THREAD – NWT6 – Part II: Lie group integrators

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- We aim at explaining the fundamentals of Lie group integrators
- For material which is more "background type" we use slides (made available to all participants)
- For material at the core of the topic we may write live on iPad
- There will be exercises every afternoon to practice the understanding of the material
- Supplementary material will be provided as documents

II.1 Introduction, motivation and historical remarks

Traditional view on solving ordinary differential equations (ODEs)

Traditionally one considered initial value problems for ODEs in a black box sense

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

- No more detail or structure was assumed on $f(t, y)$
- Later one found reason to separate "stiff" and "nonstiff"
- Then came DAE problems, mix between ODEs and algebraic equations
- Geometric or structure preserving methods became important in the numerical analysis community from ca 1990.
- Lie group integrators is a subfield of Geometric integration that was studied systematically from the early 1990's.

Consider as an example the Euler equations for the free rigid body (angular momentum equations)

$$\dot{m}(t) = m(t) \times \mathbb{I}^{-1} m(t), \quad \mathbb{I} \text{ inertia tensor}$$

Then $\frac{d}{dt}\|m(t)\|^2 = \langle m(t), m(t) \times \mathbb{I}^{-1} m(t)\rangle = 0$

Constant $\|m(t)\|$ is associated to the the sphere as a submanifold of $\mathbb{R}^3$.

Evolution of the solution should effectively be by rotations

The space of rotations is a Lie group

Stiefel manifold

- Let $M_{d,k}$ be the manifold of $d \times k$-matrices with orthonormal columns.
- and $\mathfrak{so}(d)$ the skew-symmetric $d \times d$-matrices, $A^T = -A$.

Consider matrix-differential equation

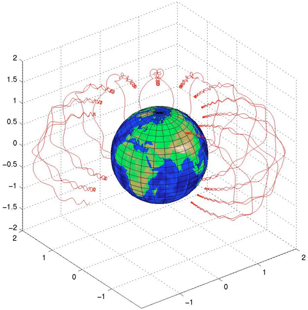
$$\dot{Y} = A(Y) \cdot Y, \quad A : M_{d,k} \to \mathfrak{so}(d)$$

Invariant: $I(Y) = Y^T Y$.
Applications

- Computation of Lyapunov exponents
- Multi-variate data analysis
- Image/signal processing

If numerical solution $Y_n \mapsto Y_{n+1}$ can be evolved by $Y_{n+1} = Q_n Y_n$ and Q_n is an orthogonal $d \times d$ matrix, then $I(Y_{n+1}) = I(Y_n)$.

Northern light



Equation for particle movement (Carl Størmer)

$$\ddot{\mathbf{x}} = \dot{\mathbf{x}} \times \mathbf{d}(\mathbf{x})$$

$\mathbf{x}$ particle position, $\mathbf{d}(\mathbf{x})$ earth magnetic field at $\mathbf{x}$.

Spiralling movement not easily followed by straight lines

Solving PDEs by means of “simpler” PDEs

We take as example a non-homogeneous heat equation

$$u_t = \nu(\mathbf{x})\Delta u$$

Fast solvers are available for the equation

$$u_t = \bar{\nu}\Delta u + f(\mathbf{x}).$$

The first problem can be approximated locally by the second, e.g. set

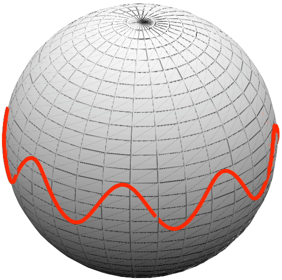
$$\bar{\nu} = \frac{\int \nu(\mathbf{x})\,\mathrm{d}\mathbf{x}}{\int \mathrm{d}\mathbf{x}}$$

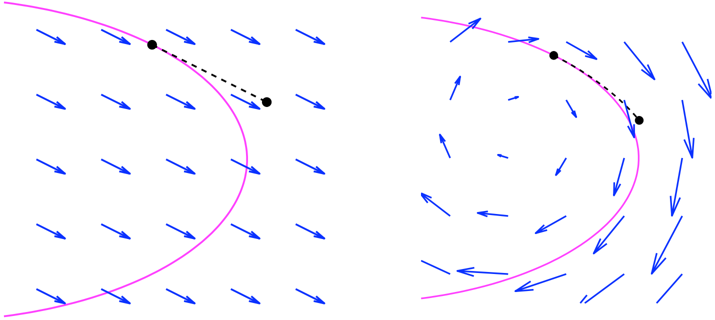
for a local known approximation $u^*(\cdot, t^*)$ let

$$f(\mathbf{x}) = (\nu(\mathbf{x}) - \bar{\nu})\Delta u^*$$

Solving the simple PDE is an action by a Lie group

- When the solution is known to be restricted to some manifold
- When it is useful to be able to move along curves rather than straight line segments





"Lie group equation"'

$$\dot{y} = A(y) \cdot y, \quad A \text{ is a matrix.}$$

Given y_n, we could approximate this equation locally by the problem

$$\dot{y} = A(y_n) \cdot y \quad \Rightarrow y_{n+1} = \mathrm{e}^{hA(y_n)} \cdot y_n$$

This is called the Lie-Euler method.

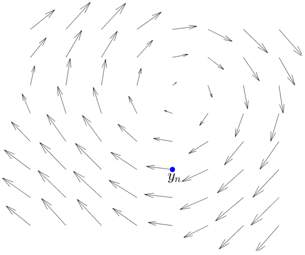
Many questions remain to be answered

1. What is the form of $A(y)$ and y?
2. Are these all the problems we can solve?
3. What does it have to do with Lie groups and manifolds?
4. How can we get higher order of convergence?

II.2 A primer on Lie group methods

$$\dot{y} = f(y),$$

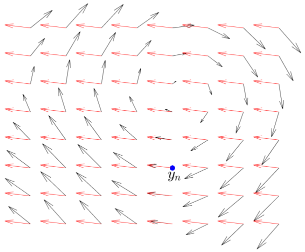
$$y_{n+1} = y_n + hf(y_n)$$



A new interpretation: Solve exactly the local problem

$$\dot{z} = f(y_n), \; z(0) = y_n$$

Set $y_{n+1} = z(h)$, $t_{n+1} = t_n + h$.



We consider the Euler free rigid body

$$\dot{m} = m \times \mathbb{I}^{-1} m, \quad \mathbb{I} = \mathrm{diag}(I_1, I_2, I_3)$$

We can rewrite this as

$$\begin{pmatrix} \dot{m}_1 \\ \dot{m}_2 \\ \dot{m}_3 \end{pmatrix} = \begin{pmatrix} 0 & \frac{m_3}{I_3} & -\frac{m_2}{I_2} \\ -\frac{m_3}{I_3} & 0 & \frac{m_1}{I_1} \\ \frac{m_2}{I_2} & -\frac{m_1}{I_1} & 0 \end{pmatrix} \cdot \begin{pmatrix} m_1 \\ m_2 \\ m_3 \end{pmatrix} = A(m) \cdot m \qquad (*)$$

Now $\|m(t)\| = \|m(0)\|$ for all t since $A(m)$ is skew-symmetric and

$$\frac{1}{2}\frac{d}{dt}(m^T m) = m^T \dot{m} = m^T A(m) m = 0$$

Inspired by the "New look" we could replace $(*)$ by

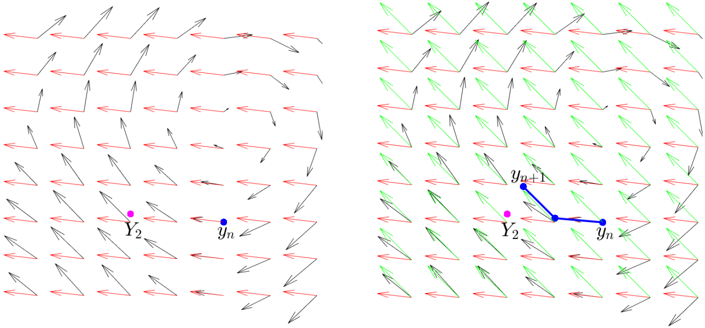
$$\dot{z} = A(m_n) z, \quad z(0) = m_n$$

Solution: $z(t) = \mathrm{e}^{tA(m_n)} m_n$ so $m_{n+1} = \mathrm{e}^{hA(m_n)} m_n$ (Lie-Euler)

$$m_{n+1} = \mathrm{e}^{hA(m_n)} \cdot m_n$$

- The exponential here is the matrix exponential
- When a matrix A is skew-symmetric then $Q = \mathrm{e}^A$ is orthogonal, $Q^T Q = I$
- Orthogonal matrices preserve the Euclidean norm $\|Qx\| = \|x\|$ for any vector x
- This means that the Lie-Euler method preserves $\|m\|$, i.e. $\|m_n\| = \|m_0\|$ for all n.

Modified Euler



$$Y_1 = y_n,$$
$$Y_2 = y_n + hf(Y_1),$$
$$y_{n+1} = y_n + \frac{h}{2}(f(Y_1) + f(Y_2))$$

Geometric interpretation is ambiguous.
Details on next slide

Step 1.

Solve $\dot{z} = f(y_n),\ z(0) = y_n$.

Set $Y_2 = z(h)$. Then

Interpretation 1

Evaluate $\bar{z} := z(h/2)$ from step 1

Solve $\dot{w} = f(Y_2),\ w(0) = \bar{z}$

Set $y_{n+1} = w(h/2)$

FRB version

$m_{n+1} = \mathrm{e}^{\frac{h}{2}A_2}\mathrm{e}^{\frac{h}{2}A_1}m_n$

Interpretation 2

Let $\bar{f} = \frac{1}{2}(f(Y_1) + f(Y_2))$

Solve $\dot{w} = \bar{f},\ w(0) = \bar{y}_n$

Set $y_{n+1} = w(h)$

FRB version

$m_{n+1} = \mathrm{e}^{\frac{h}{2}(A_1+A_2)}m_n$

Here

$$A_1 = A(m_n), \qquad A_2 = A(\mathrm{e}^{hA_1}m_n)$$

Runge–Kutta standard

$$Y_1 = y_n$$

$$Y_i = y_n + h\sum_{j=1}^{i-1} a_{ij} f(Y_j),$$

$$y_{n+1} = y_n + h\sum_{i=1}^{s} b_i f(Y_i)$$

Runge–Kutta Lie (naive)

$$M_1 = m_n$$

$$M_i = \exp\left(h\sum_{j=1}^{i-1} a_{ij} A(M_j)\right) m_n,$$

$$m_{n+1} = \exp\left(h\sum_{i=1}^{s} b_i A(M_i)\right) m_n$$

Alternatively, in the Runge–Kutta Lie, we could have defined

$$M_i = \mathrm{e}^{ha_{i,i-1}M_{i-1}} \cdot \mathrm{e}^{ha_{i,i-2}M_{i-2}} \cdots \mathrm{e}^{ha_{i,1}M_1}\, m_n$$

$$m_{n+1} = \mathrm{e}^{hb_s M_s} \cdot \mathrm{e}^{hb_{s-1}M_{i-2}} \cdots \mathrm{e}^{hb_1 M_1}\, m_n$$

Hybrids between the two RK-Lie methods can also be considered.
For the first type, no method of order higher than $p = 2$ can be achieved.

First order methods with one stage

$$m_{n+1} = \mathrm{e}^{hA(m_n)} \cdot m_n \quad \text{(Lie-Euler)}$$

Explicit methods with two stages. Write $M_1 = m_n$, $A_i := A(M_i)$

$$m_{n+1} = \mathrm{e}^{h(b_1 A_1 + hb_2 A_2)} m_n, \quad M_2 = \mathrm{e}^{ha_{21} A_1} m_n$$

or

$$m_{n+1} = \mathrm{e}^{hb_2 A_2} \mathrm{e}^{hb_1 A_1} m_n, \quad M_2 = \mathrm{e}^{ha_{21} A_1} m_n$$

Second order whenever $b_1 + b_2 = 1$ and $b_2 a_{21} = \frac{1}{2}$.

Important fact: $\mathrm{e}^{A+B} \neq \mathrm{e}^{A} \mathrm{e}^{B}$ in general for matrices A and B.

We define: Matrix commutator $[A, B] = AB - BA$ for matrices A and B.

$$
\begin{aligned}
A_1 &= hA(m_n),\\
A_2 &= hA(\exp(\tfrac{1}{2}A_1)\cdot m_n),\\
A_3 &= hA(\exp(\tfrac{1}{2}A_2 - \tfrac{1}{8}[A_1, A_2])\cdot m_n),\\
A_4 &= hA(\exp(A_3)\cdot m_n),\\
m_{n+1} &= \exp(\tfrac{1}{6}(A_1 + 2A_2 + 2A_3 + A_4 - \tfrac{1}{2}[A_1, A_4]))\cdot m_n.
\end{aligned}
$$

This is a generalisation of the "classical" Runge–Kutta method of order 4 found in all the text books.

Commutator-free Lie group method

$$
\begin{aligned}
M_1 &= m_n \\
M_2 &= \exp(\tfrac{1}{2}hA_1) \cdot m_n \\
M_3 &= \exp(\tfrac{1}{2}hA_2) \cdot m_n \\
M_4 &= \exp(hA_3 - \tfrac{1}{2}hA_1) \cdot M_2 \\
m_{n+\frac{1}{2}} &= \exp(\tfrac{1}{12}h(3A_1 + 2A_2 + 2A_3 - A_4)) \cdot m_n \\
m_{n+1} &= \exp(\tfrac{1}{12}h(-A_1 + 2A_2 + 2A_3 + 3A_4)) \cdot m_{n+\frac{1}{2}}
\end{aligned}
$$

where $A_i = f(M_i)$.

Note: one exponential is saved in computing M_4 by making use of M_2.

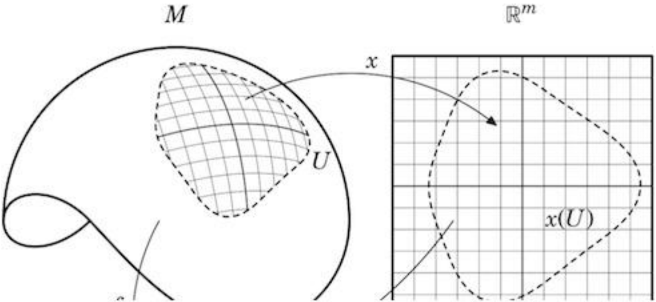
- We have consider one simple model problem of the type $\dot{m} = A(m) \cdot m$ where A is a matrix and m is a vector.
- We have naively generalised an interpretation of standard Runge–Kutta scheme, breaking them down into building blocks that consist of solving simpler differential equations exactly.
- We get away with this for methods of convergence order $p \leq 2$.
- For $p > 2$ we need to either include extra corrections (commutators) or compose together building blocks to get the right order

Several open questions remain.

II.3 Manifolds

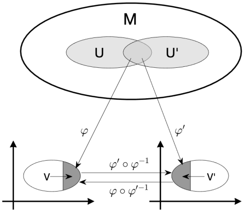
A manifold is a set M with a collection of charts (U, φ) such that

- $U \subset M$
- $\varphi : U \to \varphi(U) \subset \mathbb{R}^n$ is a bijective map
- $\varphi(m) = (x_1, \ldots, x_n)$ are called coordinates of the point m,



(U, φ), (U', φ') overlapping:

$$V = \varphi(U \cap U') \subset \mathbb{R}^n,$$
$$V' = \varphi'(U \cap U') \subset \mathbb{R}^n.$$



(U, φ) and (U', φ') compatible if

$$\varphi' \circ \varphi^{-1} : V \to V'$$
$$\varphi \circ (\varphi')^{-1} : V' \to V$$

are C^∞.

Differentiable manifold

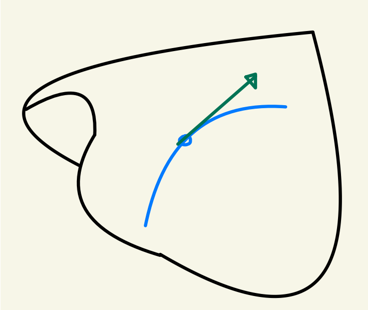
1. There is a collection of charts such that each $m \in M$ is a member of at least one chart
2. M is a union of compatible charts

Two (for us) useful definitions

1. By curves
2. By derivations

$\gamma(t),\ t \in C^1(-\varepsilon, \varepsilon)$
$v_m = \dot{\gamma}(0)$, tangent vector at $m = \gamma(0)$.

Curve



Derivation acting on function germs. A tangent vector v_m can be seen as a linear operator acting on functions on M

- $v_m[\alpha f + \beta g] = \alpha v_m[f] + \beta v_m[g]$ (linearity)
- $v_m[fg] = v_m[f]g(m) + f(m)v_m[g]$ (derivation property)

Interpretation: $v_m[f]$ is the directional derivative of f in the direction of v_m at m. In coordinates $v_m = \mathbf{v} \cdot \nabla$.

The 2-sphere S^2.
Vectors of unit norm,

$$\{x \in \mathbb{R}^3 : x_1^2 + x_2^2 + x_3^2 = 1\}.$$

Curve $\gamma(t)$ must satisfy

$$\sum_{i=1}^{3} \gamma_i(t)^2 = 1$$

Differentiating wrt. t,

$$\sum_{i=1}^{3} \dot{\gamma}_i(t)\gamma_i(t) = 0$$

Suppose $\gamma(0) = r$ and $\dot{\gamma}(0) = v$,

$$T_r S^2 = \{v \in \mathbb{R}^3 : v \perp r\}$$

The Euclidean space $\mathbb{R}^n$.

Tangent space at x: $T_x\mathbb{R}^n \simeq \mathbb{R}^n$.
Curve $x + tv$ for any $v \in \mathbb{R}^n$.

Orthogonal $n \times n$-matrices $\mathcal{O}(n)$.

Manifold contains identity matrix I.
Curve $\gamma(t)$ through I, i.e.

$$\gamma(0) = I, \quad \dot{\gamma}(0) = v.$$

Orthogonality: $\gamma(t)^T\gamma(t) = I \ \forall t$

$$\frac{\mathrm{d}}{\mathrm{d}t}\gamma(t)^T\gamma(t) = \dot{\gamma}(t)^T\gamma(t) + \gamma(t)^T\dot{\gamma}(t)$$
$$t = 0 \ \Rightarrow v^T + v = 0$$

$$T_I\mathcal{O}(n) = \{v \in \mathbb{R}^{n\times n} : v^T = -v\}$$

Linear space V, **dual space** V^*

- For $f \in V^*$, $u, v \in V$,

  $f(\alpha u + \beta v) = \alpha f(u) + \beta f(v)$

  $\alpha, \beta \in \mathbb{R}$
- Duality pairing, write

$$f(v) = \langle f, v \rangle$$

- Basis for V, $e_1, \ldots, e_d$
- Dual basis $\varepsilon_1, \ldots, \varepsilon_d$
  $\varepsilon_i(e_j) = \langle \varepsilon_i, e_j \rangle$

Cotangent space

- $T_m M$ is a linear space
- $T_m^* M$ its dual
- $v \in T_m M$ velocity vector
- $p \in T_m^* M$ momentum
- Kinetic energy

$$T = \frac{1}{2} \langle p, v \rangle$$

Smoothly glue together the (co)tangent spaces at each m

$$TM = \bigcup_{m \in M} T_m M, \qquad T^*M = \bigcup_{m \in M} T^*_m M$$

Note

- These bundles are not (generally) linear spaces, but they are manifolds in their own right.
- Local coordinate charts are induced on TM from M.

$$\phi : M \supset U \to \phi(U) \;\longrightarrow\; \phi' : TM \supset TU \to (U \times V)$$

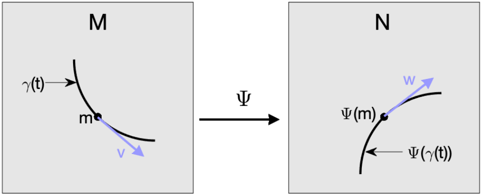
- Extra structure is needed to connect/compare $v \in T_m M$ and $v' \in T_{m'} M$.
- If it holds that e.g $TM = M \times V$ for some linear space V then the manifold is called trivial

Let M and N be manifolds and $\Psi : M \to N$ a map.
The tangent map $T\Psi_m : T_m M \to T_{\Psi(m)} N$ is defined via curves.
Let $n = \Psi(m)$.

$$\gamma(t) \in M, \quad \gamma(0) = m, \quad \dot{\gamma}(0) = v$$

The curve $\sigma(t) = \Psi(\gamma(t)) \in N$ satisfies $\sigma(0) = n$ and $w := \dot{\sigma}(0) \in T_n N$.

$$w := T\Psi_m(v)$$



One can extend the definition to all of TM, $T\Psi : TM \to TN$. Then only linear when restricted to fibers $T_m M$:

Exercise. Local coordinates $(x_1, \ldots, x_m)$ on M and similarly, $(y_1, \ldots, y_n)$ on N. Thus, $y = \Psi(x)$ can be expressed as

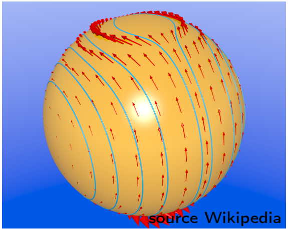
$$\begin{bmatrix} y_1 \\ \vdots \\ y_n \end{bmatrix} = \begin{bmatrix} \Psi_1(x_1, \ldots, x_m) \\ \vdots \\ \Psi_n(x_1, \ldots, x_m) \end{bmatrix}$$

Show, by using the definition of the tangent map that $T\Psi$ is just the Jacobian matrix of Ψ, i.e.

$$T\Psi = \begin{bmatrix} \frac{\partial \Psi_1}{\partial x_1} & \ldots & \frac{\partial \Psi_1}{\partial x_m} \\ \vdots & \vdots & \vdots \\ \frac{\partial \Psi_n}{\partial x_1} & \ldots & \frac{\partial \Psi_n}{\partial x_m} \end{bmatrix}$$

A vector field on M is a map

$$X : M \to TM \text{ s.t.}$$
$$\forall m : m \mapsto X|_m \in T_m M$$



A vector field on M is called a section of TM, write $X \in \mathcal{X}(M)$ or $X \in \Gamma(TM)$. We can also have sections on T^*M. They are called differential one-forms.

Example. If f is a function on M, $f : M \to \mathbb{R}$ then $Tf : TM \to T\mathbb{R}$. We have $T\mathbb{R} \equiv \mathbb{R} \times \mathbb{R}$, but often omit the first factor.

$$df|_m : T_m M \to \mathbb{R}, \quad df \in \Gamma(T^*M)$$

Vector fields as derivations of functions

- $f \in \mathcal{F}(M) := C^\infty(M)$
- Vector field $X \in \mathcal{X}(M)$
- $X : \mathcal{F}(M) \to \mathcal{F}(M)$ as

$$X[f](m) = X|_m[f]$$

In coordinates $x_1, \ldots, x_d$

$$X = \sum_{i=1}^{d} X_i(x) \partial x_i$$

Duality of vector fields and differential forms

If $X \in \Gamma(TM)$ and $\omega \in \Gamma(T^*M)$ then we have a point-wise pairing

$$\langle \omega, X \rangle \in \mathcal{F}(M)$$

For one-forms df one has

$$df(X) = \langle df, X \rangle = X[f]$$

Flow

$X \in \mathcal{X}$: vector field on M. Consider the ODE

$$\dot{x}(t) = X(x(t)), \ \ x(0) = x.$$

Solution $x(t), t \in (\alpha_x, \beta_x) \ni 0$. Write

$$x(t) = \exp(tX)x$$

$\exp(X) : M \to M$ is called the flow of X.

Domain

exp only defined on open subset

$$\exp(tX) : \mathcal{D}_t \to M$$

$$\mathcal{D}_t = \{x \in M : t \in (\alpha_x, \beta_x)\}$$

$$\bigcup_{t>0} \mathcal{D}_t = M$$

Relatedness

Let $\Psi : M \to N$ be a differentiable map and let X and Y be vector fields on M and N respectively. If

$$T\Psi \circ X = Y \circ \Psi$$

then we say that X is Ψ-related to Y.

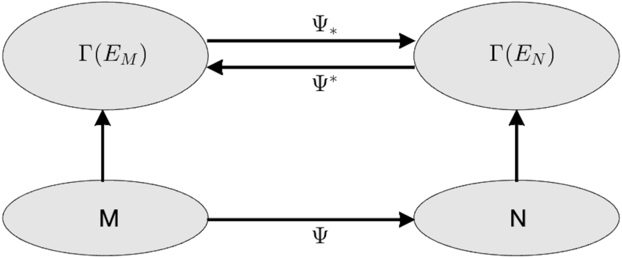
Push-forward. If Ψ is also invertible we can, for any vector field $X \in \mathcal{X}(M)$ define

$$Y = \Psi_* X = T\Psi \circ X \circ \Psi^{-1} \in \mathcal{X}(N)$$

Pull-back. $\Psi^* : \mathcal{X}(N) \to \mathcal{X}(N)$

$$X = \Psi^* Y = (T\Psi)^{-1} \circ Y \circ \Psi$$

Note. If $y(t) = \Psi(x(t))$, $\dot{x} = X(x)$, $\dot{y} = Y(y)$, then X is Ψ-related to X.



Functions. $F : N \to \mathbb{R}$

$$\Psi^* F = F \circ \Psi \text{ i.e. } \Psi^* F(x) = F(\Psi(x))$$

Differential one-forms. Let ω be a one-form on N, $X \in \mathcal{X}(M)$.

$$\langle \Psi^* \omega, X \rangle = \langle \omega, T\Psi(X) \rangle$$

Let X and Y be vector fields on M. They act as derivations on functions $f \in \mathcal{F}(M)$. We define the vector field

$$Z = [X, Y] \in \mathcal{X}(M)$$

as the derivation

$$Z[f] = X[Y[f]] - Y[X[f]] \text{ for every } f \in \mathcal{F}(M)$$

In coordinates $(x_1, \ldots, x_d)$

$$Z^i = \sum_{j=1}^{d} \left(X_j \frac{\partial Y^i}{\partial x_j} - Y_j \frac{\partial X^i}{\partial x_j} \right)$$

Pushforward homomorphism
Let $\Psi : M \to N$
$X, Y \in \mathcal{X}(M)$. Then

$$\Psi_*[X, Y] = [\Psi_* X, \Psi_* Y]$$

- The Lie-Jacobi bracket is bilinear and skew-symmetric
- One can prove that $[X, [Y, Z]] + [Y, [Z, X]] + [Z, [X, Y]] = 0$

A frame is a set of vector fields on a manifold M, say $E_1, \ldots, E_d$ such that for each $m \in M$

$$\mathrm{span}(E_1|_m, \ldots, E_d|_m\} = T_m M$$

Clearly $d \geq \dim M$. Sometimes, frames are defined only locally, on a subset $U \subset M$ and one requires $d = \dim M$.

Representing arbitrary vector fields by using a frame.
Any smooth vector field on M can be represented by means of a frame and a set of d functions $f_i \in \mathcal{F}(M)$

$$F|_m = \sum_{i=1}^{d} f_i(m) E_i|_m$$

II.4 Lie groups and Lie algebras

A Lie group G is a differentiable manifold which also has the structure of a group

$a, b, c \in G$

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

There is $e \in G$ such that

$$a \cdot e = e \cdot a = a, \ \forall a \in G$$

For every $a \in G$ there is $a^{-1} \in G$ s.t.

$$a \cdot a^{-1} = a^{-1} \cdot a = e$$

Smoothness

$(a, b) \mapsto a \cdot b$ is smooth

$a \mapsto a^{-1}$ smooth

Matrix Lie groups

$GL(n)$: invertible $g \in \mathbb{R}^{n \times n}$

$G \subset GL(n)$ closed subgroup

Commutative Lie groups

$g \cdot h = h \cdot g$ for all $g, h \in G$

$(\mathbb{R}^n, +)$ is an example

We always have *"group product" = matrix-matrix multiplication* and *neutral element=Identity matrix*.

1. $SL(n) = \{A : \det(A) = 1\}$
2. $O(n) = \{Q : Q^T Q = I\}$ (Orthogonal matrices).
   Subgroup $SO(n) = \{Q \in O(n) : \det(Q) = 1\}$.
3. $T(n) = \{\text{lower-triangular matrices}\}$
4. Special Euclidean group $SE(n)$.

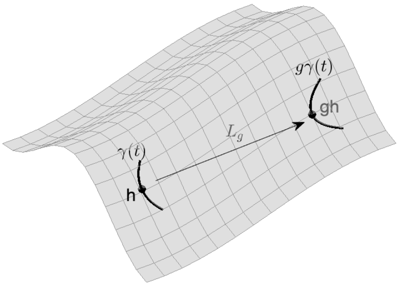
$$A = \begin{bmatrix} Q & a \\ 0 & 1 \end{bmatrix}, \quad Q \in SO(n),\ a \in \mathbb{R}^n$$

Left and right product

$g, h \in G$

$L_g : G \to G$, $L_g(h) = gh$

$R_g : G \to G$, $R_g(h) = hg$



If $TL_g \circ X = X \circ L_g$ then X is a left invariant vector field.
If $TR_g \circ X = X \circ R_g$ then X is a right invariant vector field.

The linear space of left (right) invariant vector fields on G is called the Lie algebra of G.

A left invariant vector field X is given at e as $X|_e$, then

$$X|_g = TL_g \circ X|_e$$

1. Any tangent vector $v \in T_e G$ therefore uniquely identifies a left invariant vector field.
2. Any left invariant vector field X on G defines an element $v := X|_e \in T_e G$.
3. We can take $\mathfrak{g} := T_e G$ as an alternative definition of the Lie algebra.

Lie bracket on $\mathfrak{g}$

The Lie-Jacobi bracket on $\mathcal{X}(G)$ restricted to the space of left (or right) invariant vector fields provides a Lie bracket on $\mathfrak{g}$.

$$L_{g*}[X, Y] = [L_{g*}X, L_{g*}Y] = [X, Y]$$

To the group element $g \in G$ there corresponds a map

$$A_g : G \to G, \quad A_g(h) = ghg^{-1} = L_g \circ R_{g^{-1}}(h)$$

Its tangent map $TA_g|_e$ is called the adjoint representation of G.

$$\mathrm{Ad}_g(\xi) = TA_g|_e(\xi) = TL_g \circ TR_{g^{-1}}(\xi), \quad \xi \in \mathfrak{g}.$$

For matrix groups we simply write

$$\mathrm{Ad}_g(\xi) = g\xi g^{-1}$$

Alternative definition of the Lie bracket. Let $g(t) \in G$ be such that $g(0) = e$, $\dot{g}(0) = \eta$. Then

$$[\eta, \xi] = \left.\frac{d}{dt}\right|_{t=0} \mathrm{Ad}_{g(t)}(\xi)$$

The adjoint representation of $\mathfrak{g}$

We define $\mathrm{ad}_\xi : \mathfrak{g} \to \mathfrak{g}$ for any $\xi \in \mathfrak{g}$ as

$$\mathrm{ad}_\xi(\eta) = [\xi, \eta]$$

- ad_ξ is a linear map
- The map is always singular, since $\mathrm{ad}_\xi(\xi) = 0$
- Powers of ad_ξ are iterated commutators, e.g.

$$\mathrm{ad}_\xi^2(\eta) = \mathrm{ad}_\xi([\xi, \eta]) = [\xi, [\xi, \eta]] \text{ etc}$$

- In geometric mechanics, it often happens that the "battle field" is the dual $\mathfrak{g}^*$ of a Lie algebra
- For instance, it has a natural structure as a Poisson manifold
- E.g. The heavy top has $\mathfrak{se}(3)^*$ as solution space
- The coadjoint representation can be central in these cases

Coadjoint representaton.

$$\mathrm{Ad}_g^* : \mathfrak{g}^* \to \mathfrak{g}^*, \quad g \in G.$$

$$\langle \mathrm{Ad}_g^*(\mu), \xi \rangle = \langle \mu, \mathrm{Ad}_g(\xi) \rangle, \quad \text{for all } \mu \in \mathfrak{g}^*,\ \xi \in \mathfrak{g}$$

Example $SO(3)$. Vector representation: $\mathrm{Ad}_g(\xi) = g\xi$, pairing $\langle \mu, \xi \rangle = \mu^T \xi$.

$$\langle \mathrm{Ad}_g^*(\mu), \xi \rangle = \langle \mu, g\xi \rangle = \mu^T g\xi = \langle g^T \mu, \xi \rangle$$

so $\mathrm{Ad}_g^*(\mu) = g^T \mu$.

Let $G \subset GL(n)$ be a Lie group of matrices. Lie algebra $\mathfrak{g} = T_I G$.

Take $g(t) = \mathrm{e}^{t\xi} \in G$ so that $g(0) = I$ and $\dot{g}(0) = \xi$.

$$[\xi, \eta] = \left.\frac{d}{dt}\right|_{t=0} \mathrm{e}^{t\xi} \eta \mathrm{e}^{-t\xi} = \xi\eta - \eta\xi$$

How does $T_I G$ look like for a given Lie group G?

- Look at "defining condition", such as $g^T g = I$ or $\det(g) = 1$
- Plug in a curve $g(t)$ such that $g(0) = I$.
- Differentiate and evaluate at $t = 0$
- Obtain relation for elements of Lie algebra

Example. Suppose $g(t)^T g(t) = I$. $\xi := \dot{g}(0)$. Differentiate

$$\dot{g}^T g + g^T \dot{g} = 0 \quad \Rightarrow \xi^T + \xi = 0$$

$$SO(3) = \{g \in \mathbb{R}^{3\times 3} : g^T g = I \text{ and } \det(g) = 1\}$$

Lie algebra

$$\mathfrak{so}(3) = \{\xi \in R^{3\times 3} : \xi^T + \xi = 0\}$$

Basis for $\mathfrak{so}(3)$

$$E_1 = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & -1 \\ 0 & 1 & 0 \end{pmatrix}, \; E_2 = \begin{pmatrix} 0 & 0 & 1 \\ 0 & 0 & 0 \\ -1 & 0 & 0 \end{pmatrix}, \; E_3 = \begin{pmatrix} 0 & -1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}$$

$\hat{\xi} = \xi_1 E_1 + \xi_2 E_2 + \xi_3 E_3$ and $\xi = (\xi_1, \xi_2, \xi_3)^T$.

$$\hat{\xi} = \begin{pmatrix} 0 & -\xi_3 & \xi_2 \\ \xi_3 & 0 & -\xi_1 \\ -\xi_2 & \xi_1 & 0 \end{pmatrix} \quad \text{(hat map)}$$

By using $\xi \in \mathbb{R}^3$ to represent $\hat{\xi}$, we can write ad_ξ as a matrix and we find

$$\mathrm{ad}_\xi(\eta) = [\hat{\xi}, \hat{\eta}] = \hat{\zeta}, \quad \zeta = \begin{pmatrix} 0 & -\xi_3 & \xi_2 \\ \xi_3 & 0 & -\xi_1 \\ -\xi_2 & \xi_1 & 0 \end{pmatrix} \cdot \begin{pmatrix} \eta_1 \\ \eta_2 \\ \eta_3 \end{pmatrix}$$

We can also use the cross product for the commutator

$$\zeta = \mathrm{ad}_\xi(\eta) = \xi \times \eta$$

Useful formulas

- $\widehat{g\xi} = g\hat{\xi}g^{-1} = \mathrm{Ad}_g(\hat{\xi})$, $g \in SO(3)$, $\xi \in \mathfrak{so}(3)$.
- $g(\xi \times \eta) = (g\xi) \times (g\eta)$, $g \in SO(3)$, $\xi, \eta \in \mathfrak{so}(3)$.

Unsurprisingly, the map $\exp : \mathfrak{g} \to G$ is just the flow of right- or left invariant vector fields.

$$X \in \mathfrak{g}, \quad \dot{x}(t) = X|_{x(t)},\ x(0) = e \quad \Rightarrow \quad x(1) = \exp(X) \in G$$

Properties

$\exp((t+s)X) = \exp(tX)\exp(sX)$

$\exp(X+Y) \neq \exp(X)\exp(Y)$ (in general)

$\exp$ is neither one-to-one nor onto (in general)

- Find tangent space $T_I G \equiv \mathfrak{g}$. Construct arbitrary curve $A(t),\ A(0) = I$ and let $v = \dot{A}(0) \in T_I G$.
- Define X_v and Y_v in $\mathcal{X}(G)$

$$X_v|_g = L_{g*}(v) = gv, \quad Y_v|_g = R_{g*}(v) = vg.$$

These are the left- and right invariant vector fields.

- Consider the matrix differential equation

$$\dot{g}(t) = X_v|_{g(t)} = g(t)v,\ g(0) = e, \quad \Rightarrow \quad g(t) = \mathrm{e}^{tv}$$

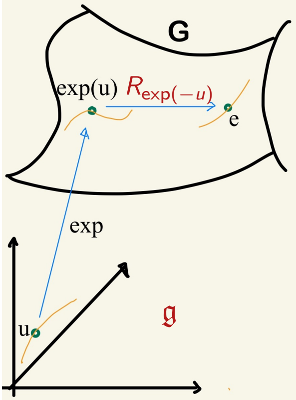
where the last expression is the matrix exponential

- $$\mathrm{e}^{tv} = \sum_{k=0}^{\infty} \frac{t^k}{k!} v^k$$

$$\exp : \quad \mathfrak{g} \to G$$
$$T\exp_u : \quad T_u\mathfrak{g} \to T_{\exp(u)}G$$

$T_u\mathfrak{g} \equiv \mathfrak{g}$ since $\mathfrak{g}$ is a linear space.
Also $T_{\exp(u)}G \equiv \mathfrak{g}$ through

$$v \in T_{\exp(u)}G \longleftrightarrow w = TR_{\exp(-u)}(v) \in T_eG \equiv \mathfrak{g}$$



We define for $u \in \mathfrak{g}$ the linear map

$$\mathrm{dexp}_u : \mathfrak{g} \to \mathfrak{g}$$

$$\mathrm{dexp}_u(v) = TR_{\exp(-u)} \circ T\exp_u(v)$$

Recall the ad-operator $\mathrm{ad}_u : \mathfrak{g} \to \mathfrak{g}$

$$\mathrm{ad}_u(v) = [u, v], \ \mathrm{ad}_u^2(v) = \mathrm{ad}_u([u, v)] = [u, [u, v]], \text{ etc.}$$

One can prove that

$$\mathrm{dexp}_u(v) = \sum_{k=0}^{\infty} \frac{1}{(k+1)!} \mathrm{ad}_u^k(v) = \left.\frac{e^z - 1}{z}\right|_{z=\mathrm{ad}_u} (v)$$

We shall see later that we need the inverse $\mathrm{dexp}_u^{-1}(v)$. This is obtained by inverting the function above, i.e.

$$\mathrm{dexp}_u^{-1}(v) = \left.\frac{z}{e^z - 1}\right|_{z=\mathrm{ad}_u} (v) = \sum_{k=0}^{\infty} \frac{B_k}{k!} \mathrm{ad}_u^k(v)$$

We shall see later that the series can be truncated after a final number of terms when used in Lie group integrators.

Let G be a Lie group and M a manifold. Lie group action $\Lambda : G \times M \to M$.

Lie group action $\Lambda : G \times M \to M$

$$\Lambda(e, m) = m, \ \forall m \in M$$

$$\Lambda(gh, m) = \Lambda(g, \Lambda(h, m)), \ \forall g, h \in G, m \in M$$

Remark

The definition above is a left action

A right action is also possible, in which case we have

$$\Lambda(gh, m) = \Lambda(h, \Lambda(g, m))$$

- If G is a Lie group and $M = G$ then set $\Lambda(g, m) = gm$
- If G is an $n \times n$ matrix group and $M = \mathbb{R}^n$, set $\Lambda(g, x) = gx$
- Let M be the set of symmetric $n \times n$-matrices and G the Lie group of orthogonal matrices. A group action is

$$\Lambda(g, m) = gmg^T$$

- $G = SL(2)$ acting on the complex plane $\mathbb{C}$ through

$$\Lambda(A, z) = \frac{az + b}{cz + d}, \quad A = \begin{pmatrix} a & b \\ c & d \end{pmatrix}, \; ad - bc = 1$$

The adjoint representation defines a left Lie group action by G on $M = \mathfrak{g}$

$$\Lambda(g, \xi) = \mathrm{Ad}_g(\xi)$$

The coadjoint representation defines a right Lie group action by G om $M = \mathfrak{g}^*$

$$\Lambda(g, \mu) = \mathrm{Ad}^*_g(\mu)$$

A left coadjoint action can be defined by replacing g by g^{-1}

$$\Lambda(g, \mu) = \mathrm{Ad}^*_{g^{-1}}(\mu)$$

Transitive. For every $x, y \in M$ there is a $g \in G$ such that $y = \Lambda(g, x)$.

Free. For any $m \in M$, $\Lambda(g, m) = m \;\Rightarrow\; g = e$.

Orbit. An orbit $\mathcal{O}_m$ containing m is $x = \{\Lambda(g, m), g \in G\}$.

Note. A group action is transitive when restricted to each of its orbits.

The stabilizer (or isotropy) subgroup of a group action is

$$H_x = \{h \in G : \Lambda(h, x) = x\}$$

Note. For a free group action any isotropy subgroup is the trivial group $H_x = \{e\}$.
Note. All isotropy groups are isomorphic to each other.

Spherical pendulum

- Configuration space S^2, phase space TS^2
- Davide Murari: adjoint action by $SE(3)$ on $\mathfrak{se}(3) \equiv \mathbb{R}^6$

$$\mathrm{Ad}_{(g,u)}(\xi, \eta) = (g\xi, u \times (g\xi) + g\eta)$$

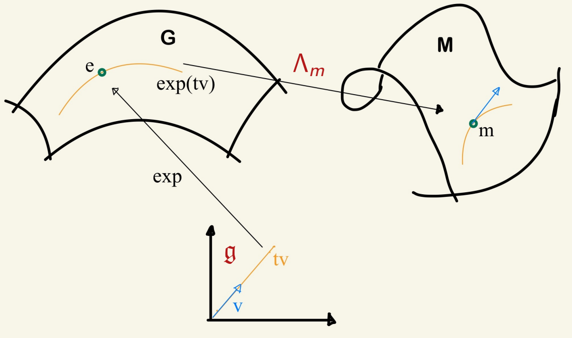
- can be restricted to

$$TS^2 \sim \{(q, v) \in \mathbb{R}^6 : |q| = 1, q^T v = 0\}$$

- So for any $q \in \mathbb{R}^3,\ |q| = 1$ and $v_q \in \mathbb{R}^3,\ q^T v = 0$ let

$$\Lambda((g, u), (q, v) = (gq, u \times gv)$$

Infinitesimal generator of a Lie group action



M manifold

G Lie group

$\mathfrak{g}$ Lie algebra

$v \in \mathfrak{g}$

$\Lambda_m(g) := \Lambda(g, m)$

Define the infinitesimal generator of the action as

$$\lambda_*(v)|_m = T\Lambda_m|_e(v)$$

$\lambda_*(v)$ is a vector field on M for every $v \in \mathfrak{g}$.

- The infinitesimal generator of the adjoint action by G on $\mathfrak{g}$

$$\Lambda(g, \xi) = \mathrm{Ad}_g(\xi)$$

Here we simply get

$$\lambda_*(\xi)\big|_\eta = \frac{d}{dt}\bigg|_{t=0} \mathrm{Ad}_{\exp(t\xi)}(\eta) = [\xi, \eta] = \mathrm{ad}_\xi(\eta)$$

- The infinitesimal generator of the left coadjoint action by G on $\mathfrak{g}^*$

$$\begin{aligned} \langle\, \lambda_*(\xi)\big|_\mu \,, \eta\rangle &= \langle\, \frac{d}{dt}\bigg|_{t=0} \mathrm{Ad}^*_{\exp(-t\xi)}(\mu), \eta\rangle \\ &= \langle \mu, \frac{d}{dt}\bigg|_{t=0} \mathrm{Ad}_{\exp(-t\xi)}(\eta)\rangle \\ &= \langle \mu, -\mathrm{ad}_\xi(\eta)\rangle = \langle -\mathrm{ad}^*_\xi(\mu), \eta\rangle \end{aligned}$$

$$\lambda_*(\xi)\big|_\mu = -\mathrm{ad}^*_\xi(\mu)$$

Free rigid body

Left coadjoint action by $SO(3)$ on $\mathfrak{so}(3)^*$

Represent $\mathfrak{so}(3)^*$ as 3-vectors μ

$$\Lambda(g,\mu) = \mathrm{Ad}^*_{g^{-1}}(\mu) = g\mu$$

Transitive on coadjoint orbits: $\{\mu : |\mu| = \text{constant}\}$

The infinitesimal action is

$$\lambda_*(\xi)|_\mu = \hat{\xi}\mu = \xi \times \mu$$

The FRB equations are

$$\dot{\mu} = \lambda_*(-\mathbb{I}^{-1}\mu)\big|_\mu$$

II.5 Lie group integrators

Writing vector fields in terms of an action

- M a differentiable manifold
- F a smooth vector field on M
- Lie group G acts transitively on M
- Lie algebra of G is $\mathfrak{g}$
- λ_* is infinitesimal generator

> Then there is a map $f : M \to \mathfrak{g}$ such that
>
> $$F|_m = \lambda_*(f(m))|_m$$
>
> This is the way vector fields on M should be represented.

Refer to previous example

Aim: Locally (near $m \in M$) convert the problem on M to a problem on $\mathfrak{g}$

Need a map λ_m from $\mathfrak{g}$ to M, can be defined using exp and $\Lambda(g, m)$

$$\lambda_m(u) = \Lambda(\exp(u), m) =: \Lambda_m \circ \exp(u)$$

Let, for $u(t) \in \mathfrak{g}$ be the solution to the problem on M be $y(t) = \lambda_m(u(t))$

$$\dot{y} = T\Lambda_m \circ T\exp_u \circ \dot{u} = F|_{\lambda_m(u)}$$

So

$$\dot{y} = T\Lambda_m \circ T\exp \circ \dot{u} = T\Lambda_m \circ TR_{\exp(u)} \circ \mathrm{dexp}_u \circ \dot{u}$$

This should be equal to

$$\dot{y} = F|_y = \lambda_*(f(y))|_y = \lambda_*(f \circ \lambda_m(u))|_{\lambda_m(u)}$$

Define for simplicity $x := \lambda_m(u)$

For any $u, v \in \mathfrak{g}$ we calculate

$$
\begin{aligned}
\lambda_*(v)|_x &= \left.\frac{\mathrm{d}}{\mathrm{d}t}\right|_{t=0} \Lambda(\exp(tv), \Lambda(\exp(u), m)) \\
&= \left.\frac{\mathrm{d}}{\mathrm{d}t}\right|_{t=0} \Lambda(\exp(tv)\exp(u), m) \\
&= \left.\frac{\mathrm{d}}{\mathrm{d}t}\right|_{t=0} (\Lambda_m \circ R_{\exp(u)})(\exp(tv)) \\
&= T(\Lambda_m \circ R_{\exp(u)})(v) = T\Lambda_m \circ TR_{\exp(u)}(v)
\end{aligned}
$$

So the last box on the previous slide becomes (copy also from previous slide)

$$
\dot{y} = F|_y = F \circ \lambda_m|_u = T\Lambda_m \circ TR_{\exp(u)} \circ f(x)
$$

$$
\dot{y} = T\Lambda_m \circ T\exp \circ \dot{u} = T\Lambda_m \circ TR_{\exp(u)} \circ \mathrm{dexp}_u \circ \dot{u}
$$

Comparing the two expressions for $\dot{y}$ a sufficient condition is

$$\mathrm{dexp}_u \circ \dot{u} = f(x) = f(\lambda_m(u))$$

True if

$$\dot{u} = \mathrm{dexp}_u^{-1}(f \circ \lambda_m(u))$$

We have thus derived the ODE vector field to be used on the Lie algebra

$$W|_u = \mathrm{dexp}_u^{-1}(f \circ \lambda_m(u))$$

One step of an RKMK method

Given y_n, h, and $f : M \to \mathfrak{g}$,

Set $m = y_n$

for $i = 1$ to s

$$U_i = h \sum_{j=1}^{i-1} a_{ij} F_j$$

$$K_i = f(\lambda_m(U_i))$$

$$F_i = \mathrm{dexp}_{U_i}^{-1}(K_i)$$

end

$$V = h \sum_{i=1}^{s} b_i F_i$$

$$y_{n+1} = \lambda_m(V) = \Lambda(\exp(V), m)$$

- First identify which manifold your solution is to evolve on
- You need a transitive Lie group action, often natural. Could be adjoint or coadjoint action, or even just left multiplication
- Derive the infinitesimal generator of the action. This allows you to express your vector field by means of the map $f : M \to \mathfrak{g}$. Might not be unique, but choice is often natural
- With f given, you are good to go

- Crouch and Grossman (1993) used frames to describe vector fields and integrators
- Recall that a frame $E_1, \ldots, E_d$ can be used to express any smooth vector field

$$F(y) = \sum_{i=1}^{d} f_i(y) E_i|_y$$

- C& G introduced the notion of frozen vector field. For any $m \in M$ define the vector field

$$F_m|_y = \sum_{i=1}^{d} f_i(m) E_i|_y$$

- The frozen vector fields form a d-dimensional subspace of $\mathcal{X}(M)$.

Assumption: The flow of any frozen vector field can be computed

Start with y_0

Crouch-Grossman method

$$
\begin{aligned}
Y_1 &= y_0, & F_1 &= F_{Y_1} \\
Y_2 &= \exp(ha_{21}F_1)(y_0), & F_2 &= F_{Y_2} \\
Y_3 &= \exp(ha_{32}F_2)\exp(ha_{31}F_1)(y_0), & F_3 &= F_{Y_3} \\
&\text{etc}
\end{aligned}
$$

$$y_1 = \exp(hb_sF_s)\exp(hb_{s-1}F_{s-1})\cdots\exp(hb_1F_1)(y_0)$$

Disadvantage: The number of exponentials grows quadratically with the number of stages.

A way to reduce the number of flow calculations without commutators is use a more general format

Commutator-free Lie group methods

$$Y_i = \exp\left(\sum_{k=1}^{i-1} \alpha_{i,J}^k F_k\right) \cdots \exp\left(\sum_{k=1}^{i-1} \alpha_{i,1}^k F_k\right) y_n$$

$$F_i = F_{Y_i}, \quad i = 1, \ldots, s$$

$$y_{n+1} = \exp\left(\sum_{k=1}^{s} \beta_J^k F_k\right) \cdots \exp\left(\sum_{k=1}^{s} \beta_1^k F_k\right) y_n$$

Can be seen as a generalisation of Runge-Kutta methods where

$$\sum_{j=1}^{J} \alpha_{i,j}^k = a_i^k, \quad \sum_{j=1}^{J} \beta_j^k = b^k$$

- Choosing the frames to be standard commutative basis for $\mathbb{R}^n$, the scheme reduces to a classical Runge-Kutta method with coefficients $A = (a_i^k)$, $b = (b^k)$.
- Therefore a method of order p must be such that (A, b) satisfy the classical order conditions. But this is not sufficient, there are also additional order conditions on $(\alpha_{i,j}^k)$, (β_j^k).
- In constructing CFREE methods, the "game" will always be to keep the number of exponentials as low as possible, often different J for different stages.
- An interesting possibility is to construct methods with exponentials that can be reused in later stages.
- A fourth order method based on the classical Runge-Kutta method can be constructed with a total of 5 exponentials.
- Commutator free methods can give some more flexibility than RKMK methods
- Commutator free methods have no interpretation as solving an ODE locally on the Lie algebra

Recall the setup with a Lie group G acting by Λ on M, let $\mathfrak{g}$ be the Lie algebra of G.

$\mathfrak{g}$ is a linear space. Let $e_1, \ldots, e_d$ be a basis for $\mathfrak{g}$.

We can define

$$E_i = \lambda_*(e_i), \quad i = 1, \ldots, d$$

If the action is transitive, then the spanning condition can be proven to hold, i.e. for every $m \in M$

$$\mathrm{span}\{E_1|_m, \ldots, E_d|_m\} = T_m M$$

More recently, it has become popular to replace both actions and frames with connections, we shall not pursue them here.

- In the RKMK methods we transformed the ODE (locally) from M to $\mathfrak{g}$ by using the map

$$\lambda_m(u) = \Lambda(\exp(u).m)$$

- exp can be expensive to compute, especially if we do not have a Rodrigues type formula at our disposal
- No other intrinsic maps than exp exists, but suppose we are allowed to introduce a basis for the Lie algebra, $e_1, \ldots, e_d$. We can use

$$\phi(\sum_i u_i e_i) = \exp(u_d e_d) \cdots \exp(u_2 e_2) \exp(u_1 e_1)$$

- Often much faster to calculate than $\exp(u)$
- Must replace $\mathrm{dexp}_u(v)$ with a corresponding $d\phi_u(v)$ that must be inverted. Can sometimes be done very efficiently, and closed form expressions can be obtained.

Some popular matrix Lie groups have a defining equation

$$G = \{g \in GL(n) : g^T J g = J, \quad \text{for some matrix } J$$

$SO(n)$ (special othogonal group)
$Sp(n)$ (symplectic group)
$SU(n)$ (special unitary group) (and several others)

For these cases, the Cayley transform $\mathrm{cay} : \mathfrak{g} \to G$

$$\mathrm{cay}(\xi) = (I - \tfrac{1}{2}\xi)^{-1}(I + \tfrac{1}{2}\xi)$$

One can easily calculate

$$d\mathrm{cay}_u^{-1}(v) = (I - \tfrac{u}{2})v(I + \tfrac{u}{2})$$

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