Chapter 12

Reversibility and Composition Methods

Main concepts: ρ-reversibility, adjoint of a method, self-adjoint methods, composition methods

Many physical processes—e.g. those on the molecular scale and on the cellestial scale—are *reversible*, a symmetry property of the flow map Φ_t. It turns out to be useful in such a case, to use a numerical method whose discrete flow map is also reversible. One reason for doing so is the simple construction of higher order methods by composition, which will be treated in this chapter. Another reason is the near preservation of invariants in integrable problems by reversible methods, which will not be treated in these notes.

12.1 ρ-Reversibility

Let ρ be a linear, invertible transformation on $\mathbb{R}^d$. The autonomous ODE (1.13) is called ρ-*reversible* if

$$\rho f(y) = -f(\rho y) \tag{12.1}$$

for all y.

For a ρ-reversible ODE, the solution operator Φ_t satisfies

$$\rho \circ \Phi_t = \Phi_{-t} \circ \rho. \tag{12.2}$$

In words, evolving the system t units in time and applying the reversal transformation, is equivalent to applying the reversal transformation and then evolving the system t units *backward* in time.

As a consequence of (12.2), and since $\Phi_{-t} = \Phi_t^{-1}$,

$$\rho^{-1} \circ \Phi_t \circ \rho \circ \Phi_t = \mathrm{id},$$

the identity map. So if one evolves the system t units in time, then applies the reversal transformation, then evolves it t more units in time and again applies the inverse reversal transformation, the system is returned to its initial state. This situation is illustrated in Figure 12.1.

Example. Mechanical systems. A large class of reversible problems are those given by Newton's second law of motion (5.2)

$$M\ddot{q} = F(q), \tag{12.3}$$

where $q \in \mathbb{R}^d$ is a position vector, $F : \mathbb{R}^d \to \mathbb{R}^d$ is a vector of forces, and M is a symmetric, positive definite (mass) matrix. Introducing the momentum $p \equiv M\dot{q}$, this becomes

$$\dot{q} = M^{-1}p, \qquad \dot{p} = F(q).$$

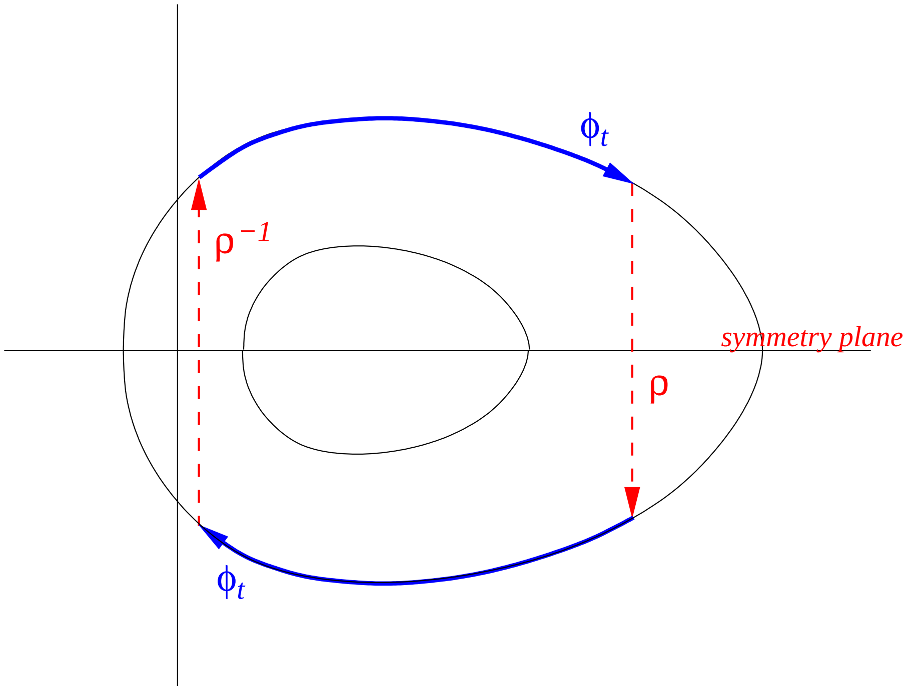

Figure 12.1: Illustration of a ρ-reversal symmetry. Here, ρ is a simple reflection about the horizontal axis. The black lines represent phase trajectories of the dynamical system in question.

This system can be written as a first order system (1.3) of dimension $2d$:

$$y = \begin{pmatrix} q \\ p \end{pmatrix}, \qquad f(y) = \begin{pmatrix} M^{-1}p \\ F(q) \end{pmatrix}$$

The time-reversal transformation just negates the momentum:

$$\rho = \begin{bmatrix} I & \\ & -I \end{bmatrix}.$$

One can easily check that (12.1) holds. Evolving a mechanical system t units in time, reversing its momentum, evolving it again t units in time, and again reversing its momentum, returns it to its initial state.

12.2 Adjoint of a Method

The **adjoint** of a one-step method Ψ_h such as a Runge-Kutta method, which takes the solution of (1.3) from t_n to t_{n+1}, i.e.

$$y_{n+1} = \Psi_h(y_n),$$

is the method $\Psi_h^* := \Psi_{-h}^{-1}$, i.e. the inverse of the method with negative time step. We can derive this method by setting $y_{n+1}^* = y_n$ with $y_n^* = y_{n+1}$ and stepping backward with stepsize $-h$,

$$y_n^* = \Psi_{-h}(y_{n+1}^*).$$

Solving for y_{n+1}^*:

$$y_{n+1}^* = \Psi_{-h}^{-1}(y_n^*) = \Psi_h^*(y_n^*).$$

Example. The adjoint of Euler's method is

$$y_n^* = y_{n+1}^* - hf(y_{n+1}^*).$$

Rearranging gives:

$$y^*_{n+1} = y^*_n + hf(y^*_{n+1}),$$

an implicit method known as *backward Euler* or *implicit Euler*.

For a general s-stage Runge Kutta method with coefficients $A = (a_{ij})$ and $b = (b_i)$, we can calculate

$$y^*_n = y^*_{n+1} - h\sum_{j=1}^{s} b_j f(Y_j),$$
$$Y_i = y^*_{n+1} - h\sum_{j=1}^{s} a_{ij} f(Y_j),$$

or,

$$y^*_{n+1} = y^*_n + h\sum_{j=1}^{s} b_j f(Y_j),$$
$$Y_i = y^*_n + h\sum_{j=1}^{s} (b_j - a_{ij}) f(Y_j).$$

However, the abscissae $c_i = \sum_j a_{ij}$ have become reversed ($c^*_i = 1 - c_i$), so we replace Y_i by Y_{s+1-i} (to recover the chronological ordering of the stage vectors) and obtain the coefficients a^*_{ij} and b^*_i of the adjoint method:

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

This is again an s-stage Runge-Kutta method. The adjoint of an explicit Runge-Kutta method is always implicit.

The order of the adjoint of method is the same as the order of the original method. In fact, the truncation error of the adjoint method satisfies

$$le^*(y,h) = (-1)^p le(y,h),$$

where p is the order of the method (i.e. $le(y,h) = \mathcal{O}(h^{p+1})$.)

A method whose adjoint is equivalent to itself ($\Psi^*_h = \Psi_h$) is called *self-adjoint*. The implicit midpoint rule (8.5) is self-adjoint. For a self-adjoint Runge-Kutta method, the coefficients satisfy

$$a_{s+1-i,s+1-j} + a_{ij} = b_j$$

for all i, j. Self-adjoint methods are necessarily implicit and have even order.

A numerical method is called *symmetric* or *time-reversible* if it satisfies $\Psi^{-1}_h = \Psi_{-h}$. Therefore, self-adjoint methods are time-reversible. More generally, if a numerical method applied to a ρ-reversible system satisfying (12.1) satisfies

$$\rho \circ \Psi_h = \Psi_{-h} \circ \rho$$

(and mostly they do), then the method is ρ-reversible if and only if Ψ_h is symmetric.

12.3 Composition Methods

Recall that the group property of flow maps $\Phi_t \circ \Phi_s = \Phi_{s+t}$ does not hold in general for numerical methods. It turns out we can use this to our "advantage" as follows:

Given a one-step method Ψ_h and a set of s real numbers γ_i, $i = 1, \ldots, s$ that sum to one $\sum_{i=1}^{s} \gamma_i = 1$, the method obtained by composing s steps of size $\gamma_i h$ is called a *composition method*

$$\bar{\Psi}_h = \Psi_{\gamma_s h} \circ \cdots \circ \Psi_{\gamma_1 h}$$

If Ψ_h is of order p, then if

$$\gamma_1^{p+1} + \cdots + \gamma_s^{p+1} = 0,$$

the composition method is at least of order $p+1$.

This relation has no real solution for p odd. For even p, there is a solution for $s = 3$. A popular choice is

$$\gamma_1 = \gamma_3 = \frac{1}{2 - 2^{1/(p+1)}}, \quad \gamma_2 = -\frac{2^{1/(p+1)}}{2 - 2^{1/(p+1)}}, \tag{12.4}$$

which is of order $p+1$. If Ψ_h is a symmetric method, then this composition is also symmetric, and the resulting method is actually of order $p+2$.

The approach can be applied recursively. For example, if Ψ_h is of order 2 and symmetric, then the $\bar{\Psi}_h$ is of order 4 and symmetric. Applying the method recursively ($3^2 = 9$ steps of Ψ_h) we obtain order 6. Applying it recursively again ($3^3 = 27$ steps of the original method) we obtain order 8. And so on.

However, other, possibly more efficient, compositions may be constructed directly (without using this recursion), and the above is really only intended to illustrate the possibilities.

Instead of composing the same methods with different stepsizes, we could also imagine composing different methods. The composition of two steps of equal size with a method Ψ_h and its adjoint Ψ_h^*, yields a self-adjoint method since

$$(\Psi_h \circ \Psi_h^*)^* = \Psi_h \circ \Psi_h^*.$$

For example, the composition of a half-step of backward Euler with a half-step of forward Euler gives either the implicit midpoint rule (8.5) or the trapezoidal rule (2.2) depending on the order of composition. Because the Euler methods are first order, the composition must also be at least first order. But since it is symmetric, it must have even order, so we conclude that it must be at least second order.

Note that (12.4) has γ_2 negative. This means that the method must regularly take backward steps. For some problems backward steps are ill-defined. For this reason, one would like to avoid them. Unfortunately it has been shown that to obtain order greater than 2, backward steps are unavoidable. For this reason, higher order composition methods are almost exclusively used only with reversible problems.

12.4 Exercises

1. Find a ρ-reversible symmetry for the Lotka-Volterra model (1.6) in the case $r = 1$.

2. Construct the adjoint of Heun's method (8.3).

3. Show that a self-adjoint Runge-Kutta method must have $|R(iy)| = 1$ on the imaginary axis. Use analyticity of the stability function to prove that a symmetric RK method with Butcher matrix A whose eigenspectrum lies strictly in the positive half of the complex plane is A-stable.

4. Discuss the relationship between a (long) numerical solution computed with implicit midpoint, and one computed with trapezoidal rule.