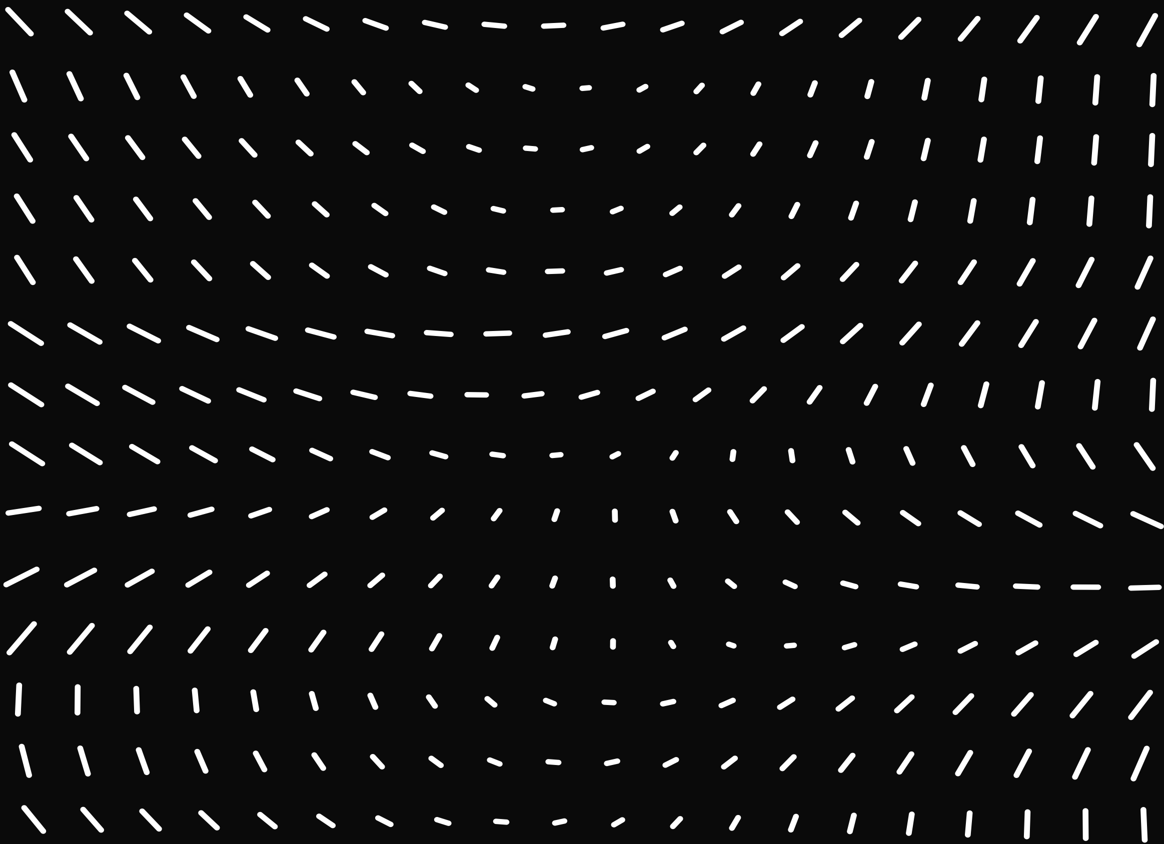
Geometric Numerical Integration

An algebrogeometric introduction



Contents:

Chapter I: The flow of an evolution differential equation

Chapter II: Splitting and composition methods

Chapter III: The Runge-Kutta approach

Chapter IV: Geometric Numerical Integration

References

Chapter I: The flow of an evolution differential equation

Let $f \in \mathcal{X}(\mathbb{R}^d)$ (vector fields on $\mathbb{R}^d$) (or $f \in \mathcal{X}(M)$, M manifold)

Assume f is Lipschitz (globally) and smooth ($\mathcal{C}^\infty$) for simplicity. The ODE
$$\begin{cases} y'(t) = f(y(t)) \\ y(0) = y_0 \end{cases} \quad (C)$$
is well defined by Cauchy-Lipschitz / Picard/Lindelöf.

We denote $\varphi_t(y_0) := y(t)$ the exact flow of (C)

Prop:
- $\varphi_0 = id$
- $\varphi_s \circ \varphi_t = \varphi_{s+t}$
- $\varphi_{-t} \circ \varphi_t = id$

$(\{\varphi_t, t \in \mathbb{R}\}, \circ)$ is a group.

Rk: recall that an ODE of the form $y'(t) = f(t, y(t))$ can be rewritten in the form (C) with $Y(t) = \begin{pmatrix} y(t) \\ t \end{pmatrix}$ and
$$F\Big(\underbrace{Y}_{= \binom{y}{t}}\Big) = \begin{pmatrix} f(t, y) \\ 1 \end{pmatrix}$$

1) Examples of differential systems

ⓐ Linear systems

→ $f(y) = Ay, \quad A \in \mathbb{R}^{d \times d}$

$\varphi_t(y) = e^{tA} y$, where $e^{tA} = \sum_{k=0}^{+\infty} \frac{tA^k}{k!}$ (power series $R = +\infty$)

→ $f(t,y) = A(t)y$ and $[A(t), A(s)] := A(t)A(s) - A(s)A(t) = 0$

then $\varphi_t(y) = e^{\int_0^t A(s)\,ds} y$

→ $f(y) = A(y)y$

↳ see DM 

Rk: if $f(y) = A(y)y$ and

↳ $A^T(y) = -A(y)$, then $\varphi_t \in SO(d)$

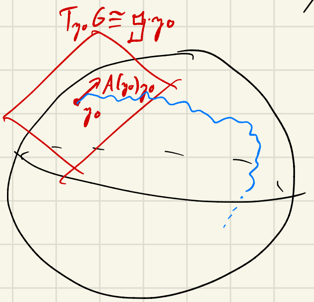
Ex: Rigid body $f\begin{pmatrix} y_1 \\ y_2 \\ y_3 \end{pmatrix} = \begin{pmatrix} 0 & -y_3 & y_2 \\ y_3 & 0 & y_1 \\ -y_2 & y_1 & 0 \end{pmatrix} \begin{pmatrix} y_1 \\ y_2 \\ y_3 \end{pmatrix}$

$$\frac{d}{dt}\left(\varphi_t^T(y)\, \varphi_t(y)\right) = \varphi_t^T(y)\left(A^T(\varphi_t(y)) + A(\varphi_t(y))\right)\varphi_t(y)$$

$$= 0$$

So that $|\varphi_t(y)| = |y|$, that is $\boxed{\varphi_t(y) \in |y|\, \mathbb{S}^{d-1}}$

↳ More generally, if $A(y) \in \mathfrak{g}$ and $y_0 \in G$ where G a Lie group and $\mathfrak{g}$ its Lie algebra, then $\varphi_t(y_0) \in G$, $\forall t$.



(b) Hamiltonian systems

Consider q the position and p the momentum (mass × speed), a force deriving from a potential $F(q) = -\nabla V(q)$, $V : \mathbb{R}^d \to \mathbb{R}$.

$$= \begin{pmatrix} -\frac{\partial V}{\partial q_1}(q) \\ \vdots \\ -\frac{\partial V}{\partial q_d}(q) \end{pmatrix}$$

Then the equations of motion are $\ddot{q}(t) = -\nabla V(q)$, or alternatively:

$$\begin{cases} \dot{q}(t) = p(t) \\ \dot{p}(t) = -\nabla V(q(t)) \end{cases} \quad (H)$$

Let the Hamiltonian $H : \mathbb{R}^{2d} \longrightarrow \mathbb{R}$
$$(q,p) \longrightarrow \frac{p^2}{2} + V(q),$$ then

(H) rewrites as
$$\begin{cases} \dot q(t) = \nabla_p H(q(t), p(t)) \\ \dot p(t) = -\nabla_q H(q(t), p(t)) \end{cases}$$

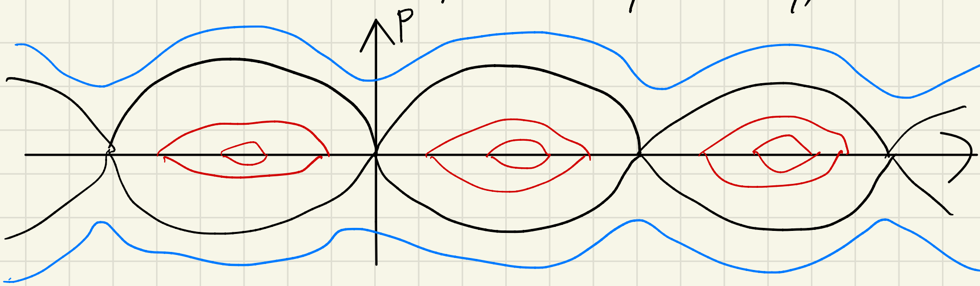
or equivalently $\gamma'(t) = J \nabla H(\gamma(t))$, $J = \begin{pmatrix} 0 & I_d \\ -I_d & 0 \end{pmatrix}$.

Ex: the simplest example is with $V(q) = \frac{q^2}{2}$, the linearised pendulum

$$\begin{cases} \dot q = p \\ \dot p = -q \end{cases} \longrightarrow \gamma'(t) = \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix} \gamma(t)$$

$$\varphi_t(\gamma_0) = e^{tJ} \gamma_0 = \begin{pmatrix} \cos(t) & \sin(t) \\ -\sin(t) & \cos(t) \end{pmatrix} \gamma^0$$

The simple pendulum corresponds to $V(q) = -\cos(q)$.



phase portrait

Prop: The solution of (H) satisfies $H(\gamma(t)) = H(\gamma_0)$, $\forall t$.

proof: $\frac{d}{dt}\left(H(\varphi_t(\gamma_0))\right) = \left\langle \nabla H(\varphi_t(\gamma_0)), \frac{d}{dt} \varphi_t(\gamma_0) \right\rangle$

$$= \langle \nabla H(\varphi_t(y_0)), J \nabla H(\varphi_t(y_0)) \rangle$$
$$= 0$$

$\square$

Rk: this type of systems appears also in molecular dynamics for instance with the Lennard-Jones potential

$$V_{ij}(|q_i - q_j|) = \frac{C_1}{r^{12}} - \frac{C_2}{r^6}$$

In this context, the dimension d is very high (theoretically, $d \sim N_{avogadro} \propto 10^{24}$).

© Constrained equations, dynamics on manifolds

Let $\zeta : \mathbb{R}^d \to \mathbb{R}^q$, $q < d$, and define

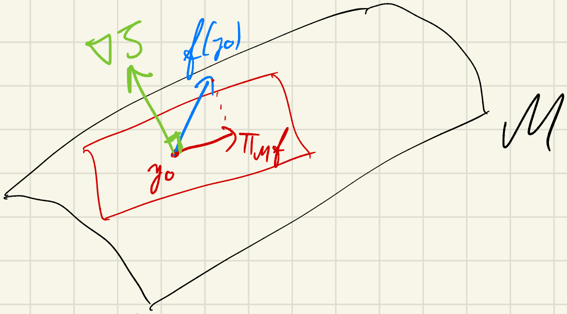
$$\mathcal{M} = \{ x \in \mathbb{R}^d, \zeta(x) = 0 \}$$

and $\Pi_{\mathcal{M}}(x) = I_d - \dfrac{\nabla\zeta \cdot \nabla\zeta^T}{\nabla\zeta^T \cdot \nabla\zeta}(x)$, assuming $|\nabla\zeta(x)| > 0, \forall x$.

Prop: the solution of

$$y'(t) = \Pi_{\mathcal{M}}(y(t)) f(y(t)) \text{ satisfies}$$

satisfies $\varphi_t(y_0) \in \mathcal{M}$, $\forall t$.



<u>proof:</u> $\frac{d}{dt}\left(\zeta(y(t))\right) = \big(\underbrace{\nabla\zeta^T \cdot \Pi_M}_{=0} f\big)(y(t))$. $\square$

One could directly define $f \in \mathfrak{X}(M)$ on any differentiable manifold M. Then the flow of $y' = f(y)$ is on M.

$\Longrightarrow$ No need for an embedding in a space of higher dimension.

Necessary tools of diff geometry

2) Geometric properties of the flow

ⓐ First integrals

def: a non-constant function $I(y)$ is called a first integral of (C) if

$$I'(y) f(y) = 0 \ , \ \forall y$$

Prop: I first integral $\Leftrightarrow \forall t, y_0, \ I(\varphi_t(y_0)) = I(y_0)$

Ex:
- H is a first integral of $y' = J \nabla H(y)$.
- rigid body $y \mapsto |y|^2$ is a first integral.
- ζ is a first integral of constrained systems.

ⓑ Volume preservation

def: the flow of an ODE $y' = f(y)$ preserves volume if for all measurable set $\Omega \subset \mathbb{R}^d$, for all $t \geq 0$, we have $\mathrm{Vol}(\varphi_t(\Omega)) = \mathrm{Vol}(\Omega)$, that is,

$$\int_{\varphi_t(\Omega)} dy = \int_{\Omega} dy .$$

Thm (Liouville): the flow of $y' = f(y)$ is VP iff $\operatorname{div}(f) = 0$.

proof: $$\int_{\varphi_t(\Omega)} dy = \int_{\Omega} \left|\det\left(\frac{\partial \varphi_t}{\partial y}\right)\right| dy$$ Jacobian

As this is valid for any Ω, we have:

$$\begin{aligned} \text{VP} &\iff \left|\det\left(\frac{\partial \varphi_t}{\partial y}(y)\right)\right| = 1, \quad \forall t, y \\ &\iff \det\left(\frac{\partial \varphi_t}{\partial y}(y)\right) = 1, \quad \forall t, y \quad (C^0 + \text{value in } t=0) \\ &\iff \frac{d}{dt}\left(\det\left(\frac{\partial \varphi_t}{\partial y}\right)\right) = 0 \end{aligned}$$

We find $\frac{d}{dt}(\varphi_t(y)) = f(\varphi_t(y))$,

so that by differentiating in y:

$$\frac{\partial}{\partial y}\left(\frac{d}{dt} \varphi_t(y)\right) = f'(\varphi_t(y)) \frac{\partial \varphi_t}{\partial y}(y)$$

By Schwarz, we find the Variational equation

$$\boxed{\frac{d}{dt}\left(\frac{\partial \varphi_t}{\partial y}\right) = f'(\varphi_t(y)) \frac{\partial \varphi_t}{\partial y}}$$

Puis la différentielle du déterminant pour une matrice inversible est : $\det'(A)(H) = \mathrm{Tr}(\mathrm{Com}(A)^T H)$

$$= \mathrm{Tr}(A^{-1} H) \det(A)$$

donc $\frac{d}{dt}\left(\det\left(\frac{\partial \varphi_t}{\partial y}\right)\right) = \det'\left(\frac{\partial \varphi_t}{\partial y}\right)\left(\frac{d}{dt}\frac{\partial \varphi_t}{\partial y}\right)$

$$= \mathrm{Tr}\left(\cancel{\left(\frac{\partial \varphi_t}{\partial y}\right)^{-1}} f'(\varphi_t(y)) \cancel{\frac{\partial \varphi_t}{\partial y}}\right) \det\left(\frac{\partial \varphi_t}{\partial y}\right)$$

$$= \mathrm{div}(f)(\varphi_t(y)) \cdot \det\left(\frac{\partial \varphi_t}{\partial y}\right)$$

Donc, $\frac{d}{dt}\left(\det\left(\frac{\partial \varphi_t}{\partial y}\right)\right) = 0 \iff \boxed{\mathrm{div}(f) = 0}$
$, \forall t, y$

$\square$

Ex : (ABC flow)

$$\dot{x} = A\sin(z) + C\cos(y)$$
$$\dot{y} = B\sin(x) + A\cos(z)$$
$$\dot{z} = C\sin(y) + B\cos(x)$$

$$\mathrm{div}(f) = 0$$

Ex : $y' = A(t)\, y$

VP $\iff \mathrm{Tr}(A(t)) = 0, \ \forall t$

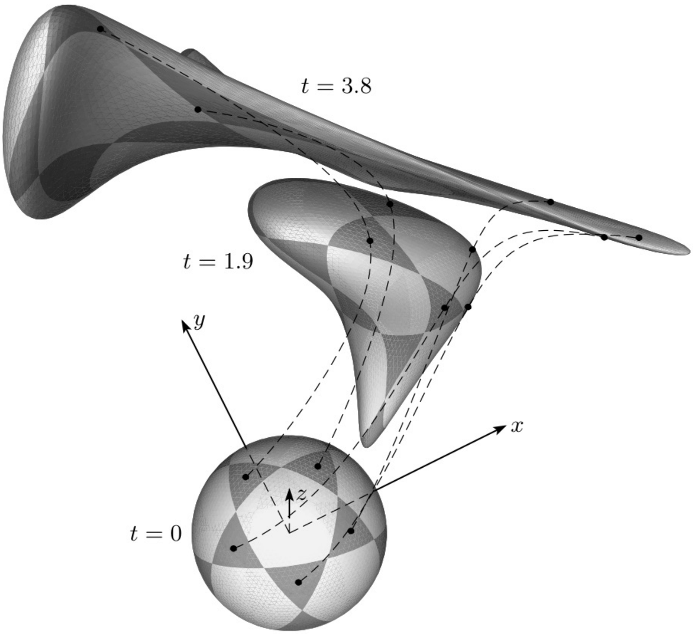
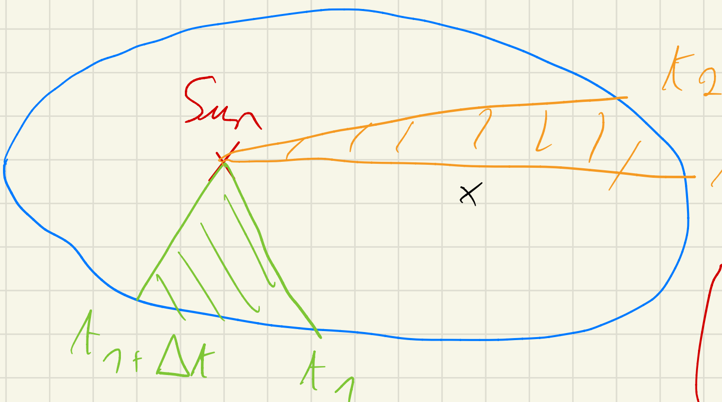


Fig. 9.1. Volume preserving deformation of the ball of radius 1, centred at the origin, by the ABC flow; $A = 1/2$, $B = C = 1$

(c) Symplecticity

Idea: Motion of the earth around the sun given by a Hamiltonian system.
Kepler second law says:
"A line segment joining a planet and the sun sweeps out equal areas during equal intervals of time."



$$\boxed{A_1 = A_2}$$

<u>def</u>: let the 2-form w be given by

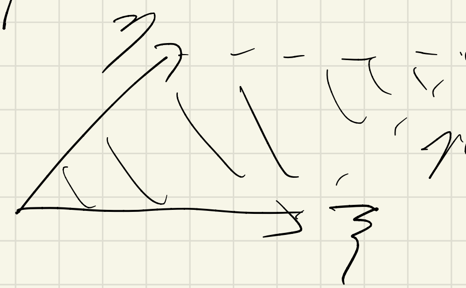
$$\begin{aligned} &\mathbb{R}^{2d} \times \mathbb{R}^{2d} \longrightarrow \mathbb{R} \\ w :\ &(\xi, \eta) \longmapsto \sum_{i=1}^{d} \det\begin{pmatrix} \xi^q_i & \eta^q_i \\ \xi^p_i & \eta^p_i \end{pmatrix} \end{aligned}$$

$$\xi = \begin{pmatrix} \xi^q \\ \xi^p \end{pmatrix}, \quad \eta = \begin{pmatrix} \eta^q \\ \eta^p \end{pmatrix}$$

↳ Matrix form $w(\xi, \eta) = \xi^T J \eta$, $J = \begin{pmatrix} 0 & Id \\ -Id & 0 \end{pmatrix}$

↳ In dim 2, $\det\begin{pmatrix} \xi^q & \eta^q \\ \xi^p & \eta^p \end{pmatrix} = \text{Area}(P)$ (oriented)

où $P =$



parallelogram

<u>def</u>: a smooth map $g : U \subset \mathbb{R}^{2d} \longrightarrow \mathbb{R}^{2d}$ is symplectic iff

$$g'(y)^T J g'(y) = J, \quad \forall y$$

that is, $w(g'(q,p)\xi, g'(q,p)\eta) = w(\xi, \eta)$, $\forall q, p, \xi, \eta$

Ex: for $g(\eta) = A\eta$, g is symplectic

$\iff \omega(A\xi, A\eta) = \omega(\xi, \eta)$

$\iff A^T J A = J$

That is, A preserves the areas
(rotation for instance)

Thm (Poincaré): let $H : \mathbb{R}^{2d} \to \mathbb{R}$ be $\mathcal{C}^2$,
then the flow of $\eta' = J \nabla H(\eta)$ is symplectic.

proof: variational equation for $\Psi_t = \frac{\partial \varphi_t}{\partial \eta}$

$$\frac{d}{dt} \Psi_t(\eta) = J \nabla^2 H(\varphi_t(\eta)) \cdot \Psi_t(\eta)$$

Then

$$\frac{d}{dt}\left(\Psi_t^T J \Psi_t\right) = \left(\frac{d}{dt}\Psi_t\right)^T J \Psi_t + \Psi_t^T J \left(\frac{d}{dt}\Psi_t\right)$$

$$= \Psi_t^T \Big[\underbrace{(\nabla^2 H)^T}_{\substack{= \nabla^2 H \\ \text{Schwarz}}} \underbrace{J^T J}_{= I_{2d}} + \underbrace{J J}_{= -I_{2d}} \nabla^2 H \Big] \Psi_t$$

$$= 0$$

$\square$

Let $I : \mathbb{R}^d \times \mathbb{R}^{d\times d} \longrightarrow \mathbb{R}^{d\times d}$, then

$$(\varphi, \psi) \longmapsto \psi^T J \psi$$

I is a $\boxed{\text{quadratic first integral}}$ of the augmented ODE:

$$\begin{cases} \frac{d}{dt}\varphi_t(y) = f(\varphi_t(y)) \\ \frac{d}{dt}\psi_t(y) = f'(\varphi_t(y)) \cdot \psi_t(y) \end{cases}$$

Thm: let $f : U \subset \mathbb{R}^{2d} \to \mathbb{R}^{2d}$ C^1,

then the flow of $y' = f(y)$ is symplectic for t small iff it is locally Hamiltonian, that is,

$\forall y_0 \in U$, $\exists \mathcal{N}(y_0)$, $\exists H : \mathcal{N}(y_0) \to \mathbb{R}$ st $f = J\nabla H$ in $\mathcal{N}(y_0)$

proof: $\Leftarrow$: OK

$\Rightarrow$: for t small enough, we have

$$\frac{d}{dt}\left(\psi_t^T J \psi_t\right) = 0$$

that is $\psi_t^T \left[\left(f'(\varphi_t)\right)^T J + J f'(\varphi_t) \right] \psi_t = 0$

$t = 0$ gives $f'(y)^T J + J f'(y) = 0, \ \forall y \in U$

that is $\boxed{J^{-1} f'(y) \text{ is symmetric}}$

($J f'$ as well)

Define $g = J^{-1} f$ and assume $y_0 = 0$ for simplicity.

let $H(y) = \int_0^1 y^T g(ty)\, dt$ for $y \in B(y_0, \varepsilon) \subset U$

then $\nabla H(y) = \int_0^1 \left(g(ty) + t\left(y^T g'(ty)\right)^T \right) dt$

$$= \int_0^1 \left(g(ty) + t\, g'(ty)\, y \right) dt$$

$$= \int_0^1 \frac{d}{dt}\left(t\, g(ty)\right) dt$$

$$= g(y)$$

that is $f(y) = J\nabla H(y), \forall y \in B(y_0, \varepsilon)$ $\square$

Rk: if U is star shaped, (for instance) H is globally defined.

Reformulation in geometry:

$$\overset{0}{\Omega} \xrightarrow{``J\nabla''} \overset{1\text{ forms}}{\Omega^1} \xrightarrow{``w''} \overset{2\text{ forms}}{\Omega^2}$$

$$H \longmapsto J\,dH \longmapsto \sum_{\cancel{i,j}} f_i\, dy_i \wedge f_j\, dy_j$$

$$J\,dH = f_1\, dy_1 + \dots + f_n\, dy_n$$

A corriger

Then $f\,dy \in \mathrm{Ker}(w) \iff f \in \mathrm{Im}(J\nabla)$

We just showed that a complex is *exact*!

The homotopy operator is (around $y_0 = 0$)

$$\Omega^0 \underset{h}{\overset{d}{\rightleftarrows}} \Omega^1$$

$$h : f \longmapsto \int_0^1 y^T f(ty)\, dt$$

Prop: 1) If g symp., then g preserves volume

2) If g_1, g_2 symp, $g_2 \circ g_1$ symp

Proof: 1) $(g')^T J g' = J$ 2) exercise

$\Rightarrow \det(g')^2 = 1$

$\Rightarrow |\det(g')| = 1$

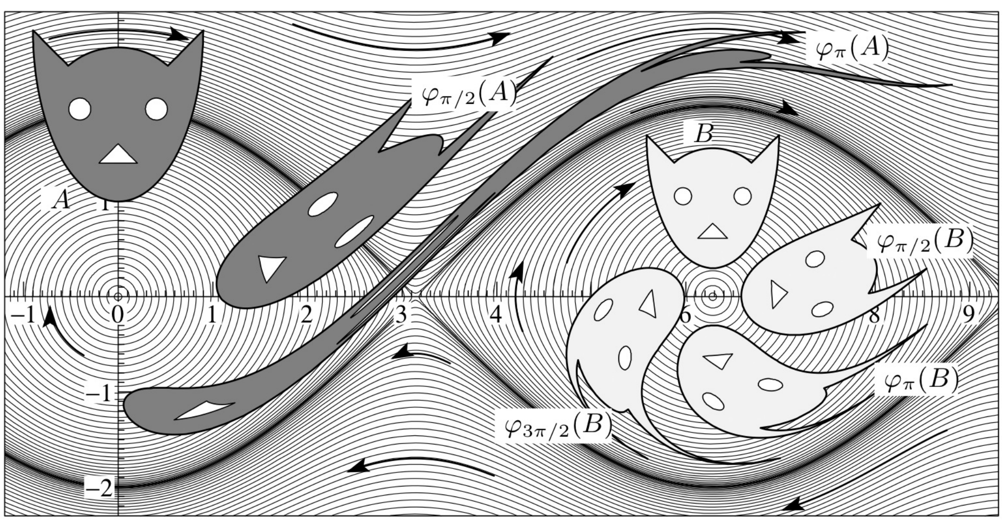
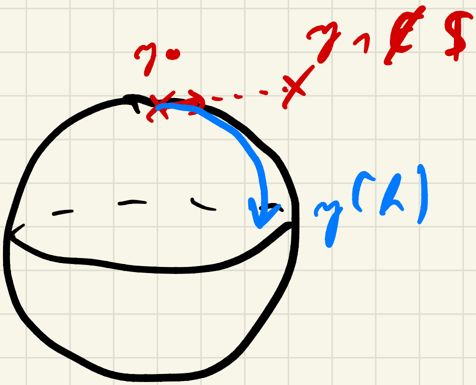
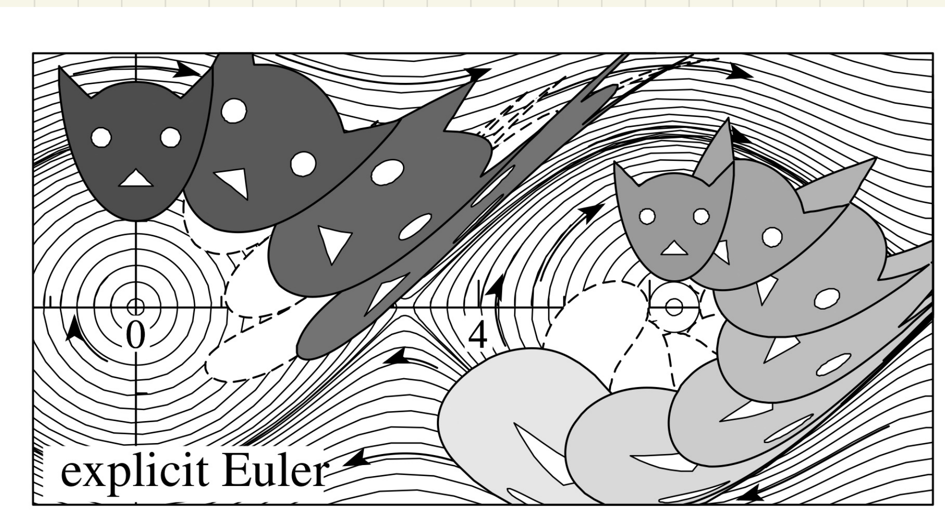


Fig. 2.2. Area preservation of the flow of Hamiltonian systems

The question: the flow satisfies a handful of geometric properties. How do we create numerical integrators that preserve these properties as well?

Example: Euler method





Chapter II: Splitting and composition methods

1) Definition and examples

ODE $\begin{cases} y' = f(y) \\ y(0) = y_0 \end{cases}$ flow $y(t) = \varphi_t(y_0)$

integrator $y_{n+1} = \Psi_h(y_n)$, $t_n = nh$, $hN = T$

If $f = f^1 + f^2 + \dots + f^P$ and we know the exact flows φ_t^p, $1 \leq p \leq P$ (a sufficiently good approximation), then a splitting method is a composition of these flows.

For simplicity, we consider $f = f^A + f^B$.

def: A splitting method is given for constants $a_1, \dots, a_s$, $b_1, \dots, b_s$ by

$$\Psi_h = \varphi^B_{b_s h} \circ \varphi^A_{a_s h} \circ \dots \circ \varphi^B_{b_1 h} \circ \varphi^A_{a_1 h}.$$

Ex: $y' = J \nabla H(y)$, $H(q,p) = T(p) + V(q)$
↳ separable Hamiltonian

Pb A

$$\begin{cases} q' = \nabla T(p) \\ p' = 0 \end{cases} \Rightarrow \varphi_t^A\left(\begin{pmatrix} q_0 \\ p_0 \end{pmatrix}\right) = \begin{pmatrix} q_0 + t\,\nabla T(p_0) \\ p_0 \end{pmatrix}$$

Pb B

$$\begin{cases} q' = 0 \\ p' = -\nabla V(q) \end{cases} \Rightarrow \varphi_t^B\left(\begin{pmatrix} q_0 \\ p_0 \end{pmatrix}\right) = \begin{pmatrix} q_0 \\ p_0 - t\,\nabla V(q_0) \end{pmatrix}$$

Idea: we split the pb into multiple simpler pbs.

def: given an integrator $\chi_h(y_0)$, a composition method is

$$\Psi_h = \chi_{\gamma_s h} \circ \cdots \circ \chi_{\gamma_1 h}$$

We obtain methods given by composition of exact/numerical flows.

$\Rightarrow$ If a geometric property is satisfied by

$y' = f(y)$, if this pty is satisfied by the flows used in the method $(\chi_h, \varphi_h^A, \varphi_h^B)$, then the splitting/composition method preserves the geometric ppties.

<u>Ex:</u> $f^A(y) = Ay$, $A^T = -A$

$f^B(y) = By$, $B^T = -B$

then $\varphi_t^A = e^{tA} y \in \mathbb{S}^d$ / for $y \in \mathbb{S}^d$

$\varphi_t^B = e^{tB} y \in \mathbb{S}^d$

<u>Ex:</u> Schrödinger equation

$$\partial_t u = i\Delta u + F(u), \quad F(u) = iP(|u|)u$$

$g: \mathbb{R} \to \mathbb{R}$

discretisation $y' = Ay + g(|y|)Jy$, $A^T = -A$

$$\partial_t |y|^2 = 2\langle y, Ay + g(|y|)Jy \rangle = 0$$

Pb A : $y' = Ay$ $\qquad \varphi_t^A : \mathbb{S}^d \to \mathbb{S}^d$

$$\varphi_t^A(y) = e^{tA} y$$

Pb B : $y' = g(|y|) J y$ $\qquad \varphi_t^B : \mathbb{S}^d \to \mathbb{S}^d$

$$\varphi_t^B(y) = e^{t\, g(|y|) J} y$$

Ex : manifold case

$$\varphi_t^A \in \mathfrak{X}(M), \quad \varphi_t^B \in \mathfrak{X}(M)$$

then the composition $\in \mathfrak{X}(M)$

1) Taylor expansion of the flow (1st time)

Let $y' = f(y)$ with $y(0) = y_0$.

Q°: what is the expansion of $y(h)$? (assuming f C^∞)

Notation: $f^{(n)} : \mathbb{R}^d \longrightarrow \mathcal{L}(\underbrace{\mathbb{R}^d \times \mathbb{R}^d \times \cdots \times \mathbb{R}^d}_{\underline{\underline{n \text{ linéaire}}}}, \mathbb{R}^d)$

We write $f^{(n)}(y)(a^1, \ldots, a^n) = \sum_{i_j = 1}^{d} \frac{\partial^n f}{\partial y_{i_1} \cdots \partial y_{i_n}} a^1_{i_1} \cdots a^n_{i_n}$

Ex: in the linear case $f(y) = Ay$,
we find $\varphi_t(y) = e^{tA} y = y + tAy + \frac{t^2}{2} A^2 y + \ldots$

Prop: the flow satisfies

$$\boxed{\varphi_t(y) = \sum_{n=0}^{+\infty} \frac{t^n}{n!} (f(y))^{\triangleright n} = \exp^{\triangleright}(tf)(y)}$$

$$= y + t f(y) + \frac{t^2}{2} (f \triangleright f)(y)$$

$$+ \frac{t^3}{6} \left(f \triangleright (f \triangleright f)\right)(y) + \frac{t^4}{24} f \triangleright (f \triangleright (f \triangleright f)) + \cdots$$

where $f \triangleright g = g'(f) \left(= \langle \nabla g, f \rangle = \nabla_f g \right)$.

The product $\triangleright : \mathcal{X}(\mathbb{R}^d) \times \mathcal{X}(\mathbb{R}^d) \to \mathcal{X}(\mathbb{R}^d)$ is non commutative and non associative. ⚠

Manifold case:

Moreover for $\phi \in \mathcal{C}^\infty(\mathcal{M}, \mathbb{R})$ and $f \in \mathcal{X}(\mathcal{M})$, we have

$$\phi(\varphi_t(y)) = \exp(f \triangleright)[\phi]$$
$$= \phi(y) + t f \triangleright \phi(y) + \frac{t^2}{2} f \triangleright (f \triangleright \phi)(y) + \dots$$

Rk: the series in the proposition are formal power series indexed by h. One needs to assume analyticity of f typically to obtain CV.

Proof: by induction

- $y(0) = y_0$
- $y'(0) = f(y_0)$
- $y''(t) = f'(y(t))(y'(t)) = (f \triangleright f)(y(t))$
- $y'''(t) = (f \triangleright f)'(y(t))(y'(t))$

$$= \big(f \triangleright (f \triangleright f)\big)\big(g(x)\big)$$

$\square$

3) Order theory of splitting methods

Denote $A = f^A \nabla = \sum f^{A,i} \frac{\partial}{\partial x_i}$ Lie operators

$B = f^B \nabla = \sum f^{B,i} \frac{\partial}{\partial x_i}$

with the identification $\frac{\partial}{\partial x_i} \simeq e_i$ basis of $\mathbb{R}^d$.

diff op order 1 $\simeq$ V.f.

def Given 2 linear operators X, Y, the Lie algebra $\mathcal{L}(X,Y)$ is the smallest vector space stable by $[-,-]$ and containing X, Y, where $[-,-]$ is a Lie bracket:

- $[-,-]$ is bilinear
- $[x,x] = 0$
- Jacobi $[x,[y,z]] + [y,[z,x]] + [z,[x,y]] = 0$

Rk: other relations could be satisfied. Eg

Recall that, we work in a general setting with a free Lie algebra.

Thm (BCH formula): there exists a map

$$BCH(X,Y) \in \mathcal{L}(X,Y) \text{ s.t.}$$

$$e^X e^Y = e^{BCH(X,Y)}, \quad [X,Y] = XY - YX$$

and the first terms are:

$$BCH(X,Y) = \overbrace{X+Y}^{(1)} + \frac{1}{2}\overbrace{[X,Y]}^{(2)}$$

$$+ \frac{1}{12}\left([X,[X,Y]] + [Y,[Y,X]]\right) \quad (3)$$

$$- \frac{1}{24}[Y,[X,[X,Y]]] \quad (4)$$

$$+ \ldots$$

The complete combinatorial formula is called the Dynkin formula.

Then $\phi(\Psi_h(y_0)) = \phi(\varphi^B_{b_0 h} \circ \dots \circ \varphi^A_{a_1 h}(y_0))$

$= (\phi \circ \dots \varphi^B_{b_1 h})(\varphi^A_{a_1 h}(y_0))$

$= e^{a_1 h A}[\phi \circ \dots \circ \varphi^B_{b_1 h}](y_0)$

$= e^{a_1 h A} e^{b_1 h B} \dots e^{b_0 h B}[\phi](y_0)$

<u>def</u>: an integrator has (local) order p for solving $y'(t) = f(y(t))$ if $\exists h_0 > 0$, $\forall h \leq h_0$, $|\varphi_h(y_0) - \Psi_h(y_0)| \leq C(y_0) h^{p+1}$

<u>Rk</u>: under stability assumptions, one can go from local to global order:

$$|\varphi_T(y_0) - \Psi_h^N(y_0)| \leq C(T, y_0) h^p$$

Thm: if $e^{a_1 h A} \cdots e^{b_s h B} = e^{h(A+B) + O(h^{p+1})}$

the splitting method Ψ_h has (at least) order p.

Proof: $e^{X + O(h^{p+1})} = e^X + O(h^{p+1})$ by Taylor.

Application:

Lie-Trotter: $\Psi_h = e^{hB} e^{hA}$ order 1

and $e^{hA} e^{hB} = e^{h(A+B) + \frac{h^2}{2}[A,B] + \cdots}$

Strang: $\Psi_h = e^{h/2 A} e^{hB} e^{h/2 A}$

$$e^{h/2 A} e^{hB} e^{h/2 A} = e^{h/2 A} e^{h(A/2 + B) + \frac{h^2}{4}[B,A] + \cdots}$$

$$= e^{h(A/2 + B) + \frac{h^2}{4}[B,A] + h/2 A + \frac{h^2}{2}[A,B] + \cdots}$$

$$= e^{h(A+B) + O(h^3)}$$

order 2

For higher orders, we need a basis of $\mathcal{L}(X,Y)$.

Lyndon words: $\{a, b, ab, abb, aab, abbb, \ldots$ based on the alphabet $A = \{a,b\}$

and $F_a = A$, $F_b = B$,

$$F_{ab} = [A, B], \quad F_{abb} = [F_{ab}, F_b],$$

$$F_{aab} = [F_a, F_{ab}],$$ (see Reutenauer, '93) and Casas and al, '24

then $\log\left(e^{a_1 h A} \cdots e^{b_s h B}\right) = \sum\limits_{w \in \text{Lyndon}(a,b)} h^{|w|} p(w) F_w$

where $p(w)$ is a polynomial in the a_i, b_i.

$$p(a) = \sum a_i, \quad p(b) = \sum b_i,$$

$$p(ab) = \frac{1}{2} p(a) p(b) - \sum_{i<j} b_i a_j,$$

$$p(abb) = \frac{1}{12} p(a)\, p(b)^2 - \frac{1}{2} \sum_{i \leq j < k} b_i a_j b_k,$$

$$p(aab) = \frac{1}{12} p(a)^2 p(b) - \frac{1}{2} \sum_{i \leq j \leq k} a_i b_j a_k$$

...

Rk: more details on the calculation of $p(w)$ in the exercises. and the algebraic structure ♡.

Then, a splitting method has

order 1 $\iff \sum a_i = 1 = \sum b_i$

order 2 $\iff p(ab) = 0$ + order 1

order 3 $\iff p(abb) = p(aab) = 0$ + order 2

etc...

Prop: if a splitting method has order three, then $\exists\, i_0, j_0$ st $a_{i_0} < 0$ and $b_{j_0} < 0$. (Blanes, Casas, '05) & Sheng, 89

proof: see exercises.

Problem: for non-reversible problems such as the heat equation:

$$\partial_t u = \underbrace{\Delta u}_{A} + \underbrace{F(u)}_{B}$$

φ^A_{-h} is not defined!

Thus, a **splitting method has max order of 2!**

Possible solutions: splitting methods with commutators

Ex: Takahashi-Imada splitting (1984)

$$\psi_h = e^{\frac{h^2}{24}[A,B]} e^{h/2\, A} e^{\frac{h}{2} B} e^{-\frac{h^3}{24}[B,[B,A]]} e^{h/2\, B} e^{h/2\, A} e^{-\frac{h^2}{24}[A,B]}$$

of order 4.

or splitting methods with complex coefficients

(Castella, Chartier, Descombes, Vilmart & Hansen, Ostermann; 2009)

4) Composition methods

Thm: let $\Psi_h = \chi_{\gamma_s h} \circ \dots \circ \chi_{\gamma_1 h}$ a composition method with χ of order r, then if $\begin{cases} \gamma_1 + \dots + \gamma_s = 1 \\ \gamma_1^{r+1} + \dots + \gamma_s^{r+1} = 0 \end{cases}$,

then Ψ_h has order at least $r+1$.

Proof: $\chi_{\gamma h}(y) = \varphi_{\gamma h}(y) + C(y)(\gamma h)^{r+1} + \dots$

$$Y_0 = y_0 \quad , \quad Y_{i+1} = \chi_{\gamma_i h}(Y_i) \quad , \quad Y_s = \Psi_h(y_0)$$

$$e_i := \chi_{\gamma_i h}(Y_i) - \varphi_{\gamma_i h}(Y_i) = C(\underbrace{Y_i}_{= y_0 + O(h)})(\gamma_i h)^{r+1} + O(h^{r+2})$$

$$= C(y_0)(\gamma_i h)^{r+1} + O(h^{r+2})$$

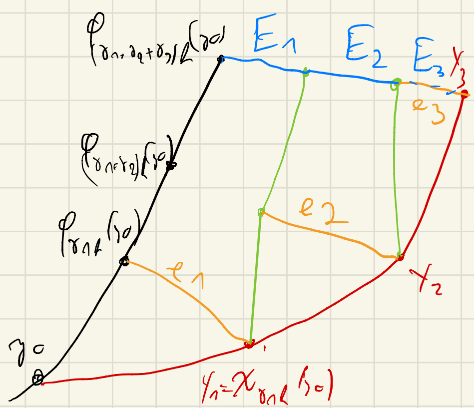
$$E_i = \varphi_{(\gamma_{i+1} + \dots + \gamma_s) h}(e_i) = (1 + O(h)) e_i \quad \text{as } \varphi_h = id + O(h)$$

$$= C(y_0)(\gamma_i h)^{r+1} + O(h^{r+2})$$

We observe that if $\sum \gamma_i = 1$

$$\Psi_h(y_0) - \varphi_h(y_0) = E_1 + \dots + E_s$$

$$= (id + O(h)) \sum e_i$$



$= C(y_0)\left(\gamma_1^{k+1} + \dots + \gamma_0^{k+1}\right) h^{k+1} + \mathcal{O}(h^{k+2})$

$\square$

def: the adjoint of a method Ψ_h is $\Psi_h^* = \Psi_{-h}^{-1}$,

that is, $\Psi_h^* \circ \Psi_h = id$

if $\Psi_h^* = \Psi_h$, the method is symmetric.

Ex: the exact flow satisfies $\varphi_h^* = \varphi_{-h}^{-1} = \varphi_{-(-h)} = \varphi_h$.

Explicit Euler: $\Psi_h(y) = y + h f(y)$

$$y_{n+1} = y_n + h f(y_n)$$

$h \leftrightarrow -h$: $\quad y_{n+1} = y_n - h f(y_n)$

$y_{n+1} \leftrightarrow y_n$: $\quad y_n = y_{n+1} - h f(y_{n+1})$

$$\boxed{y_{n+1} = y_n + h f(y_{n+1})}$$

the adjoint of Exp Euler is Imp. Euler.

Ex: $y_{n+1} = y_n + h f\left(\frac{y_n + y_{n+1}}{2}\right)$ is symmetric.

Ex: if $\tilde{\Psi}_h = \Psi_{h/2}^* \circ \Psi_{h/2}$, then $\tilde{\Psi}_h$ is symmetric

↳ try with EE, IE.

<u>Prop:</u> if Ψ_h is of order p, Ψ_h^* is of order p.

Moreover, if $\Psi_h(y) = \varphi_h(y) + C(y)\, h^{p+1} + O(h^{p+2})$

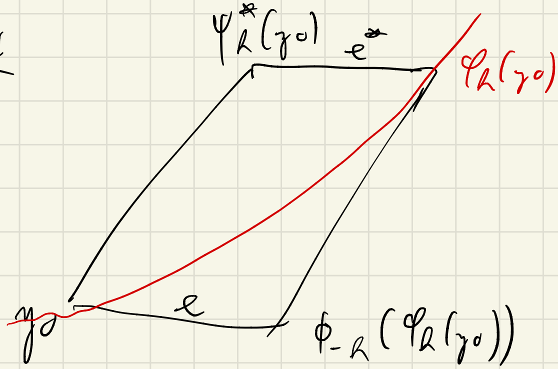
then $\Psi_h^*(y) = \varphi_h(y) + (-1)^p C(y)\, h^{p+1} + O(h^{p+2})$

In particular, if Ψ_h is symmetric, then

$$C(y) = (-1)^p\, C(y)$$

so that if p odd, then $C(y) = 0$ and the method is of order $p+1$.

<u>proof:</u>



let $\begin{cases} e^* = \Psi_h^*(y_0) - \varphi_h(y_0) \\ e = y_0 - \Psi_{-h}(\varphi_h(y_0)) \end{cases}$

$$\begin{aligned} e &= \varphi_{-h}(\varphi_h(y_0)) - \Psi_{-h}(\varphi_h(y_0)) \\ &= -C(\varphi_h(y_0))(-h)^{p+1} + O(h^{p+2}) \\ &= (-1)^p C(y_0)\, h^{p+1} + O(h^{p+2}) \quad \text{as } \varphi_h(y_0) = y_0 + O(h) \end{aligned}$$

On the other hand, $y_0 = \Psi_{-h}(\Psi_h^*(y_0))$, so $e = \Psi_{-h}(\Psi_h^*(y_0)) - \Psi_{-h}(\varphi_h(y_0))$

$= (id + O(h))\, e^*$ as $\Psi_h = id + O(h)$

so $e^* = (id + O(h))\, e = (-1)^p C(y_0)\, h^{p+1} + O(h^{p+2})$ □

Application: • there is no real solution to

$$\gamma_1 + \dots + \gamma_s = 1$$
$$\gamma_1^{r+1} + \dots + \gamma_s^{r+1} = 0 \quad \text{for } r \text{ odd.}$$

• let χ_h symmetric of order (r even), let $\gamma_1 = \gamma_3 = \dfrac{1}{2 - 2^{\frac{1}{r+1}}}$, $\gamma_2 = 1 - 2\gamma_1$

then $\Psi_h = \chi_{\gamma_3 h} \circ \dots \circ \chi_{\gamma_1 h}$ is of order $r+2$.

This procedure can be repeated: we start with a symmetric method of order 2, apply (4.4) with $p = 2$ to obtain order 3; due to the symmetry of the γ's this new method is in fact of order 4 (see Theorem 3.2). With this new method we repeat (4.4) with $p = 4$ and obtain a symmetric 9-stage composition method of order 6, then with $p = 6$ a 27-stage symmetric composition method of order 8, and so on. One obtains in this way *any* order, however, at the price of a terrible zig-zag of the step points (see Fig. 4.2).

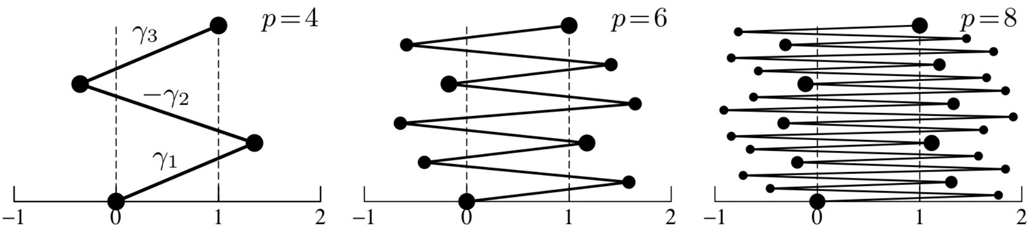


Fig. 4.2. The Triple Jump of order 4 and its iterates of orders 6 and 8

Example 4.3 (Suzuki's Fractals). If one desires methods with smaller values of γ_i, one has to increase s even more. For example, for $s = 5$ the best solution of (4.2) has the sign structure $++-++$ with $\gamma_1 = \gamma_2$ (see Exercise 7). This leads to (Suzuki 1990)

$$\gamma_1 = \gamma_2 = \gamma_4 = \gamma_5 = \frac{1}{4 - 4^{1/(p+1)}}, \qquad \gamma_3 = -\frac{4^{1/(p+1)}}{4 - 4^{1/(p+1)}} \,. \tag{4.5}$$

The repetition of this algorithm for $p = 2, 4, 6, \ldots$ leads to a fractal structure of the step points (see Fig. 4.3).

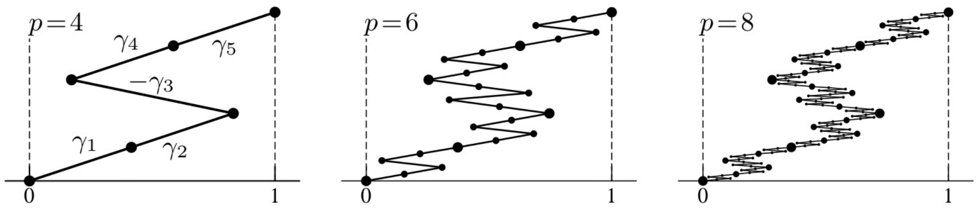


Fig. 4.3. Suzuki's "fractal" composition methods

Pb: lots of evaluations to reach high order, need for exact flows...

Can we preserve geometry with simpler / cheaper methods?

Chapter 3 : the Runge-Kutta approach

1) Definition, examples

<u>def</u> : a Runge-Kutta method for $y' = f(y)$ is of the form

$$\begin{cases} Y_i^n = y_n + h \sum_{j=1}^{s} a_{ij} f(Y_j^n) \\ y_{n+1} = y_n + h \sum_{i=1}^{s} b_i f(Y_i^n) \end{cases}$$

for given coefficients b_i, a_{ij} stored in a Butcher tableau

$$\begin{array}{c|c} c & A \\ \hline & b_1 \dots b_s \end{array} \qquad A = (a_{ij})_{i,j} \qquad c_i = \sum_{j=1}^{s} a_{ij}$$

If A is lower triangular strictly, the method is explicit (implicit else).

If A is lower triangular, the method is diagonally implicit.

Ex:

$$\begin{array}{c|c} 0 & 0 \\ \hline & 1 \end{array}$$ explicit Euler

$$\begin{array}{c|c} 1 & 1 \\ \hline & 1 \end{array}$$ Implicit Euler: $y_{n+1} = y_n + h f(y_{n+1})$

$$\begin{array}{c|c} 1/2 & 1/2 \\ \hline & 1 \end{array}$$ Midpoint

$$\begin{array}{c|cc} 0 & 0 & 0 \\ 1/2 & 1/2 & 0 \\ \hline & 0 & 1 \end{array}$$ explicit midpoint

$$\begin{array}{c|cc} 0 & 0 & 0 \\ 1 & 1/2 & 1/2 \\ \hline & 1/2 & 1/2 \end{array}$$ trapezoidal rule

$$\begin{array}{c|cccc} 0 & 0 & 0 & 0 & 0 \\ 1/2 & 1/2 & 0 & 0 & 0 \\ 1/2 & 0 & 1/2 & 0 & 0 \\ 1 & 0 & 0 & 1 & 0 \\ \hline & 1/6 & 1/3 & 1/3 & 1/6 \end{array}$$ RK4

<u>Rk</u>: for implicit methods, the system has a unique solution for h small enough as f is Lipschitz (Fixed point theorem).

<u>def</u>: partitioned RK method:

for $\begin{pmatrix} y \\ z \end{pmatrix}' = \begin{pmatrix} f(y,z) \\ g(y,z) \end{pmatrix}$, we have the method

$$Y_i^n = y_n + h \sum a_{ij} f(Y_j^n, Z_j^n)$$

$$Z_i^n = y_n + h \sum \hat{a}_{ij} g(Y_j^n, Z_j^n)$$

$$y_{n+1} = y_n + h \sum b_i f(Y_i^n, Z_i^n)$$

$$z_{n+1} = z_n + h \sum \hat{b}_i g(Y_i^n, Z_i^n)$$

Tableaux $\begin{array}{c|c} c & A \\ \hline & b \end{array}$ $\quad \begin{array}{c|c} \hat{c} & \hat{A} \\ \hline & \hat{b} \end{array}$

Ex: $\begin{array}{c|c} 0 & 0 \\ \hline & 1 \end{array} \qquad \begin{array}{c|c} 1 & 1 \\ \hline & 1 \end{array}$ Symplectic Euler

$$\begin{cases} y_{n+1} = y_n + h\, f(y_n, z_{n+1}) \\ z_{n+1} = z_n + h\, g(y_n, z_{n+1}) \end{cases}$$

2) Taylor expansion of the exact flow (2nd time)

In practice, we did not present the full expansion before. We need it now

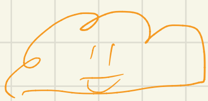
We find $\Phi_t(y) = y + tf + \frac{t^2}{2} f \triangleright f + \frac{t^3}{6} f \triangleright (f \triangleright f) + \dots$

$$= y + tf + \frac{t^2}{2} f'f + \frac{t^3}{6}\left(f'f'f + f''(f,f)\right)$$

$$+ \frac{t^4}{24}\left(f'f'f'f + f'f''(f,f) + 3f''(f,f'f) + f'''(f,f,f)\right) + \dots$$

WTH?

It looks a bit more involved. This is why we introduce Butcher series!

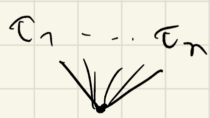


def: The set of trees $\mathcal{T}$ is defined by induction.

$\to \bullet \in \mathcal{T}$

$\to$ if $\tau_1, \dots, \tau_n \in \mathcal{T}$, $[\tau_1, \dots, \tau_n] \in \mathcal{T}$

$\|$



<u>def</u>: $F : \mathcal{C} \longrightarrow J^\infty$ is the elementary differential

→ infinite jet bundle

" = " polynomial in $f^i, f^i_j, f^i_{jk}, \dots$

→ $F_f(\bullet) = f$

→ $F_f([\tau_1, \dots, \tau_n]) = f^{(n)}(F_f(\tau_1), \dots, F_f(\tau_n))$

F is extended by linearity on $\mathrm{Span}(\mathcal{C})$.

<u>Prop</u>: let $\curvearrowright : \mathcal{C} \times \mathcal{C} \to \mathcal{C}$ be the grafting of trees, then $F_f(\tau_2) \triangleright F_f(\tau_1) = F_f(\tau_2 \curvearrowright \tau_1)$

<u>Ex</u>: $f \triangleright (f'f) = (f'f)'f = f''(f,f) + f'f'f$

$\qquad\qquad \shortparallel$

$F_f(\bullet \curvearrowright$  $) = F_f($  $)$

<u>def</u>: * the order of $\tau \in \mathcal{C}$ is $|\tau| =$ nb of nodes.

* the factorial of $\tau \in \mathcal{C}$ is

$$\begin{cases} \gamma(\bullet) = 1 \\ \gamma([\tau_1, \dots, \tau_n]) = |\tau|\, \gamma(\tau_1) \cdots \gamma(\tau_n) \end{cases}$$

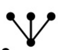
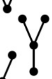
* the symmetry of $\tau \in \mathcal{T}$ is

$$\sigma(\bullet) = 1$$

$$\sigma([\underbrace{\tau_1, \dots, \tau_1}_{r_1}, \dots, \underbrace{\tau_m, \dots, \tau_m}_{r_m}]) = \prod r_i! \, \sigma(\tau_i)^{r_i}$$

Rk: $\sigma(\tau)$ is also the number of graph automorphisms of τ.

Table 1.1. Trees, elementary differentials, and coefficients

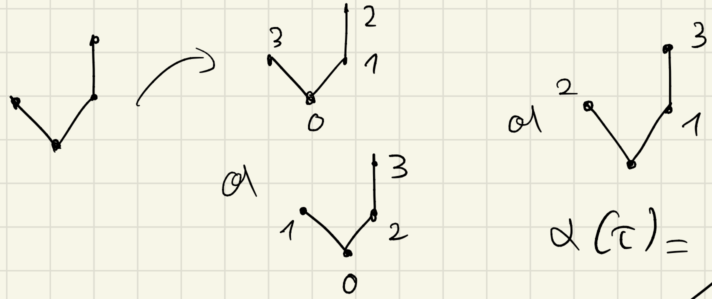
$\|\tau\|$	τ	graph	$\alpha(\tau)$	$F(\tau)$	$\gamma(\tau)$	$\phi(\tau)$	$\sigma(\tau)$
1	$\bullet$	$\bullet$	1	f	1	$\sum_i b_i$	1
2	$[\bullet]$		1	$f'f$	2	$\sum_{ij} b_i a_{ij}$	1
3	$[\bullet, \bullet]$		1	$f''(f,f)$	3	$\sum_{ijk} b_i a_{ij} a_{ik}$	2
3	$[[\bullet]]$		1	$f'f'f$	6	$\sum_{ijk} b_i a_{ij} a_{jk}$	1
4	$[\bullet, \bullet, \bullet]$		1	$f'''(f,f,f)$	4	$\sum_{ijkl} b_i a_{ij} a_{ik} a_{il}$	6
4	$[[\bullet], \bullet]$		3	$f''(f'f,f)$	8	$\sum_{ijkl} b_i a_{ij} a_{ik} a_{jl}$	1
4	$[[\bullet, \bullet]]$		1	$f'f''(f,f)$	12	$\sum_{ijkl} b_i a_{ij} a_{jk} a_{jl}$	2
4	$[[[\bullet]]]$		1	$f'f'f'f$	24	$\sum_{ijkl} b_i a_{ij} a_{jk} a_{kl}$	1

Rk:

$$\frac{\alpha(\tau)}{|\tau|!} = \frac{1}{\sigma(\tau)\gamma(\tau)}$$

where α is the number of ways to obtain τ

from grafting :



$\alpha(\tau) = 3$

Def: a B-series is a formal power series: given $a : \mathcal{C} \longrightarrow \mathbb{R}$ a one-form / the coefficient map, (Butcher)

$$B_h^f(a) = \sum_{\tau \in \mathcal{C}} \frac{h^{|\tau|}}{\sigma(\tau)} a(\tau) F_f(\tau).$$

Thm: the exact flow of $y' = f(y)$ is given by

$$\boxed{\varphi_t = id + B_t^f\left(\frac{1}{\gamma}\right)}$$

Proof: $f(y_0 + B_t^f(\gamma^{-1})(y_0))$

$$= \sum_{k=0}^{+\infty} f^{(k)}(y_0)\left(B_t^f(\gamma^{-1})^{(y_0)}, \dots, B_t^f(\gamma^{-1})^{(y_0)}\right)$$

$$= \sum_{k=0}^{+\infty} \sum_{\tau_1,\dots,\tau_k \in \mathcal{C}} \frac{t^{|\tau_1|} \cdots t^{|\tau_k|}}{k!\,\sigma(\tau_1)\cdots\sigma(\tau_k)\gamma(\tau_1)\cdots\gamma(\tau_k)} \underbrace{f^{(k)}(F_f(\tau_1), \dots, F_f(\tau_k))}_{(y_0)}$$

$$= \sum_{k=0}^{+\infty} \sum_{\tau_1, \dots, \tau_k \in \mathcal{C}} \frac{t^{|\tau|-1} \, |\tau|}{k! \, \sigma(\tau_1) \dots \sigma(\tau_k) \, \gamma(\tau)} F_f(\tau)(y_0)$$

$$= \sum_{k=0}^{+\infty} \sum_{\tau = [\tau_1, \dots, \tau_k] \in \mathcal{C}} \frac{|\tau| \, t^{|\tau|-1}}{\sigma(\tau) \, \gamma(\tau)} F_f(\tau)(y_0)$$

as going from the sum $\sum_{\tau_1, \dots, \tau_k \in \mathcal{C}}$ to $\sum_{\tau = [\tau_1, \dots, \tau_k] \in \mathcal{C}}$

yields the coefficient $\frac{k!}{r_1! \dots r_n!} = \binom{k}{r_1 \dots r_n}$ as we go from

<u>ordered</u> subtrees $\tau_1 \dots \tau_k$ to non-ordered subtrees.

Then $\frac{d}{dt}\left(y_0 + B_t^f(\gamma^{-1})(y_0)\right)$

$$= \frac{d}{dt}\left(\sum_{\tau \in \mathcal{C}} \frac{t^{|\tau|}}{\sigma(\tau) \gamma(\tau)} F_f(\tau)(y_0)\right)$$

$$= \sum_{\tau \in \mathcal{C}} \frac{|\tau| \, t^{|\tau|-1}}{\sigma(\tau) \gamma(\tau)} F_f(\tau)(y_0)$$

$\square$

3) Order theory of RK methods

Lemma: $hf\left(y_0 + B_h^f(a)(y_0)\right) = B_h^f(b)(y_0)$

where $\begin{cases} b([\tau_1, \dots, \tau_m]) = a(\tau_1)\cdots a(\tau_m) \\ b(\cdot) = 1 \end{cases}$

proof: similar as last proof with $\frac{1}{\gamma}$ replaced by a.

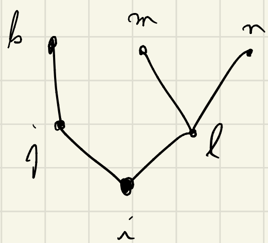
Thm: a RK method $y_{n+1} = \Psi_h(y_n)$ satisfies

$$\Psi_h(y_0) = y_0 + B_h^f(a) \text{ where}$$

$$a(\tau) = b^T \beta(\tau) \text{ and } \begin{cases} \alpha(\bullet) = \mathbb{1} = \begin{pmatrix} 1 \\ \vdots \\ 1 \end{pmatrix} \\ \alpha([\tau_1, \dots, \tau_m]) = A\left(\alpha(\tau_1) \diamond \cdots \diamond \alpha(\tau_m)\right) \\ u \diamond v = \begin{pmatrix} u_1 v_1 \\ \vdots \\ u_d v_d \end{pmatrix} \end{cases}$$

$$\text{and } \begin{cases} \beta(\cdot) = \mathbb{1} \\ \beta([\tau_1, \dots, \tau_m]) = \alpha(\tau_1) \diamond \cdots \diamond \alpha(\tau_m). \end{cases}$$

Ex:

$\tau =$ 

$$a(\tau) = \sum b_i a_{ij} a_{jk} a_{il} a_{lm} a_{ln}$$
$$= \sum b_i a_{ij} c_j a_{il} c_l^2$$

proof: if $Y_i = y_0 + B_h^f(\alpha_i)(y_0)$

then $Y_i = y_0 + \sum a_{ij}\, h f(y_0 + B_h^f(\alpha_j)(y_0))$

$$\overset{\text{(lemma)}}{=} y_0 + \sum a_{ij}\, B_h^f(\beta_j)(y_0)$$

where $\begin{cases} \beta_j([\tau_1, \dots, \tau_m]) = \alpha(\tau_1) \cdots \alpha(\tau_m) \\ \beta_j(\cdot) = 1 \end{cases}$

$$= y_0 + B_h^f\left(\sum a_{ij} \beta_j\right)(y_0)$$

then by identification $\alpha_i(\tau) = \sum a_{ij} \beta_j(\tau) = (A\beta)_i$

that is $\alpha([\tau_1, \dots, \tau_m]) = A(\alpha(\tau_1) \circ \cdots \circ \alpha(\tau_m))$

Then $y_1 = y_0 + h \sum b_i f(Y_i)$

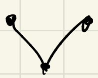
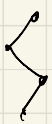
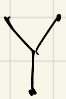
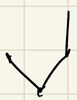
$$= y_0 + h \sum b_i f(y_0 + B_h^f(\alpha_i)(y_0))$$

$$= y_0 + \sum b_i B_h^f(\beta_i)(y_0)$$

$$= y_0 + B_h^f(b^T \beta)(y_0) \qquad \square$$

Thm: a RK method has order p iff

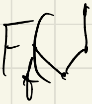
$$\forall \tau \in \mathcal{T},\ |\tau| \leq p,\ \frac{1}{\gamma(\tau)} = a(\tau).$$

$\mathcal{T}$	condition	order
	$\sum b_i = 1$	1
	$\sum b_i c_i = 1/2$	2
	$\sum b_i a_{ij} c_j = 1/6$	3
	$\sum b_i c_i^2 = 1/3$	
	$\sum b_i a_{ij} a_{jk} c_k = 1/24$	4
	$\sum b_i a_{ij} c_j^2 = 1/12$	
	$\sum b_i c_i a_{ij} c_j = 1/8$	
	$\sum b_i c_i^3 = 1/4$	

A000081
OEIS

order	1	2	3	4	5	6	7	8	9	10
Nb conditions	1	1	2	4	9	20	48	115	286	719

Rk: • degeneracies may appear

for $d = 1$, $F_f($$) = F_f($$)$

• $\forall \tau_0 \in \mathcal{T}, \exists f \in \mathcal{X}(\mathbb{R}^d)$ st

$$\begin{cases} F_f(\tau_0)(0) \neq 0 \\ F_f(\tau)(0) = 0, \ \tau \neq 0 \end{cases}$$

• A RK method is of order p <u>for all ODE pb</u> $\boxed{\text{iff}}$ $\forall |\tau| \leq p$, $1/\gamma(\tau) = a(\tau)$

<u>Extension to S-series</u>: we consider forests $\mathcal{F}$  $\cup$ with empty forest $\mathbb{1}$

as concatenation of trees.

a S series is a differential operator

$$S_h^f(a)[\phi] = \sum_{\pi \in \mathcal{F}} \frac{h^{|\pi|} a(\pi)}{\sigma(\pi)} F^f(\pi)[\phi]$$

where $a(\tau_1 \dots \tau_n) = a(\tau_1) \dots a(\tau_n)$ character

$$F^f(\pi) = \phi^{(n)}(F^f(\tau_1), \dots F^f(\tau_n))$$

4) Algebraic structure of composition

a) Deshuffle Hopf algebra: primitive elements and numerical flows

Let $\cdot$ be the commutative, associative concatenation of trees:

$\vee \; |$ is a forest with 2 trees.

Let $\mathcal{F}$ be the algebra of forests $(+, \times, \cdot)$ with the unit 1 and counit δ_1.

Define the deshuffle coproduct $\Delta_{\sqcup\!\sqcup} : \mathcal{F} \to \mathcal{F} \otimes \mathcal{F}$

$$\begin{cases} \Delta_{\sqcup\!\sqcup} 1 = 1 \otimes 1 \\ \Delta_{\sqcup\!\sqcup} \tau = \tau \otimes 1 + 1 \otimes \tau, \quad \tau \in E \\ \Delta_{\sqcup\!\sqcup} (w_1 \cdot w_2) = (\Delta_{\sqcup\!\sqcup} w_1) \cdot (\Delta_{\sqcup\!\sqcup} w_2) \end{cases}$$

Recall that $(a \otimes b) \cdot (a' \otimes b') = (a \cdot a') \otimes (b \cdot b')$.

This makes $\mathcal{F}$ a bialgebra.

morally an inverse

$\mathcal{F}$ becomes a graded Hopf algebra if there is an antipode $S : \mathcal{F} \to \mathcal{F}$

$$\text{s.t.} \quad \mu \circ (S \otimes Id) \circ \Delta = \mu \circ (Id \otimes S) \circ \Delta = 1\, \delta_1$$

Here $S_{\sqcup\!\sqcup}(\tau) = -\tau$

$S_{\sqcup\!\sqcup}(w_1 \cdot w_2) = S_{\sqcup\!\sqcup}(w_2) \cdot S_{\sqcup\!\sqcup}(w_1)$ (S is an antimorphism w.r.t. $\cdot$ but as it's commutative, it is just a morphism)

→ Note here we are not using the tree structure at all.

Ex: $\Delta_{ш}(\bullet\,|) = (\Delta_{ш}\,\bullet)\cdot(\Delta_{ш}\,|)$

$$= (\bullet\otimes 1 + 1\otimes\bullet)\cdot(|\otimes 1 + 1\otimes |)$$

$$= \bullet\,|\otimes 1 + \bullet\otimes | + |\otimes\bullet + 1\otimes\bullet\,|$$

and $(S_{ш}\otimes Id)\circ\Delta_{ш}(\bullet\,|) = \bullet\,|\otimes 1 - \bullet\otimes | - |\otimes\bullet + 1\otimes\bullet\,|$

$\mu\circ$ ——————— $= 0$ OK

def: $\pi\in\mathcal{T}$ is primitive if $\Delta\pi = \pi\otimes 1 + 1\otimes\pi$, gathered in $\mathfrak{g}$.
$\pi\in\mathcal{T}$ is group-like if $\Delta\pi = \pi\otimes\pi$, gathered in G.

Prop: ($\mathfrak{g} = \mathcal{C}$ set of trees here)

$$\exp^{\cdot}(\tau) = 1+\tau+\frac{1}{2}\tau\cdot\tau+\cdots \quad \text{formal serie}$$

$$\boxed{\exp: \mathfrak{g}\longrightarrow G}\ \boxed{\log: G\to\mathfrak{g}}$$

$\mathfrak{g}$ represents the vector fields and G represents the flows

$$\log(\pi) = \sum_{n\geq 1}\frac{(-1)^{n-1}}{n}(\pi-1)^{\cdot n}$$

proof:

Note that $\Delta\exp(\tau) = \exp(\Delta\tau)$ as $\Delta(\alpha\cdot\beta) = (\Delta\alpha)\cdot(\Delta\beta)$

$$= \exp(\tau\otimes 1 + 1\otimes\tau)$$

$$= \exp(\tau \otimes 1) \cdot \exp(1 \otimes \tau) \quad \text{as they commute}$$

$$= (\exp(\tau) \otimes 1) \cdot (1 \otimes \exp(\tau))$$

$$= \exp(\tau) \otimes \exp(\tau)$$

Then one deduces that $\log = \exp^{-1}$. $\square$

Idea: "$\log^{\star}(\pi)$ is the v.f generating the flow π for the law $\star$." Here $\exp^{\star}$ is the flow generated by the Euler method.

Rk: The dual of a Hopf algebra is a Hopf algebra.

$$(\mathcal{H}, \cdot, \Delta_{⧢}) \overset{*}{\longleftrightarrow} (\mathcal{H}^{*}, ⧢, \Delta_{\cdot})$$

$$\text{st} \begin{cases} \langle \Delta_{\cdot}\alpha, w_1 \otimes w_2 \rangle = \langle \alpha, w_1 \cdot w_2 \rangle \\ \langle \alpha ⧢ \beta, w \rangle = \langle \alpha \otimes \beta, \Delta_{⧢} w \rangle \end{cases}$$

(b) Grossman-Larson Hopf algebra and exact flow

Consider now the $\boxed{\text{composition}}$ of flows.

We observe $F(\tau_1)[F(\tau_2)[\phi]] = F[\tau_1 \tau_2 + \tau_1 \curvearrowright \tau_2][\phi]$

Define the Grossman-Larson product by

$$\pi \diamond \tilde{\pi} = \sum_{\substack{\Delta_{\sqcup\!\sqcup}\pi = \\ \pi_{(1)} \otimes \pi_{(2)}}} \pi_{(1)} \cdot (\pi_{(2)} \curvearrowright \tilde{\pi})$$

(See Guin Oudom)

This yields a new Hopf algebra called the Grossman-Larson Hopf algebra $(\mathcal{F}, \diamond, \Delta_{\sqcup\!\sqcup})$ with same primitive elements $\mathfrak{g}$.

$$\exp^{\diamond}(\tau) = 1 + \tau + \frac{1}{2}\tau \diamond \tau + \cdots$$

<u>Idea:</u> $\exp^{\diamond} : \mathfrak{g} \longrightarrow G_{GL}$

$y' = f(y)$

which amounts to $hf \longrightarrow \phi(y(h)) = \phi(y_0) + h\phi'(y_0) f(y_0) + \cdots$

$\curvearrowright$ V.f.

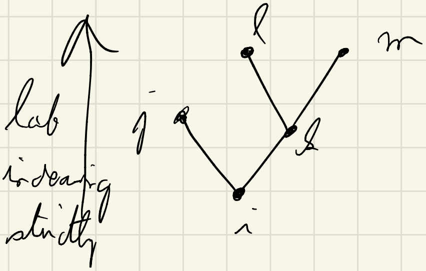
while $\exp^{\cdot} : \mathfrak{g} \longrightarrow G_{Euler}$

gives $hf \longrightarrow \phi(y_1) = \phi(y_0 + hf(y_0)) = \phi(y_0) + h \cdots$

<u>Application</u>: We deduce from $\phi(y(h)) = F^{hf}(\exp^{\diamond}(\bullet))[\phi]$

that $\dfrac{1}{(\gamma\ \sigma)(\pi)} = \dfrac{\alpha(\pi)}{|\pi|!}$

where $\alpha(\tau)$ is the number of labellings of τ:



$\mathrm{lab}: V \longrightarrow \{1, \dots, |V|\}$ bijective

s.t. lab increases strictly from bottom to top.

and $\alpha(\tau_1 \cdots \tau_n) = \alpha(\tau_1) \cdots \alpha(\tau_n)$.

- Note that all coefficient maps are characters

$$a(\pi_1 \cdot \pi_2) = a(\pi_1)\, a(\pi_2)$$

so that if $a = e$ on $\mathfrak{g}$, then

symmetric algebra

as $1 \oplus \mathfrak{g} \oplus \mathfrak{g}\cdot\mathfrak{g} \oplus \mathfrak{g}\cdot\mathfrak{g}\cdot\mathfrak{g} + \dots =: S(\mathfrak{g})$

$$\| \\ \mathcal{H}$$

then it implies $a = e$ on $\mathcal{H}$.

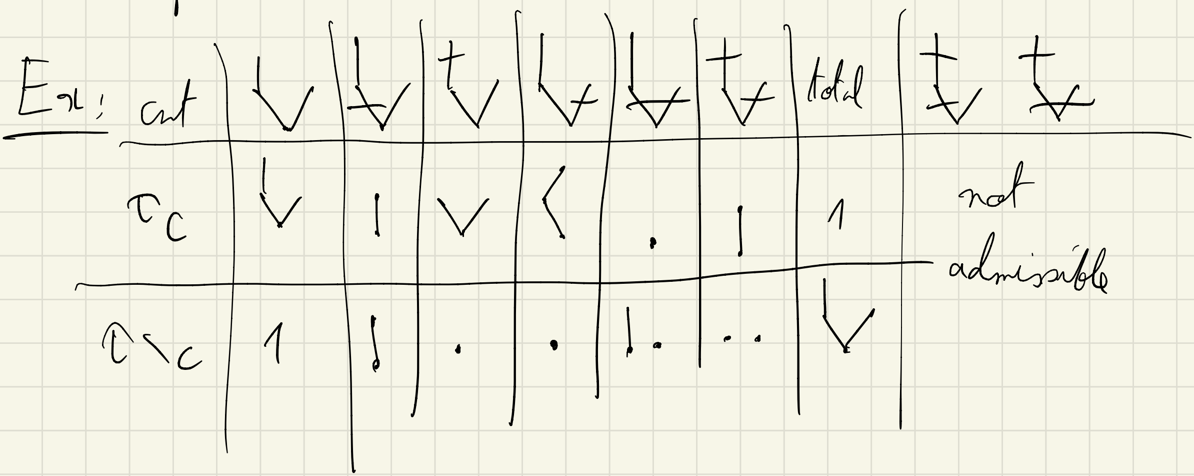
(c) Composition and Butcher-Connes-Kreimer Hopf algebra

Q: How do we compute $S_h^f(a)[S_h^f(b)[\phi]]$?

An admissible cut c is a choice of edges of a tree τ such that by removing these edges, any directed path (from bottom to top) meets at most one cutting edge.

The cut c splits the tree τ into a rooted tree τ_c (if not the total cut) and a forest $\tau \setminus c$.

Ex:



The BCK coproduct is

$$\Delta_{BCK} \tau = \sum_{c \in Adm} (\tau \setminus c) \otimes \tau_c$$

$$\Delta_{BCK}(\pi_1 \cdot \pi_2) = (\Delta_{BCK} \pi_1) \cdot (\Delta_{BCK} \pi_2)$$

Thm $(\mathcal{T}, \cdot, \Delta_{BCK})$ is a Hopf algebra with antipode S_{BCK}, detailed later.

Thm: $S_h^f(a)\left[S_h^f(b)[\phi]\right] = S_h^f(a * b)[\phi]$

where $a, b \in \mathcal{T}^*$
and the composition law is
$a * b = \mu \circ (a \otimes b) \circ \Delta_{BCK}$, $\mu(x \otimes y) = xy$

Ex: $(a * b)(\dot{\mathrm{V}}) = b(\dot{\mathrm{V}}) + a(|)\,b(|) + a(\cdot)\,b(\mathrm{V})$
$\quad + a(\cdot)\,b(>) + a(\cdot)\,a(|)\,b(\cdot) + a(\cdot)^2\,b(|) + a(\dot{\mathrm{V}})$

Rk: a similar set of algebraic tools exist for Lie-group methods, based on a left grafting operation and ordered planar forests.

Rk: The dual of the BCK Hopf algebra is isomorphic to the GL Hopf algebra.

Chapter 4: Geometric Numerical Integration

1) Preservation of quadratic invariants

<u>Prop:</u> a RK method preserves all linear invariants.

<u>Prop:</u> a RK method cannot preserve all polynomial invariants of fixed degree $p \geq 3$.
(see exercises).

<u>Thm:</u> a RK method preserves all quadratic invariants (of any ODE)
if $b_i a_{ij} + b_j a_{ji} = b_i b_j$, $\forall i, j = 1, \dots, s$. (⊛)

For PRK methods, we have the condition

$$\begin{cases} \hat{b}_i a_{ij} + b_j \hat{a}_{ji} = \hat{b}_i b_j & \forall i, j \\ \hat{b}_i = b_i \end{cases}$$

for preserving all invariants of the form $y^T D z$.

<u>Rk:</u> this is quite restrictive! An explicit RK method cannot satisfy (⊛) and have order 1. (exercise)
(Hint: consider $f = J \nabla H$, $H = \frac{p^2 + q^2}{2}$, $y_{n+1} = R(hJ)\, y_n$, $|R(hJ)| = 1 \ \forall h$, R polynomial)

proof: $I(y) = y^T C y$, C quadratic

$I'(y)(f(y)) = 0$ so that $y^T C f(y) = 0$

$y_1 = y_0 + h \sum b_i f(Y_i)$

$Y_i = y_0 + h \sum a_{ij} f(Y_j)$

$$y_1^T C y_1 = \left(y_0 + h \sum b_i f(Y_i)\right)^T C \left(y_0 + h \sum b_j f(Y_j)\right)$$

$$= y_0^T C y_0 + h^2 \sum b_i b_j f(Y_i)^T C f(Y_j)$$

$$+ h \sum b_j \underbrace{y_0^T C f(Y_j)} + h \sum b_i f(Y_i)^T C y_0$$

$$= \underbrace{Y_j^T C f(Y_j)}_{=0} - h \sum a_{ji} f(Y_i)^T C f(Y_j)$$

$$= y_0^T C y_0 + h^2 \sum (b_i b_j - b_i a_{ij} - b_j a_{ji}) f(Y_i)^T C f(Y_j)$$

$\square$

Ex: midpoint $\begin{array}{c|c} 1/2 & 1/2 \\ \hline & 1 \end{array}$ preserves quadratic invariants.

$\longrightarrow$ show simulation pendulum.

for $H(q, p) = \frac{p^2 + q^2}{2}$

2) Symplectic methods

Thm: a RK method preserving quadratic invariants is symplectic.

proof: $y_{n+1} = \Phi_h(y_n)$ RK method

We have to show that $Y_n = \dfrac{\partial y_n}{\partial y_0}$ satisfies

$$Y_n^T J Y_n = J, \ \forall n.$$

Recall the variational equation $\varphi_t(y_0)$ flow of $\begin{cases} y' = f(y) \\ y(0) = y_0 \end{cases}$ (1)

$$\begin{cases} y' = f(y), & y(0) = y_0 \\ Y' = f'(y)Y, & Y(0) = Id \end{cases} \quad (2) \qquad Y_t = \frac{\partial \varphi_t}{\partial y}$$

Claim: the following diagram commutes

$$\begin{tikzcd}[column sep=huge, row sep=huge]
y' = f(y),\ y(0) = y_0) \arrow[r, "Y_t = \frac{\partial y}{\partial y_0}\ (1)"'] \arrow[d, "y_{n+1} = \Phi_h^{(d)}(y_n)"] \arrow[dr, phantom, "\circlearrowleft"] & \begin{cases} y' = f(y),\ y(0) = y_0 \\ Y' = f'(y)Y,\ Y(0) = Id \end{cases} \arrow[d, "{(y_{n+1}, Y_{n+1}) = \Phi_h^{(d+d^2)}(y_n, Y_n)}"] \\
\{y_n\} \arrow[r, "Y_n = \frac{\partial y_n}{\partial y_0}"'] & \{y_n, Y_n\}
\end{tikzcd}$$

Indeed $(y_{n+1}, Y_{n+1}) = \Phi_h(y_n, Y_n)$ gives

$$\begin{cases} y_{n+1} = y_n + h \sum b_i f(z_i) \\ Y_{n+1} = Y_n + h \sum b_i f'(z_i) Z_i \\ z_i = y_n + h \sum a_{ij} f(z_j) \\ Z_i = Y_n + h \sum a_{ij} f'(z_j) Z_j \end{cases}$$

On the other hand,

$$\frac{\partial}{\partial y_0} \begin{cases} y_{n+1} = y_n + h \sum b_i f(z_i) \\ z_i = y_n + h \sum a_{ij} f(z_j) \end{cases}$$ yields with $Y_n = \frac{\partial y_n}{\partial y_0}$

$$\begin{cases} Y_{n+1} = Y_n + h \sum b_i f'(z_i) \frac{\partial z_i}{\partial y_0} \\ \frac{\partial z_i}{\partial y_0} = Y_n + h \sum a_{ij} f'(z_j) \frac{\partial z_j}{\partial y_0} \end{cases}$$

writing $Z_i = \frac{\partial z_i}{\partial y_0}$ yields the same thing. ✓

However, $I \begin{pmatrix} y \\ Y \end{pmatrix} = Y^T J Y$ is a quadratic invariant of the augmented method. The RK method preserves it. As it coincides with the original method, I is preserved and the method is symplectic. $\square$

Ex: Midpoint, Trapezoidal rule, Störmer-Verlet and symplectic Euler are symplectic.

→ Show simulations solar system

3) Backward error analysis

idea:

exact flow
$y'(t) = f(y(t))$ $\quad \varphi_t^f$

integrator
$y_{n+1} = \Phi_h^f(y_n)$

modified ODE
$\tilde{y}'(t) = \hat{f}(\tilde{y}(t))$ $\quad \varphi_t^{\hat{f}}$

such that $\boxed{\Phi_h^f = \varphi_h^{\hat{f}}}$

It is easier to study properties on a continuous problem.

Ex: for $y' = Ay$, the Euler method is $y_{n+1} = (I + hA)\,y_n$ and the exact flow is $y(h) = e^{hA}\,y_0$

Then we want $y_1 = e^{h\widetilde{A}_h} y_0$

that is $e^{h\widetilde{A}_h} = I + hA$

$$\boxed{\widetilde{A}_h = \frac{1}{h} \operatorname{Log}(I + hA)}$$

marche pour h petit.

$$= \sum_{k=1}^{+\infty} \frac{h^{k-1}}{k} (-1)^{k-1} A^k$$

<u>General case without B-series:</u>

Assume

$$\begin{cases} \phi_h^f(y_0) = y_0 + h f(y_0) + h^2 d_2 + h^3 d_3 + \cdots & \underline{\text{Consistent}} \\ \varphi_h^f(y_0) = y_0 + B_h^f(\gamma^{-1})(y_0) \\ \quad = y_0 + h f(y_0) + \frac{h^2}{2} f'f + \frac{h^3}{6}\left(f'f'f + f''(f,f)\right) + \cdots \\ h\tilde{f} = hf + h^2 f_2 + h^3 f_3 + \cdots \end{cases}$$

The condition $\phi_h^f = \varphi_h^{\tilde{f}}$ gives

$$\varphi_h^{\tilde{f}} = id + B_h^{\tilde{f}}(\gamma^{-1})$$

$$= y_0 + (hf + h^2 f_2 + h^3 f_3 + \cdots) + \frac{1}{2}(hf + h^2 f_2 + \cdots)'(hf + h^2 f_2 + \cdots)$$

$$+ \frac{h^3}{6}(f'f'f + f''(f,f)) + \cdots$$

$$= y_0 + hf + h^2\left(f_2 + \frac{1}{2} f'f\right)$$

$$+h^3\left(f_3+\tfrac{1}{2}f_2'f+\tfrac{1}{2}f'f_2+\tfrac{1}{6}f'f'f+\tfrac{1}{6}f''(f,f)\right)+\cdots$$

This yields the conditions:

$$f_2+\tfrac{1}{2}f'f=d_2$$

$$f_3+\tfrac{1}{2}f_2'f+\tfrac{1}{2}f'f_2+\tfrac{1}{6}f'f'f+\tfrac{1}{6}f''(f,f)=d_3$$

$$\vdots$$

That is $\boxed{f_2=d_2-\tfrac{1}{2}f'f}$

$$f_3=d_3-\tfrac{1}{2}\left(d_2-\tfrac{1}{2}f'f\right)'f-\tfrac{1}{2}f'\left(d_2-\tfrac{1}{2}f'f\right)$$
$$-\tfrac{1}{6}f'f'f-\tfrac{1}{6}f''(f,f)$$

$$f_3=d_3-\tfrac{1}{2}d_2'f-\tfrac{1}{2}f'd_2+\tfrac{1}{4}f'f'f+\tfrac{1}{4}f''(f,f)$$
$$+\tfrac{1}{4}f'f'f-\tfrac{1}{6}f'f'f-\tfrac{1}{6}f''(f,f)$$

$$\boxed{f_3=d_3-\tfrac{1}{2}d_2'f-\tfrac{1}{2}f'd_2+\tfrac{1}{3}f'f'f+\tfrac{1}{12}f''(f,f)}$$

The integrator ϕ_h^f satisfies $\left|\phi_h^f(y_0)-\tilde{y}^{[3]}(h)\right|\leq Ch^4$

where $\tilde{y}'=\Big(f+h\left(d_2-\tfrac{1}{2}f'f\right)+h^2\big(d_3-\tfrac{1}{2}d_2'f-\tfrac{1}{2}f'd_2+\tfrac{1}{3}f'f'f$
$+\tfrac{1}{12}f''(f,f)\big)\Big)(\tilde{y})$,

(under smoothness assumptions on f)

In particular for the Euler method, $d_2 = d_3 = \cdots = 0$,

we find $h\tilde{f} = hf - \frac{h^2}{2} f'f + \frac{h^3}{3}\left(f'f'f + \frac{1}{14} f''(f,f)\right) + \dots$

If $f(y) = Ay$, we find back $\hat{A}_h$. (by induction)

<u>Thm</u>: Let $f_{j+1}(y) = \lim_{h\to 0} \frac{\varphi_h^{f^{[j]}}(y) - \varphi_h(y)}{h^{j+1}}$, then

$$\left| \phi_h^f(y_0) - \varphi_h^{\tilde{f}^{[N]}}(y_0) \right| \leq C_N h^{N+1},$$

where $h\tilde{f}^{[N]} = hf_1 + \dots h^N f_N$

(under assumptions on f).

<u>Thm</u>: • If ϕ_h is of order p, then $f_j = 0$, $2 \leq j \leq p$.

• If I is an invariant of ϕ_h $(I(\phi_h(y)) = I(y))$, then $I'f = 0$

$I'(y)(f_j(y)) = 0$, $\forall j$

• If $\phi_h^* = id$, then $\tilde{f}_h = \tilde{f}_{-h}$ $(\Leftrightarrow f_{2j} = 0, \forall j)$

• If ϕ_h is symplectic, then $\forall j$, $\exists j$, $f_j = J\nabla H_j$.
and $f = J\nabla H$

• If $\mathrm{div}(f) = 0$ and ϕ_h is volume preserving, then $\mathrm{div}(\tilde{f}_h) = 0$

⋮

IDEA: the ppties of Φ_h are read on $\tilde{f}_h$.

proof: let us prove the symplectic case by induction

Initialisation: $\tilde{f}_h^{[1]} = f$ and $f = J\nabla H$ by assumption. ✓

Assume $\tilde{f}_h^{[N]} = J \nabla H_h^{[N]}$, $H_h = H + hH_2 + \dots + h^{N-1} H_N$

By definition of f_i,

$$\Phi_h(y) = \varphi_h^{\tilde{f}_h^{[N]}}(y) + h^{N+1} f_{N+1}(y) + O(h^{N+2})$$

We can differentiate: ⚠ not obvious. We can do this as we work with smooth maps.

$$\frac{\partial \Phi_h}{\partial y} = \frac{\partial \varphi_h^{\tilde{f}_h^{[N]}}}{\partial y} + h^{N+1} \frac{\partial f_{N+1}}{\partial y} + O(h^{N+2})$$

We know that $J = \frac{\partial \Phi_h}{\partial y}^T J \frac{\partial \Phi_h}{\partial y} = \frac{\partial \varphi_h^X}{\partial y}^T J \frac{\partial \varphi_h^X}{\partial y}$.

$$\text{Thus } J = \left(\frac{\partial \varphi_h^{\tilde{f}_h^{[N]}}}{\partial y} + h^{N+1} \frac{\partial f_{N+1}}{\partial y} + O(h^{N+2}) \right)^T J \left(\text{---} \right)$$

$$= J + h^{N+1}\left(\left(\frac{\partial f_{N+1}}{\partial y}\right)^T J \underbrace{\frac{\partial \varphi_h^{\hat{f}_h^{[N]}}}{\partial y}}_{= I_d + O(h)} + \left(\frac{\partial \varphi_h^{\hat{f}_h^{[N]}}}{\partial y}\right)^T J \frac{\partial f_{N+1}}{\partial y}\right) + O(h^{N+2})$$

Thus, we find $\left(\frac{\partial f_{N+1}}{\partial y}\right)^T J + J \frac{\partial f_{N+1}}{\partial y} = 0$

that is, $J^{-1} \frac{\partial f_{N+1}}{\partial y}$ is symmetric

We proved that it implies that $\exists\, H_{N+1}$ (at least locally)

st $J^{-1} f_{N+1} = \nabla H_{N+1}$ OK

$\downarrow$

true globally if domain is simply connected.

The concept of backward error analysis propagates to global error under analyticity assumption.

Thm: if f and the d_j are analytic in $B_R(y_0)$, for $h \leq h_0$ small enough, $\exists\, N = \left\lfloor \frac{h_0}{h} \right\rfloor$,

$$\left| \Phi_h(y_0) - \varphi_h^{\tilde{f}_h^{[N]}}(y_0) \right| \leq C h e^{-h_0/h}$$

Corollary: Consider $H : D \to \mathbb{R}$ with D open set of $\mathbb{R}^d$ and H analytic in D, if $f = J \nabla H$ and the integration stays in the compact $K \subset D$, then $\exists\, h_0$ st $\forall h \leq h_0$, $N = \left\lfloor \frac{h_0}{h} \right\rfloor$,

$$\begin{cases} H(y_n) = H(y_0) + O(h^p) \quad \text{order} \\ \widehat{H}(y_n) = \widetilde{H}(y_0) + O\left(e^{-h_0/2h}\right), \end{cases}$$

$$\forall\, n h \leq e^{h_0/2h}$$

(see GNI, 2006 and references therein)

→ Show simulations.

Ex: $H(q,p) = \frac{p^2}{2} - \cos(q)$

The midpoint rule is symplectic and satisfies

$$\tilde{f}_h = J \nabla \tilde{H}_h$$

$$\tilde{H}_h = H + \frac{h^2}{48}\left(\cos(2q) - 2p^2\cos(q)\right) + O(h^4)$$

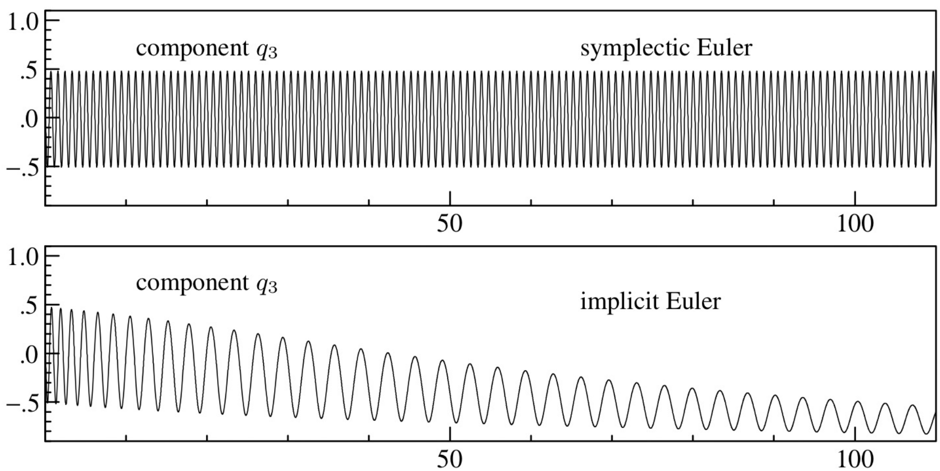


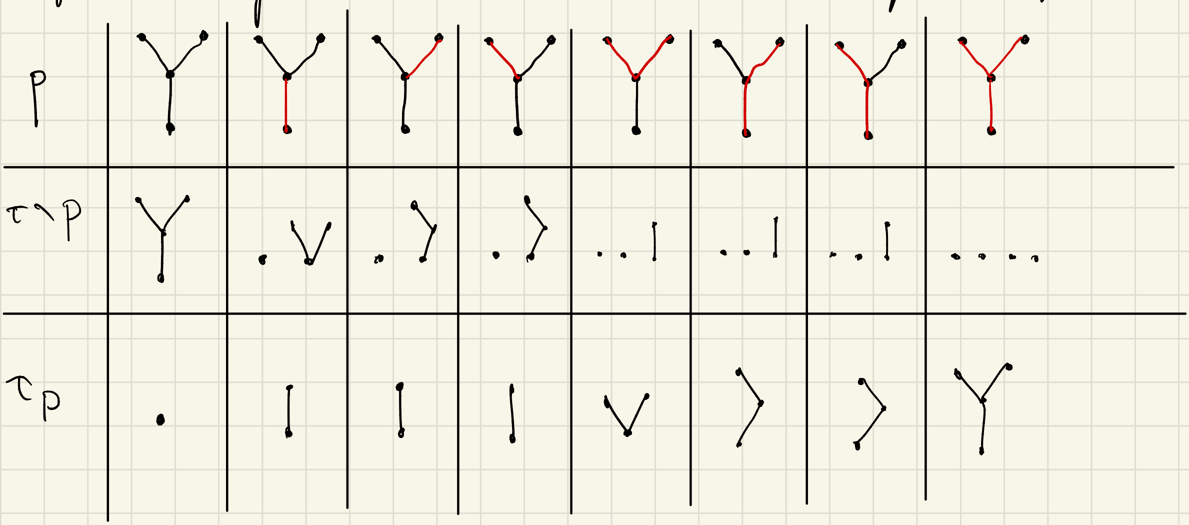
Fig. 1.2. Spherical pendulum problem solved with the symplectic Euler method (1.19)-(1.20) and with the implicit Euler method; initial value $q_0 = (\sin(1.3), 0, \cos(1.3))$, $p_0 = (3\cos(1.3), 6.5, -3\sin(1.3))$, step size $h = 0.01$

4) B-series formulation of BEA

Question: what are $B^{B_h^f(b)}(a)$ and $S^{B_h^f(b)}(a)$?

$\left(\text{where } B^{hf} = B_1^{hf} = B_h^f\right)$

a partition $p \in \mathcal{P}(\tau)$ of a tree τ is a subset of the edges of τ. $\tau \setminus p$ are the remaining forests. τ_p is the tree obtained by contracting the trees in $\tau \setminus p$ to $\bullet$ and putting the edges back.



def: the Calaque – Ebrahimi-Fard – Manchon coproduct is

$$\Delta_{CEM}(\tau) = \sum_{p \in \mathcal{P}(\tau)} (\tau \setminus p) \otimes \tau_p$$

$$\Delta_{CEM}(\pi_1 \cdot \pi_2) = \Delta_{CEM}(\pi_1) \cdot \Delta_{CEM}(\pi_2)$$

Thm: $(\mathcal{F}, \cdot, \Delta_{CEM})$ is a Hopf algebra with unit $\bullet$.

$\triangle$ $(\boxed{b(1)=0})$

Let $b \in \mathcal{C}^*$, extended as a character to $\mathcal{F}$, let $a \in \mathcal{F}^*$, then $S^{B_h^f(b)}(a) = S^f(b \star a)$ (and similar for B-series)

↳ substitution

and $b \star a = \mu \circ (b \otimes a) \circ \Delta_{CEM}$

$$\left.\begin{array}{l} b : \text{modified } \nabla f \hat{hf} \\ a : \text{integrator} \\ e : \text{exact flow } e(\tau) = \dfrac{1}{\gamma(\tau)} \end{array}\right) \text{ characters over } \mathcal{F}$$

BEA: the goal is to find b st $b \star e = a$

We write $\begin{cases} a = \exp(b) \\ b = \log(a) \end{cases}$.

Note that $\exp^{\diamond}\left(\sum \frac{b(\tau)}{\sigma(\tau)} \tau\right) = \sum \frac{a(\pi)}{\sigma(\pi)} \pi$, which is the formulation in the dual.

$$\begin{cases} \exp : & G_{\star} \longrightarrow G_{*} \\ \log : & G_{*} \longrightarrow G_{\star} \end{cases}$$

with
$$\begin{cases} G_{\star} = \{ a \in \mathcal{H}^{*}, \text{ a character}, a(1) = 0 \} \\ \\ G_{*} = \{ a \in \mathcal{H}^{*}, \text{ a character}, a(1) = 1 \} \end{cases}$$

groups

In particular, the inverse of $a \in G_{*}$ is

$$a^{\star,-1}(\tau) = \sum_{p \in \mathcal{P}(\tau)} (-1)^{|\tau_p|} a(\tau \setminus p)$$
$$= (a \circ S_{BCK})(\tau)$$

(extended as a character)

and $b \star e = a$

$$\Rightarrow b \star (e - \delta_1) = a - \delta_1$$

$$\Rightarrow b = (a - \delta_1) \star \underbrace{(e - \delta_1)^{\star,-1}}_{w}$$

where $w \star (e - \delta_1) = \delta_{\cdot} \iff w \star e = \delta_1 + \delta_{\cdot}$

5) Volume preservation and aromatic series

We saw that a method is volume-preserving for $y'=f(y)$, $\boxed{\mathrm{div}(f)=0}$, iff $\boxed{\mathrm{div}(\hat{f})=0}$.

If $f=J\nabla H$, a symplectic method preserves volume.

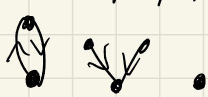
For f general, this is more difficult.

Q°: can we identify the $\tilde{f}=B_f^h(b)$ that satisfy $\mathrm{div}(\hat{f})\overset{?}{=}0$

def: (Aromatic ordered forests)

V set of nodes, E set of edges ($E \subset V\times V$), $(v,w)\in E \Rightarrow$ an edge is going from v to w.

Assume each node is the source of at most one edge. The nodes that are the source of none are called roots and are numbered from 1 to n. A connected component with root is a tree and without is an aroma. We call aromatic forests in $\mathcal{F}_n$ these graphs (up to equivalence of graphs).

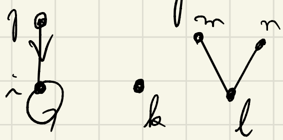
Ex:  $\in \mathcal{F}_0$,  $\in \mathcal{F}_2$

The order is the nb of nodes.

def: elem. differential

edge = derivation
node = evaluation
root j = ∂_{x_j} basis of v.f.

order 2 diff operator

 $\to \sum f^{i}_{ij}\, f^{1}\, f^{k}\, f^{l}_{mn}\, f^{m}\, f^{n}\, \partial_k \otimes \partial_l$

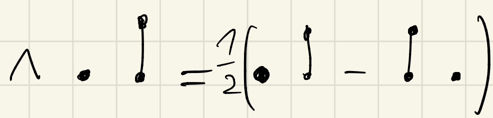
Rk: a tree represents a vf = diff operator of order 1

def: let $\gamma \in \mathcal{T}_n$, then

$$\wedge \gamma = \frac{1}{n!} \sum_{\sigma \in \mathfrak{S}_n} \varepsilon(\sigma)\, \sigma.\gamma$$

where $\sigma.\gamma$ permutes the roots following σ.

$$\boxed{\Omega_n = \wedge \mathcal{T}_n}$$

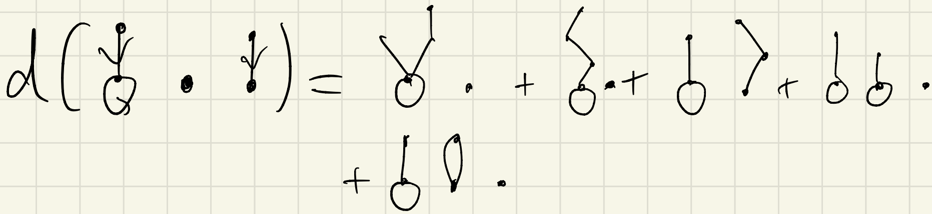
Ex: 

def: let $d : \Omega_n \to \Omega_{n-1}$ be

$$d\gamma = \sum_{v \in V} D^{r_n \to v} \gamma$$ where $D^{r_n \to v}$ grafts

r_n to v.

Ex:



Application: consider an aromatic tree γ

then $\boxed{\operatorname{div}(F_f(\gamma)) = F_f(d\gamma).}$

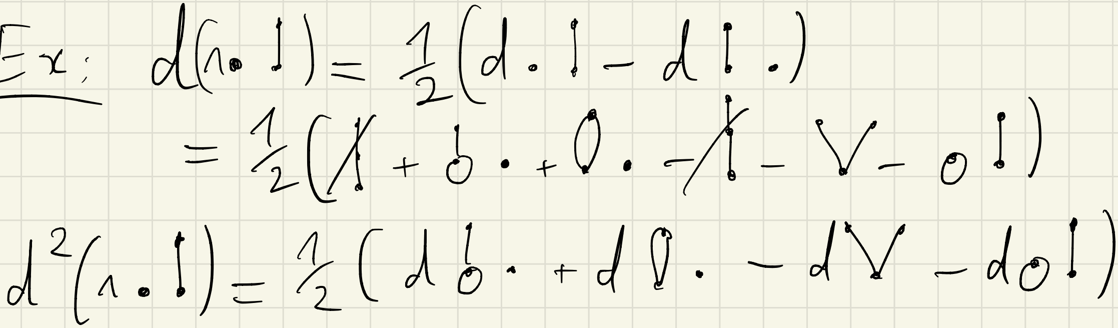
Ex:
$$\bullet \longrightarrow f^i \partial_i = f$$
$$\circ \longrightarrow f^i_i = \sum \frac{\partial f^i}{\partial x_i} = \operatorname{div}(f)$$

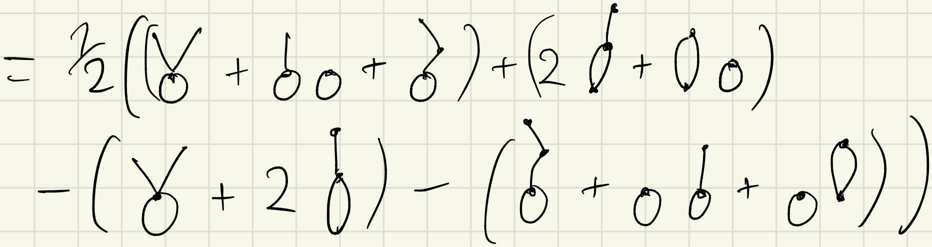
Aromatic De Rham complex:

$$\cdots \xrightarrow{d} \Omega_3 \xrightarrow{d} \Omega_2 \xrightarrow{d} \Omega_1 \xrightarrow{d} \Omega_0$$

Prop: $d^2 = 0$ on Ω_n (exercise)

Ex:





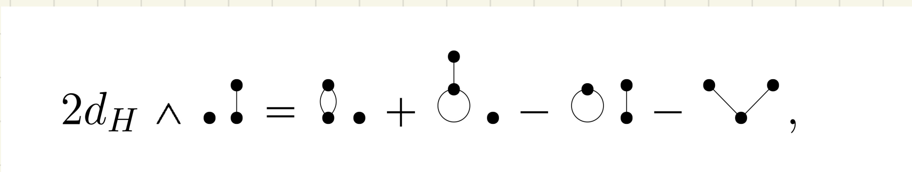
$= 0$ ✓

Thm: the aromatic De Rham complex is exact, that is, $\mathrm{Ker}(d|_{\Omega_n}) = \mathrm{Im}(d|_{\Omega_{n+1}})$

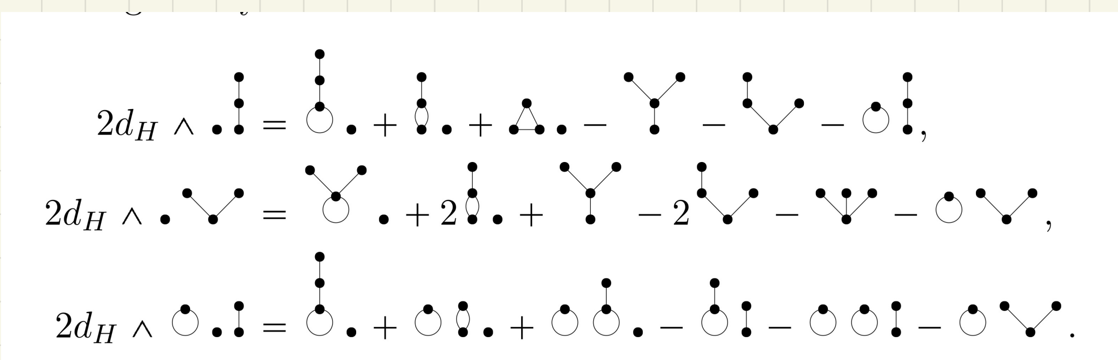
proof: difficult (see Laurent, McLachlan, MK, Verdier, 2023)

Application: basis of $\mathrm{Ker}(d|_{\Omega_1})$ is

order 3



order 4



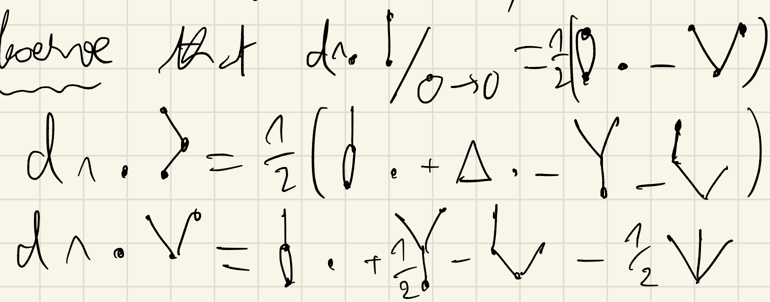
<u>Thm</u> (Iserles, Quispel, Tse, 2007 / Chartier, Murua, 2007)

No RK method preserves volume.

<u>proof:</u> (idea) assume $\operatorname{div}(f)=0$, that is $\circ, \ldots \to 0$

then $\tilde{f}$ is of the form $d\pi$, $\pi \in \Omega_2$

We <u>observe</u> that



There are aromatic trees everywhere (that can't compensate each other)

However, the $\tilde{f}$ of a RK method is made of Butcher trees only. Absurd $\square$

<u>Open problem:</u> does there exist a volume preserving aromatic RK method?

<u>Ex:</u> $y_{n+1} = y_n + h f(y_n)\left(1 + \alpha \operatorname{div}(hf)(y_n)\right)$, $\alpha \in \mathbb{R}$

see Bogfjellmo, 2019; Bronasco, Laurent, 26 for <u>Hopf algebra structure</u>.

6) Lie group methods

→ see Homeworks

References:

- Hairer, Lubich, Wanner, Geometric Numerical Integration, 2006
- Iserles, Munthe-Kaas, Nørsett, Zanna, Lie-group methods, 2000
- McLachlan, Quispel, splitting methods, 2002
- Blanes, Casas, Murua, Splitting methods for differential equations, 2024
- Chartier, Hairer, Vilmart, Algebraic structure of B-series, 2010
- Laurent, McLachlan, Munthe-Kaas, Verdier, The aromatic bicomplex for the description of divergence-free aromatic forms and volume-preserving integrators, 2023
- Foissy, an introduction to Hopf algebras of trees, 2013