1 Differential equations

The basic problem:

$$\frac{dx}{dt} = \dot{x} = f\left(x,t\right)$$

subject to given boundary conditions (may be initial or end-point values etc.). Of course we may be interested in higher-order differential equations!

2 Initial value problems

If the boundary conditions are all expressed at the same point, then we have an **initial value problem**.

$$\begin{aligned} \dot{x} &= f\left(x,t\right) \\ \Rightarrow x\left(t\right) &= x\left(0\right) + \int_0^t f\left(x,t'\right)dt' \end{aligned}$$

Unlike conventional numerical integration where we are interpolating between known end-points, we are now *extrapolating* ⟶ can lead to large errors. How do we solve this?

First we split integral into discrete blocks:

$$\begin{aligned} x\left(t\right) &= x\left(0\right) + \int_0^{\Delta t} f\left(x,t'\right)dt' + \int_{\Delta t}^{2\Delta t} f\left(x,t'\right)dt' + \\ &\quad \ldots + \int_{\mathbf{n\Delta t}}^{\mathbf{(n+1)\Delta t}} \mathbf{f\left(x,t'\right)dt'} + \ldots + \int_{t-\Delta t}^{t} f\left(x,t'\right)dt' \end{aligned}$$

Write each term $f(x,t)$ as Taylor series about lower limit

$$f(x,t) = f(x,n\Delta t) + (t-n\Delta t)\left.\frac{\partial f}{\partial t}\right|_{t=n\Delta t} + \frac{\left(t-n\Delta t\right)^2}{2}\left.\frac{\partial^2 f}{\partial t^2}\right|_{t=n\Delta t} + \ldots$$

Now we need a way to compute these small integrals.

3 Euler method

If f varies slowly over the range $n\Delta t \leq t < \left(n+1\right)\Delta t$ then we can ignore most of the terms in the Taylor series and write:

$$f(x,t) \approx f(x,n\Delta t)$$

n	t_n	x_n	analytic
0	0.0	1.0	1.0
1	0.1	0.90	0.904837
2	0.2	0.81	0.818731
$\vdots$	$\vdots$	$\vdots$	$\vdots$
10	1.0	0.348678	0.367879
$\vdots$	$\vdots$	$\vdots$	$\vdots$
50	5.0	0.005154	0.006738

Table 1: The Euler method for radioactive decay, with $\lambda = 1$ and $\Delta t = 0.1$.

i.e. replace function in each integral by the function *value* at the start:

$$\begin{aligned} \int_{n\Delta t}^{(n+1)\Delta t} f\left(x, t'\right) dt' &\approx \int_{n\Delta t}^{(n+1)\Delta t} f\left(x\left(n\Delta t\right), n\Delta t\right) dt' \\ &= f\left(x\left(n\Delta t\right), n\Delta t\right) \Delta t \end{aligned}$$

4 Example 1: radioactive decay

Can solve $\frac{dx}{dt} = -\lambda x$ analytically, but let's use Euler:

$$x_{n+1} = x_n + (-\lambda x_n)\Delta t$$

Let's see what happens for $\lambda = 1$ and $\Delta t = 0.1$ (table 1). Overall, the error doesn't seem too bad.

- Can reduce this **truncation error** by reducing $\Delta t \longrightarrow$ more steps.
- Finite precision, or **roundoff error**, limits final accuracy of *any* scheme.

5 Example 2: simple harmonic oscillator

Now we'll look at a *second-order* differential equation:

$$\frac{d^2x}{dt^2} = -\omega^2 x$$

We'll split this into two coupled first order equations:

$$\begin{aligned} \frac{dx}{dt} &= v \\ \frac{dv}{dt} &= -\omega^2 x \end{aligned}$$

n	t_n	x_n	analytic x	v_n	analytic v
0	0.0	1.0	1.0	0.0	0.0
1	0.1	1.0	0.995004	-0.1	-0.099833
2	0.2	0.99	0.980067	-0.2	-0.198669
$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\vdots$
10	1.0	0.570790	0.540302	-0.882508	-0.841471
$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\vdots$
50	5.0	0.343355	0.283662	**1.235613**	**0.958924**

Table 2: Example of the Euler method for a simple harmonic oscillator. Here $\omega = 1$ and $\Delta t = 0.1$.

so using the Euler method we have:

$$\begin{aligned} x_{n+1} &= x_n + v_n \Delta t \\ v_{n+1} &= v_n - \omega^2 x_n \Delta t \end{aligned}$$

Typical boundary conditions: $x(0) = 1; v(0) = 0$. Let's use $\omega = 1$ and $\Delta t = 0.1$ as before. The results are in table 2. The Euler method leads to a nonphysical velocity v! Clearly something has gone wrong, but what?

6 Error analysis for Euler method

Let's measure the error at step n, ϵ_n, by the residual:

$$\begin{aligned} \epsilon_n &= x_n^{true} - x_n \\ \Rightarrow x_n^{true} &= x_n + \epsilon_n \end{aligned}$$

Now according to Euler,

$$\begin{aligned} x_{n+1}^{true} &= x_n^{true} + f\left(x_n^{true}, t\right) \Delta t \\ \Rightarrow (x_{n+1} + \epsilon_{n+1}) &= (x_n + \epsilon_n) + f\left(x_n + \epsilon_n, t\right) \Delta t \end{aligned}$$

Assuming ϵ_n is small, use a Taylor expansion in x to write:

$$f\left(x_n + \epsilon_n, t\right) \approx f\left(x_n, t\right) + \epsilon_n \left.\frac{\partial f}{\partial x}\right|_{x=x_n}$$

and so we have

$$(x_{n+1} + \epsilon_{n+1}) = (x_n + \epsilon_n) + \left(f\left(x_n + \epsilon_n, t\right)\right) \Delta t$$

$$\begin{aligned} &\approx (x_n+\epsilon_n)+\left(f\left(x_n,t\right)+\epsilon_n\left.\frac{\partial f}{\partial x}\right|_{x=x_n}\right)\Delta t \\ &= \left(x_n+f\left(x_n,t\right)\Delta t\right)+\epsilon_n\left(1+\left.\frac{\partial f}{\partial x}\right|_{x=x_n}\Delta t\right) \end{aligned}$$

But Euler means

$$x_{n+1} = \left(x_n+f\left(x_n,t\right)\Delta t\right)$$

and so

$$\begin{aligned} \epsilon_{n+1} &= \epsilon_n\left(1+\left.\frac{\partial f}{\partial x}\right|_{x=x_n}\Delta t\right) \\ &= \epsilon_n G \end{aligned}$$

where G is the **error gain term**.

Provided $|G|<1$ the error term does not grow, so we have a stable scheme.

E.g. for radioactive decay we have $f\left(x,t\right)=\frac{dx}{dt}=-\lambda x$, so

$$\begin{aligned} G &= 1+\left.\frac{\partial f}{\partial x}\right|_{x=x_n}\Delta t \\ &= 1-\lambda\Delta t \end{aligned}$$

Thus the Euler method is stable if $|1-\lambda\Delta t|<1$, i.e.

$$\begin{aligned} -1< \quad & 1-\lambda\Delta t \quad <1 \\ \Rightarrow -2< \quad & -\lambda\Delta t \quad <0 \\ \Rightarrow 0< \quad & \lambda\Delta t \quad <2 \\ \Rightarrow 0< \quad & \Delta t \quad <\frac{2}{\lambda} \end{aligned}$$

7 Beyond Euler

- Predictor-corrector
- Higher-order methods (extending truncation scheme)

These schemes are generally more accurate and stable, allowing a larger Δt, but require more function evaluations per step and more computer storage.

One common scheme is 4th-order Runge-Kutta – see any text on numerical methods for lots of details!