April 28, 2020

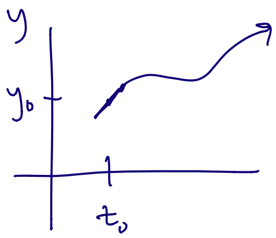
Numerical Analysis

Ordinary Differential Equations:

Initial value problem (IVP)

(*) $y'(t) = f(t,y)$

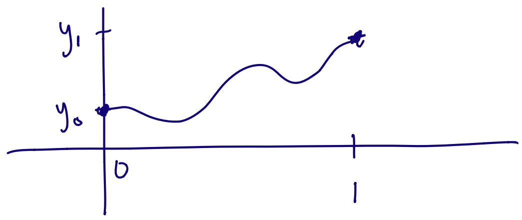
$y(t_0) = y_0$



Boundary Value Problems

$y'' + by' + cy = 0$

$y(0) = y_0 \quad , \quad y(1) = y_1$



The numerical methods used for solving these two problems are very different. We will focus only on initial value problems.

The solution to (*) can be written down formally as:

$$y(t) = y_0 + \int_{t_0}^{t} f(\tau, y(\tau))\, d\tau . \quad (**)$$

If f doesn't depend on y, we can straightforwardly evaluate: $\int_{t_0}^{t} f(\tau)\, d\tau$.

If f does depend on y, then we must solve (**) for y.

All methods for solving IVPs are merely approximating the formal solution in (**).

The local uniqueness of the solution to (*) is established by Picard's Theorem, see page 311 in the textbook. Basically, if f is continuous and bounded in a neighborhood of (t_0, y_0) (remember $f = f(t,y)$), then a unique solution exists in some neighborhood of (t_0, y_0).

Another way of viewing numerical solutions to (*) is to directly approximate the differential part:

For some small $h>0$,

$$y'(t) \approx \underbrace{\frac{y(t+h) - y(t)}{h}}_{\text{Finite Difference.}} \approx f(t, y(t))$$

$\Rightarrow$ Given $y(t)$, to approximate $y(t+h)$ we write:

$$\frac{y(t+h) - y(t)}{h} \approx f(t, y(t))$$

$$\Rightarrow \quad y(t+h) \approx y(t) + \underbrace{h \cdot f(t, y(t))}_{\approx \int_t^{t+h} f(\tau, y(\tau))\, d\tau} \qquad \text{(Compare with (**))}$$

This scheme is called the Forward Euler Method.

Let's turn to Finite Differences for a bit:

① Approximation error

② Floating point round off error.

How good is the Forward Difference at approximating y' in the presence of round-off error:

round-off error, $|\delta_i| < \epsilon$ ← machine precision

$$\frac{y(t+h) - y(t)}{h} \xrightarrow{\text{f.p.}} \frac{y(t+h)(1+\delta_1) - y(t)(1+\delta_2)}{h}$$

Ignore the round-off error in t, h, $t+h$.

$$= \frac{y(t+h) - y(t)}{h} + \frac{y(t+h)\delta_1 - y(t)\delta_2}{h}$$

$$= \frac{\left(y(t) + h\,y'(t) + \frac{h^2}{2} y''(\xi)\right) - y(t)}{h} + \frac{y(t+h)\delta_1 - y(t)\delta_2}{h}$$

$$= y'(t) + \frac{h}{2} y''(\xi) + \frac{y(t+h)\delta_1 - y(t)\delta_2}{h}$$

The total error is given as $\mathrm{Err}(h) = y'(t) - \frac{y(t+h) - y(t)}{h}$

$$\Rightarrow |\mathrm{Err}(h)| \le \left|\frac{h}{2} y''(\xi)\right| + \left|\frac{y(t+h)\delta_1 + y(t)\delta_2}{h}\right|$$

$$\le \underbrace{\left|\frac{h}{2} y''(\xi)\right|}_{O(h)} + \underbrace{\left(|y(t+h)| + |y(t)|\right)\frac{\epsilon}{h}}_{O\left(\frac{\epsilon}{h}\right)}.$$

truncation error | 1st order approximation — round-off error.

To minimize $|\mathrm{Err}(h)|$, h must be chosen to balance these terms:

$$h \sim \frac{\epsilon}{h} \Rightarrow h^2 \sim \epsilon \Rightarrow h \sim \sqrt{\epsilon}.$$

If $\epsilon \sim 10^{-16}$ (in double precision), then choosing $h \sim 10^{-8}$ minimizes the error, which is then of size:

$$|\mathrm{Err}(h)| \sim O(h) + O\left(\frac{\epsilon}{h}\right) \sim 10^{-8} + \frac{10^{-16}}{10^{-8}} \sim 10^{-8}$$

This is the best you can hope for from a forward difference approximation.

An alternative approximation, the <u>centered difference</u>, has the property that:

$$\left| y'(t) - \frac{y(t+h) - y(t-h)}{2h} \right| \leq \underbrace{\mathcal{O}(h^2)}_{\substack{\text{truncation} \\ \text{error}}} + \underbrace{\mathcal{O}\left(\frac{\epsilon}{h}\right)}_{\substack{\text{round-off} \\ \text{error}}}$$

2nd order approximation

Just like before, h must be chosen to balance these terms:

$$\Rightarrow \quad h^2 \sim \frac{\epsilon}{h}$$

$\Rightarrow \quad h \sim \epsilon^{1/3}$ in order to minimize this total error.

So if $h \sim 10^{-5}$, then the total error is

$$\mathcal{O}(h^2) + \mathcal{O}\left(\frac{\epsilon}{h}\right) \sim 10^{-10} + \frac{10^{-16}}{10^{-5}}$$

$$\sim 10^{-10} + 10^{-11}$$

$$\sim 10^{-10}$$

<u>Richardson Extrapolation</u>

What if we compute $f'(x) \approx \dfrac{f(x+h) - f(x-h)}{2h} = \varphi_0(h)$

for <u>several values</u> of h? Can we use this estimate to get a better estimate of $f'(x)$?

(Ignore round-off error for now).

The centered difference approximation is 2nd-order accurate:

$$\frac{f(x+h) - f(x-h)}{2h} = \varphi_0(h) = f'(x) + \frac{h^2}{6} f^{(3)}(x) + \mathcal{O}(h^4)$$

Compute $\varphi_0\left(\frac{h}{2}\right) = f'(x) + \frac{1}{6}\left(\frac{h}{2}\right)^2 f^{(3)}(x) + \mathcal{O}(h^4)$

$$= f'(x) + \frac{1}{6}\frac{1}{4} h^2 f^{(3)}(x) + \mathcal{O}(h^4)$$

Can we take a linear combination of $\varphi_0(h)$ and $\varphi_0(\frac{h}{2})$ to kill the $\mathcal{O}(h^2)$ term?

$$4\cdot\varphi_0(\tfrac{h}{2}) - \varphi_0(h) = 4f'(x) + \tfrac{1}{6}h^2 f^{(3)}(x) + \mathcal{O}(h^4) - f'(x) - \tfrac{1}{6}h^2 f^{(3)}(x) - \mathcal{O}(h^4)$$

$$= 3f'(x) + \mathcal{O}(h^4)$$

$$\Rightarrow \quad f'(x) = \underbrace{\frac{4\cdot\varphi_0(\frac{h}{2}) - \varphi_0(h)}{3}}_{} {}^{(***)} + \mathcal{O}(h^4)$$

4th order approximation to $f'(x)$.

We only used two 2nd order approximations to obtain a 4th order one.

If the round off error in $(***)$ is $\mathcal{O}(\frac{\epsilon}{h})$, then h must be chosen to balance $h^4 \sim \frac{\epsilon}{h}$

$$\Rightarrow h \sim \underbrace{\epsilon^{1/5}}_{\sim 10^{-3}} \text{ minimizes the total error}$$

$$= \mathcal{O}(h^4) + \mathcal{O}(\tfrac{\epsilon}{h}) \sim 10^{-12} + \frac{10^{-16}}{10^{-3}} \sim \underline{10^{-12}}$$

Richardson extrapolation can be repeated several times:

$$\varphi_1(h) \quad \frac{4\,\varphi_0(\frac{h}{2}) - \varphi_0(h)}{3} = f'(x) + \mathcal{O}(h^4)$$

$$\varphi_1(\tfrac{h}{2}) \quad \frac{4\,\varphi_0(\frac{h}{4}) - \varphi_0(\frac{h}{2})}{3} = f'(x) + \mathcal{O}\left(\frac{h^4}{16}\right)$$

$$\Rightarrow \quad \frac{16\,\varphi_1(\frac{h}{2}) - \varphi_1(h)}{15} = f'(x) + \mathcal{O}(h^6)$$

these truncation errors are specific to the original centered difference formula.