Chapter 3

Important classes of numerical methods

We present in this chapter some of the most important classes of numerical methods for systems of differential equations with initial condition of the form

$$\begin{cases} \dot{y} = f(t,y), \quad t \in [0,T], \\ y(t_0) = y_0, \end{cases} \tag{3.1}$$

where $f : [0,T] \times \mathbb{R}^d \to \mathbb{R}^d$ is a given smooth vector field, $y(0) = y_0 \in \mathbb{R}^d$ is the given initial condition, T is the final time, and $y : [0,T] \to \mathbb{R}^d$ is the solution of the system.

We shall focus on one step methods

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

where h_n denotes the stepsize (which may be constant, $h_n = h$, or may be variable at each step), to compute by induction a discrete approximation $y_0, y_1, y_2, \dots$ of the exact solution $y(t_0), y(t_1), y(t_2), \dots$ at times t_n defined as $t_{n+1} = t_n + h_n$.

Given y_n, the simplest method to compute $y_{n+1} \simeq y(t_{n+1})$ where $t_n = nh$ is obtained by substituting in (3.1) the derivative approximation $\dot{y}(t_n) \simeq \frac{y_{n+1}-y_n}{h}$, which yields the explicit Euler method

$$y_{n+1} = y_n + hf(t_n, y_n).$$

3.1 Runge-Kutta methods

3.1.1 Definition

As presented before, the explicit Euler method

$$y_{n+1} = y_n + hf(t_n, y_n),$$

Given t_0 and T, we consider the Cauchy problem

Given a stepsize h such that $T - t_0 = Nh$, we consider the time sequence $t_0 < t_1 < \dots < t_n$. The integration of (3.1) from t_n to $t_n + h = t_{n+1}$ gives

$$y(t_1) = y(t_0) + \int_{t_0}^{t_0+h} f(s, y(s))\, ds.$$

The approximation of the integral in the second term of the right hand side leads to a numerical method.

Example 3.1.1. 1. (Euler, 1768) The approximation

$$\int_{t_0}^{t_0+h} f(s, y(s)) \approx hf(t_0, y_0),$$

leads to the Euler explicit method.

2. (Cauchy, 1824) The approximation

$$\int_{t_0}^{t_0+h} f(s, y(s)) \approx hf(t_0 + h, y(t_0 + h)),$$

leads to the Euler implicit method.

Definition 3.1.2. A one step method *has order* p if for all problems (3.1) with $f(t, y)$ sufficiently differentiable we have, after one step,

$$y_1 - y(t_0 + h) = \mathcal{O}(h^{p+1}), \quad h \to 0, \tag{3.2}$$

where we start on the exact solution for the method, $y_0 = y(t_0)$.

Example 3.1.3. For a smooth y, we apply the Taylor expansion,

$$\begin{aligned} y(t_0 + h) &= y(t_0) + h\dot{y}(t_0) + \frac{h^2}{2}\ddot{y}(t_0) + ... \\ &= y(t_0) + hf(t_0, y_0) + \frac{h^2}{2}\Big(\frac{\partial f}{\partial t}(t_0, y_0) + \frac{\partial f}{\partial y}(t_0, y_0)f(t_0, y_0)\Big) + ... \end{aligned} \tag{3.3}$$

Consider the Euler explicit method

$$y_1 = y(t_0) + hf(t_0, y(t_0)).$$

Compared to (3.3) we see that $y_1 - y(t_1) = \mathcal{O}(h^2)$, $h \to 0$, so that the method is of order 1.
Consider now the Euler implicit method

$$y_1(h) = y(t_0) + h\underbrace{f(t_0 + h, y(t_0 + h))}_{\phi(h)} = y(t_0) + h\phi(h), \quad y_1(0) = y(t_0).$$

We expand ϕ :

$$\begin{aligned} \phi(h) &= \phi(0) + \phi'(0)h + \mathcal{O}(h^2), \\ \phi(h) &= f(t_0, y(t_0)) + \Big(\frac{\partial f}{\partial t}(t_0, y_0) + \frac{\partial f}{\partial y}(t_0, y_0)y_1'(h)\Big)h + \mathcal{O}(h^2) \\ &= f(t_0, y(t_0)) + \Big(\frac{\partial f}{\partial t}(t_0, y_0) + \frac{\partial f}{\partial y}(t_0, y_0)f(t_0, y_0)\Big)h + \mathcal{O}(h^2). \end{aligned}$$

Then we obtain that

$$y_1 = y(t_0) + hf(t_0, y(t_0)) + h^2\Big(\frac{\partial f}{\partial t}(t_0, y_0) + \frac{\partial f}{\partial y}(t_0, y_0)f(t_0, y_0)\Big),$$

which compared to (3.3) gives that $y_1 - y(t_1) = \mathcal{O}(h^2)$, $h \to 0$, and the method is of order 1.

Example 3.1.4. Consider now the midpoint rule for quadrature formulas

$$\int_{t_0}^{t_0+h} f(s, y(s)) \approx hf\Big(t_0 + \frac{h}{2}, y\Big(t_0 + \frac{h}{2}\Big)\Big).$$

Here, we see that we have to approximate $y(t_0 + \frac{h}{2})$. There are multiple ways to do it. First, we consider the method used by the mathematician Runge (1895) :

$$\begin{cases} y_{1/2} = y_0 + \frac{h}{2} f(t_0, y_0), \\ y_1 = y_0 + hf\Big(t_0 + \frac{h}{2}, y_{1/2}\Big). \end{cases}$$

We observe that the first line is an Euler explicit step. We rewrite this method more elegantly

$$\begin{cases} k_1 = f(t_0, y_0), \\ k_2 = f\Big(t_0 + \frac{h}{2}, y_0 + \frac{h}{2} k_1\Big), \\ y_1 = y_0 + hk_1. \end{cases}$$

We can check that this method has order 2.
A second way to approximate $y(t_0 + \frac{h}{2})$, is to use an Euler implicit step in the first line,

$$\begin{cases} y_{1/2} = y_0 + \frac{h}{2} f\Big(t_0 + \frac{h}{2}, y_{1/2}\Big), \\ y_1 = y_0 + hf\Big(t_0 + \frac{h}{2}, y_{1/2}\Big), \end{cases}$$

which rewritten gives

$$\begin{cases} k_1 = f\Big(t_0 + \frac{h}{2}, y_0 + \frac{h}{2} k_1\Big) \\ y_1 = y_0 + hk_1. \end{cases}$$

This is the so called *implicit midpoint rule*, which is of order 2 as well.

The generalization of the previous examples leads to a general family called Runge-Kutta methods.

Definition 3.1.5. (Runge, 1895 ; Kutta, 1901 ; Heun, 1900) Let $s \in \mathbb{N}^*$ and let b_i, a_{ij}, c_i, $1 \leq i, j \leq s$ be real numbers. An *s-stage Runge-Kutta method* for the integration of (3.1) is given by

$$k_i = f\Big(t_0 + c_i h,\ y_0 + h \sum_{j=1}^{s} a_{ij} k_j\Big), \qquad i = 1, ..., s, \tag{3.4}$$

$$y_1 = y_0 + h \sum_{i=1}^{s} b_i k_i. \tag{3.5}$$

Remark:

1. We usually take $c_i = \sum_{j=1}^{s} a_{ij}$. This ensures that all k_i are first order approximation, i.e. $f(t_o + c_i h, y(t_0 + c_i h)) = \mathcal{O}(h^2)$.

2. If $a_{ij} = 0$, $\forall j \geq i$, the method is explicit. Otherwise it is implicit.

3. Usually, we display such a method with its characteristic *Butcher tableau* of coefficients,

$$\begin{array}{c|ccc} c_1 & a_{11} & \dots & a_{1s} \\ \vdots & \vdots & & \vdots \\ c_s & a_{s1} & \dots & a_{ss} \\ \hline & b_1 & \dots & b_s \end{array} \tag{3.6}$$

Example 3.1.6. 1. The Euler explicit method is given by

$$\begin{aligned} k_1 &= f(t_0, y_0), \\ y_1 &= y(t_0) + hk_1. \end{aligned}$$

Its Butcher tableau is

$$\begin{array}{c|c} 0 & 0 \\ \hline & 1 \end{array} \tag{3.7}$$

2. In the same way, the Butcher tableau of the Euler implicit method

$$\begin{aligned} k_1 &= f(t_0 + h, y_0 + hk_1), \\ y_1 &= y(t_0) + hk_1, \end{aligned}$$

is given by

$$\begin{array}{c|c} 1 & 1 \\ \hline & 1 \end{array} \tag{3.8}$$

3. Consider now the Runge method given in the Example 3.1.4. Its Butcher tableau is given by

$$\begin{array}{c|cc} 0 & 0 & 0 \\ 1/2 & 1/2 & 0 \\ \hline & 0 & 1 \end{array} \tag{3.9}$$

Remark:

1. Does an implicit method exist ? If f is Lipschitz and h small enough, yes (see exercise serie 2).
2. A variable stepsize can be used :

$$\begin{aligned} y_1 &= y_0 + h_0 \sum_{i=1}^{s} b_i k_i(h_0) \\ &\vdots \\ y_{k+1} &= y_k + h_k \sum_{i=1}^{s} b_i k_i(h_k) \end{aligned}$$

3.1.2 Order theory

Global convergence

Theorem 3.1.7. *Let $y(t)$ be the solution of*

$$\begin{cases} y'(t) = f(t, y(t)), & t \in [t_0, T], \\ y(t_0) = y_0. \end{cases} \tag{3.10}$$

Assume that