Lie Group Integrators – an introduction

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Example 1 – Problem on S^2 (the sphere)

$$\begin{aligned} \dot m_1 &= \alpha_1 m_2 m_3 \\ \dot m_2 &= \alpha_2 m_1 m_3 \\ \dot m_3 &= \alpha_3 m_1 m_2 \end{aligned} \quad , \qquad \alpha_1 + \alpha_2 + \alpha_3 = 0$$

First integral.

$$\mathcal{I}(m_1, m_2, m_3) = m_1^2 + m_2^2 + m_3^2.$$

Effectively, any conservative method acts by means of rotations.

Example 2 – Stiefel manifold

Let

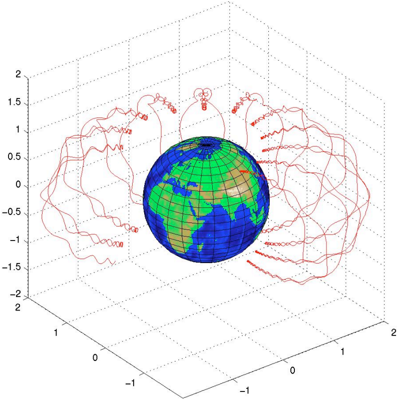
- $\mathcal{M}_{n,k}$ be the manifold of $n \times k$-matrices with orthonormal columns.
- $\mathfrak{so}(n)$ be the skew-symmetric $n \times n$-matrices, $A^T = -A$.

Consider matrix-differential equation

$$\dot{Y} = A(Y) \cdot Y, \quad A : \mathcal{M}_{n,k} \to \mathfrak{so}(n)$$

Invariant: $\mathcal{I}(Y) = Y^T Y$.
Applications

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



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 $\mathbf{x}$.

We take as example a non-homogeneous heat equation

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

Fast solvers are available for the equation

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

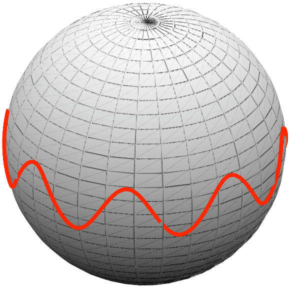
The first problem can be approximated locally by the second, e.g. set

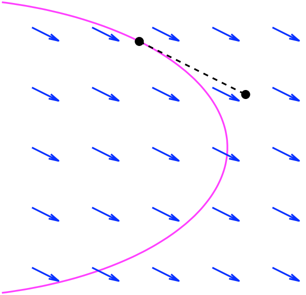
$$\bar{\nu} = \frac{\int \nu(\mathbf{x})\, \mathrm{d}\mathbf{x}}{\int \mathrm{d}\mathbf{x}}$$

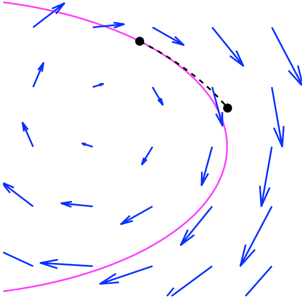
for a local known approximation $u^*(\cdot, t^*)$ let

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

- 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







- G: Lie group (manifold with smooth group structure)
- $\mathcal{M}$: Smooth manifold (could be G itself)

Left action: $\Lambda : G \times \mathcal{M} \to \mathcal{M}$

$$\begin{aligned} \Lambda(\mathrm{Id}, m) &= m, \qquad \forall m \in \mathcal{M} \\ \Lambda(g, \Lambda(h, m)) &= \Lambda(g \cdot h, m), \quad \forall g, h \in G,\ m \in \mathcal{M} \end{aligned}$$

Transitivity: $\Lambda(\cdot, m) : G \to \mathcal{M}$ onto for every $m \in \mathcal{M}$.

Orbit. $\mathcal{O}_m = \Lambda(G, m)$.

Let $\mathfrak{g} := T_{\mathrm{Id}}G$ and let $g(t)$ be any curve on G such that

$$g(0) = \mathrm{Id}, \quad \dot{g}(0) = v \in \mathfrak{g}$$

Then $\gamma(t) = \Lambda(g(t), m)$ is a curve on $\mathcal{M}$ such that

$$\gamma(0) = m, \quad \dot{\gamma}(0) := E_v(m) \in T_m\mathcal{M}$$

Thus, any $v \in \mathfrak{g}$ induces a vector field E_v on $\mathcal{M}$. One writes $E_v = \lambda_*(v)$.

Frame vector fields

A basis $\{v_1, \ldots, v_d\}$ for $\mathfrak{g}$, defines a frame, $\{E_1, \ldots, E_d\}$ on $\mathcal{M}$.

The space $\mathfrak{g} = T_{\mathrm{Id}}G$ is a linear space, but can also be used to "encode" the group operation of G.

Lie bracket (commutator)

Let $g(t)$ and $h(s)$ be two curves in G, satisfying $g(0) = h(0) = \mathrm{Id}$, $\dot{g}(0) = v$, $\dot{h}(0) = w$. Then

$$[v, w] := \frac{\partial}{\partial t}\bigg|_{t=0} \frac{\partial}{\partial s}\bigg|_{s=0} g(t)h(s)g(t)^{-1}$$

Example

The Lie algebra of a matrix group has commutator

$$[v, w] = vw - wv$$

Let $x_1, \ldots, x_\nu$ be local coordinates on $\mathcal{M}$. Vector fields $X, Y \in \mathcal{X}(\mathcal{M})$ can then be expressed as

$$X = (X_1, \ldots, X_\nu)^T, \quad Y = (Y_1, \ldots, Y_\nu)^T$$

The Lie-Poisson bracket between X and Y is $Z = (Z_1, \ldots, Z_\nu)$

$$Z_i = \sum_j \left(X_j \frac{\partial Y_i}{\partial x_j} - Y_j \frac{\partial X_i}{\partial x_j} \right)$$

Whenever $v, w \in \mathfrak{g}$ one has

$$\lambda_*([v, w]_{\mathfrak{g}}) = [\lambda_*(v), \lambda_*(w)]_{LP}$$

1. The boring one. Euclidean space $G = \mathbf{R}^d = \mathfrak{g}$ acts on itself ($\mathcal{M} = \mathbf{R}^d$) by addition. $\mathrm{Id} = \vec{0}$

$$\Lambda(g, x) = g + x, \quad E_k(m) = e_k$$

2. Matrix group acting on itself by left multiplication, $G \subseteq \mathbf{R}^{n \times n}$ (or $\mathbf{C}^{n \times n}$).

$$\Lambda : G \times G \to G, \quad \Lambda(g, h) = g \cdot h.$$

3. Orthogonal matrices $O(n)$ acting on symmetric matrices $\mathcal{S}_n$ by conjugation

$$\Lambda : O(n) \times \mathcal{S}_n \to \mathcal{S}_n, \quad \Lambda(Q, S) = QSQ^T$$

non-transitive.

Some matrix groups (and their Lie algebras)

Group	description	Algebra	description
$GL(n)$	All invertible $n \times n$ matrices	$\mathfrak{gl}(n)$	All $n \times n$ matrices
$SL(n)$	All $n \times n$ matrices with determinant 1	$\mathfrak{sl}(n)$	All trace free $n \times n$ matrices
$SO(n)$	$Q \in SL(n)$ s.t. $Q^T Q = I$	$\mathfrak{so}(n)$	All skew-symmetric $n \times n$ matrices
$SP(2n)$	$M \in SL(2n) : MJM^T = J$	$\mathfrak{sp}(2n)$	$A \in \mathfrak{sl}(2n) : AJ + JA^T = 0$

The flow of a vector field $F \in \mathcal{X}(\mathcal{M})$

is a one parameter family of maps

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

such that for any $m \in \mathcal{D}_t$,

$$\exp(tF)\, m = \gamma(t) \quad \text{where} \quad \dot{\gamma}(t) = F(\gamma(t)),\ \gamma(0) = m$$

Example

Matrix group: $G \subseteq GL(n)$,

$$F_A(g) = A \cdot g, \quad A \in \mathfrak{g},\ g \in G$$

$$\exp(tF_a)g = \mathtt{expm}(tA) \cdot g$$

Transitivity of group action implies

1. $\dim G = \dim \mathfrak{g} \geq \dim \mathcal{M}$
2. for any $m \in M$ one has $\lambda_*(\mathfrak{g})(m) = T_m\mathcal{M}$ or equivalently

$$\mathrm{span}(E_1(m), \ldots, E_d(m)) = T_m\mathcal{M}$$

ODE is a smooth vector field F on $\mathcal{M}$, $F \in \mathcal{X}(\mathcal{M})$. It follows that for any such F

1. There exists a map $f : \mathcal{M} \to G$ such that $F(m) = \lambda_*(f(m))$
2. There exist functions $f_1, \ldots, f_d$, each $f_i : \mathcal{M} \to \mathbf{R}$ such that

$$F(m) = \sum_{k=1}^{d} f_k(m) E_k(m)$$

Let $V_{\mathfrak{g}} \subset \mathcal{X}(\mathcal{M})$ be the linear space

$$V_{\mathfrak{g}} = \mathrm{span}_{\mathbf{R}}(E_1, \ldots, E_d)$$

Freeze operator $\mathrm{Fr} : \mathcal{M} \times \mathcal{X}(\mathcal{M}) \to V_{\mathfrak{g}}$

$$\mathrm{Fr}(m, F) = \sum_k f_k(m) E_k$$

Example

$$F(y) = A(y) \cdot y, \quad \mathrm{Fr}(m, F)(y) = A(m) \cdot y$$

- The most well-known Lie group integrators include flows of "arbitrary" vector fields in $V_{\mathfrak{g}}$.
- It is not necessary that $V_{\mathfrak{g}}$ is closed under the Lie-Poisson bracket, i.e. forms a Lie algebra. A linear space is sufficient.
- If $V_{\mathfrak{g}}$ is not a Lie algebra, then some Lie group integrators will assume that flows can be computed (exactly) for arbitrary vector fields in the smallest Lie algebra containing $\mathfrak{g}$.
- Exact flow calculations may sometimes be replaced by other maps which are cheaper to compute.

Let $E_1, \ldots, E_d$ be a frame on $\mathcal{M}$ and suppose that an ODE on $\mathcal{M}$ can be written in the form

$$\dot{y} = F(y) = \sum_k f_k(y)\, E_k(y)$$

Suppose that an approximation y_n to $y(t_n)$ is given.

$$y_{n+1} = \exp(\Delta t\, \mathrm{Fr}(y_n, F)) \cdot y_n$$

Example

$$\dot{y} = A(y) \cdot y, \quad y_{n+1} = \mathtt{expm}(\Delta t\, A(y_n)) \cdot y_n$$

Write $\vec{m} = (m_1, m_2, m_3)^T$.

$$\begin{aligned} \dot{m}_1 &= \alpha_1 m_2 m_3 \\ \dot{m}_2 &= \alpha_2 m_1 m_3 \\ \dot{m}_3 &= \alpha_3 m_1 m_2 \end{aligned} \quad , \quad \Rightarrow \quad \dot{\vec{m}} = \begin{bmatrix} 0 & \frac{m_3}{I_3} & -\frac{m_2}{I_2} \\ -\frac{m_3}{I_3} & 0 & \frac{m_1}{I_1} \\ \frac{m_2}{I_2} & -\frac{m_1}{I_1} & 0 \end{bmatrix} \cdot \vec{m}$$

Here we take

G: $SO(3)$ (orthogonal, $\det 1$)

$\mathfrak{g}$: $\mathfrak{so}(3)$, skew-symmetric

$\mathcal{M}$: S^2 (sphere)

Λ: $SO(3) \times SO(3) \to S^2$, $\Lambda(g, \vec{m}) = g \cdot \vec{m}$

$$\vec{m}_{n+1} = \mathtt{expm}(A(\vec{m}_n)) \cdot \vec{m}_n$$

$$
\begin{aligned}
k_1 &= \mathrm{Fr}(y_n, F) \\
k_2 &= \mathrm{Fr}(\exp(\Delta t\, k_1)\, y_n, F) \\
y_{n+1} &= \exp(\frac{\Delta t}{2}(k_1 + k_2)))y_n
\end{aligned}
$$

is of second order. However, generalizing RK as follows

$$
\begin{aligned}
&Y_r = \exp(\Delta t \textstyle\sum_j a_r^j k_j)\, y_n, \quad k_r = \mathrm{Fr}(Y_r, F) \\
&y_{n+1} = \exp(\Delta t \textstyle\sum_r b^r k_r)\, y_n
\end{aligned}
$$

leads to schemes of order at most 2.

The stage vector fields k_r belong to a Lie algebra (under the Lie-Poisson bracket). It may be included as part of the scheme

$$Y_r = \exp(\Delta t \sum_j a_r^j k_j)\, y_n, \quad \tilde{k}_r = \mathrm{Fr}(Y_r, F)$$
$$k_r = \tilde{k}_r + \Delta t \sum_j \gamma_r^j [\tilde{k}_r, \tilde{k}_j] + \dots$$
$$y_{n+1} = \exp(\Delta t \sum_r b^r k_r)\, y_n$$

By a careful choice of correction terms, arbitrary order can be obtained (also for explicit schemes).

One can also replace the one exponential with compositions. (Celledoni, O, Marthinsen, 2003)

$$
\begin{aligned}
&Y_r = \exp(\Delta t \textstyle\sum_j \alpha_{q,r}^j k_j) \cdots \exp(\Delta t \textstyle\sum_j \alpha_{1,r}^j k_j)\, y_n,\\
&k_r = \mathrm{Fr}(Y_r, F),\\
&y_{n+1} = \exp(\Delta t \textstyle\sum_r \beta_q^r k_r) \cdots \exp(\Delta t \textstyle\sum_r \beta_1^r k_r)\, y_n.
\end{aligned}
$$

4th order RKMK scheme (Munthe-Kaas & O, 1999)

$$
\begin{aligned}
Y_1 &= y_n, & k_1 &= \mathrm{Fr}(Y_1, F),\\
Y_2 &= \exp(\tfrac{\Delta t}{2} k_1)\, y_n, & k_2 &= \mathrm{Fr}(Y_2, F),\\
Y_3 &= \exp(\tfrac{\Delta t}{2} k_2 - \tfrac{\Delta t^2}{8}[k_1, k_2])\, y_n, & k_3 &= \mathrm{Fr}(Y_3, F),\\
Y_4 &= \exp(\Delta t\, k_3)\, y_n, & k_4 &= \mathrm{Fr}(Y_4, F),
\end{aligned}
$$

$$
\begin{aligned}
v &= \tfrac{\Delta t}{6}(k_1 + 2k_2 + 2k_3 + k_4) - \tfrac{\Delta t^2}{12}[k_1, k_4] \qquad ,\\
y_{n+1} &= \exp(v)\, y_n.
\end{aligned}
$$

4th order CFREE scheme (Celledoni, O, Marthinsen, 2003)

$$\begin{aligned}
Y_1 &= y_n, & k_1 &= \mathrm{Fr}(Y_1, F),\\
Y_2 &= \exp(\tfrac{\Delta t}{2} k_1)\, y_n, & k_2 &= \mathrm{Fr}(Y_2, F),\\
Y_3 &= \exp(\tfrac{\Delta t}{2} k_2)\, y_n & k_3 &= \mathrm{Fr}(Y_3, F),\\
Y_4 &= \exp(\Delta t\, (k_3 - \tfrac{1}{2} k_1))\, Y_2, & k_4 &= \mathrm{Fr}(Y_4, F),\\
y_{n+\frac{1}{2}} &= \exp(\tfrac{\Delta t}{12}(3k_1 + 2k_2 + 2k_3 - k_4))\, y_n & & ,\\
y_{n+1} &= \exp(\tfrac{\Delta t}{12}(-k_1 + 2k_2 + 2k_3 + 3k_4))\, y_{n+\frac{1}{2}} & & .
\end{aligned}$$

Note the reuse of Y_2 in Y_4.

The schemes of Munthe-Kaas may be derived by

1. making the ansatz

$$y(t) = \Lambda(\exp(\sigma(t)), y_n), \qquad \sigma(0) = 0$$

   where $\sigma(t)$ is a curve in $\mathfrak{g}$, and $\exp$ is now the map from the Lie algebra to the Lie group.
2. deriving a differential equation for σ, ($\dot{\sigma} = \cdots$), and solving with a standard (RK)-method as a DE in the linear space $\mathfrak{g}$.
3. transforming back to $\mathcal{M}$ setting $y_{n+1} = \Lambda(\exp(\Delta t\, \sigma_1), y_n)$.

- The procedure involves the derivative of the exponential mapping.
- It has an infinite expansion in commutators, which can be truncated.
- It is from here the commutators of RKMK stem.

One can think of $\exp : \mathfrak{g} \to G$ as a coordinatization of the Lie group G in a patch containing the identity element.
Idea: Replace $\exp$ by other (differentiable) map $\phi : \mathfrak{g} \to G$ and write

$$y(t) = \Lambda(\phi(\sigma(t)), y_n)$$

follow thereafter the above procedure. One would ask for ϕ to

1. be exactly computable, at least to roundoff level.
2. be inexpensive to compute (at least compared to $\exp$)
3. have a (trivialized) derivative map which can be inverted inexpensively, not necessarily exactly as long as it maps $\mathfrak{g}$ to $\mathfrak{g}$

1. Canonical coordinates of the second kind. Let $v_1, \dots, v_d$ be a basis for $\mathfrak{g}$.

$$\phi_2(\alpha_1 v_1 + \cdots + \alpha_d v_d) = \exp(\alpha_1 v_1) \cdots \exp(\alpha_d v_d)$$

   Its derivative map can be inverted by exploiting the structure theory for Lie algebras (O&Marthinsen, 1999).

2. For some matrix Lie groups, the Cayley transform is highly efficient

$$\phi_c(v) = (I - v)^{-1}(I + v)$$

   Its derivative map is easy to derive and compute

3. The notion of retractions or tangent space parametrizations has been used in papers by Celledoni et al.

Recall the previous example of the free rigid body

$$\dot{\vec{m}} = \begin{bmatrix} 0 & \frac{m_3}{I_3} & -\frac{m_2}{I_2} \\ -\frac{m_3}{I_3} & 0 & \frac{m_1}{I_1} \\ \frac{m_2}{I_2} & -\frac{m_1}{I_1} & 0 \end{bmatrix} \cdot \vec{m}$$

Can write $\dot{\vec{m}} = I^{-1}\vec{m} \times \vec{m}$. But since $\vec{m} \times \vec{m} = 0$, we can also write

$$\dot{\vec{m}} = (I^{-1}\vec{m} + g(\vec{m}) \cdot \vec{m}) \times \vec{m}$$

for an arbitrary function $g : S^2 \to \mathbf{R}$.

The choice of $g(\vec{m})$ does however affect the Lie group integrator.

To types of approaches have been studied in the literature

1. The freedom comes from the fact that the Lie group is "larger" than the manifold. One may restrict the action to a subspace of the Lie algebra. Reduces computational cost. (Celledoni & O, Krogstad ++)
2. One may make use of the extra freedom to improve the approximation. Some nice ideas suggested in (Lewis and Olver).

- Lie group integrators can be designed to preserve invariants by forcing the orbits of the group action to be contained in level sets of the invariant, but can freedom in coefficients further enhance the preservation of first integrals?
- Currently no non-trivial symplectic or volume-preserving Lie group integrators are known, but some progress recently by Munthe-Kaas.
- The problem of dealing with isotropy is still wide open, some recent progress indicates that by understanding how to deal with isotropy, we can also understand how to find non-trivial symplectic/volume preserving LGIs
- Many applications involve the orthogonal group, what about other Lie groups. We know that there is a very rich selection of group actions, we all seem to be a bit too attached to matrix$\times$matrix or matrix$\times$vector actions.
- Applying LGIs to PDEs is relatively new, exponential integrators constitute one example. Difficulty: Discretization of infinite-dimensional Lie algebras.

Thank you for listening!