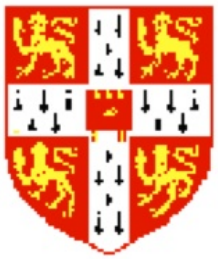

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Lie-group methods in geometric numerical integration

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OUTLINE

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1. Why geometric numerical integration?

A classical paradigm of applied mathematics:

Do rigorous, pure mathematics as far as it goes. Determine qualitative features of your problem. And then, when you've exhausted the power of analysis, resort to computation.

The problem: having spent great effort and ingenuity on finding precise qualitative information on the behaviour of our problem, which often has deep physical significance, we produce numerical solution that does not respect this qualitative information.

Invariants and geometry represent important qualitative information about the differential system: it is often vital to respect them under discretization. **This means designing numerical methods that share qualitative features of the differential system.**

This is precisely the purpose of ***geometric numerical integration (GNI)***.

Major themes in GNI:

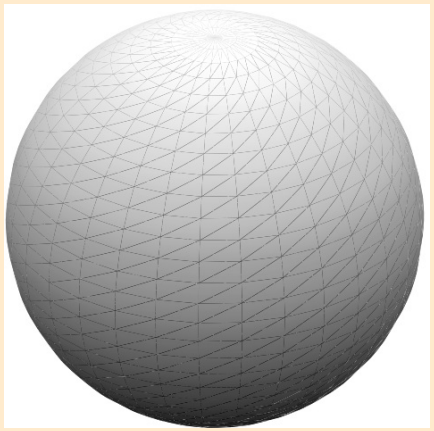
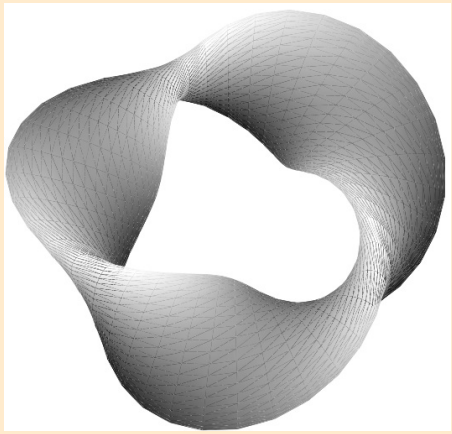
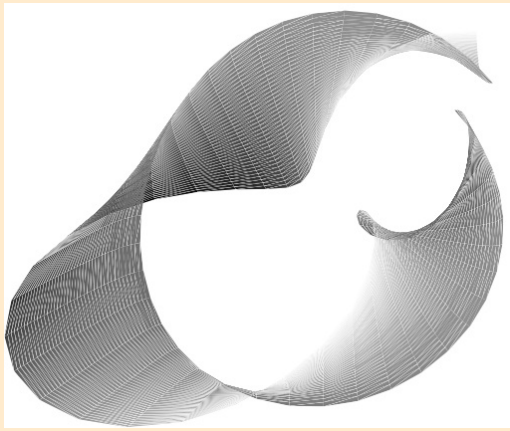
- Symplectic methods for DEs with Hamiltonian structure
  (Bennetin, Feng Kang, Gorgili, Hairer, Leimkuhler, Lubich, Newton, Sanz-Serna, Scovel, Störmer, Verlet, de Vogelaerre, . . .)
- Volume and energy conservation in DEs
  (Celledoni, Chartier, Feng Kang, McLachlan, Owren, Quispel, . . .)
- Methods respecting Lie-Poisson structure
  (Faltinsen, Leok, Lewis, Marsden, Ratiu, Simo, . . .)
- Methods replacing symplectic structure by a 'nearby' symplectic structure
  (Bridges, Hong, Leok, Marsden, Moser, Reich, Veselov, . . .)
- Methods for problems evolving on a differentiable manifold, in particular on a homogeneous manifold
  (Blanes, Casas, Crouch, AI, Munthe-Kaas, Nørsett, Owren, Zanna, . . .)

Major techniques in GNI:

- Identification of ‘classical’ methods that retain geometric invariants
  (Murua, Sanz-Serna, Scovel, Skeel,. . .)
- Splitting and composition methods
  (Blanes, Casas, McLachlan, Murua, Quispel, Sanz-Serna, Suzuki, Yošida, . . .)
- Backward error analysis
  (Bennetin, Gorgili, Hairer, Lubich, Naishtadt, Reich, . . .)
- Clever asymptotic expansions
  (Cohen, Hairer, Lubich)
- Structure-preserving projection techniques
  (Calvo, Hairer, AI, Lubich, Zanna, . . .)
- Trivializations, group actions and Lie-algebraic techniques
  (Blanes, Casas, Celledoni, Crouch, AI, Lewis, Munthe-Kaas, Nørsett, Oteo, P. Olver, Owren, Simo, Zanna, . . .)
- Ideas from abstract algebra and combinatorics
  (Bogfjellmo, Chartier, Ebrahimi-Fard, Hairer, AI, Munthe-Kaas, Murua, Owren, Quispel, Verdier, Vilmart, Zanna, . . .)

2. Elements of differential geometry

An analytic manifold is an analytic domain, embedded in an Euclidean space, which locally 'looks like' an Euclidean space: more formally, it can be covered by an atlas composed of local coordinate charts.* Conceptually, think of

A tangent vector at $p \in \mathcal{M}$ is $\mathrm{d}\rho(t)/\mathrm{d}t|_{t=0}$, where $\rho(t) \in \mathcal{M}$ is a smooth curve s.t. $\rho(0) = p$.

The linear space of all tangents at p is the tangent space $\mathsf{T}\mathcal{M}|_p$, while

$$\mathsf{T}\mathcal{M} = \cup_{p\in\mathcal{M}} \mathsf{T}\mathcal{M}|_p$$

is the tangent bundle.

*This is not the most abstract definition – but is (non-trivially) equivalent to it.

The cotangent space $\mathsf{T}^\star\mathcal{M}|_p$ consists of all linear functionals acting on elements of $\mathsf{T}\mathcal{M}|_p$.

Differential equations and tangents

A vector field on a manifold $\mathcal{M}$ is a smooth function $F(p) \in \mathsf{T}\mathcal{M}|_p$, $p \in \mathcal{M}$.

The set of all vector fields over $\mathcal{M}$ is denoted by $\mathfrak{X}(\mathcal{M})$ and is a linear space.

The differential equation

$$y' = F(y), \quad t \geq 0, \qquad y(0) = y_0 \in \mathcal{M},$$

where $F \in \mathfrak{X}(\mathcal{M})$, evolves on the manifold $\mathcal{M}$.

The flow of this DE is denoted by

$$y(t) = \Psi_{t,F}(y_0), \qquad t \geq 0.$$

Therefore

$$F(y) = \frac{\mathrm{d}}{\mathrm{d}t}\Psi_{t,F}(y_0)|_{t=0}.$$

In other words, F is the infinitisimal generator of the flow.

Noting that $\Psi_{\alpha,F} = \Psi_{1,\alpha F}$, we define

$$\Psi_{1,F} = \exp(F), \qquad \text{hence} \qquad \exp(tF) = \Psi_{t,F}.$$

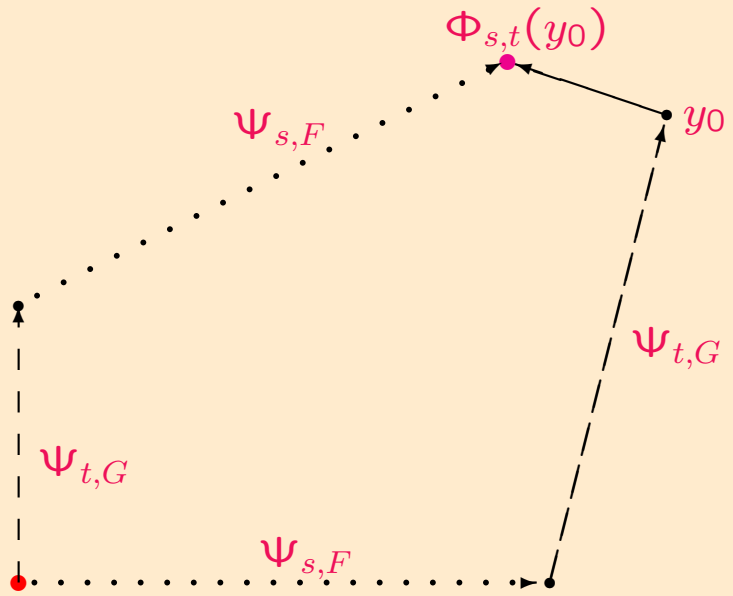
This is the exponential map.*

In general, flows fail to commute. Thus, let

$$\Phi_{s,t} = \exp(sF) \circ \exp(tG) \circ \exp(-sF) \circ \exp(-tG).$$

*This 'exponential map' should not be confused with the concept of a semigroup in PDE theory, although at a deeper abstract level the two share *some* features!

If flows commute then $\Phi_{s,t}(y) = y$, but this isn't in general true.



The local measure of this breakdown in commutativity is the Poisson bracket $H = \{F, G\}$ where (translating to the standard Euclidean coordinates in $\mathbb{R}^n$)

$$H_i(y) = \sum_{j=1}^{n} \left\{ G_j(y) \frac{\partial F_i(y)}{\partial y_j} - F_j(y) \frac{\partial G_i(y)}{\partial y_j} \right\}.$$

Note that for every $F, G, H \in \mathfrak{X}(\mathcal{M})$ and scalar α we have the following features of the bracket operation:

Skew symmetry: $\{F, G\} = -\{G, F\}$;

Bilinearity:

$$\{\alpha F, G\} = \alpha\{F, G\},$$
$$\{F + G, H\} = \{F, H\} + \{G, H\};$$

The Jacobi identity

$$\{F, \{G, H\}\} + \{G, \{H, F\}\} + \{H, \{F, G\}\} = 0.$$

Therefore, $\{\,\cdot\,,\,\cdot\,\}$ is a commutator and $\mathfrak{X}(\mathcal{M})$ is a Lie algebra.

In the important case of linear DE $y' = ay$ (where a is a matrix) we have $\Psi_{t,F}(y) = \exp(ta)y_0$, with the familiar matrix exponential

$$\mathrm{e}^{ta} = \sum_{m=0}^{\infty} \frac{1}{m!} t^m a^m.$$

In that case $\{a, b\} = [a, b] = ab - ba$.

Examples of manifolds:

- The graph $(\boldsymbol{x}, \boldsymbol{f}(\boldsymbol{x}))$, $\boldsymbol{x} \in X$, where $\boldsymbol{f} : X \to Y$ is smooth;
- The sphere $\mathbb{S}_n \subset \mathbb{R}^n$: $\boldsymbol{x} \in \mathbb{R}^n$ s.t. $\|\boldsymbol{x}\| = 1$;
- The (topological) torus $\mathbb{T}_n \subset \mathbb{R}^n$: $\boldsymbol{x} \in \mathbb{R}^n$ which are 1-periodic in each coordinate;
- The orthogonal group $\mathrm{O}(n)$ of $n \times n$ orthogonal matrices;
- The Grassmannian $\mathrm{G}_{n,m}$ of real $n \times m$ matrices, $m \leq n$, consisting of unit-length columns that are orthogonal to each other and equivalenced by orthogonal transformations;
- The isospectral orbit $\mathbb{I}_n(y_0)$ of all $n \times n$ symmetric matrices which are similar to the symmetric matrix y_0;
- The projective space $\mathbb{P}^n$ of all lines in $\mathbb{R}^n$ that pass through the origin.

Lie groups

Lie group $\mathcal{G}$ is an analytic manifold, endowed with group structure which is analytic with respect to the topology of the manifold.*

$\mathsf{O}(n,\mathbb{R})$: real $n \times n$ orthogonal matrices (*the orthogonal group*);

$\mathsf{SL}(n,\mathbb{R})$: real $n \times n$ matrices with unit determinant (the *special linear group*);

$\mathsf{SU}(n,\mathbb{C})$: complex $n \times n$ unitary matrices with unit determinant (the *special unitary group*);

$\mathsf{SO}(n,m,\mathbb{R})$: real $n \times n$ matrices a s.t. $apa^{\top} = p$, $p = \mathsf{diag}\,[\mathbf{1}_m, -\mathbf{1}_{n-m}]$, with unit determinant. ($n = 4$, $m = 1$: the Lorenz group);

$\mathsf{E}(n,\mathbb{R})$: The Euclidean group of all translations and length-preserving linear transformations in $\mathbb{R}^n$;

$\mathsf{A}(n,\mathbb{R})$: The affine group of all translations and area-preserving linear transformations in $\mathbb{R}^n$.

*Not to be confused with a topological group.

Why are Lie groups useful?

Lie groups are important since they provide an appropriate formalism to investigate symmetries, invariants and qualitative behaviour of differential equations.

There are many other good reasons why Lie groups are important. We'll see one (group actions on manifolds) but there are many others, not least in theoretical physics (string theory), number theory (the proof of FLT) and group theory (classification of finite groups).

Many physical laws are conveniently formulated with built-in Lie-group symmetries.

For example, laws of motion have $\mathrm{SO}(3)$ symmetry, $\mathrm{A}(3)$ is important in computer vision, equations of special relativity evolve in $\mathrm{SO}_{4,1}$ and theory of superstrings can be formulated in $\mathrm{SU}(32)$ and in $\mathrm{E}(8) \times \mathrm{E}(8)$.*

A finite-dimensional Lie group can be usually (but not always!) represented as a subgroup of the set of $n \times n$ nonsingular square matrices, $\mathrm{GL}_n[\mathbb{F}]$, for some $n \geq 1$ and a field $\mathbb{F}$. Such groups are called *matrix Lie groups.*

*This $\mathrm{E}(8)$ is not the Euclidean group but an exponential of the exceptional Lie algebra $\mathfrak{E}(8)$.

The tangent space of a Lie group

Let $\mathcal{G}$ be a Lie group and $\mathfrak{g} = \mathsf{T}\mathcal{G}|_I$ the tangent space at identity. Since $\mathcal{G}$ is a group, it follows at once that

$$\mathsf{T}\mathcal{G}|_X = \mathfrak{g}X \qquad \text{for all} \qquad X \in \mathcal{G}.$$

Since (as we have already seen) there is a natural isomorphism between (finite-dimensional) linear vector fields and square matrices, we deduce that

- $\mathfrak{g}$ is a Lie algebra (cf. next slide)
- The exponential map is the classical matrix exponential.
- Let ρ and σ be smooth curves on $\mathcal{G}$ s.t. $\rho(t) = I + ta + \cdots$ and $\sigma(t) = I + tb + \cdots$. Then $a, b \in \mathfrak{g}$ and

$$\{a, b\} = \frac{\partial^2}{\partial t \partial s} \rho(s)\sigma(t)\rho(-s)|_{t=s=0} = ab - ba = [a, b].$$

Lie algebras

We say that the abstract set $\mathfrak{g}$ is a Lie algebra if it is a linear space, which in addition is closed under the binary operation $[\,\cdot\,,\,\cdot\,] : \mathfrak{g} \times \mathfrak{g} \to \mathfrak{g}^*$ which obeys the following axioms:

1. Linearity: For every $a, b, c \in \mathfrak{g}$ and scalars α, β it is true that

$$[\alpha a + \beta b, c] = \alpha[a, c] + \beta[b, c].$$

2. Skew-symmetry: For every $a, b \in \mathfrak{g}$

$$[a, b] = -[b, a].$$

3. The Jacobi identity:† For every $a, b, c \in \mathfrak{g}$

$$[[a, b], c] + [[b, c], a] + [[c, a], b] = 0.$$

Lie algebras can be fairly strange objects and not all of them originate as tangent spaces of Lie groups.

*Hence, a non-associative algebra.

†Little known (and completely irrelevant) factoid: Sophus Lie and Carl Gottfried Jacobi both died on 18th February. (48 years apart.)

Examples of Lie algebras

1. Lie group: $\mathsf{O}(n,\mathbb{R}), \mathsf{SO}(n,\mathbb{R})$
   Lie algebra: The set $\mathfrak{so}(n,\mathbb{R})$ of real $n \times n$ skew symmetric matrices;

2. Lie group: $\mathsf{SL}(n,\mathbb{R})$:
   Lie algebra: The set $\mathfrak{sl}(n,\mathbb{R})$ of real $n \times n$ matrices with zero trace;

3. Lie group: $\mathsf{SO}(n,m,\mathbb{R})$:
   Lie algebra: The set $\mathfrak{so}(n,m,\mathbb{R})$ of real $n \times n$ matrices a such that $ap + pa^\top = 0$, where $p = \mathsf{diag}[1_m, -1_{n-m}]$. With greater generality, for any nonsingular symmetric p and the quadratic Lie group

$$\{x \in \mathsf{GL}(n,\mathbb{R}) \,:\, xpx^\top = p\}$$

   the corresponding Lie algebra is

$$\{a \in \mathfrak{gl}(n,\mathbb{R}) \,:\, ap + pa^\top = 0.$$

Group actions

An action of a Lie group $\mathcal{G}$ on a manifold $\mathcal{M}$ is a smooth map $\Lambda : \mathcal{G} \times \mathcal{M} \to \mathcal{M}$ s.t.

$$\begin{aligned} &\Lambda(I, y) = y, \qquad y \in \mathcal{M}, \\ &\Lambda(p, \Lambda(q, y)) = \Lambda(pq, y), \qquad p, q \in \mathcal{G},\ y \in \mathcal{M}. \end{aligned}$$

- Each group acts on itself;
- $\mathrm{O}(n, \mathbb{R})$ acts on on the sphere $\mathbb{S}_n$, $\Lambda(p, y) = py$;
- $\mathrm{SO}(n, \mathbb{R})$ acts on the Grassmannian

$$\mathbb{G}(n, m) = \mathrm{S}(n)/(\mathrm{SO}(m) \times \mathrm{SO}(n - m))$$

- . . . and on the isospectral orbit $\mathbb{I}_n(y_0)$ via

$$\Lambda(p, y) = pyp^{-1}.$$

As a matter of fact, all previous examples of manifolds are subject to transitive group action: every point in $\mathcal{M}$ is reachable from any other point via the group action. In that case $\mathcal{M}$ is a homogeneous manifold.

Differential equations and group actions

Given a homogeneous manifold $\mathcal{M}$ and a group action Λ we define $\lambda_* : \mathfrak{g} \to \mathfrak{X}(\mathcal{M})$ as

$$\lambda_*(a)(y) = \frac{\mathrm{d}}{\mathrm{d}s}\Lambda(\rho(s), y)|_{s=0},$$

where $\rho(s) = I + as + \cdots$ is a smooth curve in $\mathcal{G}$.

Suppose that $\mathcal{G}$ is a matrix group. Then, for $a \in \mathfrak{g}$ the flow of λ_*, i.e.

$$y' = \lambda_*(a)(y), \quad t \geq 0, \qquad y(0) = y_0 \in \mathcal{M},$$

can be expressed in the form

$$y(t) = \Lambda(s(t), y_0), \qquad t \geq 0,$$

where

$$s' = as, \quad t \geq 0, \qquad s(0) = I.$$

This can be generalized from fixed $a \in \mathfrak{g}$ to a sufficiently smooth function $a : \mathbb{R}_+ \times \mathcal{M} \to \mathfrak{g}$: The solution of the differential equation

$$y' = \lambda_*(a(t, y))(y), \quad t \geq 0, \qquad y(0) = y_0 \in \mathcal{M},$$

can be represented as $y(t) = \Lambda(s(t), y_0)$, where

$$s' = a(t, \Lambda(s, y_0))s, \quad t \geq 0, \qquad s(0) = I,$$

evolves in $\mathcal{G}$.

Therefore,

instead of solving the equation in $\mathcal{M}$, i.e. finding y_{N+1} given y_N, say, find a group action that takes y_N to y_{N+1}.

We conclude that

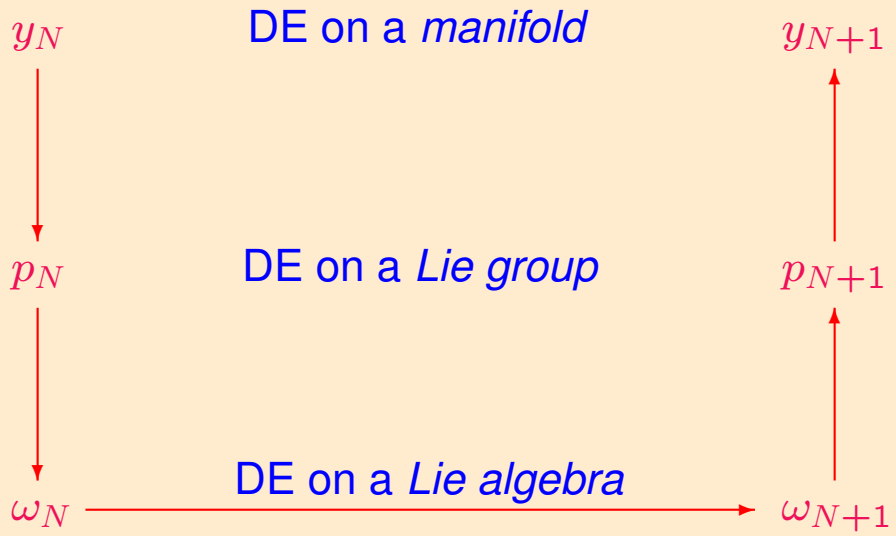
if we can devise a numerical method that respects a Lie-group structure then it can be extended to respect every homogeneous manifold structure acted upon by that group.

The main paradigm of Lie-group methods

Instead of a group action, we can consider an algebra action. Specifically, if $\mathcal{G} \ni x = \mathrm{e}^v$, where $v \in \mathfrak{g}$, then define $\mu(v, y) = \Lambda(\mathrm{e}^v, y) = \Lambda(x, y)$. Note that this is less general than a group action: it is entirely possible that there is no single $v \in \mathfrak{g}$ s.t. $x = \mathrm{e}^v$, although in a finite-dimensional $\mathcal{G}$ there always exist $v_1, v_2, \ldots, v_r \in \mathfrak{g}$ s.t. $x = \mathrm{e}^{v_1} \cdots \mathrm{e}^{v_r}$. Another way of saying this is that we *might* need to restrict the step size, although no such examples have arisen in practice.

For example, each element of $\mathrm{SL}(2)$ can be obtained as a product of at most two exponentials of elements from $\mathfrak{sl}(2)$.

We follow the pattern



Some Lie-group methods do not follow this pattern:

- The method of Crouch & Grossman represents the equation in the form $y' = \sum_{l=1}^{d} \alpha_l(t) q_l$, using a rigid frame $q_l \in \mathsf{T}\mathcal{M}|_y$, $l = 1, \ldots, d$, and composes the solution from one-dimensional 'steps'.

- The method of McLachlan, Quispel & Robidoux represents the equation in the skew-gradient form $y' = S(t, y)\nabla g(y)$, where S is skew-symmetric, and suitably discretizes the gradient.

- The approach of cannonical coordinates of the second kind (Marthinsen & Owren) writes

$$\mathcal{G} \ni y(t) = \mathrm{e}^{\theta_1(t)\phi_1}\mathrm{e}^{\theta_2(t)\phi_2}\ldots\mathrm{e}^{\theta_d(t)\phi_d}y_0,$$

  where $\dim \mathfrak{g} = d$, $\{\phi_1, \ldots, \phi_d\}$ is a basis of $\mathfrak{g}$ and $\theta_1, \ldots, \theta_d$ are scalar functions. It is then possible to derive differential equations for the unknowns θ_k. The CCSK approach is particularly useful when the basis corresponds to the root space decomposition of $\mathfrak{g}$, since this simplifies the equations a great deal.

3. The exponential and trivializations

With greater generality, an equation evolving on a homogeneous manifold $\mathcal{M}$ can be written in the form

$$y' = \mu_*(a(t,y))(y), \quad t \geq 0, \qquad y(0) = y_0 \in \mathcal{M},$$

where the function $\mu_* : \mathfrak{g} \to \mathfrak{X}(\mathcal{M})$ is a Lie-algebra homomorphism, $\mathfrak{X}(\mathcal{M})$ is the set of vector fields on $\mathcal{M}$ and $a : [0,\infty) \times \mathcal{M} \to \mathfrak{g}$.

Many such ODEs occur in applications – grouped by Lie groups,

$\mathrm{O}(n,\mathbb{R})$ *(Orthogonal group)*: mechanical systems, robotics, computer vision, computation of Lyapunov exponents, isospectral flows, numerical linear algebra;

$\mathrm{SL}(n,\mathbb{R})$ *(Special linear group)*: conservation of volume, Riccati systems, Sturm–Liouville problems, image processing;

$\mathrm{Sp}(n,\mathbb{R})$ *(Symplectic group)*: Hamiltonian and Lie–Poisson systems;

$\mathrm{SO}(1,3)$ *(Lorenz group)*: relativity theory (also $\mathrm{SO}(2,5)$);

$\mathrm{SU}(n,\mathbb{C})$ *(Unitary group)*: quantum mechanics.

Example 1: 'Classical' Lie-group equations:

$$y' = a(t, y)y, \quad t \geq 0, \qquad y(0) = y_0 \in \mathcal{G},$$

where $a : [0, \infty) \times \mathcal{G} \to \mathfrak{g}$.

Example 2: Isospectral flows (a.k.a. Lax pairs):

$$y' = [b(t, y), y], \quad t \geq 0,$$

where $y(0) = y_0 \in \mathrm{Sym}_n[\mathbb{R}]$ and $b : [0, \infty) \times \mathbb{I}[y_0] \to \mathfrak{so}(n, \mathbb{R})$.

Example 3: Equations on a sphere:

$$\boldsymbol{y}' = \boldsymbol{a}(t, \boldsymbol{y}) \times \boldsymbol{y}, \quad t \geq 0, \qquad \boldsymbol{y}(0) = \boldsymbol{y}_0 \in \mathbb{S}_2,$$

where $\boldsymbol{a} : [0, \infty) \times \mathbb{S}_2 \to \mathbb{R}^3$ and $\times$ is a vector product. E.g., the Lagrange spinning top equations of a rigid body in body coordinates are

$$\boldsymbol{\Pi}_b' = \boldsymbol{\Pi}_b \times \boldsymbol{\Omega}_b + mg\,l\,\boldsymbol{\Gamma}_b \times \boldsymbol{\chi}, \quad \boldsymbol{\Gamma}_b' = \boldsymbol{\Gamma}_b \times \boldsymbol{\Omega}_b,$$

where $\boldsymbol{\Pi}_b$ is angular momentum, $\boldsymbol{\Omega}_b$ the angular velocity ($\boldsymbol{\Omega}_b = I_b^{-1}\boldsymbol{\Pi}_b$, I_b the inertia tensor) and $\boldsymbol{\Gamma}_b$ the gravity, while m is the mass, g the gravitational constant, l the distance between the centre of mass and the centre of frame of reference and $\boldsymbol{\chi}$ the unit vector on the body axis.

Trivialization

We solve homogeneous-manifold equations by five conceptual steps, to be implemented in every time step,

1. Transform the equation from $\mathcal{M}$ to $\mathcal{G}$;
2. Transform the equation from $\mathcal{G}$ to $\mathfrak{g}$;
3. Discretize the equation in $\mathfrak{g}$;
4. Transform the outcome from $\mathfrak{g}$ to $\mathcal{G}$;
5. Transform the outcome from $\mathcal{G}$ to $\mathcal{M}$.

The advantage of this approach is that

while in general M is *nonlinear*, the Lie algebra $\mathfrak{g}$ is a *linear space.* As long as we discretize there with just linear operations and commutators, we are bound to respect its structure!

Steps 1 and 5 are already clear from our discussion, at present we focus on steps 2–4.

A trivialization is a smooth mapping $\Phi : \mathfrak{g} \to \mathcal{G}$ such that $\Phi(0) = I$. The main idea is change variables $p \to \omega$, where ω evolves in $\mathfrak{g}$,

$$p(t) = \Phi(\omega(t)), \qquad t \geq 0$$

and replace the equation for p by the Lie-algebraic equation for ω.

Formally,

$$\begin{aligned} & p' = a(t,p)p = \mathrm{d}\Phi(\omega, \omega') \\ \Rightarrow \quad & \omega' = \mathrm{d}\Phi_\omega^{-1} a(t,p) \\ \Rightarrow \quad & \omega' = \mathrm{d}\Phi_\omega^{-1} a(t, \Phi(\omega)), \end{aligned}$$

with the initial condition $\omega(0) = 0$.

Note that a trivialization might be valid only in (hopefully, large) neighbourhood of the origin: this represents a possible restriction on the step size of the discretization method.

An obvious (and most useful) trivialization is exponentiation,

$$p(t) = \mathrm{e}^{\omega(t)} p_N.$$

The outcome is the *dexpinv equation*

$$\omega' = \mathrm{dexp}_\omega^{-1} a = \sum_{m=0}^{\infty} \frac{\mathrm{B}_m}{m!} \mathrm{ad}_\omega^m a, \qquad \omega(t_N) = 0$$

(Hausdorff), where

$$\mathrm{ad}_\omega^0 a = a, \qquad \mathrm{ad}_\omega^m a = \overbrace{[\omega, [\omega, \ldots, [\omega}^{m \text{ times}}, a] \cdots]], \quad m \in \mathbb{N},$$

and $\{\mathrm{B}_m\}_{m \geq 0}$ are *Bernoulli numbers,*

$$\sum_{m=0}^{\infty} \frac{\mathrm{B}_m}{m!} z^m = \frac{z}{\mathrm{e}^z - 1} = 1 - \tfrac{1}{2} z + \tfrac{1}{12} z^2 - \tfrac{1}{720} z^4 + \tfrac{1}{30240} z^6 + \cdots.$$

Note that all the operations are consistent with a Lie algebra!

Note that the dexpinv equation is always nonlinear and consists of an infinite sum. However, infinite sums can be truncated and nonlinearity is a small price to pay...

Specifically, the dexpinv equation is

$$\omega' = a - \tfrac{1}{2}[\omega, a] + \tfrac{1}{12}[\omega, [\omega, a]] - \tfrac{1}{720}[\omega, [\omega, [\omega, [\omega, a]]]] + \tfrac{1}{30240}[\omega, [\omega, [\omega, [\omega, [\omega, [\omega, a]]]]]] + \cdots.$$

For a quadratic Lie group, i.e. $G = \{p : pqp^\top = q\}$, where $q \in \mathrm{Sym}_n[\mathbb{R}]$ is nonsingular, an intriguing alternative is the Cayley trivialization

$$\Phi(z) = \frac{1 + \frac{1}{2}z}{1 - \frac{1}{2}z}.$$

It results in the dcayinv equation

$$\omega' = a - \tfrac{1}{2}[\omega, a] + \tfrac{1}{4}\omega a \omega.$$

The Cayley trivialization has two advantages *vis-á-vis* the standard exponential: the equation is much simpler and the evaluation of $\Phi(\omega)$ *much* cheaper, in particular for large n. On the other hand, of course, it applies *only* to quadratic Lie groups.

4. Runge–Kutta–Munthe-Kaas methods

We apply a Runge–Kutta method to the dexpinv equation, rather than doing so to the original equation on a homogeneous manifold. E.g., instead of the familiar 3-stage 3rd-order scheme for $y' = a(t,y)y$,

$$\begin{aligned} k_1 &= a(t_N, y_N)y_N \\ k_2 &= a(t_{N+1/2}, y_N + \tfrac{1}{2}hk_1)(y_N + \tfrac{1}{2}hk_1) \\ k_3 &= a(t_{N+1}, y_N - hk_1 + 2hk_2)(y_N - hk_1 + 2hk_2) \\ \Delta &= h(\tfrac{1}{6}k_1 + \tfrac{2}{3}k_2 + \tfrac{1}{6}k_3) \\ y_{N+1} &= y_N + \Delta, \end{aligned}$$

we use

$$\begin{aligned} k_1 &= a(t_N, y_N) \\ k_2 &= a(t_{N+1/2}, \mathrm{e}^{\frac{1}{2}hk_1}y_N) \\ k_3 &= a(t_{N+1}, \mathrm{e}^{-hk_1+2hk_2}y_N) \\ \Delta &= h(\tfrac{1}{6}k_1 + \tfrac{2}{3}k_2 + \tfrac{1}{6}k_3) \\ y_{N+1} &= \mathrm{e}^{\Delta + \frac{1}{6}h[\Delta, k_1]}y_N. \end{aligned}$$

This is again a 3rd-order method, except that it is guaranteed to evolve on $\mathcal{G}$.

- The beauty of this approach is that we can take any RK method and convert it into a Lie-group method without any major effort.
- Each step of an explicit ν-stage RK–MK method requires ν function evaluations and ν computations of the matrix exponential. The latter can be fairly expensive for large ν.
- The number of commutators increases rapidly with order (in particular if we want really high-order methods!). This can be alleviated by techniques from graded Lie algebras, which will be considered later.
- Implicit RK–MK methods can be used, but they require the solution of underlying nonlinear algebraic equations. Owren & Welfert have presented an extension of Newton's method that respects Lie group structure but, again, it ain't cheap.
- Similar approach is valid for other trivializations, in particular for the dcay-inv equations.

5. Magnus and Magnus-type expansions

Consider the linear equation

$$y' = a(t)y, \quad t \geq 0, \qquad y(0) \in \mathcal{G}, \quad a(t) \in \mathfrak{g}.$$

Recall that $y(t) = \mathrm{e}^{\omega(t)} y_0$, where ω was given by the dexpinv equation.

Wilhelm Magnus showed that

$$\begin{aligned}\omega(t) = &\int_0^t a(\xi)\mathrm{d}\xi - \tfrac{1}{2}\int_0^t\int_0^{\xi_1} [a(\xi_2), a(\xi_1)]\mathrm{d}\xi_2\mathrm{d}\xi_1 \\ &+ \tfrac{1}{4}\int_0^t\int_0^{\xi_1}\int_0^{\xi_2} [[a(\xi_3), a(\xi_2)], a(\xi_1)]\mathrm{d}\xi_3\mathrm{d}\xi_2\mathrm{d}\xi_1 \\ &+ \tfrac{1}{12}\int_0^t\int_0^{\xi_1}\int_0^{\xi_1} [a(\xi_3), [a(\xi_2), a(\xi_1)]]\mathrm{d}\xi_3\mathrm{d}\xi_2\mathrm{d}\xi_1 \\ &+ \cdots.\end{aligned}$$

Extensive use of Magnus expansions in theoretical physics, quantum chemistry, control theory, stochastic DEs, geometric mechanics, ...

Systematic theoretical analysis and numerical implementation of the Magnus expansion by Al & Nørsett, using graph theory.

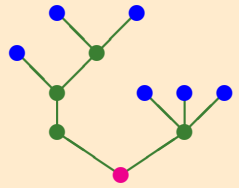
- Graph: The pair $\boldsymbol{G} = \langle \boldsymbol{V}, \boldsymbol{E} \rangle$, where $\boldsymbol{V} = \{v_1, \ldots, v_r\}$ are vertices and $\boldsymbol{E} \subseteq \boldsymbol{V} \times \boldsymbol{V}$ edges;

- Path from v_i to v_j: An ordered set $\{(v_{s_l}, v_{s_{l+1}})\}_{l=1}^{q}$ of distinct vertices s.t. $s_1 = i$ and $s_{q+1} = j$;

- A graph is connected if each two vertices are connected by a path and it is a tree if such a path is unique;

- Rooted tree: The pair $\boldsymbol{T} = (\boldsymbol{G}, w)$, where $\boldsymbol{G}$ is a tree and w (the root) is one of its vertices.

- A rooted tree admits a natural partial ordering of ancestor/successor and parent/child. (Think family tree!) Note that the root has no parent. Childless vertices are called leaves.



- a leaf
- the root

It is easy to see that all terms in a Magnus expansion of ω' are of the form

$$\left[\int \text{simpler term}, \text{another simpler term}\right].$$

This can be expressed by recursion (the proof follows by Picard iteration):

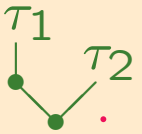
1. We commence from the integral of $a(t)$;
2. If integrals of $H_1(t)$ and $H_2(t)$ already feature in the expansion, so does the integral of

$$\left[\int_0^t H_1(\xi)\mathrm{d}\xi, H_2(t)\right].$$

We model this with *rooted binary trees,*

1. The tree $\bullet$ corresponds to $a(t)$;
2. If $H_{\tau_1} \rightsquigarrow \tau_1$, $H_{\tau_2} \rightsquigarrow \tau_2$ have been already derived, then

$$\left[\int_0^t H_{\tau_1}(\xi)\mathrm{d}\xi, H_{\tau_2}(t)\right] \rightsquigarrow$$

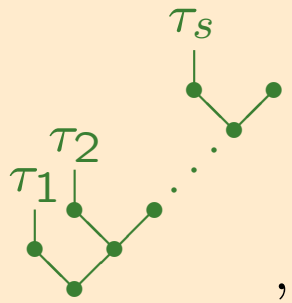


Magnus in terms of trees

Let $\mathbb{T}_m$ be the set of trees with m vertical lines (i.e., corresponding to terms with m integrals). Then

$$\omega(t) = \sum_{m=0}^{\infty} \sum_{\tau \in \mathbb{T}_m} \alpha(\tau) \int_0^t H_\tau(\xi) \mathrm{d}\xi.$$

The mapping $\tau \to H_\tau$ has been already described, while the constants $\alpha(\tau)$ are obtained recursively: any $\tau \in \mathbb{T}_m$, $m \geq 1$, can be written uniquely in the form



,

whereby

$$\alpha(\bullet) = 1,$$

$$\alpha(\tau) = \frac{\mathrm{B}_s}{s!} \prod_{l=1}^{s} \alpha(\tau_l).$$

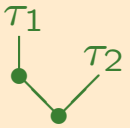
Truncation by power

Instead of grouping trees into the sets $\mathbb{T}_m$, counting integrals, we count their order p such that $H_\tau(t) = \mathcal{O}(t^p)$: we call this truncation by power.

We have

$\bullet \quad \Rightarrow \quad p = 0$ But  $\Rightarrow \quad p = 2.$

(Because $\left[\int_0^t a(x)\,\mathrm{d}x, a(t)\right] = \frac{1}{2}[a(0), a'(0)]t^2 + \mathcal{O}\left(t^3\right)$.) In general, the rule is: if

$\tau =$ 

then

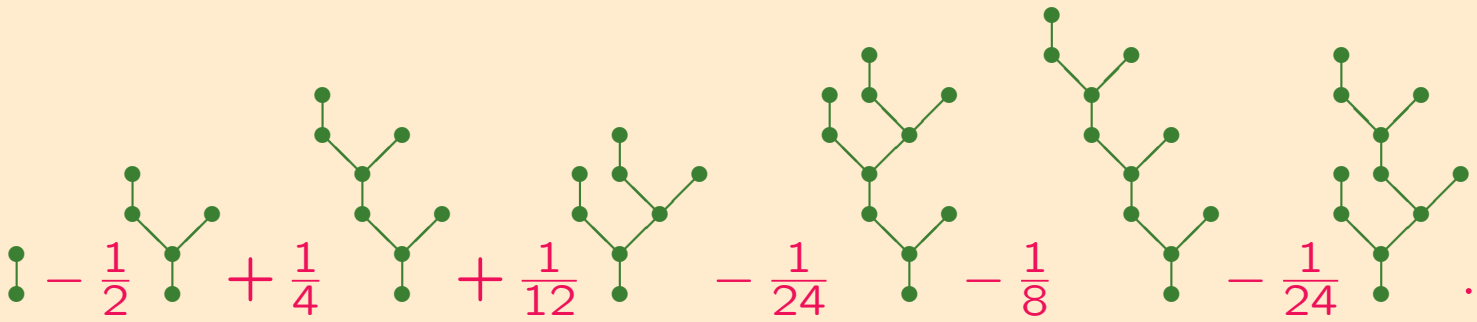
$$\tau_1 \neq \tau_2 \quad \Rightarrow \quad p(\tau) = p(\tau_1) + p(\tau_2) + 1,$$
$$\tau_1 = \tau_2 \quad \Rightarrow \quad p(\tau) = p(\tau_1) + p(\tau_2) + 2.$$

The set of all trees of order p is denoted by $\mathbb{F}_p$ and we reorder

$$\omega(t) = \sum_{m=0}^{\infty} \sum_{\tau \in \mathbb{F}_m} \alpha(\tau) \int_0^t H_\tau(\xi)\mathrm{d}\xi,$$

AI, Nørsett & Rasmussen: Once we truncate by power, a Magnus expansion $y_{n+1} = \Upsilon_h y_n$ is time symmetric, i.e. $\Upsilon_h \circ \Upsilon_{-h} = \mathrm{Id}$. Therefore $\Upsilon_h = \mathrm{e}^{\Psi_h}$, where Ψ_h is an odd function and it follows that such an expansion is *always* of an even order – if we truncate it to produce odd order, we gain for free an extra unit of order.

Thus, a sixth-order Magnus expansion:

$\omega(t) \rightsquigarrow$  .

The advantage of truncating by power is not just a smaller number of trees but the fact that the expansion is solely in odd powers of h: we will take an advantage of this fact in the sequel.

Convergence of the Magnus expansion

Theorem *The Magnus expansion converges if*

$$\int_0^t \|a(\xi)\|\mathrm{d}\xi \leq \int_0^{2\pi} \frac{\mathrm{d}\xi}{4+\xi(1-\cot\frac{\xi}{2})} \approx 1.086869.$$

Original proof by Blanes, Casas, Oteo & Ros. Shorter proof by Moan: Integration & the triangle inequality imply that

$$\|\omega(t)\| \leq \int_0^t \|\mathrm{dexp}^{-1}_{\omega(\xi)} a(\xi)\|\mathrm{d}\xi \leq \int_0^t \sum_{k=0}^{\infty} \frac{|\mathrm{B}_k|}{k!}(2\|\omega(\xi)\|)^k a(\xi)\mathrm{d}\xi$$
$$= \int_0^t g(2\|\omega(\xi)\|)\|a(\xi)\|\mathrm{d}\xi,$$

where $g(x) = 2 + \frac{x}{2}(1-\cot\frac{x}{2})$. Bihari-type inequality: Let $h, g, v \in \mathrm{C}[0, t^*)$ positive, g nondecreasing. Then $h(t) \leq \int_0^t g(h(\xi))v(\xi)\mathrm{d}\xi$ implies

$$h(t) \leq \tilde{g}^{-1}\left(\int_0^t v(\xi)\mathrm{d}\xi\right), \qquad \tilde{g}(x) = \int_0^x \frac{\mathrm{d}\xi}{g(\xi)}.$$

Letting $h(t) = 2\|\omega(t)\|$, $v(t) = \|a(t)\|$ completes the proof. □

A stronger result by Moan & Niesen is available.

The Fer expansion

Fer: We approximate the solution of $y' = a(t)y$ in the form

$$y(t) = \exp\left(\int_0^t a(\xi)\mathrm{d}\xi\right) v(t).$$

Then

$$v' = \mathrm{fer}_{\int_0^t a(\xi)\mathrm{d}\xi} a(t)\, v, \quad t \geq 0, \qquad v(0) = y(0),$$

where

$$\begin{aligned}\mathrm{fer}_b a &= \mathrm{ad}_b^{-1}[(I + \mathrm{ad}_b)\mathrm{e}^{-\mathrm{ad}_b} - I]a \\ &= \sum_{k=1}^{\infty} (-1)^k \frac{k}{(k+1)!} \mathrm{ad}_b^k a.\end{aligned}$$

This procedure can be iterated: the outcome is the Fer expansion

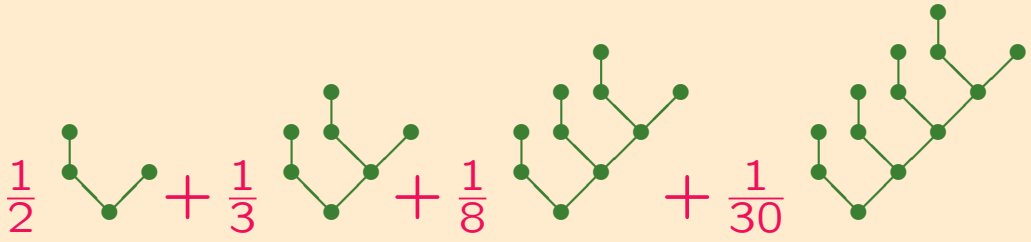
$$y(t) = \mathrm{e}^{\int_0^t \omega_0(\xi)\mathrm{d}\xi} \mathrm{e}^{\int_0^t \omega_1(\xi)\mathrm{d}\xi} \mathrm{e}^{\int_0^t \omega_2(\xi)\mathrm{d}\xi} \cdots y(0), \qquad t \geq 0.$$

Al: $\omega_m(t) = \mathcal{O}\left(t^{2^{m+2}-2}\right)$, hence the order increases very fast.

Also the Fer expansion can be expanded in rooted trees. Thus, for order 6, just two terms are required,

ω_0 :

ω_1 : $\frac{1}{2}$ + $\frac{1}{3}$ + $\frac{1}{8}$ + $\frac{1}{30}$



Detailed complexity analysis of Lie-group methods (Celledoni, AI, Nørsett & Orel) demonstrates that in general the Magnus expansion is always cheaper than the Fer expansion. A major reason is that Fer requires more evaluations of the exponential. However, Fer is useful for 'niche' computations. In particular, it is the engine of the best algorithm to compute spectra of Sturm–Liouville problems (Ramos & AI).

The Cayley expansion

For a quadratic Lie group with the Cayley trivialization we let

$$y(t) = \mathrm{cay}_{\omega(t)} y_0 = \frac{I + \frac{1}{2}\omega(t)}{I - \frac{1}{2}\omega(t)} y_0, \qquad t \geq 0,$$

consequently

$$\omega' = a - \tfrac{1}{2}[\omega, a] + \tfrac{1}{4}\omega a \omega, \quad t \geq 0, \qquad \omega(0) = 0.$$

In line with the Magnus expansion, we can show that

$$\begin{aligned}\omega(t) = &\int_0^t a(\xi)\mathrm{d}\xi - \tfrac{1}{2}\int_0^t \int_0^{\xi_1} [a(\xi_2), a(\xi_1)]\mathrm{d}\xi_2\mathrm{d}\xi_1 \\ &+ \tfrac{1}{4}\int_0^t \int_0^{\xi_1}\int_0^{\xi_2} [[a(\xi_3), a(\xi_2)], a(\xi_1)]\mathrm{d}\xi_3\mathrm{d}\xi_2\mathrm{d}\xi_1 \\ &- \tfrac{1}{4}\int_0^t \int_0^{\xi_1} a(\xi_2)\mathrm{d}\xi_2 a(\xi_1) \int_0^{\xi_1} a(\xi_2)\mathrm{d}\xi_2\mathrm{d}\xi_1 + \cdots.\end{aligned}$$

This Cayley expansion can be also expanded in rooted trees, except that we require slightly more complicated structures.

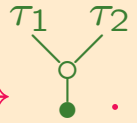
AI: Specifically, we have the following composition rules:

1. $\int_0^t a(\xi)\mathrm{d}\xi \rightsquigarrow$  is a term.

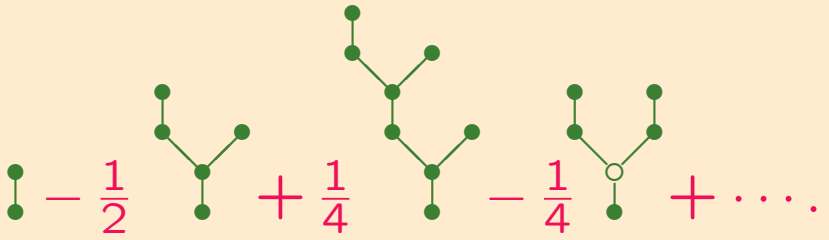
2. If $H \rightsquigarrow \tau$ is a term, then so is

$$\int_0^t [H(\xi), a(\xi)]\mathrm{d}\xi \rightsquigarrow$$  .

3. If $H_1 \rightsquigarrow \tau_1$ and $H_2 \rightsquigarrow \tau_2$ are terms, then so is

$$\int_0^t H_1(\xi)a(\xi)H_2(\xi)\mathrm{d}\xi \rightsquigarrow$$  .

We obtain

$\omega(t) \rightsquigarrow$ 

6. Multivariate quadrature

Each term in a Magnus, Fer or Cayley expansion corresponds to a multivariate integral over a different polytope. In principle, multivariate integration is very expensive: we need many function evaluations for *each and every* polytope. Fortunately, everything simplifies!

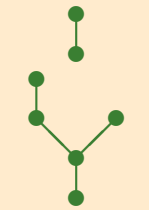
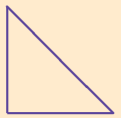
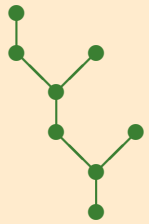
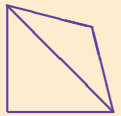
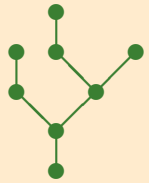
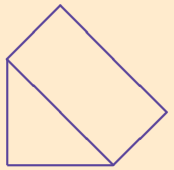
All integrals in question are of the form

$$\mathscr{I}(h) = \int_{h\mathcal{S}} \mathcal{L}(a(\xi_1), a(\xi_2), \ldots, a(\xi_r))\mathrm{d}\boldsymbol{\xi},$$

where $\mathcal{L}$ is a multilinear form and $\mathcal{S}$ is a polytope,

$$\mathcal{S} = \{\boldsymbol{x} \in \mathbb{R}^r \,:\, 0 \le x_k \le x_{i_k}, \quad k = 1, 2, \ldots, r\},$$

with $x_0 = 1$ and $i_k \le k - 1$, $x_0 = 1$, $k = 1, 2, \ldots, r$. Specifically, for the first few integrals we have the following polytopes $\mathcal{S}$ and multilinear forms $\mathcal{L}$:

Tree	r	The term	$\mathcal{L}(z_1, \ldots, z_r)$	$\mathcal{S}$
	1	$\int A(\xi)$	z_1	
	2	$\int \left[\int A(\xi_1), A(\xi_2) \right]$	$[z_2, z_1]$	
	3	$\int \left[\int \left[\int A(\xi_1), A(\xi_2) \right], A(\xi_3) \right]$	$[[z_3, z_2], z_1]$	
	3	$\int \left[\int A(\xi_1), \left[\int A(\xi_2), A(\xi_3) \right] \right]$	$[z_3, [z_2, z_1]]$	

Let $c_1, \ldots, c_\nu \in [0, 1]$ be distinct quadrature points and $a_k = a(t_N + c_k h)$. We approximate $\mathscr{I}(h)$ with

$$\mathscr{Q}(h) = h^r \sum_{\boldsymbol{i} \in C_\nu^r} \beta_{\boldsymbol{i}} \mathcal{L}(a_{i_1}, a_{i_2}, \ldots, a_{i_r}),$$

where C_ν^r are all the combinations of $\{1, 2, \ldots, \nu\}$. Note that we repeatedly recycle just ν function evaluations of a!

Theorem *(Al & Nørsett) The order of quadrature is $\nu + s$, where*

$$\int_0^1 \zeta^{i-1} q(\zeta) \mathrm{d}\zeta = 0, \qquad i = 1, 2, \ldots, s,$$

and $q(x) = \prod_{k=1}^{\nu} (x - c_k)$.

The proof is long and complicated. We'll prove instead a simpler statement. For this (and for much future use) we require the

Alekseev–Gröbner Lemma *Given the ODE $y' = f(t, y)$, suppose that u is any C^1 function s.t. $u(t_N) = y(t_N)$. Then*

$$u(t) - y(t) = \int_{t_N}^{t} \Phi(t - x, y(x))[f(x, u(x)) - u'(x)]\mathrm{d}x,$$

where Φ is the solution of the variational equation $\Phi' = \frac{\partial f}{\partial y}\Phi$, $\Phi(0) = I$.

Theorem *(Zanna) The order of the approximation to truncated Magnus expansion with the above quadrature is $\nu + s$.*

To prove this, we replace the matrix a by its interpolating polynomial $\widehat{a}$ s.t. $\widehat{a}(t_N + c_k h) = a(t_N + c_k h)$, $k = 1, \ldots, \nu$. Let $u' = \widehat{a}u$, $u(t_N) = y(t_N)$. Therefore, by the A–G Lemma

$$u(t_{N+1}) = y(t_{N+1}) + \int_{t_N}^{t_{N+1}} \Phi(t_{N+1} - x, y(x))[\widehat{a}(x) - a(x)]u(x)\mathrm{d}x.$$

The integrand vanishes at $c_1, \ldots, c_\nu$. Therefore, once we discretize the integral by the quadrature formula, all that remains is the quadrature error, i.e. $\mathcal{O}\left(h^{\nu+s+1}\right)$. □

Corollary *If $c_1, \ldots, c_\nu$ are Gauss–Legendre points in $[0, 1]$ then the order is 2ν.*

Example: A 4th-order approximantion

$$\int_0^h \int_0^{\xi_1} [a(\xi_2), a(\xi_1)]\mathrm{d}\boldsymbol{\xi} \approx \tfrac{\sqrt{3}}{6} h^2 [a_1, a_2],$$

where $c_1 = \frac{1}{2} - \frac{\sqrt{3}}{6}$, $c_2 = \frac{1}{2} + \frac{\sqrt{3}}{6}$.

To construct a quadrature formula in greater detail, let $\ell_k \in \mathbb{P}_{\nu-1}$ be the kth cardinal polynomial of Lagrangian interpolation,

$$\ell_k(c_k) = 1, \qquad \ell_k(c_j) = 0, \quad j \neq k.$$

Then

$$\beta_{\boldsymbol{i}} = \int_{\mathcal{S}} \prod_{k=1}^{r} \ell_{i_k}(\xi_k) \mathrm{d}\boldsymbol{\xi}.$$

GOOD NEWS

It takes just ν evaluations of the matrix a to compute all the integrals in the expansion to order 2ν.

BAD NEWS

The numbers of commutators increases very fast, in line with the exponential growth in the number of combinations C_ν^r. Therefore, the volume of linear algebra required in every time step becomes prohibitive for large orders.

7. Graded Lie algebras

The number of commutators can be hugely reduced using an approach due to Munthe-Kaas & Owren. Replace $ha_1, \ldots, ha_\nu$ by $b_0, b_1, \ldots, b_{\nu-1}$, where

$$\sum_{l=0}^{\nu-1} \tfrac{1}{l!}(c_k - \tfrac{1}{2})^l b_l = ha_k, \qquad k = 1, 2, \ldots, \nu.$$

Then $b_l \approx h^{l+1} a^{(l)}(\frac{1}{2}h) = \mathcal{O}(h^{l+1})$: the term b_l is of grade $l+1$. The grades propagate naturally under commutation: if the grade of x_i is w_i for $i = 1, 2$, then the grade of $[x_1, x_2]$ is $w_1 + w_2$. Therefore, the term

$$\mathcal{L}(b_{i_1}, b_{i_2}, \ldots, b_{i_r})$$

is of grade $|\boldsymbol{i}| = \sum_{l=1}^{r} i_l$. We obtain the order-$(2\nu)$ quadrature

$$\widetilde{\mathcal{Q}}(h) = \sum_{|\boldsymbol{i}| \le 2\nu} \tilde{\beta}_{\boldsymbol{i}} \mathcal{L}(b_{i_1}, b_{i_2}, \ldots, b_{i_r}),$$

where

$$\tilde{\beta}_{\boldsymbol{i}} = \int_{\mathcal{S}} \prod_{l=1}^{r} (\xi_l - \tfrac{1}{2})^{i_l} \mathrm{d}\xi_r \cdots \mathrm{d}\xi_1.$$

Because each b_i is a linear combination of $ha_1, \ldots, ha_\nu$, we are using *the same information* in $\widetilde{\mathcal{Q}}$ and $\mathcal{Q}$.

Free Lie algebras

For future use we require the concept of a free Lie algebra. Given generators $\Phi = \{\phi_1, \phi_2, \ldots, \phi_\nu\}$, we say that

$$\mathfrak{F} = \mathsf{FLA}(\phi_1, \phi_2, \ldots, \phi_\nu)$$

is the free Lie algebra generated by Φ if it is the closure of the generators under commutation and linear combinations. Trivially, it is a Lie algebra.

We attach to each ϕ_l the grade $g(\phi_l) \in \mathbb{N}$ and let grades propagate by commutation:

$$g(t_1) = \mu_1, \quad g(t_2) = \mu_2 \qquad \Rightarrow \qquad g([t_1, t_2]) = g(t_1) + g(t_2).$$

We denote by $\mathscr{K}_m^\nu$ the linear space of all terms in the FLA of grade m. Clearly, $\mathfrak{F} = \oplus\{\mathscr{K}_m^\nu \,:\, m \geq 1\}$, although we will not make much use of this.

The surprisingly small dimension of $\mathscr{K}_m^\nu$ is the key to our goal, to reduce the number of commutators.

The great commutator throw-away

Three mechanisms allow us to get rid of most terms:

1. Terms of grade $\geq 2\nu + 1$ are not required and can be thrown out.

2. It is possible to show that the discrete expansion is time symmetric, provided that $c_1, c_2, \ldots, c_\nu$ are symmetric w.r.t. $\frac{1}{2}$ (e.g. Gauss, Chebyshev or Lobatto points). Therefore sums of terms of even grade vanish and we don't need to compute them.

3. The classical Witt–Birkhoff formula gives the (surprisingly small) dimension of $\mathscr{K}_m^{\mathcal{V}}$ for unit grades $\kappa_l \equiv 1$ (corresponding to $x_l = ha_l$). Munthe-Kaas & Owren have extended the Witt–Birkhoff formula to arbitrary grades. Specifically, let λ_k, $k = 1, 2, \ldots, s = \max \kappa_l$, be the zeros of the polynomial

$$1 - \sum_{i=1}^{\nu} z^{g(\phi_l)}.$$

1. Then

$$\dim \mathscr{K}_m^{\nu} = \frac{1}{m} \sum_{d|m} \mu(d) \sum_{i=1}^{s} \lambda_i^{m/d},$$

where μ is the Möbius function,

$$\mu(d) = \begin{cases} 1, & d = 1, \\ (-1)^q, & n_i = 1,\ i = 1, 2, \ldots, q, \\ 0, & \text{otherwise}, \end{cases}$$

where $d = p_1^{n_1} p_2^{n_2} \cdots p_q^{n_q}$ is the prime-number decomposition of d.

They also gave a recursive procedure for the formation of a basis of $\mathscr{K}_m^{\nu}$ (a generalisation of Hall, Lyndon or Dynkin bases).

The number of required terms:

order:	2	4	6	8	10
Naive	1	5	80	3304	1256567
Clever	1	2	7	22	73

Is this the optimal Magnus expansion?

Further economy is possible by clever algorithmic tricks and aggregating terms.
This has been worked out for even orders 4–8 by Blanes, Casas & Ros.

For example, for order 6, we compute

$$c_1 = \tfrac{1}{2} - \tfrac{\sqrt{15}}{10}, \quad c_2 = \tfrac{1}{2}, \quad c_3 = \tfrac{1}{2} + \tfrac{\sqrt{15}}{10},$$
$$a_k = ha(t_N + c_k), \quad k = 1, 2, 3,$$
$$b_0 = ha_2, \qquad b_1 = \tfrac{\sqrt{15}}{3}(a_3 - a_1), \qquad b_2 = \tfrac{10}{3}(a_3 - 2a_1 + a_1),$$
$$v_1 = [b_0, b_1],$$
$$v_2 = [b_0, 2b_2 + v_1],$$
$$v_3 = [-20b_0 - b_2 + v_1, b_1 - \tfrac{1}{60}v_2],$$
$$\omega_N = b_0 + \tfrac{1}{12}b_2 + \tfrac{1}{240}v_3,$$
$$y_{N+1} = \mathrm{e}^{\omega_N} y_N.$$

Thus,

just three function evaluations, three commutators and one exponential!

8. The matrix exponential

It is not enough to "approximate" the exponential: we must do so while mapping an element from $\mathfrak{g}$ to $\mathcal{G}$! Otherwise all the hard work in designing Lie-group methods would be in vain!

Standard methods for the calculation of the matrix exponential:

- Eigenvalue/eigenvector decomposition:
  Exceedingly expensive (in particular for large systems) and ill conditioned.
- Polynomial and rational approximations*:
  We cannot expect the result to live in $\mathcal{G}$, with one exception: when the Lie group is quadratic and we use diagonal Padé approximations (Feng Kang) †. On the other hand, no rational approximation can map $\mathfrak{sl}(n)$ to $\mathrm{SL}(n)$ for $n \geq 3$.
- Krylov subspace approximation:
  Very effective means for large matrices (Hochbruck & Lubich). However, again, they map an algebra to 'its' group only for orthogonal and unitary groups.

*That's, essentially, how MATLAB computes the exponential, with the scaling-and-squaring algorithm.

†But in that case we can alternatively use the Cayley trivialisation.

Krylov subspace methods (Tal-Ezer & Kosloff; Gallopoulos & Saad; Hochbruck & Lubich)

The mth Krylov subspace generated by $\{A, \boldsymbol{v}\}$, where $A \in \mathsf{M}_{n\times n}[\mathbb{R}]$ and $\boldsymbol{v} \in \mathbb{R}^n$, is

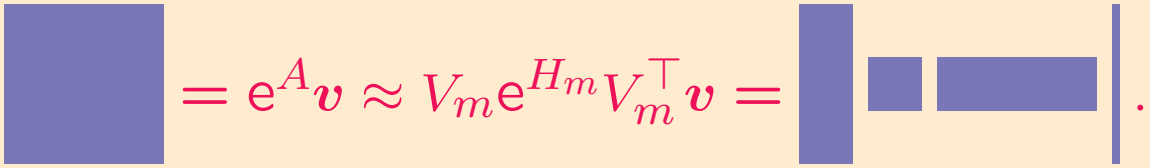
$$\mathcal{K}_m(A, \boldsymbol{v}) = \mathsf{Sp}\{\boldsymbol{v}, A\boldsymbol{v}, A^2\boldsymbol{v}, \ldots, A^{m-1}\boldsymbol{v}\}.$$

Then $\dim \mathcal{K}_m(A, \boldsymbol{v}) \leq m$ and its orthonormal basis can be generated by the Arnoldi process

$\boldsymbol{v}_1 = \boldsymbol{v}/\|\boldsymbol{v}\|_2$,
for $j = 1, \ldots, m-1$ **do**
  $\boldsymbol{t} = A\boldsymbol{v}_j$,
  for $i = 1, \ldots, j$ **do**
    $h_{i,j} = \boldsymbol{v}_i^\top \boldsymbol{t}, \qquad \boldsymbol{t} = \boldsymbol{t} - h_{i,j}\boldsymbol{v}_i$,
  end for
  $h_{j+1,j} = \|\boldsymbol{t}\|_2, \qquad \boldsymbol{v}_{j+1} = \boldsymbol{t}/h_{j+1,j}$
end for

results in $V_m \in \mathsf{M}_{n\times m}[\mathbb{R}]$ whose columns are an orthogonal basis of $\mathcal{K}_m$ and an upper Hessenberg $H_m \in \mathsf{M}_{n\times n}[\mathbb{R}]$.

Typically $m \ll n$: V_m is 'long and skinny'. We approximate



$$= \mathrm{e}^{A}\boldsymbol{v} \approx V_m \mathrm{e}^{H_m} V_m^\top \boldsymbol{v} =$$

.

- $V_m^\top \boldsymbol{v} = \|\boldsymbol{v}\|_2 \boldsymbol{e}_1$, hence
- $\mathrm{e}^{H_m} V_m^\top \boldsymbol{v}$ is just the first column of e^{H_m}, scaled by $\|\boldsymbol{v}\|_2$.
- H_m being $m \times m$ and $m \ll n$, it is in general very easy to compute e^{H_m} to high precision – we thus need to compute just a small exponential and a matrix-vector product.
- If $A \in \mathfrak{so}_n$ then $H_m \in \mathfrak{so}_m$ and is tridiagonal.
- For $A \in \mathfrak{so}_n$ we have

$$\|\mathrm{e}^{A}\boldsymbol{v} - V_m \mathrm{e}^{H_m} V_m^\top \boldsymbol{v}\|_2 \leq 12 \mathrm{e}^{-\|A\|^2/(4m)} \left(\frac{\mathrm{e}\|A\|}{2m}\right)^m, \qquad m \geq \|A\|$$

(Hochbruck, Lubich & Selhofer).

Splitting methods (Celledoni & Al)

Given $a \in \mathfrak{g}$, we split its exponential,

$$\mathrm{e}^{ta} \approx \mathrm{e}^{tb_1}\mathrm{e}^{tb_2}\dots\mathrm{e}^{tb_s}$$

such that

1. $\sum_k b_k = a$, each b_k lives in $\mathfrak{g}$;

2. It is easy to evaluate each e^{tb_k} exactly; and

3. The overall error is consistent with the order of the Lie-group method

Note that automatically $\mathrm{e}^{tb_1}\mathrm{e}^{tb_2}\dots\mathrm{e}^{tb_s} \in \mathcal{G}$.

If $b_k = b_{s+1-k}\ \forall k$ then the approximation is time symmetric. In that case the order can be further enhanced with the Yošida device.

Practical splittings decompose a into low-rank matrices, using the following explicit formula for the matrix exponential. Suppose that u and v are both $n \times r$ matrices, $r \ll n$, and $c = uv^\top$. Then

$$\mathrm{e}^{tc} = I + tud^{-1}(\mathrm{e}^{td} - I)v^\top,$$

where $d = v^\top u$ is $r \times r$, hence 'small'.

For example, for $\mathfrak{g} = \mathfrak{so}(n)$ we let $r = 2$, $s = n - 1$, set

$$b^{[0]} = a = [\boldsymbol{b}_1^{[0]}, \boldsymbol{b}_2^{[0]}, \ldots, \boldsymbol{b}_n^{[0]}]$$

and choose

$$b_1 = \boldsymbol{b}_1^{[0]} \boldsymbol{e}_1^\top - \boldsymbol{e}_1 \boldsymbol{b}_1^{[0]\top} \in \mathfrak{so}(n)$$

and $b^{[1]} = b^{[0]} - b_1$. Observe that the first row and column of $b^{[1]}$ vanish. We continue in this manner, similar to LU factorization, letting $b^{[i]} = b^{[i-1]} - b_i$ and

$$b_i = \boldsymbol{b}_i^{[i-1]} \boldsymbol{e}_i^\top - \boldsymbol{e}_i \boldsymbol{b}_i^{[i-1]\top} \in \mathfrak{so}_n, \quad i = 1, \ldots, n-1.$$

Note that $\operatorname{rank} b_i \equiv 2$.

The Yošida device

Let Φ_h be a time-symmetric numerical method of order p for the solution of $y' = f(t, y)$.

Time symmetry implies that p is even.

We consider a new method,

$$\Psi_h = \Phi_{\alpha h} \circ \Phi_{\beta h} \circ \Phi_{\alpha h}.$$

1. The method Ψ_h is time reversible.

2. Suppose that

$$\alpha = \frac{1}{2 - 2^{1/(p+1)}}, \qquad \beta = -\frac{2^{1/(p+1)}}{2 - 2^{1/(p+1)}}.$$

   Then Ψ_h is of order $p + 2$.

This approach (originally developed by Haruo Yošida for symplectic methods) can be used to improve the order of our approximation to the exponential.

Canonical coordinates of the second kind (Celledoni & Al)

Let $d = \dim \mathfrak{g}$ and let $\{\phi_1, \phi_2, \ldots, \phi_d\}$ be its basis. We seek scalar functions $\theta_1, \theta_2, \ldots, \theta_m$ s.t.

$$\mathrm{e}^{ta} = \mathrm{e}^{\theta_1(t)\phi_1}\mathrm{e}^{\theta_2(t)\phi_2}\ldots\mathrm{e}^{\theta_d(t)\phi_d}.$$

Such functions always exist for small $t > 0$ but their practical evaluation in closed form is virtually impossible for $d \geq 3$ (Wei & Norman). Alternatively, we approximate the functions θ_k to requisite order.

Let $\{\phi_1, \phi_2, \ldots, \phi_d\}$ be a basis of $\mathfrak{g}$. The structure constants of $\mathfrak{g}$ are numbers

$$c_{k,l}^j, \quad k, l, j = 1, \ldots, d, \qquad \text{such that} \qquad [\phi_k, \phi_l] = \sum_{j=1}^{d} c_{k,l}^j \phi_j.$$

The Taylor expansion of each θ_k can be derived explicitly in terms of the structure constants (which, of course, depend on the choice of the basis). Let

$$a = \sum_{k=1}^{d} \alpha_k \phi_k.$$

We have

$$\theta_k(0) = 0,$$
$$\theta_k'(0) = \alpha_k,$$
$$\theta_k''(0) = \sum_{l=1}^{d} \sum_{j=1}^{l-1} \alpha_l c_{l,j}^k \alpha_j,$$
$$\theta_k'''(0) = 2 \sum_{l=1}^{d} \sum_{j=1}^{l-1} c_{l,j}^k [\theta_l''(0)\alpha_j + \theta_j''(0)\alpha_l] + 2 \sum_{l=1}^{d} \sum_{j=1}^{l-1} \sum_{i=1}^{j-1} \sum_{m=1}^{d} c_{l,j}^m c_{i,m}^k \alpha_l \alpha_j \alpha_i + \sum_{l=1}^{d} \sum_{j=1}^{d} \sum_{i=1}^{l-1} c_{l,i}^j c_{i,j}^k \alpha_l \alpha_i^2$$

and so on. More and longer summations!

Assume, though, that the structure constants are sparse: they are almost all zero. In that case the cost reduces a very great deal! This can be accomplished systematically by choosing as our basis the root space decomposition of $\mathfrak{g}$: the number of summations typically drops by a factor of two and the cost of a second-order approximation in $\mathfrak{so}(n)$ is just $\mathcal{O}(n)$.

Generalized polar decomposition (Munthe-Kaas, Quispel & Zanna)

An involutory automorphism of a Lie group $\mathcal{G}$ is a one-to-one map $\sigma : \mathcal{G} \to \mathcal{G}$ s.t.

$$\begin{aligned} &\sigma(x \cdot y) = \sigma(x) \cdot \sigma(y), \qquad x, y \in \mathcal{G}, \\ &\sigma(\sigma(x)) = x, \qquad x \in \mathcal{G}. \end{aligned}$$

Each $\mathcal{G}$-automorphism can be lifted to the underlying Lie algebra, resulting in a $\mathfrak{g}$-automorphism,

$$\mathrm{d}\sigma(a) = \frac{\mathrm{d}\sigma(\mathrm{e}^{ta})}{\mathrm{d}t}\Big|_{t=0}.$$

We use $\mathrm{d}\sigma$ to define the sets

$$\begin{aligned} \mathfrak{K} &= \{a \in \mathfrak{g} \,:\, \mathrm{d}\sigma(a) = a\}, \\ \mathfrak{P} &= \{a \in \mathfrak{g} \,:\, \mathrm{d}\sigma(a) = -a\}. \end{aligned}$$

While $\mathfrak{K}$ is a Lie subalgebra, $\mathfrak{P}$ is a Lie triple system: a linear space s.t.

$$a, b, c \in \mathfrak{g} \qquad \Rightarrow \qquad [a, [b, c]] \in \mathfrak{g}.$$

We have

$$\mathfrak{g} = \mathfrak{K} \oplus \mathfrak{P}.$$

Specifically, $\mathfrak{g} \ni a = p + k$, where

$$p = \tfrac{1}{2}[a - \mathrm{d}\sigma(a)], \qquad k = \tfrac{1}{2}[a + \mathrm{d}\sigma(a)].$$

Note that

$$\begin{aligned} a, b \in \mathfrak{K} &\Rightarrow [a, b] \in \mathfrak{K}, \\ a, b \in \mathfrak{P} &\Rightarrow [a, b] \in \mathfrak{K}, \\ a \in \mathfrak{K}, b \in \mathfrak{P} &\Rightarrow [a, b] \in \mathfrak{P}, \\ a \in \mathfrak{P}, b \in \mathfrak{K} &\Rightarrow [a, b] \in \mathfrak{P}. \end{aligned}$$

It is possible to prove that the Lie group can be factorized into generalized polar decomposition

$$\mathcal{G} \ni z = xy, \qquad \sigma(y) = y, \quad \sigma(x) = x^{-1}.$$

At the algebra level, this corresponds to

$$\mathcal{G} \ni \mathrm{e}^a = \mathrm{e}^c \mathrm{e}^b, \qquad c \in \mathfrak{P}, \quad b \in \mathfrak{K}.$$

The main idea is to generate the leading terms of b, c from p, k.

We have

$$\begin{aligned}\mathfrak{P} \ni c &= pt - \tfrac{1}{2}[p,k]t^2 - \tfrac{1}{6}[k,[p,k]]t^3 \\ &\quad + (\tfrac{1}{24}[p,[p,[p,k]]] - \tfrac{1}{24}[k,[k,[p,k]]])t^4 + \mathcal{O}\left(t^5\right), \\ \mathfrak{K} \ni b &= kt - \tfrac{1}{12}[p,[p,k]]t^3 + \mathcal{O}\left(t^5\right).\end{aligned}$$

Suppose now that $\dim \mathfrak{P}$ is very small. In that case e^c is very cheap to compute. This is not the case with e^b, but recall that $\mathfrak{K}$ is a subalgebra! Hence, we can go on splitting it!

We thus obtain a sequence of algebra authomorphisms and low-dimensional Lie triple systems $\mathfrak{P}_k$ for $k = 1, 2, \ldots, m$, such that

$$\mathrm{e}^a = \mathrm{e}^{p_1}\mathrm{e}^{p_2}\ldots\mathrm{e}^{p_m}, \qquad p_k \in \mathfrak{P}_k.$$

Back to the case $a \in \mathfrak{so}(n)$

A convenient way of generating such $\mathrm{d}\sigma_k$ is through involutory inner authomorphisms

$$\sigma(x) = sxs^\top, \qquad \mathrm{d}\sigma(a) = sas^\top,$$

where $s \in \mathcal{G} \cap \mathrm{O}(n)$.

Let $s_j = \mathrm{diag}(1 - 2\mathrm{e}_j)$. Then elements in each $\mathfrak{p}_j$ are nonzero just along the j row and column, hence $\mathrm{rank}\,\mathfrak{P}_j \equiv 2$. We are 'peeling' the matrix a from the top down.

Al & Zanna: Suppose that we have brought a to an upper Hessenberg form, $a = q\tilde{a}q^\top$, where $q \in \mathrm{O}(n)$. The above algorithm does not respect this form. But suppose that we 'peel' the matrix from the bottom, not from the top! In that case, moving to each subsequent subalgebra $\mathfrak{K}_j$ 'contaminates' just few elements under the first subdiagonal, at the bottom of the matrix, which can be 'cleaned' with few Givens rotations.

This yields an algorithm which is competitive with classical methods to compute the matrix exponential, even when the conservation of Lie-group structure is not at issue!

9. An example: Sturm–Liouville spectra

Let $q \in \mathsf{C}[a,b]$ be piecewise-analytic, $-\infty < q_{\min} \leq q(x) \leq q_{\max} < \infty$. The Sturm–Liouville problem is to determine $\lambda \in \mathbb{R}$ and $y_\lambda \in \mathsf{C}^2[a,b]$ s.t.

$$-y_\lambda'' + q y_\lambda = \lambda y_\lambda,$$

subject to

$$\alpha_1 y_\lambda(a) + \alpha_2 y_\lambda'(a) = \beta_1 y_\lambda(b) + \beta_2 y_\lambda'(b) = 0, \qquad \alpha_1^2 + \alpha_2^2, \beta_1^2 + \beta_2^2 > 0.$$

General theory: there exists a countable number of eigenpairs $(\lambda_m, y_{\lambda_m})$ such that $\lambda_m < \lambda_{m+1}$, $\lambda_m \overset{m\to\infty}{\longrightarrow} \infty$, each y_{λ_m} has exactly m zeros in (a,b) and $\{y_{\lambda_m}\}_{m\in\mathbb{Z}_+}$ is an orthogonal basis of $\mathsf{L}[a,b]$.*

Standard methods are good in calculating the first few λ_ms but their accuracy breaks down as m grows. **The challenge:** devise a method whose accuracy is high and independent of the size of λ_m.

*Hence, for $m \gg 1$, y_λ is a rapidly oscillating function.

We reformulate the problem in a vector form,

$$y'_\lambda = \begin{bmatrix} 0 & 1 \\ q(x) - \lambda & 0 \end{bmatrix} y_\lambda, \quad t \in [a, b], \qquad y(0) = I.$$

Note that $y_\lambda \in \mathfrak{sl}(2)$. The eigenvalues are the solutions of the scalar transcendental equation

$$\det\left(\begin{bmatrix} \alpha_1 & \alpha_2 \\ 0 & 0 \end{bmatrix} + \begin{bmatrix} 0 & 0 \\ \beta_1 & \beta_2 \end{bmatrix} y_\lambda(b) \right) = 0$$

(Zettl). Recall the Fer expansion: for every $x \in [c_k, c_{k+1}]$

$$y_\lambda(x) = \mathrm{e}^{\phi_0(x)} \mathrm{e}^{\phi_1(x)} \mathrm{e}^{\phi_2(x)} \cdots y_\lambda(c_k),$$

where

$$\beta_0(x) = \begin{bmatrix} 0 & 1 \\ q(x) - \lambda & 0 \end{bmatrix}, \qquad \phi_0(x) = \int_{c_k}^{x} \beta_0(\xi)\, \mathrm{d}\xi,$$

$$\beta_n(x) = \sum_{j=1}^{\infty} \frac{(-1)^j j}{(j+1)!} \mathrm{ad}^j_{\phi_{n-1}(x)} \beta_{n-1}(x), \qquad \phi_n(x) = \int_{c_k}^{x} \beta_n(\xi)\, \mathrm{d}\xi.$$

Note that $\beta_n(x) = \mathcal{O}\Big((c_{k+1} - c_k)^{2^{n+1}-2} \Big)$ (Al).

Fer streamers (Ramos & Al): The idea is to calculate all these quantities explicitly by mapping $\pi : \mathfrak{sl}(2) \to \mathbb{R}^3$. Thus,

$$\pi\left(\begin{bmatrix} x_1 & x_2 \\ x_3 & -x_1 \end{bmatrix}\right) = \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix}, \qquad \rho(x) = 2\sqrt{-\det x},$$

$$\mathcal{C}_x = \begin{bmatrix} 0 & -x_3 & x_2 \\ -2x_2 & 2x_1 & 0 \\ 2x_3 & 0 & -2x_1 \end{bmatrix} \qquad \Rightarrow \qquad \mathrm{ad}_x Y = \mathcal{C}_x \pi(Y),$$

$$\mathcal{C}_x^{2m-1} = \rho^{2(m-1)}(x)\mathcal{C}_x, \qquad \mathcal{C}_x^{2m} = \rho^{2(m-1)}(x)\mathcal{C}_x^2.$$

Therefore, any function in the Banach algebra of $\mathcal{C}_x$ (i.e., any "ad-expansion" in $\mathfrak{sl}(2)$) can be computed explicitly as Fer streamers. In particular,

$$\pi(\beta_n) = \theta(\rho(\phi_{n-1}))\mathcal{C}_{\phi_{n-1}}\pi(\beta_{n-1}) + \psi(\rho(\phi_{n-1}))\mathcal{C}^2_{\phi_{n-1}}\pi(\beta_{n-1}),$$

where

$$\theta(z) = \frac{\cosh z - 1 - z\sinh z}{z^2}, \qquad \psi(z) = \frac{z\cosh z - \sinh z}{z^3}.$$

Both θ and ψ are uniformly bounded along the imaginary axis. This allows to compute eigenvalues with uniform error bounds by partitioning the interval of interest into three subintervals,

$$\lambda \in [q_{\max} - h_{\max}^{-2}, q_{\min} - 1], \quad \lambda \in [q_{\min} - 1, q_{\max} + 1], \quad \lambda \in [q_{\max} + 1, \infty),$$

where $h_{\max} = \max\{c_{k+1} - c_k\}$ is $\leq (q_{\max} - q_{\min})^{-1/2}$ for $\lambda \geq q_{\min}$, otherwise $\leq (q_{\max} - \lambda)^{-1/2}$.

All this is accompanied by many technicalities: computing the highly oscillatory integrals F_n, deriving strict and realistic upper error bounds in all regimes, computing the zeros of the transcendental equation, ... (Ramos). Numerical results are spectacular.

10. An example: the semiclassical Schrödinger equation

The Schrödinger equation

$$\mathrm{i}\hbar\frac{\partial u}{\partial t} = H(\boldsymbol{x}, t, u)u,$$

where u is the wave function, H a Hamiltonian operator and $\hbar$ the (ridiculously small) Planck constant is fundamental to quantum mechanics and chemistry. The Born–Oppenheimer approximation for a non-relativistic particle in an electric field $\Rightarrow H(\boldsymbol{x}) = -[\hbar^2/(2m)]\nabla^2 - V(\boldsymbol{x})$, where V is the interaction potential and m the mass.

The outcome (for simplicity, in 1D) is the semiclassical Schrödinger equation

$$\frac{\partial u}{\partial t} = \mathrm{i}\varepsilon\frac{\partial^2 u}{\partial x^2} + \mathrm{i}\varepsilon^{-1}V(x)u, \qquad x \in [-1, 1], \quad t \geq 0,$$

with periodic boundary conditions. $\varepsilon > 0$, related to the ratio of the masses of the smallest particle (typically, an electron) and the system itself, it usually in the range $[10^{-8}, 10^{-4}]$: small, but not ridiculously so!

Why is semiclassical Schrödinger difficult? (1) Because the small ε generates oscillations at a frequency $\mathcal{O}\left(\varepsilon^{-1}\right)$ (known in quantum mechanics as wave packets), (2) The solution operator is unitary and this implies conservation in L_2 norm. It is vital to preserve this under discretisation, (3) the underlying physics is complicated (quantum tunnelling, quantum scattering, ...) and we want the numerics to model this faithfully.

Standard approach: Semidiscretise (either with a spectral method or with Hagedorn packets), resulting in the ODE

$$\boldsymbol{u}' = (\mathsf{i}\varepsilon\mathcal{D} + \mathsf{i}\varepsilon^{-1}\mathcal{V})\boldsymbol{u}, \qquad t \geq 0,$$

where $\mathcal{D}$ and $\mathcal{V}$ are discretisation matrices of the second derivative and of a multiplication by the potential, respectively. Its exact solution is

$$\boldsymbol{u}^{n+1} = \mathsf{e}^{\mathsf{i}\Delta t(\varepsilon\mathcal{D}+\varepsilon^{-1}\mathcal{V})}\boldsymbol{u}^n, \qquad n \in \mathbb{Z}_+,$$

except that we have a problem. The argument is very large and unstructured and our only hope is to use a Krylov subspace method. But large ε^{-1} renders such methods totally ineffective.

Splitting methods:

Strang's splitting: $S(\tau) = \mathrm{e}^{\frac{1}{2}\varepsilon\tau\mathcal{D}}\mathrm{e}^{\varepsilon^{-1}\tau\mathcal{V}}\mathrm{e}^{\frac{1}{2}\varepsilon\tau\mathcal{D}} = \mathrm{e}^{\mathrm{i}\tau(\varepsilon\mathcal{D}+\varepsilon^{-1}\mathcal{V})} + \mathcal{O}\left(\tau^3\right).$

Each individual exponential can be evaluated fast, e.g. with spectral collocation $\mathcal{D}$ is a circulant, whose exponential can be computed with FFT, while $\mathcal{V}$ is diagonal. Moreover, palindromy implies unitarity.

Yošida's splitting: $S(\alpha\tau)S((1-2\alpha)\tau)S(\alpha\tau) = \mathrm{e}^{\mathrm{i}\tau(\varepsilon\mathcal{D}+\varepsilon^{-1}\mathcal{V})} + \mathcal{O}\left(\tau^5\right)$

for $\alpha = 1/(2 - \sqrt[3]{2})$. Again, all exponentials can be evaluated fast and the splitting is palindromic, hence unitarity is preserved.

We can continue in this vain but... While the order increases linearily, the number of exponentials grows exponentially. Moreover, error constants become rapidly very large and they are typically $\mathcal{O}\left(\varepsilon^{-1}\right)$ – practical higher-order methods are ruled out!

Zassenhaus's splitting (Bader, AI, Kropielnicka & Singh) **:** Don't discretise yet! Let $\Delta t = \mathcal{O}(\varepsilon^\sigma)$ for $\sigma > 0$ and, since ultimately we'll need $\mathcal{O}\left(\varepsilon^{-1}\right)$ spatial degrees of freedom to resolve high oscillation, $\partial_x = \mathcal{O}\left(\varepsilon^{-1}\right)$. We seek

$$\mathrm{e}^{\tau(\varepsilon\partial_x^2+\varepsilon^{-1}V)} \approx \mathrm{e}^{\mathcal{R}_0}\mathrm{e}^{\mathcal{R}_1}\dots\mathrm{e}^{\mathcal{R}_s}\mathrm{e}^{\mathcal{T}_{s+1}}\mathrm{e}^{\mathcal{R}_s}\dots\mathrm{e}^{\mathcal{R}_1}\mathrm{e}^{\mathcal{R}_0}$$

where $\tau = \mathrm{i}\Delta t$, $\mathcal{R}_k = \mathcal{O}(\varepsilon^{\alpha_k})$, $\mathcal{T}_{s+1} = \mathcal{O}(\varepsilon^{\alpha_s+1})$ and $\alpha_0 \le \alpha_1 < \alpha_2 \cdots$, $\alpha_s \to \infty$. Note that everything is palindromic, hence unitary.

To derive Zassenhaus, let

$$\mathcal{T}_0 = \overbrace{\tau\varepsilon\partial_x^2}^{\mathcal{O}(\varepsilon^{\sigma-1})} + \overbrace{\tau\varepsilon^{-1}V}^{\mathcal{O}(\varepsilon^{\sigma-1})}, \qquad \mathcal{R}_0 = \tfrac{1}{2}\tau\varepsilon^{-1}V.$$

Having derived $\mathcal{T}_q$, set $\mathcal{R}_q$ to half the $\mathcal{O}(\varepsilon^{\alpha_q})$ term of $\mathcal{T}_q$ and let

$$\mathrm{e}^{\mathcal{T}_q} = \mathrm{e}^{\mathcal{R}_q}\mathrm{e}^{\mathcal{T}_{q+1}}\mathrm{e}^{\mathcal{R}_q} \;\Rightarrow\; \mathcal{T}_{q+1} = \log\left(\mathrm{e}^{-\mathcal{R}_q}\mathrm{e}^{\mathcal{T}_q}\mathrm{e}^{-\mathcal{R}_q}\right) = \mathsf{sBCH}(-2\mathcal{R}_q, \mathcal{T}_q),$$

where sBCH is the symmetric BCH operator.

Symmetric Baker–Campbell–Hausdorff operator:

$\mathrm{e}^{\frac{1}{2}X}\mathrm{e}^{Y}\mathrm{e}^{\frac{1}{2}X} = \mathrm{e}^{\mathsf{sBCH}(X,Y)}$ where

$$\mathsf{sBCH}(X,Y) = (X+Y) - \left(\tfrac{1}{24}[[Y,X],X] + \tfrac{1}{12}[[Y,X],X]\right)$$
$$+\Big(\tfrac{7}{5760}[[[[Y,X],X],X],X] + \tfrac{7}{1440}[[[[Y,X],X],X],Y] + \tfrac{1}{180}[[[[Y,X],X],Y],Y]$$
$$+\tfrac{1}{720}[[[[Y,X],Y],Y],Y] + \tfrac{1}{480}[[[Y,X],X],[Y,X]] - \tfrac{1}{360}[[[Y,X],Y],[Y,X]]\Big) + \cdots.$$

Note that $X, Y \in \mathfrak{g}$ ($\mathfrak{g}$ being a Lie algebra) implies that $\mathsf{sBCH}(X,Y) \in \mathfrak{g}$.*

Practical derivation of Zassenhaus splitting requires plenty of technical steps:
(1) Commutators are converted to linear combinations of derivatives: this process is accompanied by 'height reduction' – the highest derivative just goes away – and this is what renders Zassenhaus possible. For example, $[\partial_x^2, V] = (\partial_x^2 V) + 2(\partial_x V)\partial_x$, $[V,[\partial_x^2,V]] = -2(\partial_x^2 V)^2$,

(2) Terms need to be 'massaged' so that the approximation is unitary, and

(3) We need to choose optimal $\sigma > 0$.

*The first ten million terms and their coefficients have been listed by Murua.

Letting $\sigma = 1$, we obtain

$$
\begin{aligned}
\mathcal{R}_0 &= \tfrac{1}{2}\tau\varepsilon^{-1}V = \mathcal{O}(1),\\
\mathcal{R}_1 &= \tfrac{1}{2}\tau\varepsilon\partial_x^2 = \mathcal{O}(1),\\
\mathcal{R}_2 &= \tfrac{1}{24}\tau^3\varepsilon^{-1}(\partial_x V)^2 - \tfrac{1}{12}\tau^3\varepsilon\{(\partial_x^2 V)\partial_x^2 + \partial_x^2[(\partial_x^2 V)\cdot]\} = \mathcal{O}\left(\varepsilon^2\right),\\
\mathcal{R}_3 &= \tfrac{1}{120}\tau^5\varepsilon^{-1}(\partial_x^2 V)(\partial_x V)^2 + \tfrac{1}{24}\tau^3\varepsilon(\partial_x^4 V)\\
&\quad + \tfrac{1}{240}\tau^5\varepsilon\left(7\{(\partial_x^2 V)^2\partial_x^2 + \partial_x^2[(\partial_x^2 V)^2\cdot] + \{(\partial_x^3 V)(\partial_x V)\partial_x^2\right.\\
&\quad \left. + \partial_x^2[(\partial_x^3 V)(\partial_x V)\cdot]\}\right) - \tfrac{1}{120}\tau^5\varepsilon^{-3}\{(\partial_x^4 V)\partial_x^4 + \partial_x^4[(\partial_x^4 V)\cdot]\}\\
&= \mathcal{O}\left(\varepsilon^4\right)
\end{aligned}
$$

and so on. All matrices are skew-Hermitian, hence their exponentials are unitary. Moreover, using spectral collocation, $\mathcal{R}_0$ is diagonal, $\mathcal{R}_1$ a Toeplitz circulant (hence its exponential can be computed with FFT), while $\mathcal{R}_2$ and $\mathcal{R}_3$ can be computed to $\mathcal{O}\left(\varepsilon^6\right)$ in 3 and 2 Krylov iterations respectively.

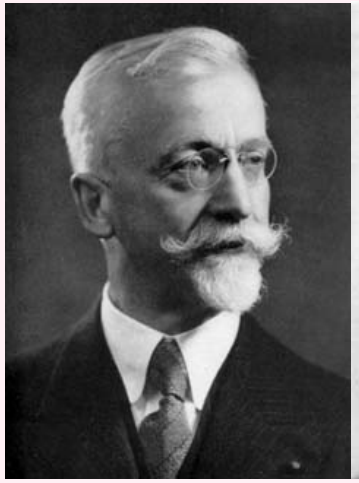
All this can be generalised to other settings.

11. A take-home lesson

- Wishing to discretise a differential equation, ask yourself *"what do I know about the qualitative behaviour of the solution?"* A good numerical method takes this into account and attempts to respect underlying qualitative features (whether dynamical or geometric) of the exact solution.
- Geometric features are best formulated in the language of differential geometry but (numerical analysts being the ultimate mathematical magpies) feel free to use any kind of mathematics – from abstract algebra to algebraic topology to graph theory, from nonlinear dynamics to functional analysis and beyond.
- It is not enough to discretise: you must understand your discretisation *as a mathematical object.*

Mathematics doesn't stop once you discretise – it just becomes more difficult!

Putting faces to names 1. *Theoretical foundations*


Elié Cartan


Felix Hausdorff


Hermann Grassmann


Peter Lax


Wilhelm Magnus

Putting faces to names 2. *Geometric numerical integration*

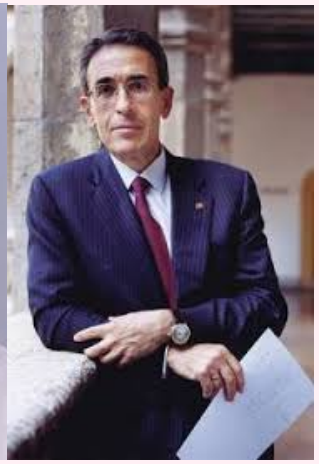

Ernst Hairer


Feng Kang


Christian Lubich


Jerry Marsden


Robert McLachlan


Chus Sanz-Serna

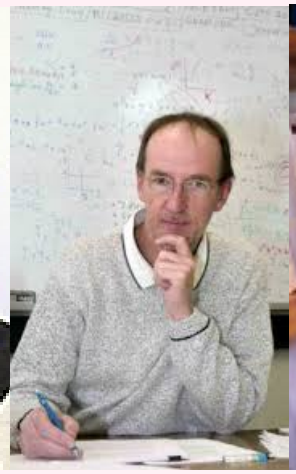
Putting faces to names 3. *Lie-group methods*


Elena Celledoni


Hans Munthe-Kaas


Brynjulf Owren

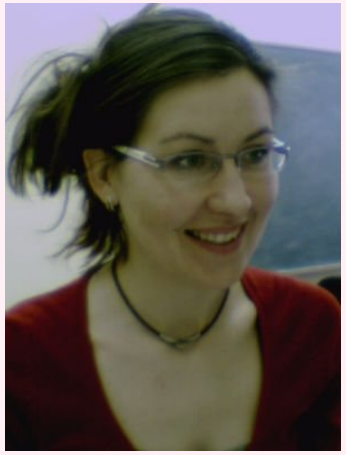

Syvert Nørsett

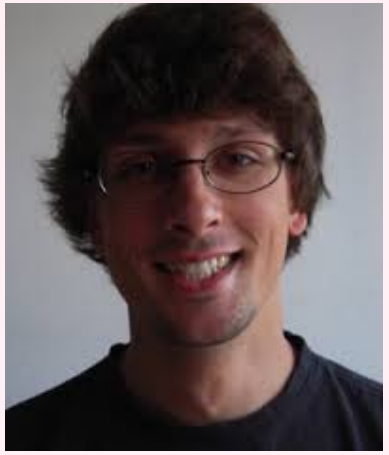

Reinout Quispel


Antonella Zanna

Putting faces to names 4. *Our examples*


Philipp Bader


Karolina Kropielnicka


Gil Ramos


Pranav Singh