

Chapter 13

Splitting Methods

Main concepts: Linear systems, nonlinear systems, BCH theorem, order conditions

In this section, we present a natural approach to “method building” which is based on splitting a vector field into integrable parts. This approach is remarkably general and can be used to construct methods with properties very similar to those of the flow map of the dynamical system.

13.1 Introduction to Splitting Methods

The idea is simple: *divide et impera* (divide and conquer). It is probably the most important systematic technique for the development of algorithms in general. Suppose we wish to solve the differential equation

$$dz/dt = f(z) \equiv f_1(z) + f_2(z),$$

where each of two differential equations

$$dz/dt = f_1(z)$$

and

$$dz/dt = f_2(z)$$

happen to be completely integrable (i.e. analytically solvable). [Note that $dz/dt = f(z)$ is *not* solvable just because the two pieces are!]

The way this is done is diagrammed in Figure 13.1, below. We first note that at any point in phase space, the vector field (hence the tangent vector to the solution curve) can be broken up into the two components f_1 and f_2 . A method can then be constructed by stepping forward along first one, then a second, solution curve, each time for a small timestep h .

That is, we start from some point z_n and solve first the initial value problem

$$dz/dt = f_1(z), \quad z(0) = z_n$$

for a time h . This means to compute the exact solution of this part of the system, which is possible, since f_1 is assumed integrable. This takes us to a point $z^* = z_1(h; z_n)$, where z_1 represents the exact solution of the differential equations on vector field f_1 .

Next we start from z^* and solve the second differential equation initial value problem

$$dz/dt = f_2(z), \quad z(0) = z^*$$

for a time h . This takes us to the point $z_{n+1} = z_2(h; z^*)$. Denoting the flow maps of the vector fields f_1 and f_2 as Φ_{t,f_1} and Φ_{t,f_2} , we have just computed $z_{n+1} = \Phi_{h,f_2}(\Phi_{h,f_1}(z_n)) = (\Phi_{h,f_2} \circ \Phi_{h,f_1})(z_n)$. Such a method is referred to as a *splitting method*.

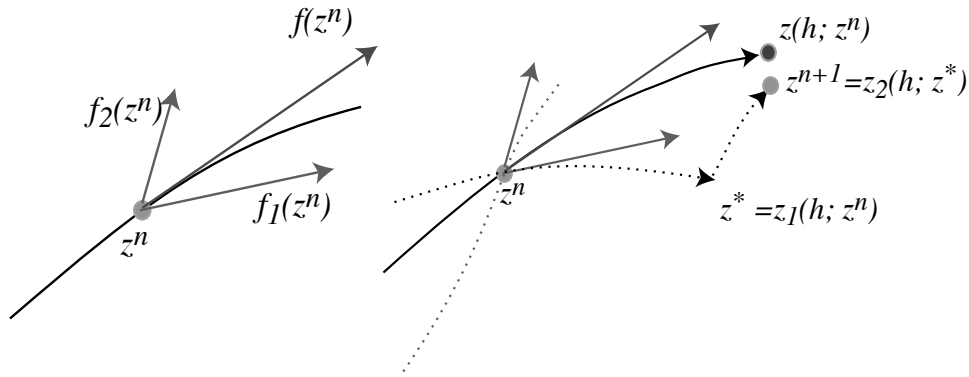


Figure 13.1: Divide and Conquer: An approximation to the solution is constructed by following the solutions of the two parts of the vector field

13.1.1 Linear ODEs

As a first step to understanding splitting methods, consider the linear ODE

$$\frac{dy}{dt} = Ay$$

Let $A = B + C$, then the splitting method defined by solving first

$$\frac{dy}{dt} = By$$

followed by

$$\frac{dy}{dt} = Cy$$

can be written

$$\Psi_h(y) = e^{Ch}e^{Bh}$$

The local error is

$$le(y; h) = \Psi_h(y) - \Phi_h(y) = e^{Ch}e^{Bh} - e^{Ah}$$

Let us work out these formulas in order to estimate the local error. Using the exponential series, we have

$$\begin{aligned} le(y; h) &= (I + Ah + \frac{1}{2}A^2h^2 + \dots) - (I + Ch + \frac{1}{2}C^2h^2 + \dots)(I + Bh + \frac{1}{2}B^2h^2 + \dots) \\ &= (I + Ah + \frac{1}{2}A^2h^2) - (I + h(B + C) + h^2(CB + \frac{1}{2}C^2 + \frac{1}{2}B^2)) + O(h^3) \\ &= h^2(\frac{1}{2}(C + B)^2 - (CB + \frac{1}{2}C^2 + \frac{1}{2}B^2)) + O(h^3) \\ &= h^2[\frac{1}{2}C^2 + \frac{1}{2}CB + \frac{1}{2}BC + \frac{1}{2}B^2 - CB - \frac{1}{2}C^2 - \frac{1}{2}B^2] + O(h^3) \\ &= \frac{h^2}{2}(BC - CB) + O(h^3) \\ &= \frac{h^2}{2}[B, C] + O(h^3) \end{aligned}$$

the matrix $[B, C] = BC - CB$ is called the “commutator” of the matrices B and C . If the commutator is zero, we say that the matrices commute. In that case, it can be shown that not

only the 2nd order term in the local error vanishes, but moreover

$$e^{hB}e^{hC} = e^{Ah}$$

i.e. the splitting method is exact. However, this is a rare situation and in general we expect that a splitting method defined in this way is convergent by Theorem 6.2.1 with $p = 1$.

More complicated splitting methods for linear systems can be constructed in several ways. First, we could imagine splitting the into more parts: $A = B + C + D + \dots$. Second, we could imagine writing

$$B = \sum_{i=1}^s \beta_i B$$

$$C = \sum_{i=1}^s \gamma_i C$$

then we could define a splitting method that is based on solving successively

$$\frac{dy}{dt} = \beta_1 B y$$

$$\frac{dy}{dt} = \gamma_1 C y$$

$$\frac{dy}{dt} = \beta_2 B y$$

$$\frac{dy}{dt} = \gamma_2 C y$$

etc., each for a step of size h .

This is equivalent to approximating the exponential e^{hA} by

$$e^{\gamma_s C h} e^{\beta_s B h} e^{\gamma_{s-1} C h} e^{\beta_{s-1} B h} \dots e^{\gamma_1 C h} e^{\beta_1 B h}$$

It turns out that this composition gives at least a first order method, but the order can be higher. For example, it can be shown that the so-called Strang splitting (named for the mathematician Gil Strang)

$$\Psi_h(y) = e^{\frac{h}{2}C} e^{hB} e^{\frac{h}{2}C} y$$

defines a 2nd order method.

13.1.2 Nonlinear ODEs

Now let $f = f_1 + f_2$ be a real-valued function. We will denote the flow map on f by $\Phi_{h,f}$ and on each of the two parts by Φ_{h,f_1} and Φ_{h,f_2} . The question we would like to answer is: what is the local error associated to the map

$$\Psi_{h,f} = \Phi_{h,f_2} \circ \Phi_{h,f_1}?$$

As before, let $z(h) = (\Phi_{h,f_2} \circ \Phi_{h,f_1})(y) = \Phi_{h,f_2}(\Phi_{h,f_1}(y))$. Noting that $\Phi_{0,\bullet}(y) = y$, we see that

$$z(0) = y$$

We know that

$$\Phi_{h,f_1}(y) = y + h f_1(y) + \frac{1}{2} h^2 f_1'(y) f_1(y) + \dots$$

and

$$\Phi_{h,f_2}(y) = y + h f_2(y) + \frac{1}{2} h^2 f_2'(y) f_2(y) + \dots$$

Hence,

$$\begin{aligned}\Phi_{h,f_2}(\Phi_{h,f_1}(y)) &= [y + hf_1(y) + \mathcal{O}(h^2)] + hf_2[y + hf_1(y) + \mathcal{O}(h^2)] + \mathcal{O}(h^2) \\ &= y + hf_1(y) + hf_2(y) + \mathcal{O}(h^2),\end{aligned}$$

that is,

$$z(h) = y + hf(y) + \mathcal{O}(h^2)$$

This shows that the method is at least first order.

More generally, it is possible to prove the following result:

Theorem 13.1.1 (Splitting Methods) *The splitting method $\Phi_{h,f_2} \circ \Phi_{h,f_1}$, where $f = f_1 + f_2$ has local error*

$$le(y; h) = \frac{h^2}{2}[f_1, f_2] + \mathcal{O}(h^3)$$

where $[f, g]$ is the commutator of the vector fields f and g , which is another vector field

$$[f, g] = \frac{\partial f}{\partial y}g - \frac{\partial g}{\partial y}f$$

The more general form of this result follows from the Baker-Campbell-Hausdorff theorem, which tells how to compute all the terms in the expansion of the product of the two flow maps. In fact, one can show

Theorem 13.1.2 (Baker-Campbell-Hausdorff) *The splitting method $\Phi_{h,f_2} \circ \Phi_{h,f_1}$, where $f = f_1 + f_2$ has local error*

$$le(y; h) = \frac{h^2}{2}[f_2, f_1] + \frac{h^3}{12}([f_2, [f_2, f_1]] - [f_1, [f_2, f_1]]) + \dots$$

If the vector fields commute, i.e. $[f_2, f_1] = 0$, then the splitting is again exact (however, such flow are not usually very interesting).

Consider the vector field obtained by writing the second order equation $\ddot{x} = g(x)$ in first order form:

$$f(x, u) = \begin{bmatrix} u \\ g(x) \end{bmatrix}.$$

Let f_1 and f_2 be defined by

$$f_1(x, u) = \begin{bmatrix} 0 \\ g(x) \end{bmatrix}, \quad f_2(x, u) = \begin{bmatrix} u \\ 0 \end{bmatrix},$$

It is easy to see that each of the differential equation systems

$$\frac{d}{dt} \begin{bmatrix} x \\ u \end{bmatrix} = f_1(x, u)$$

and

$$\frac{d}{dt} \begin{bmatrix} x \\ u \end{bmatrix} = f_2(x, u)$$

is integrable (Euler's method gives the exact solution). A first order method arises by composing the two flows.

With the same vector field decomposition, we can construct a second order method based on Strang splitting by solving successively

$$\frac{d}{dt} \begin{bmatrix} x \\ u \end{bmatrix} = \frac{1}{2}f_1(x, u)$$

and, then

$$\frac{d}{dt} \begin{bmatrix} x \\ u \end{bmatrix} = f_2(x, u)$$

and, finally,

$$\frac{d}{dt} \begin{bmatrix} x \\ u \end{bmatrix} = \frac{1}{2} f_1(x, u)$$

This method is referred to as the Leapfrog method. Note that by reversing the order of the flows, we are actually composing a half-step of the first order splitting with its adjoint (the adjoint of an exact flow is the flow itself), so the Leapfrog method (and Strang splitting in general) is self-adjoint.

Example. For u the population of predators and v the population of prey, an alternative Lotka-Volterra model can be written

$$u' = u(v - 2), \quad v' = v(1 - u)$$

A simple splitting with $y = (u, v)^T$ is

$$f(y) = \begin{pmatrix} u(v - 2) \\ 0 \end{pmatrix}, \quad g(y) = \begin{pmatrix} 0 \\ v(1 - u) \end{pmatrix}$$

The exact solution of $y' = f(y)$ on $[0, h]$ is

$$u(h) = e^{h(v(0)-2)}u(0), \quad v(h) = v(0).$$

The exact solution of $y' = g(y)$ on $[0, h]$ is

$$u(h) = u(0), \quad v(h) = e^{h(1-u(0))}v(0).$$

Combining these flows gives the first order method

$$\begin{aligned} u_{n+1} &= e^{h(v_n-2)}u_n, \\ v_{n+1} &= e^{h(1-u_{n+1})}v_n \end{aligned}$$

A second order, self-adjoint method can be derived by composing a half step of the above method with its adjoint. Noting that the exact solution of a subproblem is self-adjoint:

$$\begin{aligned} u_{n+1/2} &= e^{\frac{h}{2}(v_n-2)}u_n, \\ v_{n+1} &= e^{h(1-u_{n+1/2})}v_n, \\ u_{n+1} &= e^{\frac{h}{2}(v_{n+1}-2)}u_{n+1/2}. \end{aligned}$$

With initial conditions $u(0) = 6$ and $v(0) = 2$, the solution is periodic with approximate period $T = 6.336$. The solution at time $t = 6.4$ is $u(6.4) \approx 5.89200351$, $v(6.4) \approx 1.45888866$. In Figure 13.2, the solution is illustrated using the 2nd order splitting with $h = 0.1$. Also the error behavior for the first and second order splittings is shown.

Clearly, a multiple term splitting is also possible. For example, for the ODE

$$y' = f_1(y) + \cdots + f_k(y),$$

the splitting method

$$y_{n+1} = \Phi_{f_k}^h \circ \cdots \circ \Phi_{f_1}^h y_n \tag{13.1}$$

is first order in general.

It is not necessary that the split subproblems be solved exactly. Since the composition is only first order, the subproblems may also be approximated by a first order method. However, one often looks for an exactly solvable splitting.

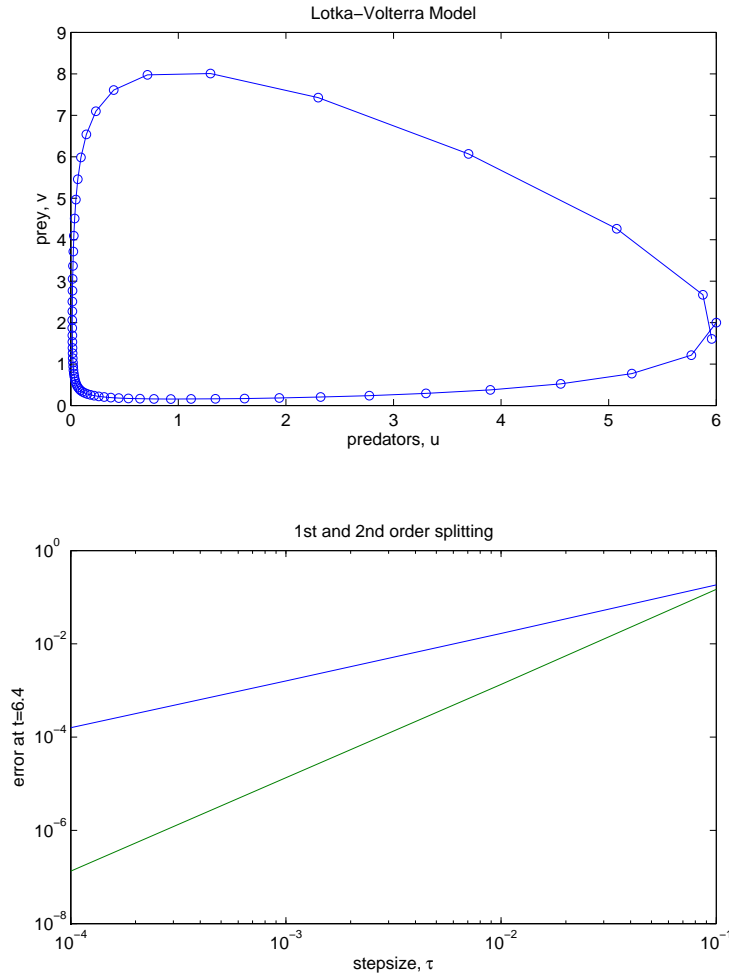


Figure 13.2: One-period of the Lotka-Volterra model: solution (top) and error (bottom).

The prudent choice of the splitting can make or break a splitting method. For one thing, if the splitting is such that the exact solution of a subproblem is not known, then it must be approximated with, for example, an RK method, and there will be approximation errors in addition to the splitting errors. Furthermore, if two terms are strongly coupled, then splitting them apart could cause large errors. For example, consider a mechanical system with two strong opposing forces that nearly balance each other out. The combined effect of the forces is small. However, each force by itself is large and would cause big accelerations if split apart. Normally one chooses the splitting based on physical or other (structural) considerations.

13.2 Exercises

1. Write out the formulas for the splitting method for the differential equation system

$$\frac{dy}{dt} = ay + \begin{bmatrix} 0 & -1 \\ 1 & 0 \end{bmatrix} y$$

where a is a scalar, based on solving

$$\frac{dy}{dt} = ay$$

followed by

$$\frac{dy}{dt} = \begin{bmatrix} 0 & -1 \\ 1 & 0 \end{bmatrix} y$$

Comment on the order of the resulting method. Repeat the exercise for

$$\frac{dy}{dt} = \begin{bmatrix} a & 0 \\ 0 & b \end{bmatrix} y + \begin{bmatrix} 0 & -1 \\ 1 & 0 \end{bmatrix} y$$

solving first

$$\frac{dy}{dt} = \begin{bmatrix} a & 0 \\ 0 & b \end{bmatrix} y$$

followed by

$$\frac{dy}{dt} = \begin{bmatrix} 0 & -1 \\ 1 & 0 \end{bmatrix} y$$

2. Prove that the Strang splitting gives a 2nd order integrator (for nonlinear problems).
3. Discuss the preservation of equilibrium points by splitting methods. Can you think of a splitting that preserves equilibrium points exactly?
4. Compare the first and second order splittings for the Lotka-Volterra model and Heun's method (8.3) for a long numerical simulation (say, 10 to 100 periods). Can you discern any qualitative differences in the solutions? Use a range of step sizes.

