Bootstrapping bases of the Lie algebra of rooted trees

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Lie algebra of vector fields

Let $VF(\mathbb{R}^n)$ be the vector space of smooth vector fields on $\mathbb{R}^n$.
Lie bracket on $VF(\mathbb{R}^n)$:

$$[v, w] = v * w - w * v,$$

where $*$ is the composition of differential operators, in the associative algebra $DO(\mathbb{R}^n)$ of smooth differential operators on $\mathbb{R}^n$.

The product $v * w$ (differential operators of order 1) is a differential operator of order 2.

The Lie bracket is of order 1 because the leading terms of $v * w$ and $w * v$ are the same and cancel each other.

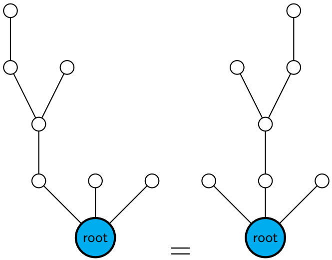
Dictionary

We want to make the following analogy :

- Vector field $\leftrightarrow$ Rooted tree
- Differential operator $\leftrightarrow$ Forest of rooted trees
- Product of differential operators $\leftrightarrow$ Product of forests
- Lie bracket of vector fields $\leftrightarrow$ Lie bracket of rooted trees

Trees and forests of rooted trees

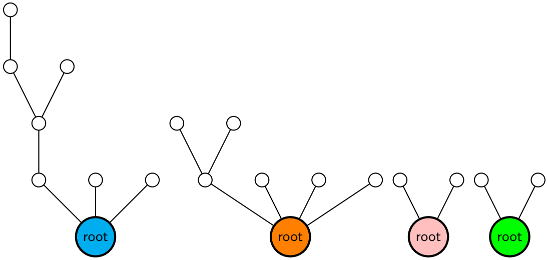
A rooted tree is a connected, simply-connected finite graph, with a distinguished vertex, called the root.



The planar embedding is not important.

Trees and forests of rooted trees

A forest of rooted trees is a finite set of rooted trees.



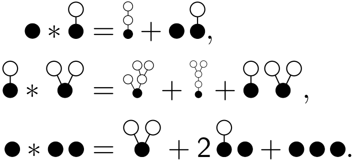
Associative algebra of forests of rooted trees

Let $U(\mathrm{PL})$ be the vector space spanned by forests of rooted trees.

Combinatorics (R. Grossman and R. Larson, 1989)

The product $F * G$ of two forests is a sum over possible (partial) graftings of G on top of F. Sum over all maps from $\{\text{roots of } G\}$ to $\{\text{vertices of } F\} \sqcup \{\text{Ground}\}$

For example, one has



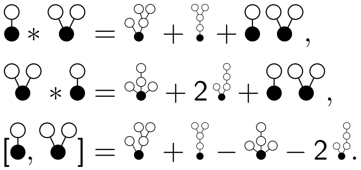
This is an associative product $*$, not commutative.

Lie bracket on rooted trees

Let PL be the subspace of $U(\mathrm{PL})$ spanned by rooted trees.
We claim that there is a Lie bracket on PL given by

$$[S, T] = S * T - T * S.$$

The product $S * T$ of two rooted trees is a sum of rooted trees and forests made of two trees.
The forest parts of $S * T$ and of $T * S$ are the same, given by the disjoint union $S \sqcup T$. They cancel each other in the bracket.
For example,



Analogy again

Recall the analogy

- Vector field $\leftrightarrow$ Rooted tree
- Differential operator $\leftrightarrow$ Forest of rooted trees
- Product of differential operators $\leftrightarrow$ Product of forests
- Lie bracket of vector fields $\leftrightarrow$ Lie bracket of rooted trees

There is more, as both Lie brackets can be cut into two parts.

Halves of brackets

For vector fields, $v * w$ is a differential operator of order 2. Define $v \curvearrowleft w$ to be the projection of $v * w$ on the space of vector fields, by annihilating the leading term. (Not diffeo invariant)

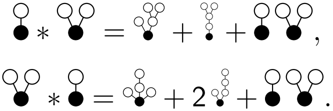
For rooted trees, $S * T$ is a sum of trees and forests of two trees. Define $S \curvearrowleft T$ to be the projection on the space of trees by annihilating forests of two trees.

In both cases, one has

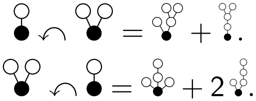
$$[x, y] = x * y - y * x = x \curvearrowleft y - y \curvearrowleft x.$$

Pre-Lie products

For example, recall that



Therefore one has



These "half-of-bracket" operations both satisfy :

$$(x \curvearrowleft y) \curvearrowleft z - x \curvearrowleft (y \curvearrowleft z) = (x \curvearrowleft z) \curvearrowleft y - x \curvearrowleft (z \curvearrowleft y).$$

This is the definition of a pre-Lie product (pre-Lie algebra).
For experts : more than an analogy, rooted trees give free pre-Lie algebras, etc.

Flow of vector fields

Let v be a vector field on $\mathbb{R}^n$. One can consider the flow of the vector field v at time t.
This can be seen as a vector field $E_t(v)$: at each point x, the difference between the initial position x at $t = 0$ and the position at time t.

We therefore have a map E_t from vector fields to vector fields.

Through the analogy above, there is a perfect analog of this map. For a rooted tree S, one can define

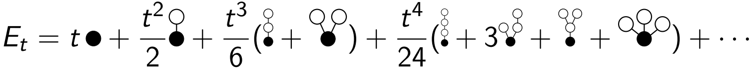
$$E_t(S) = \sum_{n \geq 1} \frac{t^n}{n!} S(\curvearrowleft S)^{n-1} = tS + \frac{t^2}{2} S \curvearrowleft S + \frac{t^3}{6} (S \curvearrowleft S) \curvearrowleft S + \dots.$$

Formal flow and inverse

Let us therefore introduce the **element**

$$E_t = \sum_{n\geq 1} \frac{t^n}{n!} \bullet (\curvearrowleft \bullet)^{n-1} = t\bullet + \frac{t^2}{2}\bullet \curvearrowleft \bullet + \frac{t^3}{6}(\bullet \curvearrowleft \bullet) \curvearrowleft \bullet + \dots .$$

This is a formal infinite sum of rooted trees :

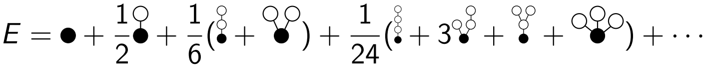


This series belong to a group, which is a kind of analog of the diffeomorphism group acting on vector fields.

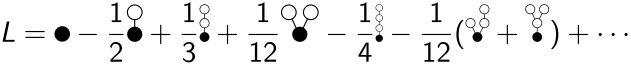
The inverse L of $E = E_{t=1}$ in this group is sometimes called the backward error analysis character.

Practical computation

One therefore has two interesting series



and its inverse



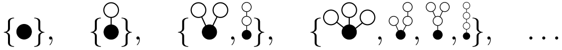
Maybe useful, for algorithms in numerical analysis, to answer

Question (K. Ebrahimi-Fard)

What is the minimal number of operations $\curvearrowleft$ needed to compute the first N terms of E and L, starting from $\bullet$?

Monomials versus trees

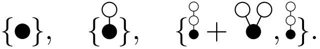
The Lie algebra PL of rooted trees comes with a natural basis :



The first few dimensions are $1, 1, 2, 4, 9, 20, 48, 115, 286, \ldots$.
Let us look for other bases, consisting of pre-Lie monomials, *i.e.* expressions using only parentheses, $\bullet$ and $\curvearrowleft$. For example :

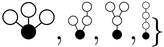
$$\{\bullet\}, \quad \{\bullet \curvearrowleft \bullet\}, \quad \{(\bullet \curvearrowleft \bullet) \curvearrowleft \bullet, \bullet \curvearrowleft (\bullet \curvearrowleft \bullet)\}.$$

This corresponds to the following linear combinations of trees :



So far, no choice, one needs every monomial to get a basis.

Too many monomials

At the next stage, there are 4 trees with 4 vertices :
{}. But there are five monomials :

$$((\bullet \curvearrowleft \bullet) \curvearrowleft \bullet) \curvearrowleft \bullet, \quad (\bullet \curvearrowleft (\bullet \curvearrowleft \bullet)) \curvearrowleft \bullet,$$
$$\bullet \curvearrowleft ((\bullet \curvearrowleft \bullet) \curvearrowleft \bullet), \quad \bullet \curvearrowleft (\bullet \curvearrowleft (\bullet \curvearrowleft \bullet)),$$
$$(\bullet \curvearrowleft \bullet) \curvearrowleft (\bullet \curvearrowleft \bullet).$$

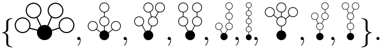
The axiom of pre-Lie algebras gives one relation :

$$\begin{aligned}(\bullet \curvearrowleft (\bullet \curvearrowleft \bullet)) \curvearrowleft \bullet - \bullet \curvearrowleft ((\bullet \curvearrowleft \bullet) \curvearrowleft \bullet) \\ = (\bullet \curvearrowleft \bullet) \curvearrowleft (\bullet \curvearrowleft \bullet) - \bullet \curvearrowleft (\bullet \curvearrowleft (\bullet \curvearrowleft \bullet)).\end{aligned}$$

Therefore there are 4 different bases made of pre-Lie monomials.

Which monomials ?

At the next stage, there are 9 trees with 5 vertices :



But there are 14 monomials ! How to choose among them to define a basis ?

There are many linear relations between monomials.

There are 438 different monomial bases here.

There is a general procedure, working for every n, to choose monomials that form a basis.

This procedure gives many monomial bases but not all of them.

Idea : see Baron Münchhausen

The idea is to define by induction an ordered basis $\mathrm{B}_{\leq n}$ of the subspace of PL spanned by rooted trees with at most n vertices, consisting of monomials of degree less than n.

More precisely, we will define, for every $n \geq 1$, an ordered basis $\mathrm{B}_{\leq n}$ of the subspace of PL spanned by rooted trees with at most n vertices, such that

- The elements of $\mathrm{B}_{\leq n}$ are pre-Lie monomials.
- For every $n \geq 1$, $\mathrm{B}_{\leq n} \subset \mathrm{B}_{\leq n+1}$ as an ordered set.

This construction is not unique, and depends on choices made at each step of the induction.

General principle

algebra $U(\mathrm{PL})$ of forests = universal enveloping algebra of Lie algebra PL of rooted trees

The induction step has two intermediate steps :

(1)
from Lie algebra PL to universal enveloping algebra $U(\mathrm{PL})$ using Poincaré-Birkhoff-Witt theorem.

(2)
back from universal enveloping algebra to Lie algebra using an isomorphism of graded vector spaces $\mathrm{PL} \simeq U(\mathrm{PL})$.

Recipe : first ingredient

From Lie algebra to universal enveloping algebra :
Assume that we have an ordered monomial basis $\mathrm{B}_{\leq n}$ of the subspace of PL spanned by rooted trees with at most n vertices, for some $n \geq 1$.

By the Poincaré-Birkhoff-Witt theorem, the increasing products give an **unordered** basis of the subspace of the universal enveloping algebra $U(\mathrm{PL})$ of degree less than n.

Recipe : second ingredient

From universal enveloping algebra to Lie algebra :

There is an isomorphism from $U(\mathrm{PL})$ to PL given by $x \mapsto \bullet \curvearrowleft x$, such that $x \curvearrowleft (y * z) = (x \curvearrowleft y) \curvearrowleft z$.

Using this isomorphism and the known **unordered** basis of the subspace of the universal enveloping algebra $U(\mathrm{PL})$ of degree less than n, one gets an **unordered** basis $\mathrm{B}_{\leq n+1}$ of the space spanned by rooted trees with at most $n+1$ vertices.

Recipe : how-to

One start from an ordered basis $\mathrm{B}_{\leq n}$ of the Lie algebra PL up to degree n.

One applies the two steps.

One gets **unordered** basis $\mathrm{B}_{\leq n+1}$ of the Lie algebra PL up to degree $n+1$.

The **unordered** basis $\mathrm{B}_{\leq n+1}$ contains the previous basis $\mathrm{B}_{\leq n}$.

One then chooses a total order on $\mathrm{B}_{\leq n+1}$ extending the total order on $\mathrm{B}_{\leq n}$.

First steps

In degree one, the ordered basis $\mathrm{B}_{\leq 1}$ of PL is $\{\bullet\}$.

Step 1

PBW gives the basis $\{1, \bullet\}$ in U(PL).

Right-action on $\bullet$ gives a basis $\{\bullet, \bullet \curvearrowleft \bullet\}$ in PL.

One can choose $\mathrm{B}_{\leq 2}$ to be the ordered basis $\{\bullet \leq \bullet \curvearrowleft \bullet\}$ in PL.

Step 2

PBW gives the basis $\{1, \bullet, \bullet \curvearrowleft \bullet, \bullet * \bullet\}$ in U(PL).

Right-action on $\bullet$ gives the basis

$\{\bullet, \bullet \curvearrowleft \bullet, \bullet \curvearrowleft (\bullet \curvearrowleft \bullet), (\bullet \curvearrowleft \bullet) \curvearrowleft \bullet\}$ in PL.

One can choose $\mathrm{B}_{\leq 3}$ to be the ordered basis

$\{\bullet \leq \bullet \curvearrowleft \bullet \leq (\bullet \curvearrowleft \bullet) \curvearrowleft \bullet \leq \bullet \curvearrowleft (\bullet \curvearrowleft \bullet)\}$ in PL.

Summary

We have therefore obtained ordered bases $\mathrm{B}_{\leq 1}, \mathrm{B}_{\leq 2}, \mathrm{B}_{\leq 3}$, each contained in the next one as an ordered subset :

$$\mathrm{B}_{\leq 1} = \{\bullet\},$$

$$\mathrm{B}_{\leq 2} = \{\bullet \leq \bullet \curvearrowleft \bullet\},$$

$$\mathrm{B}_{\leq 3} = \{\bullet \leq \bullet \curvearrowleft \bullet \leq (\bullet \curvearrowleft \bullet) \curvearrowleft \bullet \leq \bullet \curvearrowleft (\bullet \curvearrowleft \bullet)\}.$$

One can go on in that way, and obtain many different monomial bases, depending on the choice of order made at every step. Let us call them bootstrap bases.

Systematic choices

There are several systematic ways to make the choices required at each step.

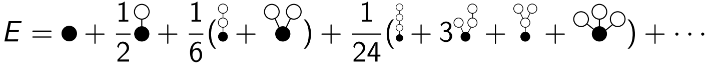
One can describe 8 different manners to define orders, using only degree and lexicographic ordering, that provide at each step an extension of the previous order.

For some of these 8 choices, one recovers bases studied by

- A. Agrachev and R. Gamkrelidze (1980)
- D. Segal (1994)
- A. Dzhumadildaev and C. Löfwall (2002)

How many terms for E?

Let us return to the series E :



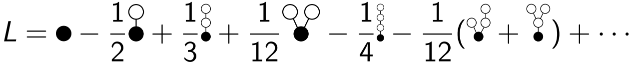
How can we choose the basis so as to minimize the number of monomials in the expression of E?
Recall the following formula for E :

$$E = \sum_{n\geq 1} \bullet \curvearrowleft \frac{1}{n!}\left(\bullet\right)^{*n-1} = \bullet + \frac{1}{2}\bullet \curvearrowleft \bullet + \frac{1}{6}(\bullet \curvearrowleft \bullet) \curvearrowleft \bullet + \dots$$

This gives an expression with only one monomial in each degree.
By the way, these monomials belong to every bootstrap basis.

How many terms for L?

Let us return to the series L, inverse of E :



Coefficients are complicated fractions involving Bernoulli numbers, and there is no simple formula.
The number of monomials in the expression of L depends on the monomial basis.

Best bootstrap bases for L

Here are the number of monomials in L, for some "taylor-made" bootstrap monomial bases, up to degree 6 :

Ambient dim.	1, 1, 2, 4, 9, 20
basis I	1, 1, 2, 2, 8, 15
basis II	1, 1, 2, 3, 7, 16
basis III	1, 1, 2, 3, 8, 14

On the other hand, the systematic choices gives the following numbers of terms, up to degree 8 :

Ambient dim.	1, 1, 2, 4, 9, 20, 48, 115
choice A	1, 1, 2, 3, 7, 18, 43, 110
choice B	1, 1, 2, 3, 7, 18, 43, 111
choice C	1, 1, 2, 2, 8, 16, 43, 110
choice D	1, 1, 2, 2, 8, 16, 42, 110