Lie group methods

Part 4, Order analysis

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Vector fields as derivations

Suppose we have local coordinates $x_1, \ldots, x_m$ on $\mathcal{M}$.
Let $\psi \in C^\infty(\mathcal{M}, \mathbb{R})$ be a function and $F \in \mathcal{X}(\mathcal{M})$ a vector field.
$x(t)$: Integral curve $x(t) = \exp(tF)\, x$. Now expand $\psi(x(t))$ in Taylor series (using local coordinates).

$$\left.\frac{d}{dt}\right|_{t=0} \psi(x(t)) \quad = \quad \sum_i \frac{\partial \psi}{\partial x_i} \cdot \dot{x}_i(0) = \sum_i F_i(x) \frac{\partial}{\partial x_i}[\psi] = (F \cdot \nabla)[\psi]$$

Arnold notation: Operator $\mathbf{L}_F = F \cdot \nabla$
Our convention: Let F be the operator and write

$$\left.\frac{d}{dt}\right|_0 \psi \circ \exp(tF)\, x \quad = \quad F[\psi](x)$$

$$\left.\frac{d^2}{dt^2}\right|_0 \psi \circ \exp(tF)\, x \quad = \quad \left.\frac{d}{dt}\right|_0 F[\psi](x)(\exp(tF)\, x) = F[F[\psi]](x) := F^2[\psi](x)$$

etc

Exponential series and Leibniz' rule

For $\psi \in C^\infty(\mathcal{M}, \mathbb{R})$ and $x \in \mathcal{M}$ it holds (formally)

$$\psi(\exp(tF)x) = \psi(x) + tF[\psi](x) + \frac{1}{2}t^2F^2[\psi](x) + \cdots$$

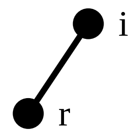
Leibniz' rule. From the local coordinate expression we infer

$$F[\psi \cdot \phi] = \psi \cdot F[\phi] + F[\psi] \cdot \phi$$

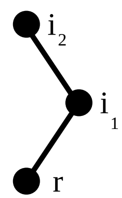
This is just Leibniz' rule for differentiation.

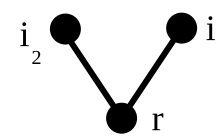
Working out the powers

In the setting of frames, ODE vector field is

$F[\psi] = \sum_i f_i E_i[\psi]$ 

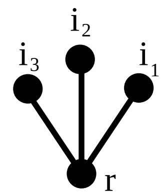
and

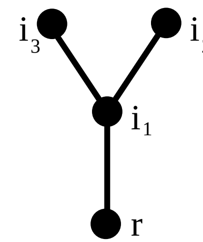




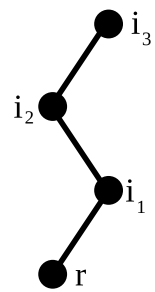
$$F^2[\psi] = \sum_{i_1,i_2} f_{i_2} E_{i_2}[f_{i_1}] E_{i_1}[\psi] + f_{i_1} f_{i_2} E_{i_1} E_{i_2}[\psi]$$

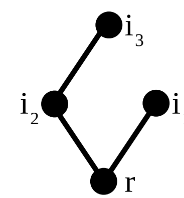
F^3



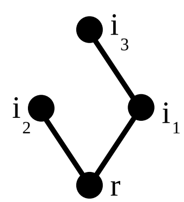


$$F^3[\psi] = \sum_{i_1,i_2,i_3} f_{i_3} f_{i_2} f_{i_1} E_{i_3} E_{i_2} E_{i_1}[\psi] + f_{i_3} f_{i_2} E_{i_3} E_{i_2}[f_{i_1}] E_{i_1}[\psi]$$





$$+ f_{i_3} E_{i_3}[f_{i_2}] E_{i_2}[f_{i_1}] E_{i_1}[\psi] + f_{i_3} E_{i_3}[f_{i_2}] f_{i_1} E_{i_2} E_{i_1}[\psi]$$



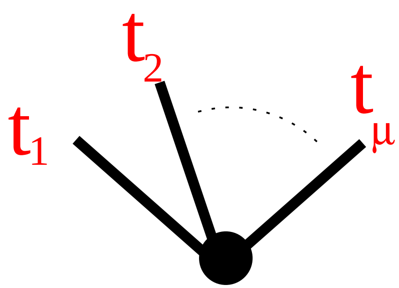
$$+ 2 f_{i_3} E_{i_3}[f_{i_2}] f_{i_1} E_{i_1} E_{i_2}[\psi]$$

Notation for trees

The terms of F^k correspond precisely to the set of all ordered rooted trees with $k+1$ nodes.

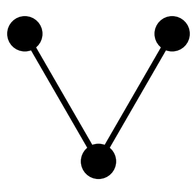
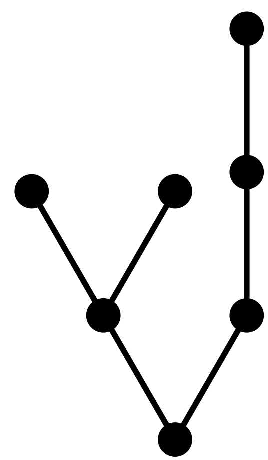
Notation. Denote by T_O the set of all ordered rooted trees.

Write $\tau :=$  and

$[t_1, \dots, t_\mu] :=$ 

each $t_i \in T_O$

Example. $t = [t_1, t_2]$, where $t_1 = [\tau, \tau]$ and $t_2 = [[\tau]]$, that is

$t_1 =$  , $t_2 =$  , $t =$ 

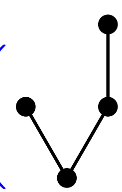
Elementary operators

Recursive definition

$$\begin{aligned} \mathbb{F}(\bullet) &= 1, \\ \mathbb{F}([t_1, \ldots, t_\mu]) &= \sum_{i_1, \ldots, i_\mu} \mathbb{F}(t_1)[f_{i_1}] \cdots \mathbb{F}(t_\mu)[f_{i_\mu}]\, E_{i_1} \cdots E_{i_\mu} \end{aligned}$$

So formally it holds that

$$\psi(e^{hF} p) = \sum_{t \in T_O} \frac{h^{\rho(t)-1}}{(\rho(t)-1)!}\, \alpha(t)\, \mathbb{F}(t)[\psi](p)$$

where for instance $\alpha\Big($  $\Big) = 2$.

Frozen elementary operators

Define $\mathbb{F}_p(\bullet) = \mathbb{F}(\bullet) = 1$ and

$$\mathbb{F}_p([t_1, \ldots, t_\mu]) = \sum_{i_1, \ldots, i_\mu} \mathbb{F}_p(t_1)[f_{i_1}](p) \cdots \mathbb{F}_p(t_\mu)[f_{i_\mu}](p)\, E_{i_1} \cdots E_{i_\mu}$$

This has the particular effect that

$$\mathbb{F}(t)[\psi](p) = \mathbb{F}_p(t)[\psi](p)$$

for every tree t, so we get (again formally)

$$\psi(e^{hF} p) = \sum_{t \in T_O} \frac{h^{\rho(t)-1}}{(\rho(t)-1)!}\, \alpha(t)\, \mathbb{F}_p(t)[\psi](p)$$

$\alpha(t)$

$\alpha(t)$: # ways to distribute ordered labels $1, \ldots, \rho(t)$ on the nodes of the tree t according to

a. parent $<$ child

b. right sibling $<$ left sibling

Strategy: Suppose $t = [t_1, \ldots, t_\mu]$

1. Assign 1 to the root node of t.
2. Assign 2 to root of sth (rightmost) subtree.
3. Choose $\rho(t_\mu) - 1$ labels from remaining $\rho(t) - 2$ in all possible ways
4. For each choice, assign chosen labels to subtree t_μ in $\alpha(t_\mu)$ different ways.
5. Proceed to subtree $t_{\mu-1}$ and repeat procedure.

$$\alpha(t) = \prod_{k=1}^{\mu} \binom{\sum_{i=1}^{k} \rho_i - 1}{\rho_k - 1} \alpha(t_k)$$

Numerical methods

Similarly, numerical methods have expansion of the form

$$\psi(y_1) = \sum_{t \in T_O} h^{\rho(t)-1} \, \beta(t) \, \mathbb{F}(t)[\psi](p)$$

Here $\beta : T_O \to \mathbb{R}$ is a method dependent coefficient.

We consider here commutator free methods, i.e. methods of the form

$$\begin{aligned}
Y_i &= \exp\Big(\overbrace{\sum_r \alpha^r_{i,J} K_r}^{G_{iJ}}\Big) \cdots \exp\Big(\overbrace{\sum_r \alpha^r_{i,1} K_r}^{G_{i,1}}\Big)\, p \\
K_i &= h F_{Y_i} = h \sum_\ell f_\ell(Y_i) E_\ell \\
y_1 &= \exp\Big(\sum_r \beta^r_J K_r\Big) \cdots \exp\Big(\sum_r \beta^r_1 K_r\Big)\, p
\end{aligned}$$

Ansatz

Assume that we have (formal) expansions

$$\psi \circ Y_i = \sum_{t \in T_O} h^{\rho(t)-1} \mathbf{Y}_i(t) \mathbb{F}_p(t)[\psi](p), \; i = 1, \ldots, s.$$

and

$$\psi \circ y_1 := \psi \circ Y_{s+1} := \sum_{t \in T_O} h^{\rho(t)-1} \mathbf{Y}_{s+1}(t) \mathbb{F}_p(t)[\psi](p)$$

Thus

$$\begin{aligned} K_i &= h \sum_{\ell} f_\ell(Y_i) E_\ell = \sum_{t \in T_O} h^{\rho(t)} \mathbf{Y}_i(t) \mathbb{F}_p(t)[f_\ell] E_\ell \\ &= \sum_{t \in T_O} h^{\rho(t)} \mathbf{Y}_i(t) \mathbb{F}_p([t]), \; i = 1, \ldots, s. \end{aligned}$$

Calculating. . .

$$G_{ij} \quad = \quad h \sum_r \alpha^r_{ij} \sum_{t \in T_O} h^{\rho(t)-1} \mathbf{Y}_r(t) \mathbb{F}_p([t]) = \sum_{t \in T_O} \mathbf{G}_{ij}(t) h^{\rho(t)} \mathbb{F}_p([t])$$

where

$$\mathbf{G}_{ij}(t) = \sum_r \alpha^r_{ij} \mathbf{Y}_r(t)$$

Now use contragredient property of $\exp$,

$$\psi(\exp(G_{iJ}) \cdots \exp(G_{i2}) \exp(G_{i1})\, p) = \exp(G_{i1}) \cdot \exp(G_{i2}) \cdots \exp(G_{iJ})[\psi](p).$$

Expand each exponential in its infinite (formal) series, and use the following concatenation product on frozen operators

$$\mathbb{F}_p([t_1]) \cdot \mathbb{F}_p([t_2]) = \mathbb{F}_p([t_1, t_2])$$

. . . and calculating

Leads to formal expression

$$\psi(Y_i) = \psi(p) + \sum_{t \in T_O+} h^{\rho(t)-1} \sum_{\mathbf{j}<} \iota(\mathbf{j}) \mathbf{G}_{ij_1}(t_1) \cdots \mathbf{G}_{ij_m}(t_m) \mathbb{F}_p(t)$$

where $t = [t_1, \ldots, t_m]$. Here $\iota(\mathbf{j})$ is a factorial expression coming from the factorials in the $\exp$ series.

Summation

$$\sum_{\mathbf{j}<} = \sum_{j_1=1}^{J} \sum_{j_2=j_1}^{J} \cdots \sum_{j_m=j_{m-1}}^{J}$$

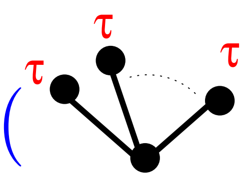
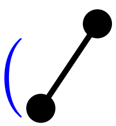
. . . and finally

Comparing with ansatz for Y_i we get recursive formula for each $Y_i([t_1, \ldots, t_m])$

$$
\begin{aligned}
\mathbf{Y}_r(\tau) &= 1, \\
\mathbf{G}_{ij}(t) &= \sum_r \alpha_{ij}^r \mathbf{Y}_r(t) \\
\mathbf{Y}_i([t_1, \ldots, t_m]) &= \sum_{\mathbf{j}<} \iota(\mathbf{j}) \mathbf{G}_{ij_1}(t_1) \cdots \mathbf{G}_{ij_m}(t_m)
\end{aligned}
$$

Bialgebra

Example. Suppose y_1 is calculated as a flow of some vector field. Then

$\beta($  $) = \beta([\tau^{\mu}]) = \frac{1}{\mu!}\Big(\beta($  $)\Big)^{\mu}$

Bialgebra

In general, there is a number of shuffle relations relating coefficients of various trees.

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Bialgebra structure on T_O

- Impose structure of (free) vector space on T_O.
- Furnish T_O with associative product and coproduct
- Extend to whole vector space by linearity.

Product

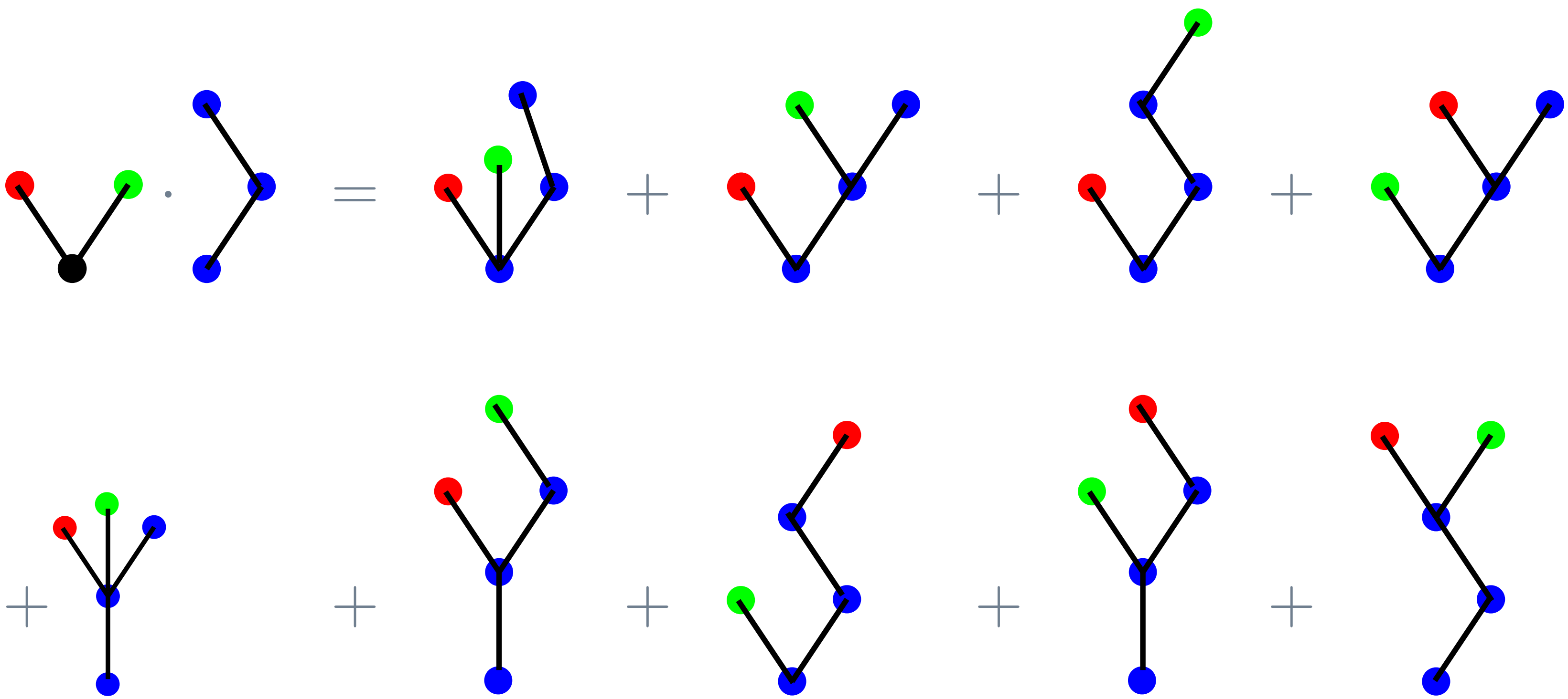
Let $1 := \tau$ (unit, grade 0) $\mathbb{S}(t)$: set of subtrees of t.

$$t_1 \cdot t_2 = \sum_d t_2 \leftarrow_d \mathbb{S}(t_1)$$

where $\sum$ is over all “attachment maps” d of $\mathbb{S}$ to tree t_2.

Product

Example



Coproduct

$\Delta : T_O \to T_O \otimes T_O$ Let $\mathbb{S}(t)$ be the forest of subtrees of t,

$$\Delta(t) = \sum_{s \subseteq \mathbb{S}(t)} [s] \otimes [s^c]$$

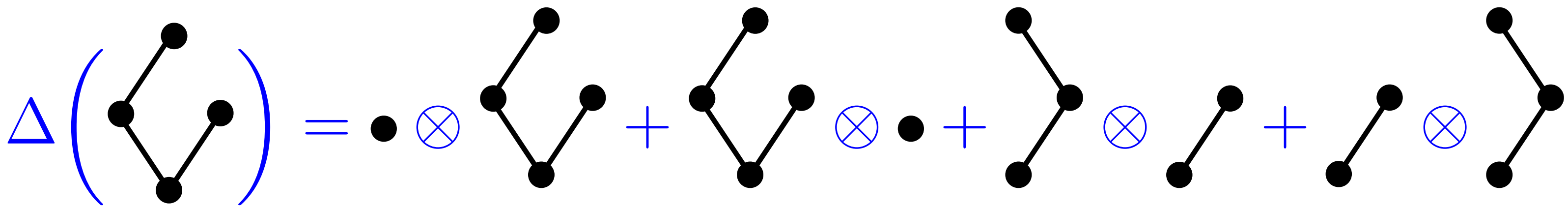
Sum over all subsets of $\mathbb{S}(t)$ and join to new root. s^c is the complement of s in $\mathbb{S}(t)$.

Coproduct

$$\Delta(t) = \sum_{s \subseteq \mathbb{S}(t)} [s] \otimes [s^c]$$

Example.

1. Trees of the form $t = [t'] \rightsquigarrow \Delta(t) = 1 \otimes t + t \otimes 1$
2.



Remarks

- The linear map defined by $t \mapsto \mathbb{F}(t)$ is a homomorphism from the associative algebra into the algebra of elementary operators on $C^\infty(\mathcal{M}, \mathbb{R})$.
- There is a Lie algebra contained in the above bialgebra, consisting of precisely those elements x which satisfy

$$\Delta(x) = 1 \otimes x + x \otimes 1.$$

Remarks

- There is a Lie algebra contained in the above bialgebra, consisting of precisely those elements x which satisfy

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- Dependency of coefficients in expansions.

$$S = \sum_{t \in T_O} h^{\rho(t)-1} \beta(t) \cdot t \quad \Rightarrow \quad \Delta(S) = S \otimes S$$