Numerical Methods for Differential Equations

Ferran Arqué

2018

Contents

ORDINARY DIFFERENTIAL EQUATIONS

1 Ordinary Differential Equations. Basic concepts

1.1 Introduction and some notation

Given $y' = f(x, y)$, where $\begin{cases} y(x) \in \mathbb{R}^n \\ f : \mathbb{R} \times \mathbb{R}^n \to \mathbb{R}^n \end{cases}$

Definition. We denote by $y(x)$ the exact solution of the ODE system above.

Definition. y_k is the approximation of $y(x_k)$ (after k steps).

Objective. We want to approximate $y(x)$ within a given interval $[x_0, x_n]$.

$$\text{We know} \begin{cases} x_0 \\ x_1 \\ x_2 \\ \vdots \\ x_n \end{cases} \qquad \text{We'd like to know} \begin{cases} y(x_0) \\ y(x_1) \\ y(x_2) \\ \vdots \\ y(x_n) \end{cases} \qquad \text{We find} \begin{cases} y_0 \\ y_1 \\ y_2 \\ \vdots \\ y_n \end{cases} \quad \text{(given by a method)}$$

Definition. $\|y(x_n) - y_n\|$ is the **global error**.

Definition. We define the **local truncation error** as the error caused by one iteration, i.e.

$$LTE = \|y(x_k) - y_k\| \qquad \big(\text{assuming the } \textit{localizing assumption}\text{: } y_{k-1} = y(x_{k-1})\big)$$

1.2 Euler's method

1.3 Enhanced Euler's method

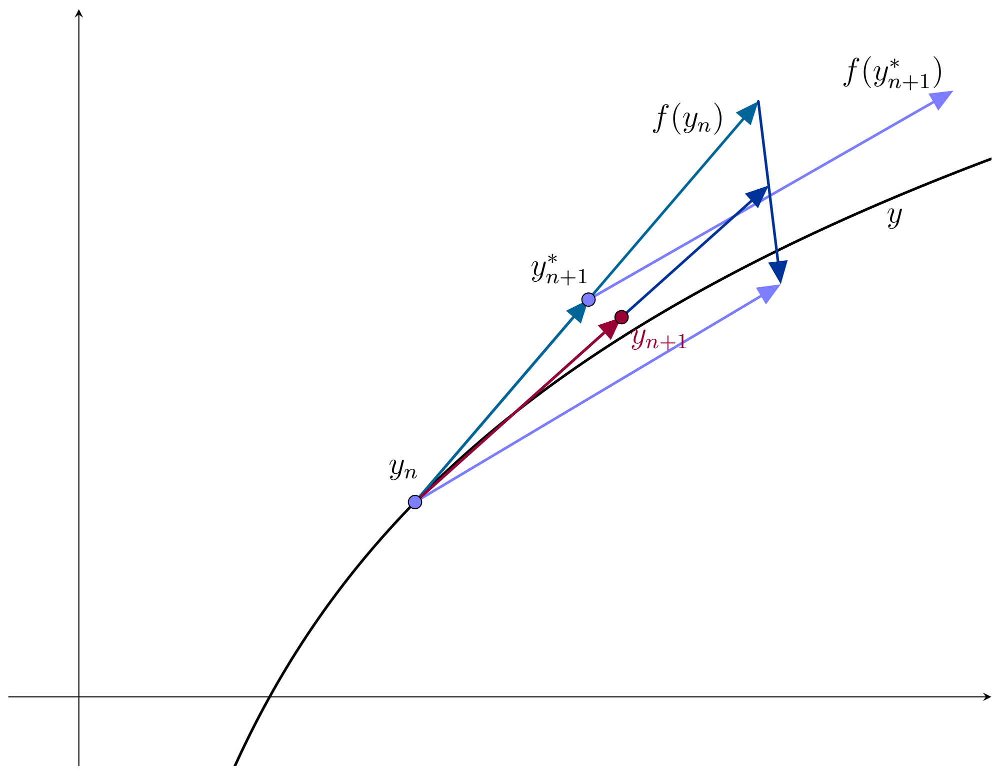


Figure 1.1: One step of the enhanced Euler's method

Given $y'(x) = f(y(x)), \quad y : \mathbb{R} \to \mathbb{R}, \quad f : \mathbb{R} \to \mathbb{R}$, we'll go through the steps to deduce the enhanced Euler's method with the help of the scheme in Figure 1.1.

The auxiliary point y^*_{n+1} can be found doing one step of the standard Euler's method, so

$$y^*_{n+1} = y_n + h \cdot f(y_n)$$

To get the point y_{n+1} we compute the average vector of $f(y^*_{n+1})$ and $f(y_n)$, and with this new vector, we can apply again a step of Euler's method, ending up with our method

$$\boxed{y_{n+1} = y_n + \frac{h}{2} \cdot \big(f(y^*_{n+1}) + f(y_n)\big)}$$

Let's find the LTE:

The Local Truncation Error is given by:

$$LTE = \|method - exact\ solution\|$$

Then

$$LTE = \|y_{n+1} - y(x_{n+1})\| = \left\| y_n + \frac{h}{2} f(y_n) + \frac{h}{2} f(y^*_{n+1}) - \underbrace{y(x_{n+1})}_{y(x_n+h)} \right\| = (*)$$

Applying Taylor on $f(y^*_{n+1}) = f\left(y_n + hf(y_n)\right)$, we have

$$f\left(y_n + hf(y_n)\right) = f(y_n) + hf(y_n)f'(y_n) + \mathcal{O}(h^2)$$

and on $y(x_n + h)$ we have

$$y(x_n + h) = y(x_n) + h \cdot y'(x_n) + \frac{h^2}{2} \cdot y''(x_n) + \mathcal{O}(h^3)$$

(In this case, we expand to second order for later simplifications)

$$(*) = \left\| y_n + \frac{h}{2} f(y_n) + \frac{h}{2}\left(f(y_n) + hf(y_n)f'(y_n) + \mathcal{O}(h^2)\right) - \left(y(x_n) + h \cdot y'(x_n) + \frac{h^2}{2} \cdot y''(x_n) + \mathcal{O}(h^3) \right) \right\| \quad (1)$$

Now, given $y'(x) = f(y(x))$, we have

$$\begin{aligned} y''(x) &= f'(y(x)) \cdot y'(x) \\ &= f'(y(x)) \cdot f(y(x)) \end{aligned}$$

and we can rewrite the following expression as:

$$\frac{h^2}{2} f(y(x))f'(y(x)) = \frac{h^2}{2} y''(x)$$

With that and the localising assumption ($y_n = y(x_n)$), we can simplify most of the terms in (1) and we end up with

$$\left\| \cancel{y_n} + \cancel{\frac{h}{2} f(y_n) + \frac{h}{2} f(y_n)} + \cancel{\frac{h^2}{2} f(y_n)f'(y_n)} + \mathcal{O}(h^3) - \left(\cancel{y(x_n)} + \cancel{h \cdot y'(x_n)} + \cancel{\frac{h^2}{2} \cdot y''(x_n)} + \mathcal{O}(h^3) \right) \right\| = \mathcal{O}(h^3)$$

So LTE $= \mathcal{O}(h^3)$

Remark. Of course, this method also works for $y : \mathbb{R} \to \mathbb{R}^n$, $f : \mathbb{R}^n \to \mathbb{R}^n$

1.4 Final remarks

- There's an improved Euler's method of order 2 similar to the previous one:

$$\boxed{y_{n+1} = y_n + hf\left(\frac{y^*_{n+1} + y_n}{2}\right)}$$

- If we have a method of order ≥ 2, and we want the value of $y(x^*)$, with x^* off the mesh ($x^* \neq k \cdot h$), we have some options:

  -Step back and take a step with the right h.

  -Interpolate with the right order.

  -Use a continuous Runge-Kutta method.

2 Runge-Kutta and Linear Multistep Methods

2.1 General Runge-Kutta methods

2.1.1 Embedded R-K

2.2 Linear multistep methods

2.2.1 Generalities

2.2.2 Predictor-Corrector method

2.2.3 Richardson's extrapolation

2.2.4 Convergence of a linear multistep method

Let's see an example of divergence using a linear multistep method:

Example

Given the method

$$\boldsymbol{y_{n+2} + a_1 y_{n+1} + a_0 y_n = h(b_1 f_{n+1} + b_0 f_n)}$$

1) Find $\boldsymbol{a_0, a_1, b_0, b_1}$ so that the method above has the highest possible order.

2) Try it on

$$\boldsymbol{\begin{cases} y' = -y \\ y(0) = 1 \end{cases} \qquad (y_0 = 1, y_1 = e^{-h})}$$

and prove the method diverges.

1) We want $y(x_n + 2h) - y_{n+2}$

We assume $y_{n+1} = y(x_n + h), y_n = y(x_n)$ (localizing assumption).

$$\begin{aligned} y(x_n + 2h) - y_{n+2} &= y(x_n + 2h) - \Big[- a_1 y_{n+1} - a_0 y_n + h\big(b_1 f(y_{n+1}) + b_0 f(y_n)\big)\Big] \underset{\text{loc.as.}}{=} \\ &= y(x_n + 2h) - \Big[- a_1 y(x_n + h) - a_0 y(x_n) + hb_1 \underbrace{f\left(y(x_n + h)\right)}_{y'(x_n+h)} + hb_0 \underbrace{f\left(y(x_n)\right)}_{y'(x_n)} \Big] \end{aligned}$$

As usual, we expand in powers of h. We'll expand to order 3

$$\begin{aligned} & y(x_n) + 2hy'(x_n) + \frac{4h^2}{2} y''(x_n) + \frac{8h^3}{6} y'''(x_n) + o(h^4) - \\ & - \Bigg[- a_1 \left(y(x_n) + hy'(x_n) + \frac{h^2}{2} y''(x_n) + \frac{h^3}{6} y'''(x_n) + o(h^4) \right) - \\ & \quad - a_0 y(x_n) \\ & \quad + hb_1 \left(y'(x_n) + hy''(x_n) + \frac{h^2}{2} y'''(x_n) + o(h^3) \right) + \\ & \quad + hb_0 y'(x_n) \Bigg] \end{aligned}$$

Let's group by powers of h and assume the right conditions to obtain the highest possible order:

$h^0 \longrightarrow y(x_n) + a_1 y(x_n) + a_0 y(x_n) = 0$

$h^1 \longrightarrow 2hy'(x_n) + a_1 hy'(x_n) - hb_1 y'(x_n) - hb_0 y'(x_n) = 0$

$h^2 \longrightarrow 2h^2 y''(x_n) + a_1 \frac{1}{2} h^2 y''(x_n) - b_1 h^2 y''(x_n) = 0$

$h^3 \longrightarrow \frac{8h^3}{6} y'''(x_n) + a_1 \frac{h^3}{6} y'''(x_n) - b_1 h \left(\frac{h^2}{2} y'''(x_n) \right) = 0$

With that, we get the system of equations

$$\begin{cases} 1 + a_1 + a_0 = 0 \\ 2 + a_1 - b_1 - b_0 = 0 \\ 2 + \dfrac{a_1}{2} - b_1 = 0 \\ \dfrac{8}{6} + \dfrac{a_1}{6} - \dfrac{b_1}{2} = 0 \end{cases}$$

And we end up with

$$a_0 = -5, \quad a_1 = 4, \quad b_0 = 2, \quad b_1 = 4$$

2) Our method is

$$y_{n+2} + 4y_{n+1} - 5y_n = h(4f_{n+1} + 2f_n)$$

and with

$$\begin{cases} y' = -y \\ y(0) = 1,\ y(h) = e^{-h} \end{cases} \qquad (y(x) = e^{-x})$$

we have

$$y_{n+2} + 4y_{n+1} - 5y_n = h(-4y_{n+1} - 2y_n)$$

We'll find a solution of the form

$$y_n = c_1(\quad)^n + c_2(\quad)^n$$

and we'll see that it diverges.

$$\lambda^2 + 4\lambda - 5 + 4h\lambda + 2h = 0$$
$$\lambda^2 + (4(1+h))\lambda + (2h - 5) = 0$$

$$\lambda = \frac{-4(1+h) \pm \sqrt{4^2(1+h)^2 - 4(2h-5)}}{2}$$

Let's expand the discriminant

$$\begin{aligned}
\sqrt{4^2(1+2h+h^2) - 8h + 20} = \sqrt{36 + 24h + 16h^2} = 6\sqrt{1 + \frac{4}{6}h + \frac{4^2}{6^2}h^2} \underset{\text{Taylor}}{=} \\
= 6\left(1 + \frac{1}{2}\left(\frac{4}{6}h + \frac{4^2}{6^2}h^2\right) + o(h^2)\right) = \\
= 6\left(1 + \frac{1}{3}h + o(h^2)\right)
\end{aligned}$$

So

$$\lambda = \frac{-4 - 4h \pm (6 + 2h + o(h^2))}{2} = \begin{cases} \nearrow 1 - h + o(h^2) \\ \searrow -5 - 3h + o(h^2) \end{cases}$$

$$\implies y_n = c_1\big(1 - h + o(h^2)\big)^n + c_2\big(-5 - 3h + o(h^2)\big)^n$$

Let's find c_1 and c_2 imposing the initial conditions

$$\begin{cases} 1 = c_1 + c_2 \implies c_1 = 1 - c_2 \\ e^{-h} = c_1\big(1 - h + o(h^2)\big) + c_2\big(-5 - 3h + o(h^2)\big) \end{cases}$$

$$\implies e^{-h} = (1 - h + o(h^2)) + c_2\big(\underbrace{-5 - 3h + o(h^2) - 1 + h + o(h^2)}_{-6-2h+o(h^2)}\big)$$

$$\implies c_2 = \frac{e^{-h} - 1 + h + o(h^2)}{-6 - 2h + o(h^2)} \underset{\text{Taylor } e^{-h}}{=} \frac{1 - h + o(h^2) - 1 + h + o(h^2)}{-6 - 2h + o(h^2)} \simeq \frac{-1}{6 + 2h}$$

$$\implies c_1 \simeq 1 + \frac{1}{6 + 2h} = \frac{7 + 2h}{6 + 2h}$$

So

$$y_n = \frac{7 + 2h}{6 + 2h}\big(1 - h + o(h^2)\big)^n + \frac{-1}{6 + 2h}\big(-5 - 3h + o(h^2)\big)^n$$

and the term $(-5)^n$ will cause the solution to diverge.

3 Stiff Problems

PARTIAL DIFFERENTIAL EQUATIONS

4 Partial Differential Equations. Generalities on their solution

4.1 Finite differences

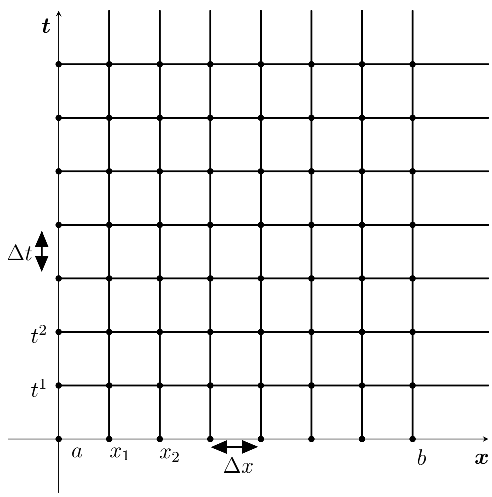
Example (1D Heat equation)

Our problem is:

$$\begin{cases} U_t - U_{xx} = f \\ U(x,0) = U_0(x) & \longleftarrow \text{Initial condition (IC)} \\ \left.\begin{matrix} U(a,t) = U_a \\ U(b,t) = U_b \end{matrix}\right\} & \longleftarrow \text{Boundary conditions (BC)} \end{cases}$$

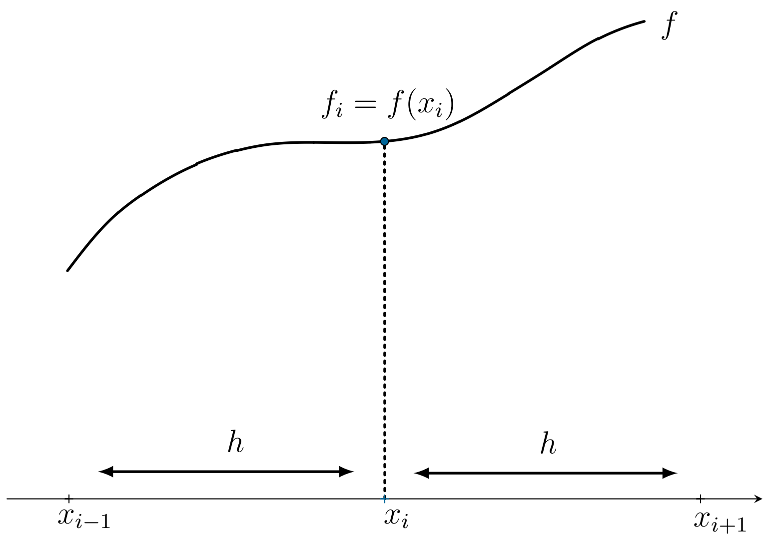
With $t \geq 0$, $x \in [a,b]$

We discretize x and t:



Idea: We'll impose $U_t(x_i, t^n) - U_{xx}(x_i, t^n) = f(x_i, t^n)$

4.1.1 Numerical derivatives



5 Numerical Solution of PDEs with the Finite Difference Method

6 Introduction to Boundary Value Problems

7 Quality Control of Solutions