Reversibility and Symmetric Integration

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Motivation

Conservative mechanical systems: Invert initial velocity $\longrightarrow$ same solution (with inverted direction of motion).

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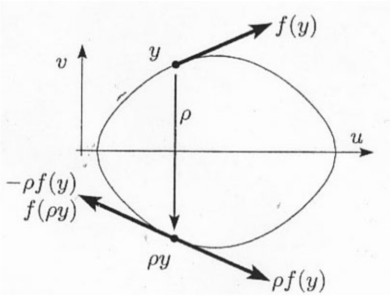

Figure: The system is invertible

Contents

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- Reversible differential equations/reversible maps

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- Symmetric numerical (one-step) methods
- Symmetric Runge-Kutta methods

Reversible Differential Equations

Definition

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

$$\rho f(y) = -f(\rho y) \quad \textit{for all } y.$$

Illustration

We need

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Satisfied in the mechanical system

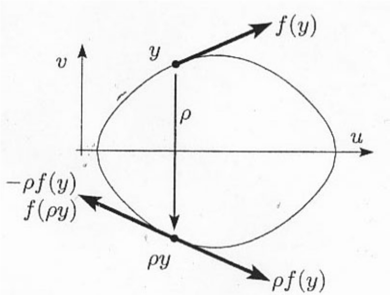

Figure: Reversible vector field

Reversible maps

Notice that for ρ-reversible differential eqns, the flow ϕ_t satisfies

$$\rho \circ \phi_t = \phi_{-t} \circ \rho = \phi_t^{-1} \circ \rho$$

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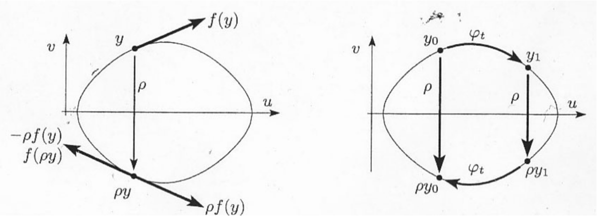

Figure: Reversible vector field and reversible map

Reversible maps

The equality

$$\rho \circ \phi_t = \phi_{-t} \circ \rho = \phi_t^{-1} \circ \rho$$

motivates the following

Definition

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

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Example

$\rho(u, v) = (u, -v)$, $\rightarrow$ invertion of initial velocity in a mechanical system

If we just say "reversible", we mean reversible wrt this ρ.

Important Example

We often encounter partitioned systems

$$\dot{u} = f(u, v), \qquad \dot{v} = g(u, v),$$

where $f(u, -v) = -f(u, v)$ and $g(u, -v) = g(u, v)$.
And ρ is given by $\rho(u, v) = (u, -v)$.

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For scalar u, v: Reversible and cross u-axis twice $\rightarrow$ periodic motion.

Symmetric Numerical Methods

Definition

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

$$\Phi_h \circ \Phi_{-h} = id \qquad \text{or equivalently} \qquad \Phi_h = \Phi_{-h}^{-1}.$$

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$\longrightarrow$ Example: Implicit midpoint rule

Symmetric Methods $\leftrightarrow$ Reversible Flows

Theorem (Criterion for Reversibility of the Numerical Flow)

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

$$\rho \circ \Phi_h = \Phi_{-h} \circ \rho \qquad (*)$$

then the numerical flow Φ_h is a ρ-reversible map iff Φ_h is a symmetric method.

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Compared to the symmetry of the method, $(*)$ is much less restrictive. It is satisfied by most numerical methods. For example

Methods that satisfy $(*)$

- Runge-Kutta methods (explicit or implicit, also partitioned ones)
- Composition methods $\Phi_h \circ \Psi_h$, if Φ_h and Ψ_h do.
- Projection methods on manifolds, if the basic method does and ρ maps the manifold unto itself and is an orthogonal matrix
- ...

Symmetric Runge-Kutta Methods

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Theorem (Symmetry of Collocation Methods)

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

$$c_i^* = 1 - c_{s+1-i}.$$

In the case that $c_i = 1 - c_{s+1-i} \forall i$*, the collocation method is symmetric.*

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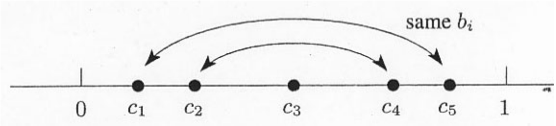

Figure: Symmetry of collocation methods

Example

The Gauss formulas and the Lobatto IIIA and IIIB formuals are symmetric integrators

$$
\begin{array}{c|cc}
\frac{1}{2}-\frac{\sqrt{3}}{6} & \frac{1}{4} & \frac{1}{4}-\frac{\sqrt{3}}{6} \\
\frac{1}{2}+\frac{\sqrt{3}}{6} & \frac{1}{4}+\frac{\sqrt{3}}{6} & \frac{1}{4} \\
\hline
 & \frac{1}{2} & \frac{1}{2}
\end{array}
$$

$$
\begin{array}{c|ccc}
\frac{1}{2}-\frac{\sqrt{15}}{10} & \frac{5}{36} & \frac{2}{9}-\frac{\sqrt{15}}{15} & \frac{5}{36}-\frac{\sqrt{15}}{30} \\
\frac{1}{2} & \frac{5}{36}+\frac{\sqrt{15}}{24} & \frac{2}{9} & \frac{5}{36}-\frac{\sqrt{15}}{24} \\
\frac{1}{2}+\frac{\sqrt{15}}{10} & \frac{5}{36}+\frac{\sqrt{15}}{30} & \frac{2}{9}+\frac{\sqrt{15}}{15} & \frac{5}{36} \\
\hline
 & \frac{5}{18} & \frac{4}{9} & \frac{5}{18}
\end{array}
$$

Figure: Gauss methods of order 4 and 6

Symmetry for s-stage RK-Methods

Theorem

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

$$a^*_{ij} = b_{s+1-j} - a_{s+1-i,s+1-j}, \qquad b^*_i = b_{s+1-i}$$

If

$$a_{s+1-i,s+1-j} + a_{ij} = b_j \;\; \forall i,j, \qquad (*)$$

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Explicit Runge-Kutta methods cannot fulfill $(*)$ with i=j and no explicit Runge-Kutta method is symmetric.

DIRK's

The simplest case of symmetric RK-methods: DIRK's (Diagonally implicit RK methods) $\rightarrow$ Non-zero diagonal elements allowed, but $a_{ij} = 0$ for $i \geq j+1$ $\rightarrow$ Condition for symmetry becomes

$$a_{ij} = b_j = b_{s+1-j} \quad \text{for} \quad i \geq j+1, \qquad a_{jj} + a_{s+1-j,s+1-j} = b_j.$$

Sample Butcher diagram 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

with $a_{33} = b_3/2$, $a_{44} = b_2 - a_{22}$, and $a_{55} = b_1 - a_{11}$

Partitioned Runge-Kutta Methods

Consider the partitioned system

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

A partitioned RK method applied to this system is symmetric only if both are symmetric ($\dot{y} = f(y)$, $\dot{z} = g(z)$ are special cases of $(*)$).

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$\ddot{y} = g(y)$, written $\dot{y} = z, \dot{z} = g(y)$, as well as Hamiltonian systems with separable Hamiltonian $H(p, q) = T(p) + V(q)$ have this structure.

Störmer/Verlet: symmetric *and* implicit

Example

0	0	0
1	1/2	1/2
	1/2	1/2

1/2	1/2	0
1/2	1/2	0
	1/2	1/2

Figure: Störmer/Verlet scheme

Apply this to $\dot{y} = f(z), \quad \dot{z} = g(y)$. We get:

$$\begin{aligned} z_{1/2} &= z_0 + h/2g(y_0) \\ y_1 &= y_0 + hf(z_{1/2}) \\ z_1 &= z_{1/2} + h/2g(y_1) \end{aligned}$$