Reversibility and Symmetric Methods

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Reversibility. Suppose that ρ is an invertible differentiable map $\rho : M \to M$. In many applications, ρ is also involutive, meaning that $\rho \circ \rho = \mathrm{Id}$ (or $\rho = \rho^{-1}$), but that will not be required here. Later on, we shall however restrict the discussion to the case that M is a linear space and ρ a linear map. But for now, define any invertible map Φ to be ρ-reversible if the following relation holds

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

Of particular interest to us is when Φ is the flow φ_t of a vector field, or a numerical method, Φ_h, approximating this flow.

$$\dot{y} = f(y) \tag{2}$$

Let us first show that the flow of (2) satisfies (1) with $\varphi_t = \Phi$ if it is true that

$$T\rho \circ f = -f \circ \rho \tag{3}$$

We compute

$$\frac{\mathrm{d}}{\mathrm{d}t}(\rho \circ \varphi_t(y_0)) = T\rho \circ f \circ \varphi_t(y_0) = -f \circ \rho \circ \varphi_t(y_0)$$

On the other hand, since $\varphi_t^{-1} = \varphi_{-t}$

$$\frac{\mathrm{d}}{\mathrm{d}t}(\varphi_{-t} \circ \rho(y_0)) = -f \circ \varphi_{-t} \circ \rho(y_0)$$

So we conclude that the two functions

$$w(t) = \rho \circ \varphi_t(y_0) \quad \text{and} \quad z(t) = \varphi_{-t} \circ \rho(y_0)$$

satisfy the same differential equation ($\dot{w}(t) = -f(w(t))$, $\dot{z}(t) = -f(z(t))$) with the same initial value $w(0) = z(0) = y_0$ they must be the same function, so $w(t) = z(t)$. We call vector fields which satisfy (3) *ρ-reversible differential equations.*

Example 1 A simple example of a linear, involutive automorphism ρ of the linear space $\mathbb{R}^{2d}$ is obtained by splitting the $2d$-vector y into two d-vectors q and p, $y = (q, p)$ and define

$$\rho : \begin{pmatrix} q \\ p \end{pmatrix} \mapsto \begin{pmatrix} q \\ -p \end{pmatrix} = \begin{pmatrix} I & 0 \\ 0 & -I \end{pmatrix} \cdot \begin{pmatrix} q \\ p \end{pmatrix}$$

□

Adjoint of a method, symmetric methods. To every invertible method map Φ_h there exist another method called the *adjoint method*, denoted Φ_h^* defined by the relation

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

Obviously, this implies that $(\Phi_h^*)^* = \Phi_h$.

Since numerical methods are often implicitly defined, it is useful to have the following recipe in mind when constructing the adjoint of a method. Interchange y_0 and y_1 and replace h by $-h$, if possible solve for y_1 or write it in a standard form.

Example 2 The Euler method: $y_1 = \Phi_h(y_0) = y_0 + hf(y_0)$ then leads to $y_0 = y_1 - hf(y_1)$ so the implicit Euler method $y_1 = y_0 + hf(y_1)$ results. So the explicit and implicit Euler methods are the adjoint of each other. □

A method is called *symmetric* if $\Phi_h = \Phi_h^*$. This can also be written as

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

a property shared by the exact flow of the differential equation. In fact, the exact flow even has the group property, i.e. $\varphi_{t+s} = \varphi_t \circ \varphi_s$ and one may set $t = h = -s$.

Exercise 1 Show that the implicit midpoint rule is symmetric. □

Composition methods. It is possible to use simple integrators to construct more advanced methods by composition. If $\Phi_h^{[1]}$ and $\Phi_h^{[2]}$ are two methods, their composition

$$\Phi_{h/2}^{[1]} \circ \Phi_{h/2}^{[2]}$$

If the set of all maps with a certain structure preserving property form a group under composition, then we have at our disposal a very powerful tool for designing advanced structure preserving integrators. Suppose for instance that ϕ and ψ are symplectic maps such that $\phi^*\omega = \omega$ and $\psi^*\omega = \omega$. Then we find[1]

$$(\phi \circ \psi)^*\omega = \psi^* \circ \phi^*\omega = \psi^*\omega = \omega.$$

A consequence of this is that any composition of symplectic methods is again symplectic.

But let us get back to symmetric methods, method maps with $\Psi_h = \Psi_h^*$ do not have such a group property. However, one way of designing a symmetric methods by composition is to consider methods

$$\Psi_h = \Phi_{h/2} \circ \Phi_{h/2}^* \quad \text{or} \quad \Psi_h' = \Phi_{h/2}^* \circ \Phi_{h/2}$$

Exercise 2 Prove that both Ψ_h and Ψ_h' above are symmetric methods □

Exercise 3 Let Φ_h^E and Φ_h^{IE} be the explicit and implicit Euler methods respectively. Show that

$$\Phi_{h/2}^E \circ \Phi_{h/2}^{IE} \quad \text{and} \quad \Phi_{h/2}^{IE} \circ \Phi_{h/2}^E$$

[1] See Appendix 1

are the implicit midpoint rule and the trapezoidal rule respectively. $\square$

Suppose that we $\Phi_h.$ is symmetric. We can compose it with itself in a symmetric fashion to obtain another symmetric method, the general format is

$$\Psi_h = \Phi_{b_0 h} \circ \Phi_{b_1 h} \circ \cdots \circ \Phi_{b_{s-1} h} \circ \Phi_{b_s h}$$

and we must have $b_i = b_{s-i}$ for all i. For consistency one should have $\sum_i b_i = 1$.

Adjoint of Runge-Kutta methods. You have shown that the implicit mid point rule is symmetric. This method can be written as a Runge-Kutta method with Butcher tableau

$$\begin{array}{c|c} \frac{1}{2} & \frac{1}{2} \\ \hline & 1 \end{array}$$

In general we can construct the adjoint of a Runge-Kutta method resulting, in fact, in anothe Runge-Kutta method.

Theorem 1. *Suppose a Runge-Kutta method has Butcher tableau*

$$\begin{array}{c|ccc} c_1 & a_{11} & \cdots & a_{1s} \\ \vdots & \vdots & & \vdots \\ c_s & a_{s1} & \cdots & a_{ss} \\ \hline & b_1 & \cdots & b_s \end{array}$$

Then the coefficents (a^*_{ij}, b_i) *of its adjoint method are given by*

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

If it happens that

$$a_{s+1-i,s+1-j} + a_{ij} = b_j, \text{ for all } i, j$$

then the method is symmetric.

The proof is left as an exercise.

Symmetric methods and reversible maps. In this paragraph we shall assume that ρ is a linear map on a linear space. This means in particular that the condition (3) for a differential equation to be ρ-reversible is simply

$$\rho \circ f = -f \circ \rho \tag{4}$$

Theorem 2. *If a numerical method applied to a ρ-reversible differential equation satisfies*

$$\rho \circ \Phi_h = \Phi_{-h} \circ \rho \tag{5}$$

then Φ_h is a reversible map if and only if it is symmetric.

Proof. This is an obvious consequence of the definitions of a reversible map and symmetric methods. $\square$

One may ask if the condition (5) is a plausible one, this is indeed true. We show in Appendix 2 that it automatically holds for every Runge–Kutta method. There are also many other relevant methods for which the condition holds.

Appendix 1. The composition of pullbacks, we show the formula

$$(\phi \circ \psi)^* = \psi^* \circ \phi^*.$$

Recall the definition of pullback of a two-form

$$(\phi^*\omega)_m(u, v) = \omega_{\phi(m)}(T_m\phi(u), T_m\phi(v)).$$

Note also the chain rule for tangent maps

$$T(\phi \circ \psi) = T\phi \circ T\psi$$

We then compute

$$\begin{aligned}((\phi \circ \psi)^*\omega)(u, v) &= \omega(T(\phi \circ \psi)u, T(\phi \circ \psi)v) = \omega(T\phi \circ T\psi(u), T\phi \circ T\psi(v)) \\ &= (\phi^*\omega)(T\psi(u), T\psi(v)) = \psi^*\phi^*\omega(u, v)\end{aligned}$$

□

Appendix 2.

Theorem 3. *All Runge–Kutta methods (Φ_h) satisfy the condition*

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

of Theorem 2 for any linear invertible map ρ when applied to a reversible differential equation.

Proof. We write the Runge–Kutta method in the following way ($y_1 = \Phi_f(y_0)$)

$$Y_i = y_0 + h\sum_{j=1}^{s} a_{ij} f(Y_j),$$

$$y_1 = y_0 + h\sum_{i=1}^{s} b_i f(Y_i)$$

□

It is convenient to define $z_0 = \rho \circ y_0$, $Z_i = \rho \circ Y_i$. We compute

$$Z_i = \rho \circ Y_i = \rho \circ y_0 + h\sum_{j=1}^{s} a_{ij}\rho \circ f(Y_j) = z_0 - h\sum_{j=1}^{s} a_{ij} f(Z_j)$$

$$z_1 = \rho \circ y_1 = \rho \circ y_0 + h\sum_{i=1}^{s} b_i\rho \circ f(Y_i) = z_0 - h\sum_{i=1}^{s} b_i f(Z_i)$$

But this is precisely the Runge–Kutta method applied to the initial value z_0 with step size $-h$, therefore

$$\rho \circ \Phi_h(y_0) = \rho \circ y_1 = z_1 = \Phi_{-h}(z_0) = \Phi_{-h} \circ \rho(y_0)$$