{(n-1)!} X_2 + \cdots + t^n \sum_{m_1 + \cdots + m_{N-1} = n-1} \frac{\mathrm{ad}_{X_1}^{m_1} \cdots \mathrm{ad}_{X_{N-1}}^{m_{N-1}}}{m_1! \cdots m_{N-1}!} X_N.$$

The Second Generalization: Kimura

Notice that the mould $S_{\mathcal{N}}$ is still symmetral, the mould $T_{\mathcal{N}} = \log S_{\mathcal{N}}$ is still alternal, whence

$$\log \Psi = T_{\mathcal{N}} \mathfrak{D} = T_{\mathcal{N}}[\mathfrak{D}], \tag{3}$$

i.e.

$$\log(\mathrm{e}^{tX_1} \cdots \mathrm{e}^{tX_N}) = \sum_{r \geq 1} \sum_{n_1, \ldots, n_r = 1}^{\infty} \frac{1}{r} T_{\mathcal{N}}^{n_1 \cdots n_r} [\mathfrak{D}_{n_1}, [\cdots [\mathfrak{D}_{n_{r-1}}, \mathfrak{D}_{n_r}] \cdots]]$$

which thus belongs to $\mathrm{Lie}(X_1, \ldots, X_N)[[t]]$, in accordance with the BCH theorem.

Outline

Two Kinds of Moulds in Dynkin and Kimura

- The first kind involves an N-element alphabet $\Omega := \{x_1, \ldots, x_N\}$ and the comould generated by the family $(B_\omega)_{\omega\in\Omega}$ defined by $B_{x_i} := tX_i \in A[[t]]$.
- For the second one, the alphabet is $\mathcal{N} := \mathbb{N}^*$ and the comould is generated by the family $(\mathfrak{D}_n)_{n\in\mathcal{N}}$ and boils down to the D_n's when $N = 2$.
- A natural question is: What is the relation between both kinds of mould expansion?
- *i.e.* can one pass from the representation of the product Ψ as $S_\Omega B$ to its representation as $S_\mathcal{N}\mathfrak{D}$, or from $\log\Psi = T_\Omega B$ to $\log\Psi = T_\mathcal{N}\mathfrak{D}$?

Two Kinds of Moulds in Dynkin and Kimura

- We can define a new operation on moulds, which allows one to pass directly from $S_{\mathcal{N}}$ to S_{Ω}, or from $T_{\mathcal{N}}$ to T_{Ω}.
- We take $N = 2$ for simplicity but the generalization to arbitrary N is easy.

Two Kinds of Moulds in Dynkin and Kimura

Let $\Omega := \{x, y\}$. The formula

$$\underline{\omega} \in \underline{\Omega} \mapsto U^{\underline{\omega}} := \begin{cases} 1 & \text{if } \underline{\omega} = x \\ \dfrac{(-1)^q}{p!q!} & \text{if } \underline{\omega} \text{ is of the form } x^p y x^q \text{ for some } p, q \in \mathbb{N} \\ 0 & \text{else} \end{cases}$$

defines an alternal mould $U \in \mathbf{Q}^{\underline{\Omega}}$ such that

$$D_n = U_n B \quad \text{for each } n \in \mathbb{N}^*,$$

where the RHS is the mould expansion associated with

$$U_n := \text{restriction of } U \text{ to the words of length } n.$$

Two Kinds of Moulds in Dynkin and Kimura

In fact $U = \mathrm{e}^{\mathrm{ad}_{I_x}}(I_x + I_y) = \mathrm{e}^{I_x} \times (I_x + I_y) \times \mathrm{e}^{-I_x}$, which allows us to relate D-mould expansions and B-mould expansions:

Let $\mathcal{N} := \mathbb{N}^*$. Define a linear map $M \in \mathbf{Q}^{\underline{\mathcal{N}}} \mapsto M \odot U \in \mathbf{Q}^{\underline{\Omega}}$ by

$$(M \odot U)^{\varnothing} := M^{\varnothing}, \tag{4}$$

$$(M \odot U)^{\underline{\omega}} := \sum_{s \geq 1} \sum_{\substack{\underline{\omega} = \underline{\omega}^1 \cdots \underline{\omega}^s \\ \underline{\omega}^1, \ldots, \underline{\omega}^s \in \underline{\Omega} \setminus \{\varnothing\}}} M^{r(\underline{\omega}^1) \cdots r(\underline{\omega}^s)} U^{\underline{\omega}^1} \cdots U^{\underline{\omega}^s} \quad \text{for } \underline{\omega} \in \underline{\Omega} \setminus \{\varnothing \tag{5}$$

Then

$$MD = (M \odot U)B \quad \text{for any } M \in \mathbf{Q}^{\underline{\mathcal{N}}}.$$

Two Kinds of Moulds in Dynkin and Kimura

The relations $S_{\mathcal{N}}D = S_{\Omega}B$ (which coincides with Ψ) and $T_{\mathcal{N}}D = T_{\Omega}B$ (which coincides with $\log\Psi$) now appear as a manifestation of above Theorem and the following

Theorem

$$S_{\mathcal{N}} \odot U = S_{\Omega}, \qquad T_{\mathcal{N}} \odot U = T_{\Omega}.$$

Outline

Further Problems

- BCH for L_∞ algebras
- Deformation Quantization
- Kashiwara-Vergne Lie Algebra

THANK YOU