Symmetric and Symplectic integration

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Oversigt

Introduction

- Invariants
  - Lotka-Volterra
  - Dynamical systems
  - Mass conservation
- Time reversibility
- Symplectic methods

Invariants

Definitions

Consider the autonomous IVP:

$$\dot{y} = f(y), \quad y(t_0) = y_0 \tag{1.1}$$

where y is a vector or possibly a matrix

Definition (Invariants)

A non-constant function $I(y)$ is called an invariant of the IVP if:

$$I'(y)f(y) = 0, \quad \forall y, \tag{1.2}$$

which is the same as saying that every solution satisfies $I(y(t)) = I(y_0) =$ constant. Synonymously with invariant, the terms first integral, conserved quantity and constant of motion are also used.

Linear Invariants

Theorem (Conservation of Linear Invariants)

All explicit and implicit Runge-Kutta methods conserve linear invariants. Partitioned Runge-Kutta methods conserve linear invariants if $b_i = \hat{b}_i$ for all i, or if the invariant depend only on p or q.

Proof.

Let $I(y) = d^T y$ then $d^T f(y) = 0$ for all y. Thus also $d^T k_i = 0$ and consequently $d^T y_1 = d^T y_0 + 0 = d^T y_0$ □

Quadratic Invariants (For Runge-Kutta Methods)

Consider the quadratic function:

$$Q(y) = y^T C y \tag{1.3}$$

where C is a symmetric square matrix. If $y^T C f(y) = 0$ then it is an invariant of the previous IVP.

Theorem

The collocation methods based upon the Gauss methods conserve quadratic invariants

Recall that all collocation methods are also Runge-Kutta methods. Further we have:

Theorem (Cooper 1987)

If the coefficients of a Runge-Kutta method satisfy

$$b_i a_{ij} + b_j a_{ji} = b_i b_j, \quad \forall i, j = 1, \ldots, s, \tag{1.4}$$

then the method conserves quadratic invariants.

Quadratic Invariants (for Partitioned Runge-Kutta Methods)

Consider the quadratic function:

$$Q(y) = y^T Dz \tag{1.5}$$

where D is of the appropriate dimensions. Note that the angular momentum of N-body problems are of this form.

Theorem

The Lobatto IIIA- IIIB pair conserves all quadratic invariants all invariants of the above form.

Theorem

If the coefficients of a Partitioned Runge-Kutta method satisfy

$$b_i \hat{a}_{ij} + \hat{b}_j a_{ji} = b_i \hat{b}_j, \quad \forall i, j = 1, \ldots, s, \tag{1.6}$$

$$b_i = \hat{b}_i, \quad \forall i = 1, \ldots, s, \tag{1.7}$$

then it conserves quadratic invariants.

Quadratic Invariants (Composition Methods)

Theorem (Compositions Methods)

If a methods conserves quadratic invariants, then so does the composition method

$$\Psi_h = \phi_{\lambda_s h} \circ \cdots \circ \phi_{\lambda_1 h} \tag{1.8}$$

This obvious property is one of the most important motivations for considering composition methods.

Polynomial Invariants

Theorem

for $n \geq 3$, no Runge-Kutta method can conserve all polynomial invariants of degree n.

Proof.

It is enough to consider linear problems $\dot{Y} = AY$, and applying a Runge-Kutta method to such a problem implies that $R(hA)Y_0 = Y_1$, where R is the stability function. To conserve all polynomial invariants we therefore need $R(hA) = 1$ for all A with $trace(A) = 0$. Which is not possible. □

Weak invariants

Definition (Weak invariant)

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

$$\mathcal{M} = \{y|g(y) = 0\} \tag{1.9}$$

$(g : \mathbb{R}^n \to \mathbb{R}^m)$ *and a differential equation* $\dot{y} = f(y)$ *with the property that:*

$$y_0 \in \mathcal{M} \implies y(t) \in \mathcal{M}, \quad \forall t \tag{1.10}$$

then $g(y)$ *is said to be a weak invariant.*

In physics this is typically due to generalized coordinates e.g. the length of a pendulum is a weak invariant

Projection Method

The standard method is to use projection

Algorithm (Standard Projection Method)

Assume that $y_n \in \mathcal{M}$. One step $y_n \mapsto y_{n+1}$ is defined as follows:

- *Compute $\tilde{y}_{n+1} = \Phi_h(y_n)$, where Φ_h is an arbitrary one step method*
- *Project the value $\tilde{y}_{n+1}$ onto the manifold $\mathcal{M}$*

$$\min \|y_{n+1} - \tilde{y}_{n+1}\|, \textit{Subject to } g(y_{n+1}) = 0 \qquad (1.11)$$

Warning: Using this method wrongly, one might destroy existing good behaviour.

Another method is to use local coordinates.

Symmetric Integration

Exact flow

Definition

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

$$\rho f(y) = -f(\rho y) \quad \forall y \tag{2.1}$$

Definition

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

$$\rho \circ \Phi = \Phi^{-1} \circ \rho \tag{2.2}$$

Numerical flow

Definition

A numerical one-step method is called symmetric if it satisfies:

$$\Phi_h = \Phi_{-h}^{-1} =: \Phi^* \tag{2.3}$$

Theorem

If a numerical method applied to a ρ-reversible differential equation satisfies:

$$\rho \circ \Phi_h = \Phi_{-h} \circ \rho, \tag{2.4}$$

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

Note that apart from the method to be symmetric this is a very weak demand:

Numerical flow

- Runge-Kutta Methods - No restrictions
- Partitioned Runge-Kutta methods - $\rho(u, v) = (\rho_1(u), \rho_2(v))$ invertible
- Composition methods - The basic method have to fulfil it
- Splitting methods - For the normal splitting, no restrictions

Adjoint of a Collocation Method

Theorem

The adjoint of a collocation method based on $c_1, \ldots, c_s$ is a collocation method based on $c_1^*, \ldots, c_s^*$, where

$$c_i^* = 1 - c_{s+1-i} \tag{2.5}$$

In the case where $c_i = 1 - c_{s+1-i}$, then the collocation method is symmetric

Proof.

Exchange (t_0, y_0) with $(t_0 + h, y_1)$ and h with $-h$, yields the result. □

Lemma

The Gauss formulas as well as the Lobatto IIIA and Lobatto IIIB are symmetric integrators (then also Störmer Verlet is symmetric)

Recall that all collocation methods are Runge-Kutta methods.

Adjoint of a Runge-Kutta method

Theorem (Stetter 1973, Wanner 1973)

The adjoint of an s-stage Runge-Kutta method is again an s-stage Runge-Kutta method. Its coefficients are given by:

$$a_{ij}^* = b_{s+1-j} - a_{s+1-i,s+1-j}, \quad b_i^* = b_{s+1-i} \tag{2.6}$$

In the case where $a_{s+1-i,s+1-j} + a_{ij} = b_j$ then the Runge-Kutta method is symmetric

Proof.

As before by exchanging y_0 with y_1 and h with $-h$ we get the result □

Lemma

No explicit Runge-Kutta method can be symmetric.

Diagonally Implicit Runge-Kutta methods (DIRK)

Then the above conditions changes to:

$$a_{ij} = b_j = b_{s+1-j} \quad i > j, \quad a_{jj} + a_{s+1-j,s+1-j} = b_j \quad (2.7)$$

Example for $s = 5$

c_1	a_{11}				
c_2	b_1	a_{22}			
c_3	b_1	b_2	a_{33}		
$1-c_2$	b_1	b_2	b_3	a_{44}	
$1-c_1$	b_1	b_2	b_3	b_2	a_{55}
	b_1	b_2	b_3	b_2	b_1

Composition of θ-Methods

Definition (θ-Method)

A θ-method is a one step methods which fulfils that:

$$\Phi_h^{\theta}(y_0) = y_1, \tag{2.8}$$

where

$$y_1 = y_0 + h\left((1-\theta) f(t_n, y_n) + \theta f(t_{n+1}, y_{n+1})\right) \tag{2.9}$$

note that $\Phi_h^{\theta *} = \Phi_h^{1-\theta}$

Theorem

A diagonally implicit Runge-Kutta method satisfying the symmetry condition and $b_i \neq 0$ is equivalent to a composition of θ-methods

$$\Phi_{b_1 h}^{\alpha_1 *} \circ \Phi_{b_2 h}^{\alpha_2 *} \circ \cdots \circ \Phi_{b_2 h}^{\alpha_2} \circ \Phi_{b_1 h}^{\alpha_1} \tag{2.10}$$

where $\alpha_i = a_{ii}/b_i$

Example

Modified midpoint rule for partitioned Runge-Kutta method (introduction of constant).

Algorithm

$$q_i^{n+1} = q_i^n \frac{h}{m_i} p_i^{n+1/2} \tag{2.11}$$

$$p_i^{n+1} = p_i^n + h \sum_{j=1}^{N} \sigma(q_i^{n+1/2} - q_j^{n+1/2}) \tag{2.12}$$

where $p_i^{n+1/2}$ is the average of p_i^n and p_i^{n+1}, and for $i > j$,

$$\sigma_{ij} = \sigma_{ji} = \frac{V_{ij}(r_{ij}^{n+1}) - V_{ij}(r_{ij}^n)}{r_{ij}^{n+1} - r_{ij}^n} \frac{1}{r_{ij}^{n+1/2}}, \tag{2.13}$$

further r_{ij} is the distance between particle i and j and $\sigma_{ii} = 0$

Example

Theorem (LaBudde and Greenspan 1974)

The above method is a second order symmetric implicit method which conserves the total linear momentum, the total angular momentum, and the total energy for N-body problems.

Symplectic Integration

A Bit of Classical Mechanics

Suppose that the position of a mechanical system with d degrees of freedom is described by $q = (q_1, \ldots, q_d)$ as generalized coordinates. We now have a function

$$T = T(q, \dot{q}), \tag{3.1}$$

which is the kinetic energy, typically it is of the form $\frac{1}{2}\dot{q}^T M(q)\dot{q}$, where $M(q)$ is symmetric and positive definite. We also have a function

$$U = U(q) \tag{3.2}$$

which is the potential energy.

A Bit of Classical Mechanics

Definition (Lagrangian)

We can now define the Lagrangian

$$L = T - U \tag{3.3}$$

such that the coordinates must obey the differential equation (known as Lagrange's equations)

$$\frac{d}{dt}\left(\frac{\partial L}{\partial \dot{q}}\right) = \frac{\partial L}{\partial q} \tag{3.4}$$

A Bit of Classical Mechanics

First introducing the momenta

$$p_k = \frac{\partial L}{\partial \dot{q}_k}(q, \dot{q}) \tag{3.5}$$

Definition (Hamiltonian)

We can now define the Hamiltonian:

$$H := p^T \dot{q} - L(q, \dot{q}) \tag{3.6}$$

Theorem

Lagrange's equations are equivalent to Hamilton's equations:

$$\dot{p}_k = -\frac{\partial H}{\partial q_k}(p, q), \quad \dot{q}_k = \frac{\partial H}{\partial p_k}(p, q) \tag{3.7}$$

A Bit of Classical Mechanics

Lemma (Case of Quadratic T (typical case))

In the case where $T = \frac{1}{2}\dot{q}^T M(q)\dot{q}$ and $M(q)$ is symmetric and positive definite, we have the Hamiltonian:

$$H(p, q) = \frac{1}{2}p^T M(q)^{-1}p + U(q) = T + U \tag{3.8}$$

Example:
For a mass point in $\mathbb{R}^3$, we have that $M(q) = m$ which is the mass. The kinetic energy is $T = \frac{1}{2}m\|\dot{x}\|_2^2$ then the momenta is $p_k = m\dot{x}_k$. If it moves in a conservative force field $F = -\nabla U(x)$ then the Lagrange's equations (and Hamilton's equations) becomes Newtons second law of motion

$$F = m\ddot{x}, \quad (\dot{x} = \dot{x}) \tag{3.9}$$

Symplectic Transformations

Definition

A linear mapping $A : \mathbb{R}^{2d} \to \mathbb{R}^{2d}$ *is called symplectic if:*

$$A^T J A = J, \quad J = \begin{pmatrix} 0 & I \\ -I & 0 \end{pmatrix} \tag{3.10}$$

or, equivalently, if $\omega(A\xi, A\eta) = \omega(\xi, \eta)$ *where*

$$\omega(\xi, \eta) := \sum_{i=1}^{d} det \begin{pmatrix} \xi_i^p & \eta_i^p \\ \xi_i^q & \eta_i^q \end{pmatrix} \tag{3.11}$$

Definition (Non-Linear Maps)

A differential map $g : U \to \mathbb{R}^{2d}$ *(where* $U \subset \mathbb{R}^{2d}$ *is an open set)is called symplectic if the Jacobian matrix of* g *is everywhere symplectic.*

Connection to Hamiltonian Systems

Theorem (Poincaré 1899)

Let the Hamiltonian be a twice continuously differentiable function on $U \subset \mathbb{R}^{2d}$. Then, for each fixed t, the flow ϕ_t is a symplectic transformation wherever it is defined.

Definition (Locally Hamiltonian)

Consider a differential equation, $\dot{y} = f(y)$, then if there for every $y_0 \in U$ exists a neighbourhood where $f(y) = J^{-1}\nabla H(y)$ for some function H. Then we call the differential equation locally Hamiltonian.

Theorem

Let $f : U \to \mathbb{R}^{2d}$ be a continuously differentiable. Then, $\dot{y} = f(y)$ is locally Hamiltonian if and only if its flow $\phi_t(y)$ is symplectic for all $y \in U$ and for all sufficiently small t

Connection to Hamiltonian Systems

Theorem (Change of Coordinates)

Let $\psi : U \rightarrow V$ be a change of coordinates such that it and its inverse are continuously differentiable functions. If ψ is symplectic, the Hamiltonian system $\dot{y} = J^{-1}\nabla H(y)$ becomes in the new variables $z = \psi(y)$:

$$\dot{z} = J^{-1}\nabla K(z) \quad \text{with} \quad K(z) = H(y) \tag{3.12}$$

Symplectic integrators

Definition (Symplectic One-step Method)

A numerical one-step method is called symplectic if the one-step map:

$$y_1 = \Phi_h(y_0) \tag{3.13}$$

is symplectic whenever the method is applied to a smooth Hamiltonian system.

Symplectic solvers:

- Symplectic euler (first order), shown by "de Vogelaere" 1956
- Störmer Verlet (second order, symmetric)
- Implicit midpoint rule (second order, symmetric)

Symplectic integrators

Theorem

Let Φ_h denote the symplectic Euler method. Then, the composition method is symplectic for every choice of the parameters, α_i and β_i.
If $\hat{\Phi}_h$ is symplectic and symmetric then the composition method is symplectic (and symmetric) too.

Theorem

Assume that the Hamiltonian is given by $H(y) = H_1(y) + H_2(y)$, and consider the splitting:

$$\dot{y} = J^{-1}\nabla H(y) = J^{-1}\nabla H_1(y) + J^{-1}\nabla H_2(y) \qquad (3.14)$$

The splitting method is then symplectic

Criteria

Theorem (Bochev and Scovel 1994)

The symplecticity is a quadratic invariant

Lemma

Any Runge-Kutta method that preserve quadratic invariants are symplectic

- For DIRK methods, use $\theta = \frac{1}{2}$ for efficiency.
- If the system is separable recall that a partitioned Runge-Kutta method can be symmetric, explicit and (now) symplectic.
- Partitioned DIRK method applied to a separable Hamiltonian system is equivalent to the splitting scheme and a composition of symplectic Euler steps.

Characterization of Symplectic Methods

Theorem

Consider a B-series method $\Phi_h(y) = B(a, y)$ and problems $\dot{y} = f(y)$ having $Q(y) = y^T C y$, with symmetric C, as first integral. If the coefficients $a(\tau)$ satisfy:

$$a(u \circ v) + a(v \circ u) = a(u) \cdot a(v) \qquad (3.15)$$

then the method exactly conserves $Q(y)$ and it is symplectic

Recall that $u \circ v = [u_1, \ldots, u_m, v]$

Characterization of Symplectic Methods

Theorem

Consider a P-series method and a separable problem $(\dot{p} = f_1(p, q),\ \dot{q} = f_2(p, q))$ *having* $Q(p, q) = p^T Eq$ *as invariant. Then it is symplectic if:*

- *it for general systems fulfil:*

$$a(u \circ v) + a(v \circ u) = a(u) \cdot a(v) \tag{3.16}$$

  and that

  $a(\tau)$ *is independent of the colour of the root of* τ

- *or for separable Hamiltonian systems fulfil:*

$$a(u \circ v) + a(v \circ u) = a(u) \cdot a(v) \tag{3.17}$$

Characterization of Symplectic Methods

Theorem

Using the previous seen invariants for respectively Runge-Kutta methods and partitioned Runge-Kutta methods. Then the method is symplectic if and only if such quadratic invariants are exactly conserved.