LAB3: ONE-STEP AND MULTISTEP METHODS
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We aim to approximate the solution of

$$\mathbf{y}'(t) = \mathbf{f}(t, \mathbf{y}(t)), \quad t > t_0; \quad \mathbf{y}(t_0) = \mathbf{y}_0, \tag{1}$$

where $\mathbf{f} : [t_0, \infty) \times \mathbb{R}^d \to \mathbb{R}^d$, $\mathbf{y}_0 \in \mathbb{R}^d$ is a given vector.

The theta method. A family of one-step approximation procedures can be derived as follows. Let $\theta \in [0, 1]$ and $h > 0$. Integrate (1) from t_0 to $t_0 + h$ and approximate the integral to get

$$\mathbf{y}(t_0+h) = \mathbf{y}(t_0)+\int_{t_0}^{t_0+h} \mathbf{f}(\tau, \mathbf{y}(\tau))\,\mathrm{d}\tau \approx \mathbf{y}_0+h\mathbf{f}(t_0, \mathbf{y}_0)\theta+h\mathbf{f}(t_0+h, \mathbf{y}(t_0+h))(1-\theta).$$

Motivated by this, given a sequence of equidistant time-instances $t_0, t_1 = t_0+h, t_2 = t_0 + 2h, \ldots$ we define the approximation

$$\mathbf{y}_1 = \mathbf{y}_0 + \theta h\mathbf{f}(t_0, \mathbf{y}_0) + (1 - \theta)h\mathbf{f}(t_1, \mathbf{y}_1),$$

or, more generally,

$$\mathbf{y}_{n+1} = \mathbf{y}_n + \theta h\mathbf{f}(t_n, \mathbf{y}_n) + (1 - \theta)h\mathbf{f}(t_{n+1}, \mathbf{y}_{n+1}), \quad n = 0, 1, 2, \ldots \tag{2}$$

The family of methods defined by (2) is called the *theta method*. We highlight some special cases:

(1) When $\theta = 1$, we get

$$\mathbf{y}_{n+1} = \mathbf{y}_n + h\mathbf{f}(t_n, \mathbf{y}_n), \quad n = 0, 1, 2, \ldots \tag{3}$$

which is the *Euler method*.

(2) When $\theta = 0$, we get

$$\mathbf{y}_{n+1} = \mathbf{y}_n + h\mathbf{f}(t_{n+1}, \mathbf{y}_{n+1}), \quad n = 0, 1, 2, \ldots$$

which is called the *implicit Euler*, or *backward Euler* method.

(3) When $\theta = \frac{1}{2}$, we get

$$\mathbf{y}_{n+1} = \mathbf{y}_n + \frac{1}{2}h\mathbf{f}(t_n, \mathbf{y}_n) + \frac{1}{2}h\mathbf{f}(t_{n+1}, \mathbf{y}_{n+1}), \quad n = 0, 1, 2, \ldots$$

which is called the *Crank-Nicolson* method or the *trapezoidal rule* (c.f. quadrature for numerical integration).

The Adams-Bashford method. Let $h > 0$ and denote $\mathbf{y}_n$ the numerical approximation of $\mathbf{y}(t_n)$, where $t_n = t_0 + nh$. Let $s \geq 1$ be an integer and suppose that we have already obtained the first s approximations $\mathbf{y}_m$ of $\mathbf{y}(t_m)$, $m = 0, 1, \ldots, s-1$. We wish to advance the solution from t_{n+s-1} to t_{n+s}, $n = 0, 1, \ldots$. Therefore, we integrate (1) from t_{n+s-1} to t_{n+s} to get

$$\mathbf{y}(t_{n+s}) = \mathbf{y}(t_{n+s-1}) + \int_{t_{n+s-1}}^{t_{n+s}} \mathbf{f}(\tau, \mathbf{y}(\tau))\,\mathrm{d}\tau. \tag{4}$$

To derive an example of an algorithm that uses the past s approximation values we use Lagrange interpolation of the function $t \mapsto \mathbf{f}(t, \mathbf{y}(t))$ on the interval $[t_n, t_{n+s-1}]$ with respect to s points t_m, $m = n, n+1, \ldots, n+s-1$:

$$\mathbf{f}(t, \mathbf{y}(t)) \approx \mathbf{p}(t) = \sum_{m=0}^{s-1} L_m(t)\mathbf{f}(t_{n+m}, \mathbf{y}(t_{m+n})),\ t \in [t_n, t_{n+s-1}] \tag{5}$$

where L_m denotes the Lagrange polynomial

$$L_m(t) = \prod_{\substack{l=0 \\ l \neq m}}^{s-1} \frac{t - t_{n+l}}{t_{m+n} - t_{n+l}}.$$

Next, if we assume that $\mathbf{y}$ is sufficiently smooth there is a good chance that (5) still provides a good approximation on the interval $[t_{n+s-1}, t_{n+s}]$ which we then insert to (4) to obtain the approximation

$$\mathbf{y}(t_{n+s}) \approx \mathbf{y}(t_{n+s-1}) + \sum_{m=0}^{s-1} \mathbf{f}(t_{n+m}, \mathbf{y}(t_{m+n})) \int_{t_{n+s-1}}^{t_{n+s}} L_m(\tau)\, \mathrm{d}\tau.$$

Let

$$b_m := \frac{1}{h}\int_{t_{n+s-1}}^{t_{n+s}} L_m(\tau)\, \mathrm{d}\tau = \frac{1}{h}\int_0^h L_m(t_{n+s-1} + \tau)\mathrm{d}\tau,\ m = 0, 1, ..., s-1.$$

We therefore arrive at the method defined by

$$\mathbf{y}_{n+s} = \mathbf{y}_{n+s-1} + h\sum_{m=0}^{s-1} b_m \mathbf{f}(t_{n+m}, \mathbf{y}_{m+n}),\ n = 0, 1, ...$$

This scheme is referred to as the *s-step Adams-Bashford method*. When $s = 2$, we have

$$L_0(t) = \frac{t - t_{n+1}}{t_n - t_{n+1}} = \frac{t_{n+1} - t}{h}$$

and

$$L_1(t) = \frac{t - t_n}{t_{n+1} - t_n} = \frac{t - t_n}{h}.$$

Then

$$b_0 = \frac{1}{h}\int_0^h \frac{-\tau}{h}\, \mathrm{d}\tau = -\frac{1}{2}$$

and

$$b_1 = \frac{1}{h}\int_0^h \frac{\tau + h}{h}\, \mathrm{d}\tau = \frac{1}{h^2}\left[\frac{(\tau + h)^2}{2}\right]_0^h = \frac{3}{2}.$$

Thus, the 2-step Adams-Bashford method reads as

$$\mathbf{y}_{n+2} = \mathbf{y}_{n+1} + h[\frac{3}{2}\mathbf{f}(t_{n+1}, \mathbf{y}_{n+1}) - \frac{1}{2}\mathbf{f}(t_n, \mathbf{y}_n)],\ n = 0, 1, ... \tag{6}$$

Exercise 1 (Lotka-Volterra or predator-prey system)**.** We consider a system of differential equations that describe the time-evolution of the sizes of two populations. Let $x(t)$ denote the size of a rabbit population at time t and $y(t)$ denote the size of a fox population at time t. The foxes prey on the rabbits. Suppose that the size of the initial populations are given by $x(0)$ and $y(0)$, respectively. A simple mathematical model that describes the time-evolution of the sizes of the two populations is as follows:

$$\begin{aligned} x'(t) &= ax(t) - bx(t)y(t), \quad t > 0; \\ y'(t) &= cx(t)y(t) - dy(t), \quad t > 0; \\ x(0) &= x_0; \\ y(0) &= y_0. \end{aligned} \tag{7}$$

Such a system is called *Lotka-Volterra* or *predator-prey system.* The parameters in the equation have the following interpretation: a is the birth rate of the rabbits, d is the death rate of the foxes, while c and d characterize the number of rabbit/fox and fox/rabbit encounter per unit time. In this lab we'll use the following parameters for the functions $a = b = c = d = 1$, and the input parameters for the solvers are: $f(x, y)$, which returns x' and y', $x_0 = 5, y_0 = 1, T = 50$ and N is free of choice if not defined.

(a) Write a function which solves (7) with the Euler method (3) on the time interval $[0, T]$ with step-size h. The input parameters should be

$$x_0, y_0, T, N,$$

where $h = T/N$. Put the approximations x_i and y_i of $x(ih)$ and $y(ih)$, respectively, $i = 0, 1, ..., N$, in vectors, or a matrix. *(Output: No output needed from this task.)*

(b) Write a function which solves (7) with the 2-step Adams-Bashford method (6) on the time interval $[0, T]$ with step-size h. The input parameters should be

$$f, x_0, y_0, T, N$$

where $h = T/N$. Put the approximations x_i and y_i of $x(ih)$ and $y(ih)$, respectively, $i = 0, 1, ..., N$, in vectors or a matrix. Use the Crank-Nicholson method to determine the approximation (x_1, y_1). *(Output: No output needed from this task.)*

(c) Solve (7) with the Euler method and the 2-step Adams-Bashford method, implemented in (b) with $N = 10^7$ and take (x_N, y_N) as the exact solution of the whole population $(x(T) + y(T))$. Solve (7) with the Euler method and the 2-step Adams-Bashford method implemented in (b), and determine the rate of convergence of the method at $T = 50$ as $N = 2^{10} \to 2^{18}$. *(Output: Either a plot where y axis is the error rate and x axis is about the step; or a list of these numbers printed out.)*

(d) The solution of this system is a periodic function, write a function which determines the maximum and minimum values (of every peak) of the whole population $(x(t) + y(t))$. Do it for both Euler and Adam-Bashford methods, how does it change? *(Output: either plot or print out the maximums and the minimums)*