On the substitution law for B-series

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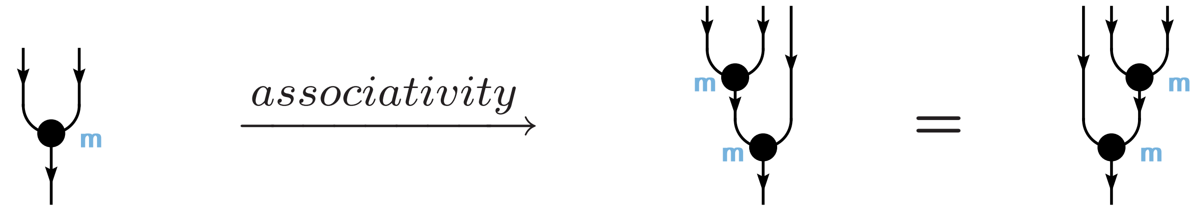
Associative algebra

Definition: We denote an associative $\mathbb{K}$-algebra by the triple (A, m, η) where A is a $\mathbb{K}$-vector space with a product $m : A \otimes A \to A$, supposed to be associative:

$$m \circ (m \otimes \mathrm{id}) = m \circ (\mathrm{id} \otimes m)$$

and $\eta : \mathbb{K} \to A$ is the unit map.



$a \cdot b = c$ $\qquad\qquad$ $(a \cdot b) \cdot c = a \cdot (b \cdot c)$

$$\begin{tikzcd}
A \otimes A \arrow[r, "\tau"] \arrow[d, "m"'] & A \otimes A \arrow[dl, "m"] \\
A &
\end{tikzcd}
\qquad
\begin{tikzcd}
A^{\otimes 3} \arrow[r, "m \otimes \mathrm{id}"] \arrow[d, "\mathrm{id} \otimes m"'] & A \otimes A \arrow[d, "m"] \\
A \otimes A \arrow[r, "m"] & A
\end{tikzcd}$$

Coassociative coalgebra

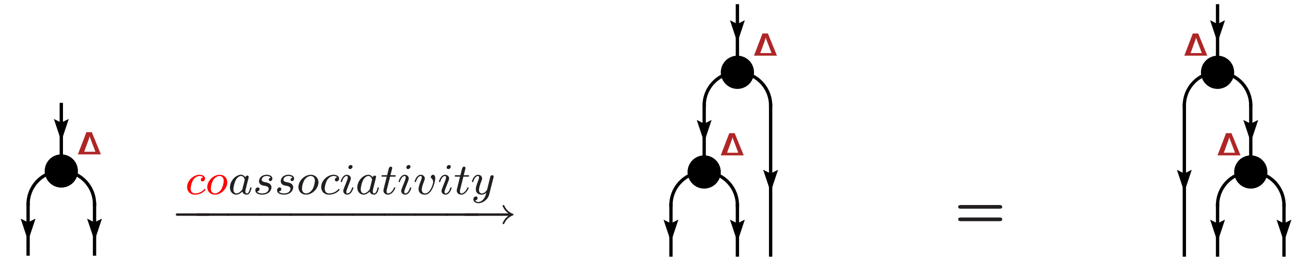
A $\mathbb{K}$-coalgebra is obtained by reversing the arrows in the diagrams.

Definition: A $\mathbb{K}$-*coalgebra* is a triple (C, Δ, ϵ), where the coproduct map $\Delta : C \to C \otimes C$ is coassociative:

$$(\Delta \otimes \mathrm{id}) \circ \Delta = (\mathrm{id} \otimes \Delta) \circ \Delta$$

$\epsilon : C \to \mathbb{K}$ is the counit map: $(\epsilon \otimes \mathrm{id}) \circ \Delta(x) = x = (\mathrm{id} \otimes \epsilon) \circ \Delta(x)$

For $x \in C$, we use the notation $\Delta(x) = \sum_{(x)} x_{(1)} \otimes x_{(2)} = x' \otimes x''$.



$$\Delta(c) \qquad c'_{(1)} \otimes c'_{(2)} \otimes c'' = c' \otimes c''_{(1)} \otimes c''_{(2)}$$

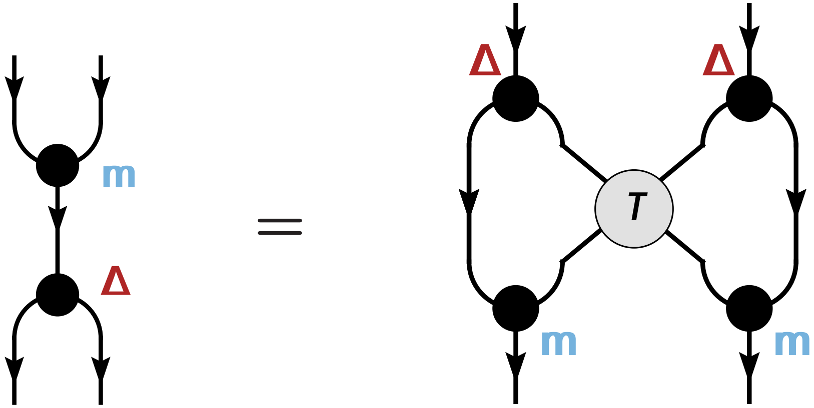
$$\begin{tikzcd}
C \arrow[r, "\Delta"] \arrow[d, "\Delta"'] & C \otimes C \arrow[dl, "\tau"] \\
C \otimes C &
\end{tikzcd}
\qquad
\begin{tikzcd}
C \arrow[r, "\Delta"] \arrow[d, "\Delta"'] & C \otimes C \arrow[d, "\mathrm{id}\otimes\Delta"] \\
C \otimes C \arrow[r, "\Delta\otimes\mathrm{id}"] & C^{\otimes 3}
\end{tikzcd}$$

Bialgebra

(B, m, η) algebra: $m : B \otimes B \to B$ and unit $\eta : \mathbb{K} \to B$

(B, Δ, ϵ) coalgebra: $\Delta : B \to B \otimes B$ and counit $\epsilon : B \to \mathbb{K}$

$$\Delta(ab) = \Delta(a)\Delta(b)$$



$\tau(a \otimes b) := b \otimes a$

$$\Delta m(a \otimes b) \quad = \quad m \otimes m(\mathrm{id} \otimes \tau \otimes \mathrm{id})\Delta \otimes \Delta(a \otimes b)$$

... the *coproduct of the product is the product of the coproducts.*

Graded connected bialgebra

A bialgebra B is called a *graded bialgebra* if there are $\mathbb{K}$-vector subspaces $B^{(n)}$, $n \geq 0$ of B such that

1. $B = \bigoplus_{n\geq 0} B^{(n)}$,
2. $m(B^{(n)} \otimes B^{(m)}) \subseteq B^{(n+m)}$,
3. $\Delta(B^{(n)}) \subseteq \bigoplus_{p+q=n} B^{(p)} \otimes B^{(q)}$.

Elements $x \in B^{(n)}$ are given a degree $\deg(x) = |x| = n$.

B is called *connected* if $B^{(0)} = \mathbb{K}$.

A graded bialgebra $B = \bigoplus_{n\geq 0} B^{(n)}$ is said to be of *finite type* if each of its homogeneous components $B^{(n)}$ is a $\mathbb{K}$-vector space of finite dimension.

Let B be a connected graded $\mathbb{K}$-bialgebra. For any element $x \in B$

$$\Delta(x) = x \otimes 1 + 1 \otimes x + \sum x' \otimes x'',$$

where $\sum x' \otimes x'' \in \ker(\epsilon) \otimes \ker(\epsilon)$, where $\ker(\epsilon) = \bigoplus_{n>0} B^{(n)}$

Convolution product

For a $\mathbb{K}$-algebra A and a $\mathbb{K}$-coalgebra C, we define the *convolution product* of two linear maps f, g in $\mathrm{Hom}(C, A)$ to be the linear map $f \star g \in \mathrm{Hom}(C, A)$ given by the composition

$$C \xrightarrow{\Delta} C \otimes C \xrightarrow{f \otimes g} A \otimes A \xrightarrow{m} A.$$

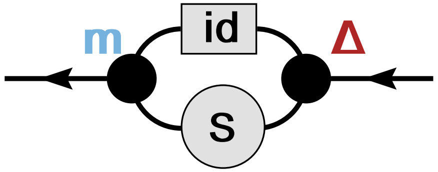
In other words, for $a \in C$, we define

$$(f \star g)(a) = \sum f(a')\, g(a'').$$

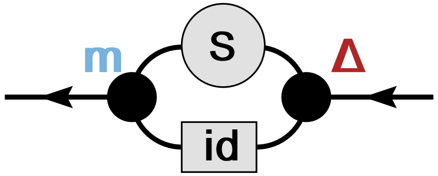
Antipode and Hopf algebra

Let $(H, m, \eta, \Delta, \epsilon)$ be a $\mathbb{K}$-bialgebra. A $\mathbb{K}$-linear endomorphism S of H is called an *antipode* for H if it is the inverse of id under the convolution product

$$\mathrm{id} \star S = m \circ (\mathrm{id} \otimes S) \circ \Delta = \eta \circ \epsilon = m \circ (S \otimes \mathrm{id}) \circ \Delta = S \star \mathrm{id}.$$



$a = \quad \eta \circ \epsilon(a) \quad =$



a

$$\sum a' S(a'') \quad = \quad \eta \circ \epsilon(a) \quad = \quad \sum S(a') a''$$

A *Hopf algebra* is a $\mathbb{K}$-bialgebra $(H, m, \eta, \Delta, \epsilon, S)$ with an antipode S, which is unique.

For a connected graded bialgebra the antipode S is defined by the geometric series $\mathrm{id}^{\star(-1)} = \Big(\eta \circ \epsilon - (\eta \circ \epsilon - \mathrm{id})\Big)^{\star(-1)}$

$$S(x) = \sum_{k \geq 0} (\eta \circ \epsilon - \mathrm{id})^{\star k}(x).$$

The antipode preserves the grading, $S(H^{(n)}) \subseteq H^{(n)}$.

The projector $P := \mathrm{id} - \eta \circ \epsilon$ maps H to its augmentation ideal, $\ker(\epsilon)$.

The antipode S for connected graded Hopf algebras may also be defined recursively in terms of either of the following two formulae

$$\begin{aligned} S(x) = -S \circ P \star \mathrm{id}(x) &= -x - \sum S(x')x'', \\ S(x) = -\mathrm{id} \star S \circ P(x) &= -x - \sum x'S(x''), \end{aligned}$$

for $x \in \ker(\epsilon)$, following readily from

$$S \star \mathrm{id} = \mathrm{id} \star S$$

by recalling that $\ker(\epsilon) = \bigoplus_{n>0} H^{(n)}$, and $S(1) := 1$.

Graded connected Hopf algebra:

$$H = \bigoplus_{n \geq 0} H^{(n)},$$

$$H^{(0)} = \mathbb{K}, \;\; H^{(n)} H^{(m)} \subseteq H^{(n+m)}$$

$$\epsilon(T) := \begin{cases} 0 & , \; T \in \bigoplus_{n \geq 1} H^{(n)} \\ 1 & , \; else. \end{cases}$$

$$\Delta(H^{(n)}) \subseteq \bigoplus_{k=0}^{n} H^{(n-k)} \otimes H^{(k)}$$

$$\Delta(T) = T \otimes 1 + 1 \otimes T + \sum T' \otimes T''$$

$$S(T) = -T - \sum S(T')T'', \qquad S(T) = -T - \sum T' S(T''),$$

Examples:

Shuffle algebra

Let V be a $\mathbb{K}$-vector space: $T(V) = \mathbb{K} \oplus \bigoplus_{n>0} V^{\otimes n}$.

$a_0,\ b_0 \in \mathbb{K},\ a_i,\ b_j \in V$

$$\begin{aligned} a_0 ш (b_1 \otimes b_2 \otimes \ldots \otimes b_n) &= a_0 b_1 \otimes b_2 \otimes \ldots \otimes b_n, \\ (a_1 \otimes a_2 \otimes \ldots \otimes a_m) ш b_0 &= b_0 a_1 \otimes a_2 \otimes \ldots \otimes a_m, \end{aligned}$$

and

$$\begin{aligned} &(a_1 \otimes \ldots \otimes a_m) ш (b_1 \otimes \ldots \otimes b_n) \\ &\quad = a_1 \otimes \Big((a_2 \otimes \ldots \otimes a_m) ш (b_1 \otimes \ldots \otimes b_n) \Big) \\ &\qquad + b_1 \otimes \Big((a_1 \otimes \ldots \otimes a_m) ш (b_2 \otimes \ldots \otimes b_n) \Big). \end{aligned}$$

$$\begin{aligned} a_1 ш (b_1 \otimes b_2) &= a_1 \otimes b_1 \otimes b_2 + b_1 \otimes a_1 \otimes b_2 + b_1 \otimes b_2 \otimes a_1 \\ (a_1 \otimes a_2) ш (b_1 \otimes b_2) &= a_1 \otimes (a_2 ш (b_1 \otimes b_2)) + b_1 \otimes (a_1 \otimes a_2 ш b_2) \end{aligned}$$

Quasi-shuffle Hopf algebra

Consider an assoc. algebra $(A,\cdot)$ over $\mathbb{C}$: $T(A) = \mathbb{K} \oplus \bigoplus_{n>0} T^n(A)$

$u = u_1 \cdots u_n, w = w_1 \cdots w_m \in T(A),\ a,b \in A$

$$au * bw := a(u * bw) + b(au * w) + (a \cdot b)(u * w)$$

$$\begin{aligned} u_1 * (v_1 \otimes w_2) &= u_1 \otimes v_1 \otimes w_2 + v_1 \otimes u_1 \otimes w_2 + v_1 \otimes w_2 \otimes u_1 \\ &\quad + (u_1 \cdot v_1) \otimes w_2 + v_1 \otimes (u_1 \cdot w_2) \end{aligned}$$

$u = u_1 \cdots u_n \in T(A)$

$$\Delta(u_1 \cdots u_n) = u \otimes 1 + 1 \otimes u + \sum_{p=1}^{n-1} u_1 \cdots u_p \otimes u_{p+1} \cdots u_n$$

$\epsilon(1) = 1,\ \epsilon(u) = 0,\ u \in T^{n>0}(A)$

$$S(u) = -\sum_{p=0}^{n-1} S(u_1 \cdots u_p) * u_{p+1} \cdots u_n, \quad u \in T^n(A)$$

Convolution product: $H \xrightarrow{\text{Hom}(H,\mathbb{K})} \mathbb{K}$

$$\phi_1 \star \phi_2 := m_{\mathbb{K}}(\phi_1 \otimes \phi_2)\Delta : H \xrightarrow{\Delta} H \otimes H \xrightarrow{\phi_1 \otimes \phi_2} \mathbb{K} \otimes \mathbb{K} \xrightarrow{m_{\mathbb{K}}} \mathbb{K}$$

$$\phi_1 \star \phi_2(x) \;=\; \phi_1(x)\phi_2(1) + \phi_1(1)\phi_2(x) + \sum \phi_1(x')\phi_2(x'')$$

We denote its unit by $e := \eta \circ \epsilon$

Group of **regularized characters** $G(\mathbb{K}) \ni \; \phi : H \to \mathbb{K}$

$$\phi(x_1 x_2) = \phi(x_1)\phi(x_2), \qquad \phi(1) = 1_{\mathbb{K}}$$

Lie algebra of **infinitesimal characters** $g(\mathbb{K}) \ni \; \alpha : H \to \mathbb{K}$

$$\alpha(x_1 x_2) = \alpha(x_1)e(x_2) + e(x_1)\alpha(x_2)$$

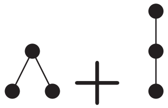
Remark: $G \subset G_1 = e + g_1$, where $\alpha \in g_1$ $\alpha(1) = 0$.

Butcher series (B-series)

$$\dot{y}(s) = f(y(s)), \quad y(0) = y_0, \quad f : \mathbb{R}^n \to \mathbb{R}^n$$

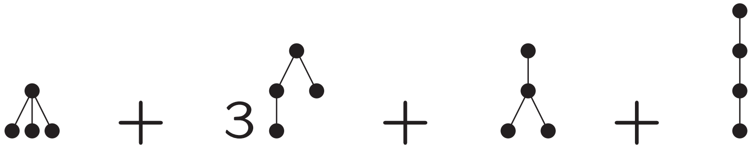
$$\frac{d^2}{ds^2} y^i = \frac{d}{ds} f^i(y) = f^i_j f^j \sim$$

$$\frac{d^3}{ds^3} y^i = f^i_{jk} f^k f^j + f^i_j f^j_k f^k \sim$$



$$\frac{d^4}{ds^4} y^i = f^i_{jkl} f^k f^j f^l + 3 f^i_{jk} f^k_l f^j f^l + f^i_k f^k_{jl} f^j f^l + f^i_j f^j_k f^k_l f^l$$

$\sim$

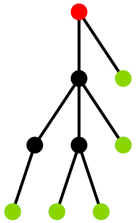


Taylor expansion:

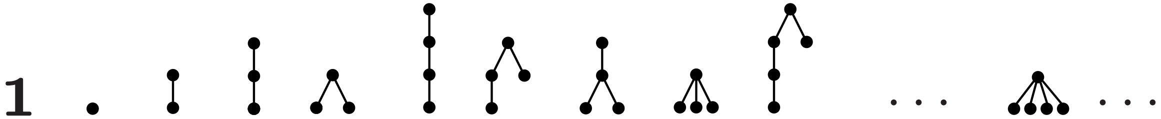
$$y(s+h) = y_0 + \sum_{t \in \mathcal{T}} \frac{h^{|t|}}{|t|!} a(t) F_f(t)$$

$F_f(\bullet) = f$, $F_f($  $) = f'f$, $F_f($  $) = f''ff...$

Rooted trees:



edges ‖, root-vertex 🔴 and leaf-vertices 🟢.



Elementary differential:

For every tree $t = [t_1 t_2 \dots t_n] \in \mathcal{T}$ the elementary differential $F_f(t)$ is a mapping from $\mathbb{R}^n$ to $\mathbb{R}^n$, defined by:

$$F_f(t)(y) = F_f([t_1 t_2 \dots t_n])(y) := f^{(n)}(y)(F_f(t_1)(y), \dots, F_f(t_n)(y))$$

$t = [t_1 t_2 \dots t_n]$:

1. The number of vertices $|t| = \sum_{j=1}^{n} |t_j|$.

2. The number of edges $e(t) = \sum_{j=1}^{n} e(t_j)$.

3. The tree factorial $\bullet! = 1$ and :

$$[t_1 \cdots t_n]! = |[t_1 \cdots t_n]| \prod_{j=1}^{n} t_j! = \left(1 + \sum_{j=1}^{n} |t_j|\right) \prod_{j=1}^{n} t_j!.$$

4. The internal symmetry factor $\sigma(t) = \prod_{j=1}^{n} |\,\mathrm{Aut}\, t_j|$.

5. The Connes–Moscovici coefficient of a tree t: $\mathrm{CM}(t) = \frac{|t|!}{t!\sigma(t)}$.

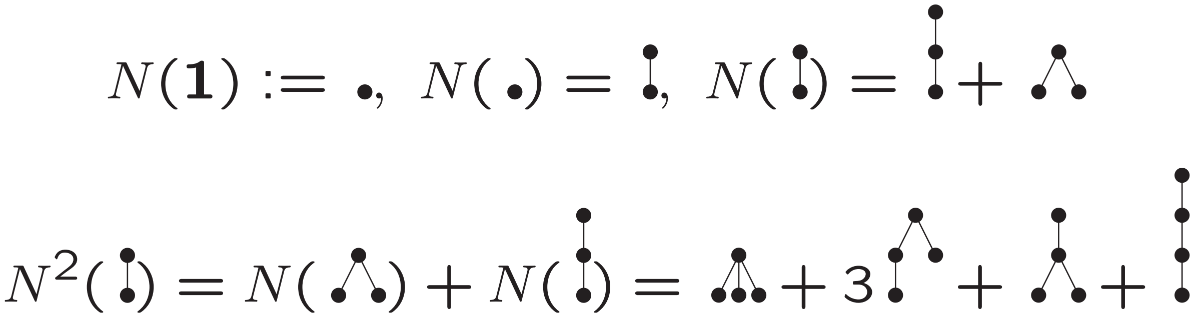
B-series: $\alpha : \mathcal{T} \to \mathbb{R}$

$$B(\alpha, hf, y) := \alpha(\mathbf{1})y + \sum_{t \in \mathcal{T}} \frac{h^{|t|}}{\sigma(t)} \alpha(t) F_f(t)(y)$$

Taylor expansion: $\gamma(t) = \frac{1}{t!}$

$$y(s+h) = B(\gamma, hf, y) = y_0 + \sum_{t \in \mathcal{T}} \frac{h^{|t|}}{t!\sigma(t)} F_f(t)$$

Natural growth: $\frac{d}{ds} \sim N$ on rooted trees and $\bullet \sim f$



Product of trees: $L_{\triangleright}[\bullet](t) := \bullet \triangleright t := N(t)$

$$N(\bullet) := \bullet \triangleright \bullet, \;\; N^2(\bullet) = \bullet \triangleright (\bullet \triangleright \bullet), \;\; N^3(\bullet) = \bullet \triangleright (\bullet \triangleright (\bullet \triangleright \bullet))$$

$$y = y_0 + \int_0^h du \exp(uL_{\triangleright}[\bullet])(\bullet) = y_0 + \frac{\exp(hL_{\triangleright}[\bullet]) - 1}{L_{\triangleright}[\bullet]}(\bullet)$$

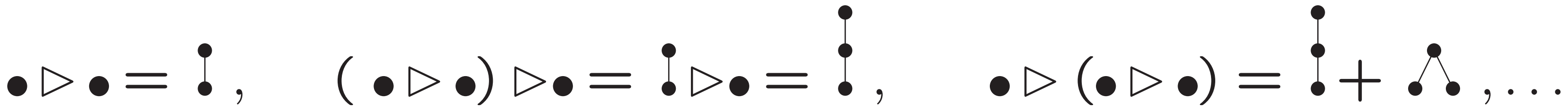
Pre-Lie Algebra

Recall: A left **pre-Lie algebra** P is a vector space, together with a bilinear pre-Lie product $\rhd : P \otimes P \to P$, satisfying the left pre-Lie relation

$$(a \rhd b) \rhd c - a \rhd (b \rhd c) = (b \rhd a) \rhd c - b \rhd (a \rhd c), \qquad a, b, c \in P,$$

The commutator $[a, b] := a \rhd b - b \rhd a$ for $a, b \in P$ satisfies the *Jacobi* identity. Hence L_P is a Lie algebra.

The pre-Lie structure on rooted trees is naturally linked to a particular connected graded commutative Hopf algebra structure on rooted non-planar trees: **Connes-Kreimer-Butcher Hopf algebra**

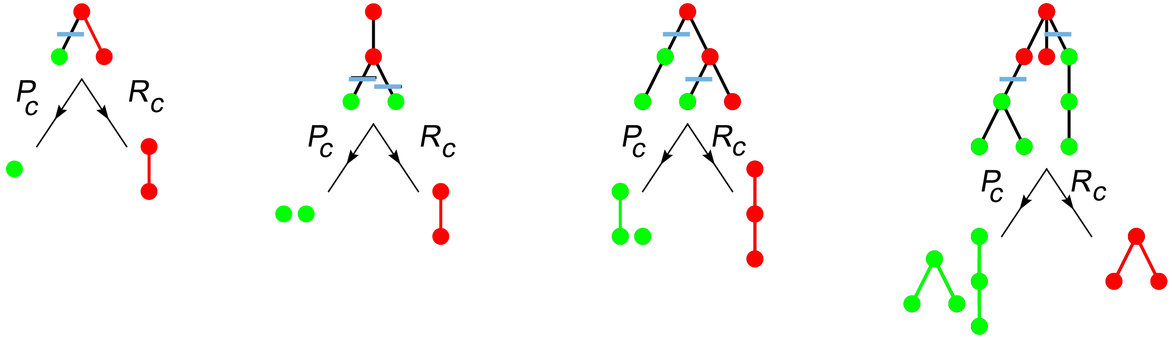


Connes-Kreimer-Butcher Hopf algebra

Let $\mathcal{T}$ be the $\mathbb{K}$-vector space generated by rooted tree, which is graded by the number of vertices, denoted by $|t| := |E(t)|$ with the convention that $\deg(\mathbf{1}) = 0$.

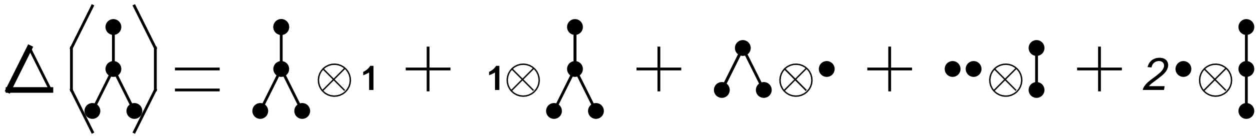
$H_{\mathcal{T}}$ is the connected graded commutative polynomial algebra of finite type over $\mathbb{K}$ generated by $\mathcal{T}$. Monomials of trees are called forests.

Coproduct: Cutting rooted trees



The *coproduct* is then defined as follows. Let C_t be the set of all admissible cuts of the rooted tree $t \in \mathcal{T}$. We exclude the empty cut $c^{(0)}(t)$, $P_{c^{(0)}}(t) = \emptyset$, $R_{c^{(0)}}(t) = t$ and the full cut $c^{(1)}(t)$, $P_{c^{(1)}}(t) = t$, $R_{c^{(1)}}(T) = \emptyset$.

$$\boxed{\Delta(T) = T \otimes \mathbf{1} + \mathbf{1} \otimes T + \textstyle\sum_{c_T \in C_T} P_{c_T} \otimes R_{c_T}}$$



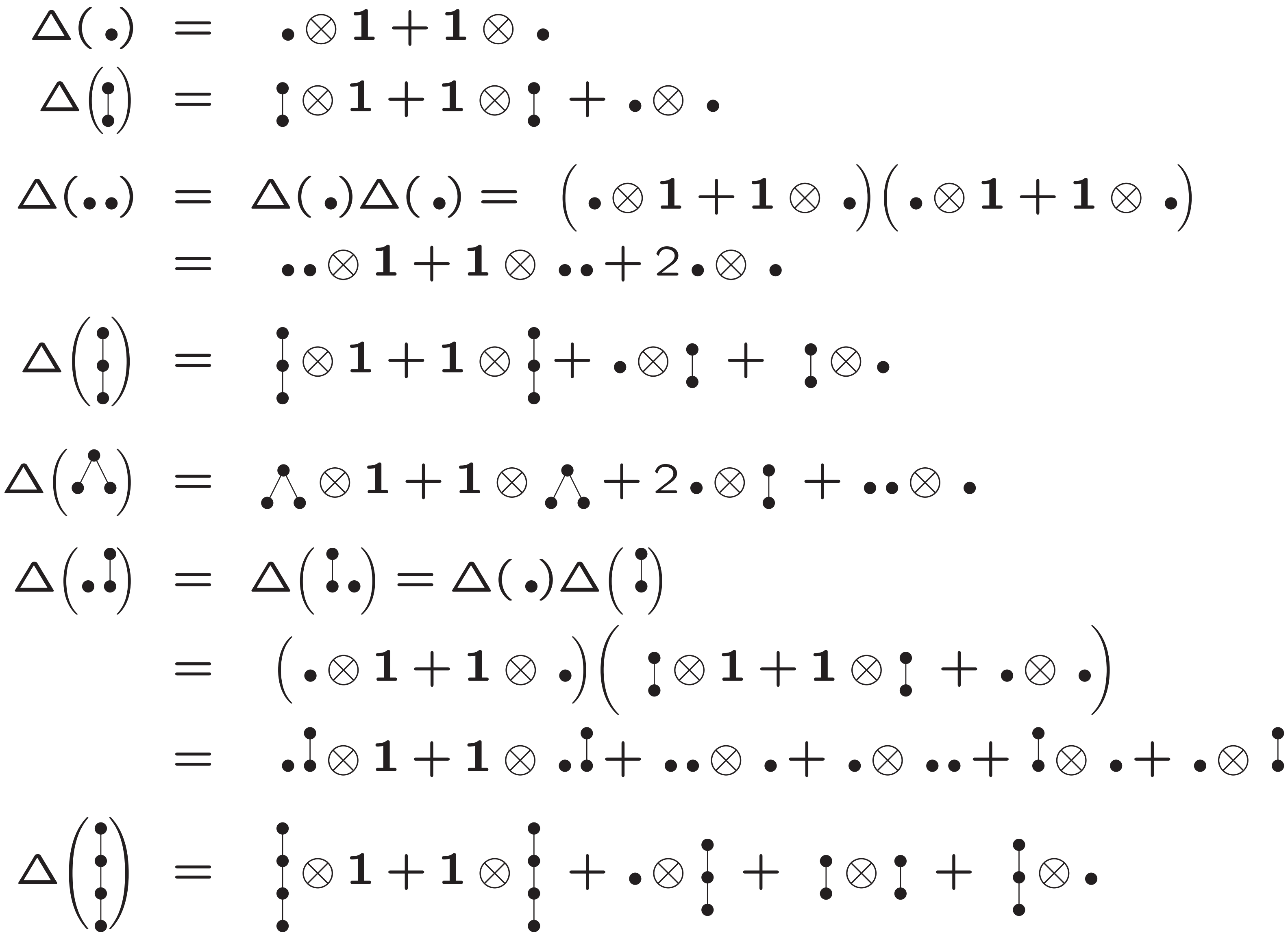
This map is extended by definition to an algebra morphism on $H_{\mathcal{T}}$

$$\Delta\Big(\prod_{i=1}^{n} T_i\Big) := \prod_{i=1}^{n} \Delta(T_i).$$

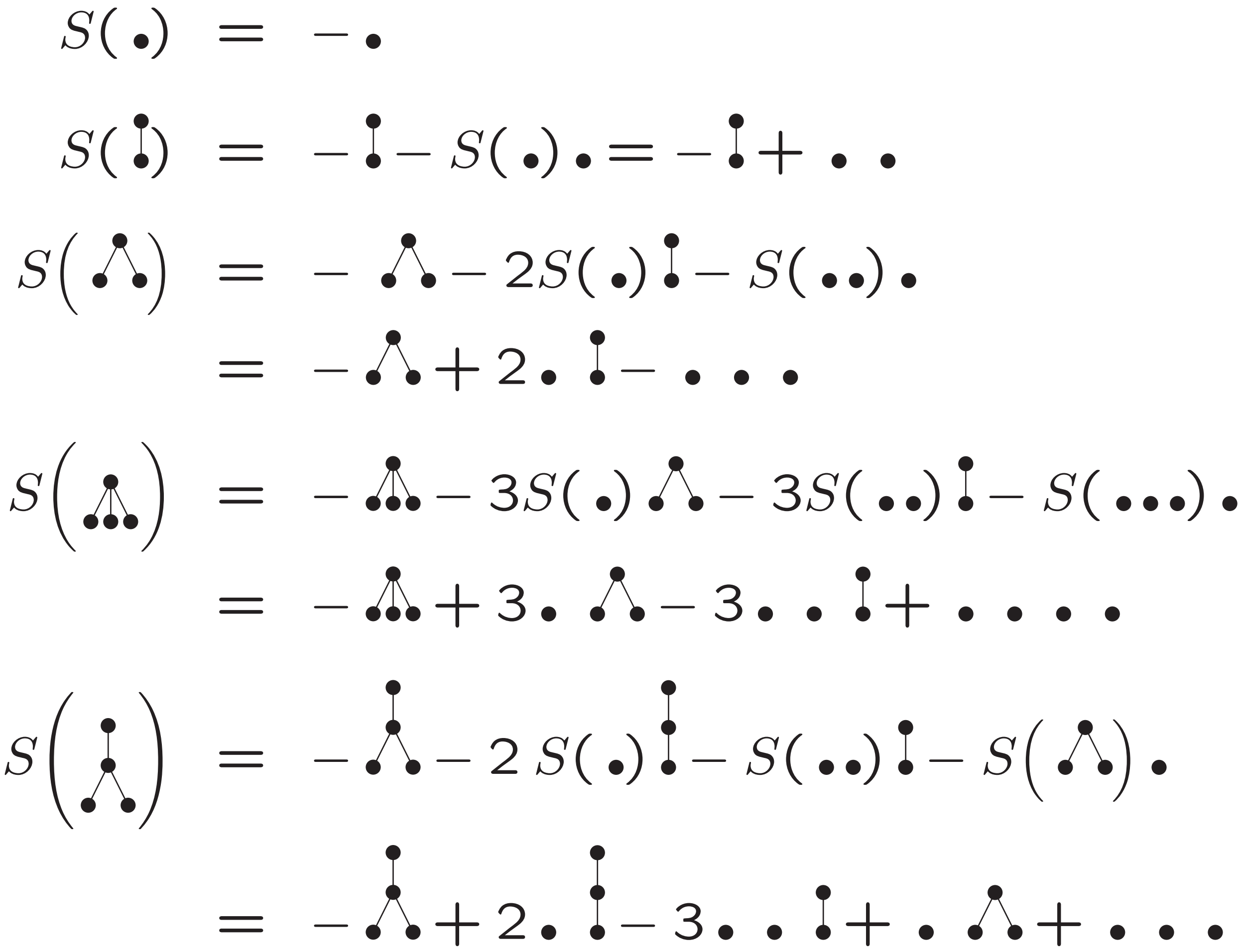
Antipode S

$$m(S \otimes id)\Delta(T) = 0 \rightarrow S(T) = -T - \sum_{c_T \in C_T} S(P_{c_T}) R_{c_T}.$$

Examples:



$$S(T) = -T - \sum_{c_T \in C_T} S({\color{green}P_{c_T}})\,{\color{red}R_{c_T}}.$$



Composition of B-series

B-series: $\alpha : \mathcal{T} \to \mathbb{R}$, $\alpha \in G$

$$B(\alpha, hf, y) := \alpha(\mathbf{1})y + \sum_{t\in\mathcal{T}} \frac{h^{|t|}}{\sigma(t)} \alpha(t) F_f(t)(y)$$

composing with another $B(\beta, hf, y)$, $\beta \in G$:

$$\begin{aligned} B(\alpha, hf, B(\beta, hf, y)) &= B(\beta \star \alpha, hf, y) \\ &= \beta\star\alpha(\mathbf{1})y + \sum_{t\in\mathcal{T}} \frac{h^{|t|}}{\sigma(t)} \beta\star\alpha(t) F_f(t)(y) \end{aligned}$$

with

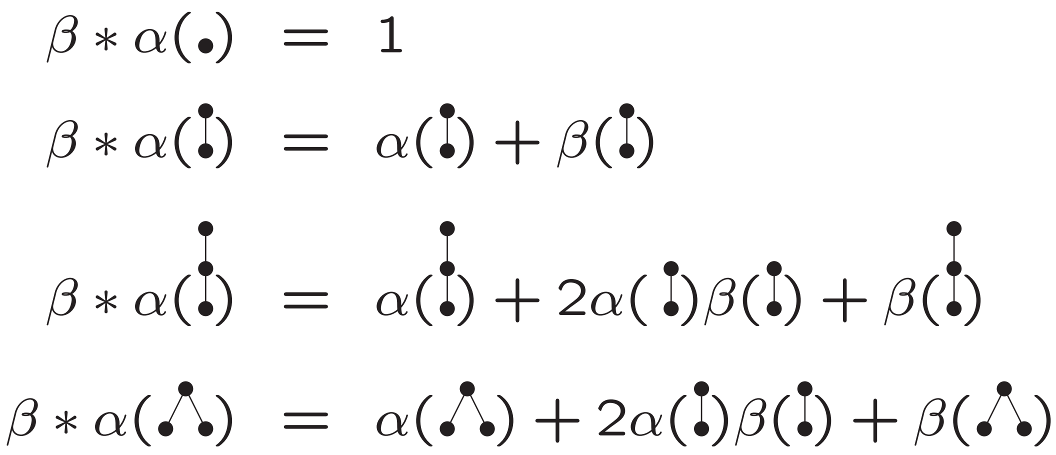
$$\begin{aligned} \beta\star\alpha(t) &= m_{\mathbb{K}}(\beta\otimes\alpha)\Delta(t) \\ &= \beta(t) + \alpha(t) + \sum \beta(t')\alpha(t'') \end{aligned}$$

Substitution of B-series

B-series: $\alpha : \mathcal{T} \to \mathbb{R}$, $\alpha \in G$, $\alpha(\bullet) = 1$, $B(\alpha, hf, y)$ composing with another $B(\beta, hf, y)$, where $b(\mathbf{1}) = 0$ and $b(\bullet) = 1$, i.e.:

$$B(\beta, hf, y) := hf(y) + \sum_{t \in (\mathcal{T}')} \frac{h^{|t|}}{\sigma(t)} \beta(t) F_f(t)(y)$$

$$B(\alpha, B(\beta, hf, \cdot), y) = B(\color{red}{\beta * \alpha}, hf, y)$$



Motivation: Backward error analysis

Theorem: initial value problem

$$\dot{y} = f(y), \quad y(0) = y_0, \quad f : \mathbb{R}^n \to \mathbb{R}^n$$

numerical solution $y_1 = \Phi_f^h(y_0) = B(\alpha, hf, y)$. Then there exists a field $hg(y) = B(\beta, hf, y)$ s.t. $\widehat{y} = \Phi_f^h(y_0)$ is the exact solution of the initial value problem

$$\dot{\widehat{y}} = g(\widehat{y}), \quad \widehat{y}(0) = y_0$$

and $\beta * \gamma = \alpha$, $\beta(\mathbf{1}) = 0, \beta(\bullet) = 1$.

Recall: Taylor expansion: $\dot{y} = B(\gamma, hf, y)$

$$\widehat{y} = B(\gamma, hg, y) = B(\beta * \gamma, hf, y_0) = B(\alpha, hf, y)$$

$\mathcal{T} = T' \oplus k\,\bullet$ rooted trees excluding the empty tree

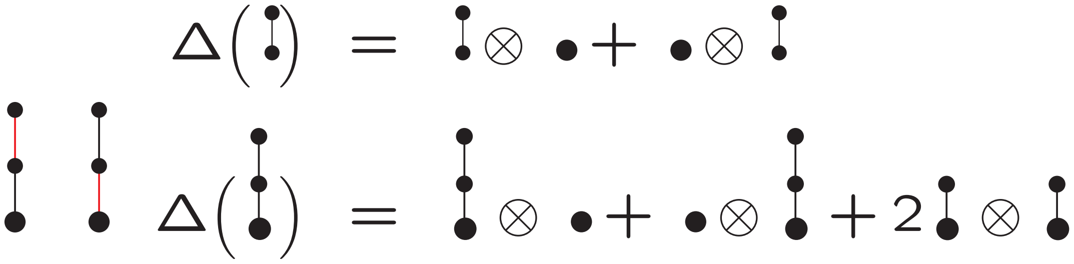
polynomial algebra $\mathcal{H} = \mathcal{S}(T')$, grading in terms of the number of edges

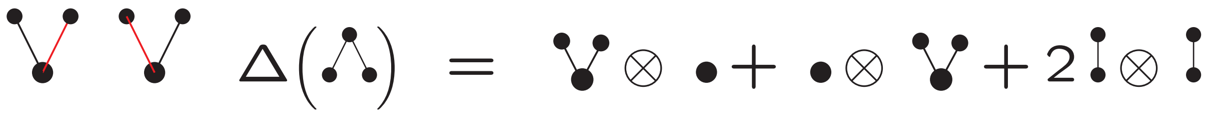
unit: $\bullet$

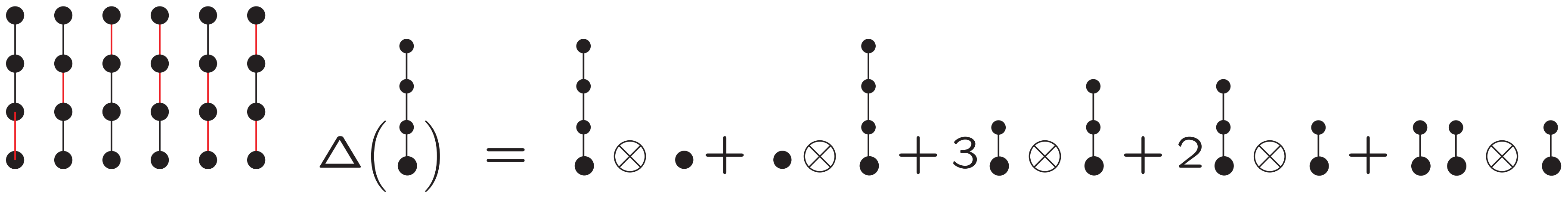
A *subforest* of a tree t is either the trivial forest $\bullet$, or a collection $(t_1, \ldots, t_n)$ of pairwise disjoint subtrees of t, each of them containing at least one edge. In particular two subtrees of a subforest cannot have any common vertex.

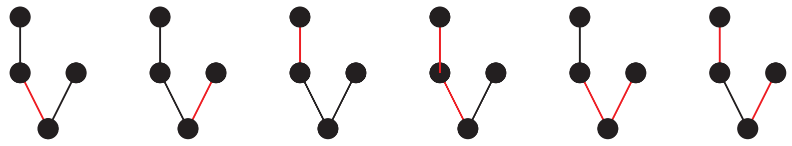
$$\Delta(t) = \sum_{s \subseteq t} s \otimes t/s,$$

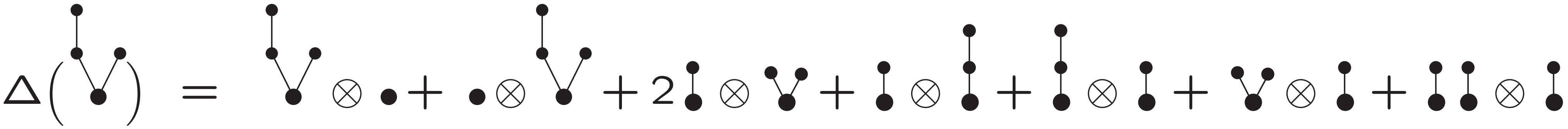
$$\Delta(\bullet) = \bullet \otimes \bullet$$











$$S(t) = -t - \sum_{s,\ \bullet \neq s \subsetneq t} S(s)\ t/s$$

$\mathcal{H}$-bicomodule structure on the Connes–Kreimer Hopf algebra $\mathcal{H}_{\mathsf{CK}}$:

Φ: $\mathcal{H}_{\mathsf{CK}} \to \mathcal{H} \otimes \mathcal{H}_{\mathsf{CK}}$, $t \neq \mathbf{1}$

$$\Phi(t) = \Delta(t) \in \mathcal{H} \otimes \mathcal{H}_{\mathsf{CK}}$$

for the unit tree $\mathbf{1}$: $\Phi(\mathbf{1}) = \bullet \otimes \mathbf{1}$.

Let φ be a character of $\mathcal{H}$, let α be any linear map from $\mathcal{H}$ into k, and let b, c be linear maps form $\mathcal{H}_{\mathsf{CK}}$ into k. Let $\varepsilon = \delta_\emptyset$ be the co-unit of $\mathcal{H}_{\mathsf{CK}}$ and $\delta_\bullet$ on H_{CK} the infinitesimal character corresponding to $\bullet$, and $Z_\bullet$ the one on $\mathcal{H}$. Then:

$$\begin{aligned}
\alpha * \varepsilon &= \varepsilon * \alpha = \alpha(\bullet)\varepsilon \\
\alpha * Z_\bullet &= Z_\bullet * \alpha = \alpha \\
Z_\bullet * b &= b * Z_\bullet = b \\
\varphi * (b \star c) &= (\varphi * b) \star (\varphi * c) \\
(\varphi * b)^{*-1} &= \varphi * b^{*-1}.
\end{aligned}$$

Recall: character H_{CK} on $\delta(\mathbf{1}) = \delta(\bullet) = 1$ zero otherwise. Define the character:

$$\gamma = \exp^\star \delta_\bullet$$

and its $*$-inverse: $L = E \circ S$. Hence $E * \delta = \exp^\star \delta_\bullet$

We show that the infinitesimal character for the explicit Euler method:

$$\omega := L * \delta_\bullet = \log^\star \delta.$$

$$\begin{aligned} E * \log^\star \delta &= \log^\star(E * \delta) \\ &= \log^\star \exp^\star \delta_\bullet \\ &= \delta_\bullet. \end{aligned}$$

Hence $E * \log^\star \delta = E * L * \delta_\bullet = \delta_\bullet$

And $\omega(t_1 \circ t_2 + t_2 \circ t_1 + t_1 \times t_2) = 0$

and Magnus' expansion is: $\Omega' = \sum_{\emptyset \neq t \in \mathcal{T}} \frac{\log^\star(\delta)(t)}{\sigma(t)}\ t$

COCO2010

Trimester

COMBINATORICS AND CONTROL

Madrid

April - June, **2010**

Workshop at Madrid

School at Zaragoza

Research in teams

Conference at Madrid

THANK YOU!!