Geometric Inegration and Multirating Schemes I

—

the $I\!\!R^n$-case

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Contents

- ODEs & first integrals
- Geometric integration schemes
- Symplecticity and symplectic schemes
- Weak invariants and projection schemes
- Time reversibility and symmetrical schemes
- Adaptivity
- Multirate schemes

ODEs & first integrals

Definition

Consider the ODE-IVP

$$\dot{y} = f(y),\ y(0) = y_0 \quad \text{with } y \in \mathbb{R}^n(\mathbb{R}^{n\times n}).$$

A non-constant function $I(y)$ is called a first integral (invariant, conserved quantity, constant of motion) if

$$I'(y)f(y) = 0 \quad \forall y \in \mathbb{R}^n(\mathbb{R}^{n\times n}).$$

This implies that every ODE solution satisfies $I(y(t)) = I(y_0) =$const.

Important special cases:

- linear invariant: $I(y) = d^\top y$ with $d \in \mathbb{R}^n$ constant;
- quadratic invariant: $I(y) = y^\top Cy$ with $C \in \mathbb{R}^{n\times n}$ (skew-)symmetric;
- polynomial invariants: $I(y)$ is a polynomial of degree n;
- positivity : $I(y) = \text{sign}(y)$

A first example for linear and quadratic invariants

Conservation of total linear and angular momentum of N-body systems

Hamiltonian:

$$H(p,q) = \frac{1}{2}\sum_{i=1}^{N}\frac{1}{m_i}p_i^\top p_i + \sum_{i=2}^{N}\sum_{j=1}^{i-1} V_{ij}\left(||q_i - q_j||\right)$$

Equation of motion:

$$\dot{q}_i = \frac{1}{m_i}p_i, \quad \dot{p}_i = \sum_{j=1}^{N}\nu_{ij}(q_i - q_j)$$

with $\nu_{ij} = \nu_{ji} = -V_{ij}'(r_{ij})/r_{ij}$, $r_{ij} = ||q_i - q_j||$

A first example for linear and quadratic invariants

Conservation of total linear momentum $P = \sum_{i=1}^{N} p_i$:

$$\frac{\mathrm{d}}{\mathrm{d}t} \sum_{i=1}^{N} p_i = \sum_{i=1}^{N} \sum_{j=1}^{N} \nu_{ij}(q_i - q_j) = 0$$

$\Leftrightarrow P = \mathbb{1}^\top p =$ const is a linear invariant

Conservation of angular momentum $L = \sum_{i=1}^{N} q_i \times p_i$:

$$\frac{\mathrm{d}}{\mathrm{d}t} \sum_{i=1}^{N} q_i \times p_i = \sum_{i=1}^{N} \frac{1}{m_i} p_i \times p_i + \sum_{i=1}^{N} \sum_{j=1}^{N} q_i \times \nu_{ij}(q_i - q_j) = 0$$

$\Leftrightarrow L$ is a quadratic invariant

A first example for polynomial invariants: isospectral flow

The flow defined by the matrix ODE-IVP

$$\dot{L} = [B(L), L], \quad L(0) = L_0$$

with L_0 symmetric and $B(L)$ skew-symmetric for all L preserves the spectrum of L_0

$\Rightarrow$ $\det(L - \lambda I) = \sum_{i=0}^{n} a_i \lambda^i$ does not depend on t

$\Rightarrow$ all $n+1$ coefficients a_i are polynomial invariants!

More appropriate: consider matrix ODE-IVP

$$\dot{U} = B(L(t))U, \quad U(0) = I$$

with quadratic invariant $U^\top U = I$

Both systems related by $L(t) = U(t) L_0 U(t)^{-1}$

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Geometric integration schemes

Consider an ODE-IVP

$$\dot{y} = f(y), \quad y(0) = y_0$$

with invariant $g(y)$=const.

A numerical (one-step) scheme

$$y_1 = \Phi_h(y_0)$$

is said to conserve this invariant, if applied to the ODE-IVP, it holds $g(y_1) = g(y_0)$.

We will now investigate under which conditions

- (Partitioned) RK schemes, and
- Composition schemes

conserve all linear, nonlinear and polynomial invariants.

RK schemes

Let $b_i, a_{ij} (i, j = 1, \dots, s)$ be real numbers. An s-stage Runge-Kutta method for the ODE-IVP $\dot{y} = f(y), \quad y(0) = y_0$ is given by

$$\begin{aligned} k_i &= f(y_0 + h \sum_{j=1}^{s} a_{ij} k_j), \quad i = 1, \dots, s \\ y_1 &= y_0 + h \sum_{i=1}^{s} b_i k_i \end{aligned}$$

- all linear invariants: conserved by all RK schemes;
- all quadrativ invariants: conserved if

$$b_i a_{ij} + b_j a_{ji} = b_i b_j \quad \forall i, j = 1, \dots, s$$

- all polynomial invariants with $n > 2$: cannot be conserved by RK schemes

Partitioned RK schemes

$$\begin{aligned}\dot{y} &= f(y, z), \quad y(0) = y_0 \\ \dot{z} &= g(y, z), \quad z(0) = z_0\end{aligned}$$

Let b_i, a_{ij} and $\widehat{b}_i, \widehat{a}_{ij} (i = 1, \ldots, s)$ be the coefficients of two RK methods. A partitioned RK method for the solution of the partitioned ODE-IVP is given by

$$\begin{aligned}k_i &= f(y_0 + h\sum_{j=1}^{s} a_{ij}k_j, z_0 + h\sum_{j=1}^{s} \widehat{a}_{ij}l_j), \\ l_i &= g(y_0 + h\sum_{j=1}^{s} a_{ij}k_j, z_0 + h\sum_{j=1}^{s} \widehat{a}_{ij}l_j), \\ y_1 &= y_0 + h\sum_{i=1}^{s} b_i k_i, \quad z_1 = z_0 + h\sum_{i=1}^{s} \widehat{b}_i l_i\end{aligned}$$

Partitioned RK schemes

We have:

- linear invariants: conserved if $b_i = \widehat{b}_i (i = 1, \ldots, s)$ or $I = I(y)$ or $I = I(z)$;
- quadrativ invariants of the type $I(y, z) = y^\top Dz.$: conserved if

  $b_i \widehat{a}_{ij} + \widehat{b}_j a_{ji} = b_i \widehat{b}_j \quad \forall i, j = 1, \ldots, s$ and $b_i = \widehat{b}_i \quad \forall i = 1, \ldots, s$
- all polynomial invariants with $n > 2$: cannot be conserved by RK schemes

Composition methods

Definition

Let Φ_h be (any) basic method and $\gamma_1, \ldots \gamma_s$ real numbers. Then we call its composition with step sizes $\gamma_1 h, \gamma_2 h, \ldots, \gamma_s h$, i.e.,

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

the corresponding composition method.

We have:

- linear invariant conserved, if conserved by the underlying basic method;
- quadratic invariants are conserved, if conserved by the underlying basic method;

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Symplecticity as a quadratic invariant

Let $H(p, q)$ be a twice continuously differentiable function on $U \subset \mathbb{R}^{2d}$. With $y := (p, q)$, the associated Hamiltonian system reads

$$\dot{y} = J^{-1} \nabla H(y) \quad \text{with } J = \begin{pmatrix} 0 & I \\ -I & 0 \end{pmatrix}$$

and $\nabla H(y) = H'(y)^\top$.

The flow φ_t of the Hamiltonian system is a symplectic transformation, i.e.,

$$\underbrace{\left(\frac{\partial \varphi_t}{\partial y_0}\right)}_{\Psi :=}^{\top} J \underbrace{\left(\frac{\partial \varphi_t}{\partial y_0}\right)}_{\Psi :=} = J \quad \forall t \, \forall y_0.$$

Symplecticity as a quadratic invariant

The symplecticity condition $\Psi^\top J \Psi = J$ is a quadratic invariant of the following augmented system:

$$\begin{aligned} \dot{y} &= J^{-1}\nabla H(y), \\ \dot{\Psi} &= J^{-1}\nabla^2 H(y)\Psi, \end{aligned}$$

as seen as follows $(J^\top = -J!)$:

$$\begin{aligned} \frac{\mathrm{d}}{\mathrm{d}t}(\Psi^\top J \Psi) &= (J^{-1}\nabla^2 H(y)\Psi)^\top J\Psi + \Psi^\top J(J^{-1}\nabla^2 H(y)\Psi) = 0, \\ \Psi(0)^\top J \Psi(0) &= J. \end{aligned}$$

Symplectic numerical schemes

RK schemes

Symplecticity condition is a quadratic invariant $\Longrightarrow$

Rk method symplectic $\Leftrightarrow$ $b_i a_{ij} + b_j a_{ji} = b_i b_j \, \forall i, j = 1, \dots, s$

Partioned RK scheme

Symplecticity condition can be rewritten into the form $I(y,z) = y^\top D z \Longrightarrow$

Partitioned RK method symplectic $\Leftrightarrow$

$b_i \widehat{a}_{ij} + \widehat{b}_j a_{ji} = b_i \widehat{b}_j, b_i = \widehat{b}_i \, \forall i, j = 1, \dots, s$

Composition schemes

Composition schemes are symplectic if the basic scheme is symplectic.

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Weak invariants and ODEs on manifolds

Definition

Suppose we have an $(n-m)$-dimensional submanifold of $\mathbb{R}^n$,

$$\mathcal{M} = \{y : g(y) = 0\} \text{ with } g : \mathbb{R}^n - \mathbb{R}^m,$$

and an ODE-IVP $\dot{y} = f(y)$, $y(0) = y_0$ with the property that

$$y_0 \in \mathcal{M} \text{ implies } y(t) \in \mathcal{M} \, \forall t.$$

Then we call $g(y)$ a weak invariant , and we say that $\dot{y} = f(y)$ is a differential equation on the manifold $\mathcal{M}$.

Note the differences:

- invariant $\Leftrightarrow g'(y)f(y) = 0 \, \forall y \in \mathbb{R}^n$;
- weak invariant $\Leftrightarrow g'(y)f(y) = 0 \, \forall y \in \mathcal{M}$;

Invariants and weak invariants

Consider mathematical pendulum in minimal coordinates:

$$\dot{y} = f(y) \Leftrightarrow \begin{pmatrix} \dot{q}_1 \\ \dot{q}_2 \\ \dot{p}_1 \\ \dot{p}_2 \end{pmatrix} = \begin{pmatrix} p_1 \\ p_2 \\ -q_1\lambda \\ -1 - q_2\lambda \end{pmatrix}$$

with $\lambda = (p_1^2 + p_2^2 - q_2)/(q_1^2 + q_2^2)$.

Quadratic invariant : $g(y) = q_1 p_1 + q_2 p_2$

$$\begin{aligned} g'(y) f(y) &= (p_1 \, p_2 \, q_1 \, q_2) \cdot \begin{pmatrix} p_1 \\ p_2 \\ -q_1\lambda \\ -1 - q_2\lambda \end{pmatrix} \\ &= p_1^2 + p_2^2 - q_2 - \lambda(q_1^2 + q_2^2) = 0 \quad \forall y \in I\!R^4; \end{aligned}$$

Invariants and weak invariants

Weak quadratic invariant : $g(y) = q_1^2 + q_2^2$

$$
\begin{aligned}
g'(y)f(y) &= (2q_1\, 2q_2\, 0\, 0) \cdot \begin{pmatrix} p_1 \\ p_2 \\ -q_1\lambda \\ -1 - q_2\lambda \end{pmatrix} \\
&= 2(q_1p_1 + q_2p_2) = 0 \quad \forall y \in \mathcal{M} := \{y : q_1^2 + q_2^2 = const\};
\end{aligned}
$$

Note: Method which conserve quadratic invariants do not conserve weak quadratic invariants!

Way-out: Projection schemes

- first compute $\widetilde{y}_1 = \Phi_h(y_0)$ using any arbitrary one step scheme
- project then the value $\widetilde{y}_1$ onto the manifold $\mathcal{M}$ to obtain $y_1 \in \mathcal{M}$

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Time reversibility and symmetry

Definitions

Let ρ be an invertible linear transformation in the phase space of $\dot{y} = f(y)$. This ODE and the vector field $f(y)$ are called ρ-reversible if

$$\rho f(y) = -f(\rho y)\,\forall y.$$

A map $\Phi(y)$ is called ρ-reversible if

$$\Phi \circ \rho \circ \Phi = \rho.$$

A numerical one-step method Φ_h is called symmetric or time reversible, if it satisfies

$$\Phi_h = \Phi_h^\star \qquad (\Phi_h^\star := \Phi_{-h}^{-1}).$$

Example: Hamiltonian system $\dot{y} = J^{-1}\nabla H(y)$ is ρ-reversible with $\rho(p,q) = (-p,q)$.

Symmetrical methods

If a numerical method, applied to a ρ-reversible differential equation, satfisfies

$$\rho \circ \Phi_h = \Phi_{-h} \circ \rho,$$

then the numerical flow Φ_h is a ρ-reversible map if and only if Φ_h is a symmetric method.

This condition is satisfied by most numerical methods, e.g., for

- all RK schemes,
- all partitioned RK schemes if $\rho(y, z) = (\rho_1(y), \rho_2(z))$ with invertible ρ_1, ρ_2,
- all composition methods if the basic schemes satisfy the condition.

Symmetrical methods

RK schemes

symmetric $\Leftrightarrow$ $a_{s+1-i,s+1-j} + a_{ij} = b_j \, \forall i, j.$

Partitioned RK schemes

symmetric $\Leftrightarrow$ above condition satisfied for both coefficient sets

Composition methods

symmetric, e.g., if

$$\Psi_h = \Phi_{\alpha_s h} \circ \Phi^\star_{\beta_s h} \circ \cdots \circ \Phi^\star_{\beta_2 h} \circ \Phi_{\alpha_1 h} \circ \Phi^\star_{\beta_1 h},$$

where Φ_s any arbitraty first order method and $\alpha_s = \beta_1, \alpha_{s-1} = \beta_2$, etc.

Examples

RK scheme

Gauß formulas are symmetric and symplectic. Lobatto schemes such as the trapezoidal rule are symmetric, but not symplectic.

Partioned RK scheme

The Störmer-Verlet is both symmetric and symplectic.

Composition schemes

Any composition scheme $\Phi_{\gamma_1 h} \circ \Phi_{\gamma_2 h}$ of symplectic methods is symplectic but symmetric only if $\gamma_1 = \gamma_2$.

Stömer-Verlet again

$$\begin{aligned} \dot{y} &= f(y,z), \quad y(0) = y_0 \\ \dot{z} &= g(y,z), \quad z(0) = z_0 \end{aligned}$$

Störmer-Verlet (Partitioned DIRK scheme) reads

$$\begin{aligned} k_1 &= f(y_0, z_0 + \frac{h}{2} l_1), \\ l_1 &= g(y_0, z_0 + \frac{h}{2} l_1), \\ k_2 &= f(y_0 + \frac{h}{2}(k_1 + k_2), z_0 + \frac{h}{2} l_1), \\ l_2 &= g(y_0 + \frac{h}{2}(k_1 + k_2), z_0 + \frac{h}{2} l_1), \\ y_1 &= y_0 + \frac{h}{2}(k_1 + k_2) \\ z_2 &= z_0 + \frac{h}{2}(l_1 + l_2) \end{aligned}$$

Störmer-Verlet again

For separable systems $f = f(z), g = g(y)$ Störmer-Verlet reads

$$\begin{aligned} k_1 &= f(z_0 + \frac{h}{2} l_1), \\ l_1 &= g(y_0), \\ k_2 &= f(z_0 + \frac{h}{2} l_1), \\ l_2 &= g(y_0 + \frac{h}{2}(k_1 + k_2)), \\ y_1 &= y_0 + \frac{h}{2}(k_1 + k_2) \\ z_2 &= z_0 + \frac{h}{2}(l_1 + l_2) \end{aligned}$$

⇒ explicit leap-frog scheme

Higher-order schemes

RK schemes

Symmetric diagonally implicit RK schemes are equivalent to a composition of Θ-schemes. Symplectic diagonally implicit RK schemes are equivalent to a composition of implicit midpoint schemes.

$\Rightarrow$ Higher-order symmetric and symplectic schemes are either composition schemes or fully implicit (such as Gauß formulas)

Partitioned RK schemes

Symmetric and symplectic partitioned diagonally implicit RK schemes (with $a_{ii}\widehat{a}_{ii} = 0$) are equivalent to a composition of the symplectic Euler methods.

$\Rightarrow$ Higher-order symmetric and symplectic schemes are either composition schemes or implicit.

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Time transformations & adaptivity

Idea: for solving ODE $\dot{y} = f(y)$, non-equidistant time grid with step sizes $h = \varepsilon\sigma(y)$ produced by a time transformation $t \leftrightarrow \tau := t/\sigma(y)$

$$y' = \sigma(y) f(y), \qquad t' = \sigma(y) \qquad \left(' := \frac{\mathrm{d}}{\mathrm{d}\tau}\right)$$

Transformation structure preserving?

- preserve ρ-reversibility for ρ-reversible systems: $\sigma(\rho y) = \sigma(y)$ $\surd$
- preserve symplecticity: $\sigma(y) = \text{const}$???

  Way-out: consider new Hamiltonian

  $$K(y) = \sigma(y)(H(y) - H_0) \quad \text{with } H_0 = H(y_0),$$

  which yields corresponding Hamiltonian system

  $$y' = \sigma(y) J^{-1} \nabla H(y) + (H(y) - H_0) J^{-1} \nabla \sigma(y).$$

  Perturbed system, but perturbation vanishes along the solution!

Choices of step size functions

- $\sigma(y) = ||f(y)||^{-1}$
  - no a-priori knowledge of the solution needed
  - arc-length paramterization ($||y'(\tau)|| = 1$)
  - approximations are nearly equidistant in the phase space
- for separable Hamiltonians $H(p,q) = \frac{1}{2} \cdot p^\top M^{-1} p + U(q)$:

$$\sigma(p,q) = \left(\frac{1}{2} p^\top M^{-1} p + \nabla U(q)^\top M^{-1} \nabla U(q) \right)^{-1/2}$$

  - invariant with respect to linear coordinate changes
  - exploiting the fact that the Hamiltonian is constant along the solution, one may use instead

$$\sigma(q) = \big((H_0 - U(q)) + \nabla U(q)^\top M^{-1} \nabla U(q) \big)^{-1/2}$$

  - to get an approximately equidistant output in the q-space:

$$\sigma(q) = (H_0 - U(q))^{-1/2}$$

Reversible controllers

Aim:

- no a-priori knowledge of $\sigma(y)$ should be needed
- but adaptive step size control should be time-reversible

Problem: standard step size controllers are not reversible

Way-out: in contrast to standard step size control, demand equality of error estimate and tolerance

Simple example: trapezoidal rule

$$
\begin{aligned}
y_{n+1} &= y_n + \frac{h}{2}\left(f(y_n) + f(y_{n+1})\right) \\
0 &= \left\| \frac{h}{2}\left(f(y_{n+1}) - f(y_n)\right) \right\| - \mathrm{tol}
\end{aligned}
$$

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Multirate behaviour

Multirate behaviour may be due to

- different slow/fast dynamics in solution components
  $\Rightarrow$ multirate schemes which use different step sizes for slow/fast components
- computationally expensive parts of the right-hand side with slow dynamics
  $\Rightarrow$ multiple time stepping which evaluates the expensive part less often then the rest
- different time scales in all solution components
  $\Rightarrow$ multirate PDE approach which transforms the ODE system into a PDE system in all time scales and solves this transformed system very efficiently

Multirate schemes

Starting point: partitioned system

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

Solve slow part y with stepsize h, and fast part z with step size h/N

- interpolation/extrapolation: replace z in f and y in g by some extrapolation/interpolation formulas
- generalized multirating: replace evaluation of z in f and y in g by internal RK stages in different time scales
- detect partitioning and appropriate time scales on the fly by subsequent integration steps

Overall problem: maintain stability and order of convergence in H

Fast-slow splitting

$$\dot{y} = f(y) = f^S(y) + f^F(y)$$

Multiple time stepping is defined by the fast-slow splitting

$$\Phi_h := \left(\Phi^S_{h/2}\right)^\star \circ \left(\Phi^F_{h/N}\right)^N \circ \left(\Phi^S_{h/2}\right)$$

with numerical integration schemes Φ^S_h and Φ^F_h consistent with $\dot{y} = f^S(y)$ and $\dot{y} = f^F(y)$, respectively.

It holds:

- For Φ^S_h arbitrary method of order 1 and Φ^F_h symmetric method of order 2, the fast-slow splitting is symmetric and of order 2.
- If $f^S(y)$ and $f^F(y)$ are Hamiltionian and both Φ^S_h and Φ^F_h are symmetric, the fast-slow splitting is also symplectic.

Fast-slow splitting for separable Hamiltonian systems

$$H(p,q) = T(p) + U(q) = \underbrace{T(p) + U^F(q)}_{\text{fast}} + \underbrace{U^S(q)}_{\text{slow}}$$

Multiple time stepping is defined by the fast-slow splitting

$$\varphi_h := \varphi^S_{h/2} \left(\varphi^F_{h/2N} \circ \varphi^T_{h/N} \circ \varphi^F_{h/2N} \right)^N \circ \varphi^S_{h/2}$$

with numerical integration schemes φ^T_h, φ^S_h and φ^F_h consistent with Hamiltonian systems for $T(p), U^S(q)$ and $U^F(q)$, respectively.

Note: N Störmer-Verlet steps (equivalent to Strang splitting!) are used for the fast part!