2. Symmetric integration

Motivation: Conservative systems are "symmetric" wrt the transformation $t \leftrightarrow -t$.

Notation: Consider $\begin{cases} y' = f(y) \\ y(0) = y_0 \end{cases}$.

Then we call the map $\varphi_t : \mathbb{R}^d \to \mathbb{R}^d$ the <u>flow</u> of the ODE if

$$\varphi_t(y_0) = y(t).$$

In general, $\varphi_t(y(s)) = y(t+s)$.

Observe that φ_t forms a group wrt its argument t and the operation of composition:

$$\varphi_t \circ \varphi_s = \varphi_{t+s} \qquad \varphi_{-t} \circ \varphi_t = \varphi_0 = Id$$

$$\varphi_0 = Id \qquad \Rightarrow \varphi_{-t} = (\varphi_t)^{-1}$$

Defn: (ρ-reversible)

Let $\rho : \mathbb{R}^d \to \mathbb{R}^d$ be a linear and invertible map. Then $y' = f(y)$ is ρ-reversible if

$$\rho(f(y)) = -f(\rho(y)) \qquad (\rho \circ f = -f \circ \rho) \quad \forall y \in \mathbb{R}^d.$$

Example: Consider a second order ODE $q'' = F(q)$ and rewrite it as:

$$\begin{cases} p' = F(q) \\ q' = p \end{cases}$$

Then the ODE is ρ-reversible with

$$\rho(p, q) = (-p, q) \qquad \text{(Exercise)}$$

<u>Rem:</u> $y' = f(y)$ is ρ - reversible $\Longleftrightarrow$

$$\frac{d}{dt}\rho(y(t)) = -f(\rho(y(t))).$$

Indeed, $\frac{d}{dt}\rho(y(t)) \overset{\downarrow \rho \text{ linear transformation}}{=} \rho(y'(t)) = \rho(f(y(t))$

$$\underset{\uparrow \rho\text{-reversible}}{=} -f(\rho(y(t))).$$

<u>Lemma:</u> For ρ-reversible problems, the flow φ_t satisfies:

$$\rho \circ \varphi_t = \varphi_{-t} \circ \rho = \varphi_t^{-1} \circ \rho.$$

<u>Proof:</u> We have

$$\frac{d}{dt}\varphi_t(y_0) = \frac{d}{dt}y(t) = f(y(t)) = f(\varphi_t(y_0))$$

$$\Rightarrow \frac{d}{dt}\varphi_t = f \circ \varphi_t .$$

Moreover,

$$\frac{d}{dt}\varphi_{-t}(y_0) = \frac{d}{dt}y(-t) = -f(y(-t)) = -f(\varphi_{-t}(y_0))$$

$$\Rightarrow \frac{d}{dt}\varphi_{-t} = -f \circ \varphi_{-t}$$

Now let $v(t) = \rho \circ \varphi_t(y_0)$, $u(t) = \varphi_{-t} \circ \rho(y_0)$

Observe that $v(0) = u(0) = \rho(y_0)$.

Moreover,

$$v'(t) = \rho \circ \frac{d}{dt}\varphi_t(y_0) = \rho \circ f \circ \varphi_t(y_0)$$

$$= -f \circ \underbrace{\rho \circ \varphi_t(y_0)}_{v(t)} = -f \circ v(t)$$

$$u'(t) = \frac{d}{dt}\varphi_{-t} \circ \rho(y_0) = -f \circ \overbrace{\varphi_{-t} \circ \rho(y_0)}^{=u(t)} = -f \circ u(t)$$

$\Rightarrow$ $v(t)$ and $u(t)$ satisfy the same ODE

$$u'(t) = -f(u(t)) \qquad (\text{resp. } v)$$

with the same initial condition $v(0) = u(0) = \rho(y_0)$.

Hence, $u(t) = v(t) \quad \forall t \geq 0$.

$$\Rightarrow \rho \circ \varphi_t = \varphi_{-t} \circ \rho .$$

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In general:

Defn: (ρ-reversible map)

A map $\phi : \mathbb{R}^d \to \mathbb{R}^d$ is ρ-reversible if

$$\rho \circ \phi = \phi^{-1} \circ \rho .$$

Hence, φ_t is a ρ-reversible map, if $y' = f(y)$ is ρ-reversible.

How about numerical methods?

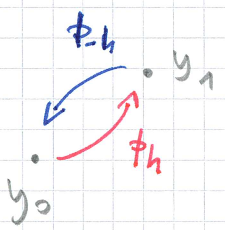
Defn.: (numerical flow)

The map $\Phi_h : \mathbb{R}^d \to \mathbb{R}^d$ s.t. $y_1 = \Phi_h(y_0)$ is called numerical flow of a one-step method.

Defn.: (symmetric numerical method)

A one-step method is symmetric if

$$\Phi_h \circ \Phi_{-h} = \mathrm{Id}.$$



Connection symmetric $\rightsquigarrow$ ρ-reversible:

Theorem:

Suppose for a ρ-reversible ODE that it holds

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

for a one-step method Φ_h.
Then Φ_h is ρ-reversible $\Longleftrightarrow$ Φ_h is symmetric.

Proof: From $(*)$ we just need to verify that

$$\Phi_{-h} \circ \rho = \Phi_h^{-1} \circ \rho .$$

Since ρ is invertible (by defn.), apply ρ^{-1} to the right:

$$\Phi_{-h} = \Phi_h^{-1} .$$

This is satisfied by symmetric methods. The result follows.

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Lemma: Condition $(*)$ (see above) is satisfied by all RK methods.
For PRK methods, $(*)$ is satisfied if

$$\rho(y,z) = (\rho_1(y), \rho_2(z)).$$

Proof: Exercises.

How do we know whether a RK method is symmetric or not?

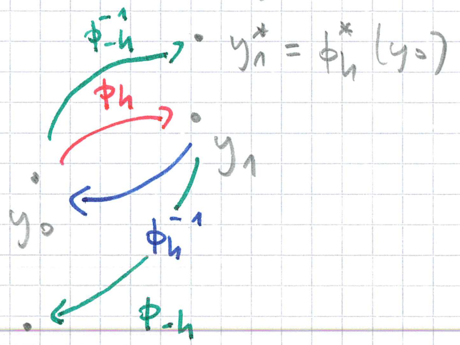
$\Rightarrow$ We need the adjoint!

Defn.: (adjoint method)

The adjoint of a one-step method Φ_h is the one-step method corresponding to

$$\Phi_h^* = \Phi_{-h}^{-1}.$$

Rem: A method is symmetric $\Leftrightarrow$ $\Phi_h^* = \Phi_h$



Properties of the adjoint:

(i) $(\Phi_h^*)^* = \Phi_h$

(ii) $(\Phi_h \circ \Psi_h)^* = \Psi_h^* \circ \Phi_h^*$ (follows from the defn of the adjoint).

Examples:

$$\boxed{\begin{matrix} (y_0, y_1) \leftrightarrow (y_1^*, y_0) \\ h \leftrightarrow -h \end{matrix}}$$ Rule to compute the adjoint

① **Explicit Euler:** $y_1 = y_0 + h f(y_0) = \Phi_h(y_0)$

We look for $\Phi_h^* = \Phi_{-h}^{-1}$

$$y_1^* = \Phi_h^*(y_0) = \Phi_{-h}^{-1}(y_0) \xRightarrow{\text{apply } \Phi_{-h}} y_0 = \Phi_{-h}(y_1^*) = y_1^* - h f(y_1^*)$$

$$\Rightarrow y_1^* = y_0 + h f(y_1^*)$$

$\Rightarrow$ Implicit Euler is the adjoint of explicit Euler.

$\Rightarrow$ Neither Explicit Euler nor Implicit Euler are symmetric!

likewise, the adjoint of Implicit Euler is Explicit Euler.

② Implicit Midpoint Rule:

$$y_1 = y_0 + h f\left(\frac{y_0+y_1}{2}\right)$$

$$\Rightarrow y_0 = y_1^* - h f\left(\frac{y_1^* + y_0}{2}\right)$$

$$\Rightarrow y_1^* = y_0 + h f\left(\frac{y_0 + y_1^*}{2}\right) \quad \Rightarrow \Phi_h = \Phi_h^*$$

$\Rightarrow$ IMR is symmetric!

In general:

Theorem: The adjoint of a consistent RK method (b_i, a_{ij}) is a RK method with coefficients (b_i^*, a_{ij}^*) given by

(characterisation)
$$a_{ij}^* = b_{s+1-j} - a_{s+1-i,\, s+1-j}$$
$$b_i^* = b_{s+1-i} \qquad \text{for } i,j = 1,2,\dots,s$$

Moreover, if $a_{ij} \overset{(\Delta)}{=} b_j - a_{s+1-i,\, s+1-j}$ for $i,j = 1,2,\dots,s$ then the method is symmetric.

Proof: Exercises.

Corollary: Explicit RK methods cannot be symmetric.

Proof: Exercises.

Theorem: Let (b_i, a_{ij}), $(\hat{b}_i, \hat{a}_{ij})$ define a PRK method for

$$\begin{cases} y' = f(y,z) \\ z' = g(y,z) \end{cases}$$

If both methods satisfy (Δ), then the PRK method is symmetric.

Rem.: If $y' = f(z)$, $z' = g(y)$, then one can build PRK that are symmetric and explicit.

Example: Störmer-Verlet for separable Hamiltonian systems, $H(p,q) = T(p) + V(q)$.

Theorem: The adjoint of a collocation method based on $c_1, c_2, \dots, c_s$ is a collocation method based on $c_1^*, c_2^*, \dots, c_s^*$ given by

$$c_i^* = 1 - c_{s+1-i} \quad \text{for } i = 1, 2, \dots, s.$$

Moreover, if $c_i = 1 - c_{s+1-i}$, then the collocation method is symmetric.

Proof: $(t_0, y_0) \leftrightarrow (t_1, y_1^*)$ (substitutions)
$h \leftrightarrow -h$ adjoint rule

$$\begin{cases} y_0 = u(t_0) \\ u'(t_0+hc_i) = f(u(t_0+hc_i)) \\ y_1 = u(t_0+h) \end{cases}$$

$$\Updownarrow$$

$$\begin{cases} y_1^* = u(t_1) \\ u'(t_1-hc_i) = f(u(t_1-hc_i)) \\ y_0 = u(t_1-h) \end{cases}$$

$\to t_1 - hc_i = t_0 + h - hc_i$
$= t_0 + (1-c_i)h$

$$\Rightarrow \begin{cases} y_0 = u(t_0) \\ u'(t_0+(1-c_i)h) = f(u(t_0+(1-c_i)h)) \\ y_1^* = u(t_0+h) \end{cases}$$

Reordering $1-c_i$ to be in ascending order

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

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Corollary: Gauss methods are symmetric.

Proof: Recall c_i zeros of $\phi_G^s(x) = \frac{d^s}{dx^s}(x^s(1-x)^s)$

Denote $q(x) = x^s(1-x)^s \Rightarrow q(1-x) = q(x)$.

$\Rightarrow \quad \frac{d^s}{dx^s} q(x) = (-1)^s \frac{d^s}{dx^s} q(1-x)$

Since $\frac{d^s}{dx^s} q(c_i) = \phi_G^s(c_i) = 0 \Rightarrow \frac{d^s}{dx^s} q(1-c_i) = 0$

$\Rightarrow \quad 1-c_i$ is a zero

which yields the desired result up to a reordering.

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AB NIPS

What properties does the adjoint have as a stand-alone RK method?

Theorem: Let φ_t be the exact flow of $y' = f(y)$ and Φ_h the numerical flow of a RK method.

If the RK method is of order p, then

(*) $$\Phi_h(y_0) = \varphi_h(y_0) + C(y_0)h^{p+1} + \mathcal{O}(h^{p+2})$$

The adjoint Φ_h^* satisfies:

$$\Phi_h^*(y_0) = \varphi_h(y_0) + (-1)^p C(y_0) h^{p+1} + \mathcal{O}(h^{p+2}).$$

Proof: (formal)

Observe that $\varphi_{-h}(y_0) = y_0 + \mathcal{O}(h)$ (problem with smooth Lipschitz RHS)

$$\Rightarrow \frac{\partial}{\partial y_0}\varphi_{-h}(y_0) = I + \mathcal{O}(h)$$

Further, from (*) it follows

$$\frac{\partial}{\partial y_0}\Phi_{-h}(y_0) = I + \mathcal{O}(h)$$

The implicit fct thm yields:

$$\frac{\partial}{\partial y_0}\Phi_h^*(y_0) = \frac{\partial}{\partial y_0}\left(\Phi_{-h}^{-1}(y_0)\right) = I + \mathcal{O}(h) \quad (**)$$

If one takes (*) and $h \leftrightarrow -h$, $y_0 \leftrightarrow \varphi_h(y_0)$:

$$\Phi_{-h}(\varphi_h(y_0)) = \varphi_{-h}(\varphi_h(y_0)) + C(\varphi_h(y_0))(-h)^{p+1} + \mathcal{O}(h^{p+2})$$

$$= y_0 - (-1)^p C(\varphi_h(y_0)) h^{p+1} + \mathcal{O}(h^{p+2})$$

Applying $\Phi_{-h}^{-1} = \Phi_h^*$ on both sides:

$$\varphi_h(y_0) = \Phi_h^*\left(y_0 - (-1)^p C(\varphi_h(y_0))h^{p+1} + \mathcal{O}(h^{p+2})\right)$$

$$= \Phi_h^*(y_0) + \frac{\partial \Phi_h^*}{\partial y_0}(y_0)\left(-(-1)^p C(\varphi_h(y_0))h^{p+1} + \mathcal{O}(h^{p+2})\right) + \mathcal{O}(h^{p+2})$$

expanding 1st order

Notice formally that since $\varphi_h(y_0) = y_0 + O(h)$

$$\Rightarrow C(\varphi_h(y_0)) = C(y_0) + O(h)$$

$$\overset{(**)}{\Rightarrow} \quad \varphi_h(y_0) = \phi_h^*(y_0) - (-1)^p C(y_0) h^{p+1} + O(h^{p+2}).$$

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<u>Rem:</u> A necessary condition for ϕ_h to be symmetric is therefore,

$$(-1)^p C(y_0) = C(y_0) \qquad (\phi_h^* = \phi_h)$$

$\Rightarrow$ <u>Symmetric</u> methods have <u>even order</u>.

How can one construct symmetric methods?

<u>Lemma:</u> Let ϕ_h be a RK method. Then

$$\phi_h^S = \phi_{h/2} \circ \phi_{h/2}^* \qquad \text{is symmetric.}$$

<u>Proof:</u>
$$(\phi_h^S)^* \underset{\substack{\uparrow \\ \text{properties adjoint}}}{=} (\phi_{h/2}^*)^* \circ \phi_{h/2}^* = \phi_{h/2} \circ \phi_{h/2}^* = \phi_h^S$$

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<u>Take-Home Message:</u> Symmetric methods are

1) the go-to for reversible systems, because they
   a) mimic the "physics" of the problem
   b) allow long-time good approximation of reversible systems (see Hairer, Lubich, Wanner Chapt. XI)

2) often implicit, unless PRK + some structure in the coupled ODE (e.g. separable Hamiltonian).

3) theory is based extensively on the adjoint.