

MAS212 Scientific Computing and Simulation

Dr. Sam Dolan

School of Mathematics and Statistics,
University of Sheffield

Autumn 2019

<http://sam-dolan.staff.shef.ac.uk/mas212/>

G18 Hicks Building
s.dolan@sheffield.ac.uk

Today's lecture

- Explicit methods for solving ODEs
 - ① The midpoint method (review)
 - ② The ratio test
 - ③ Runge-Kutta methods
- Linear multi-step methods:
 - ① A two-step method
 - ② Adams-Bashforth methods
- Implicit methods:
 - ① The Backward Euler method
 - ② Adams-Moulton methods

Recap: Euler's method

$$\frac{dx}{dt} = f(x, t) \quad x(t_0) = x_0$$

Euler's method

$$x_{k+1} = x_k + h f(x_k, t_k)$$

Algorithm:

- Divide the domain $[t_0, t_f]$ into n equally-spaced intervals:

$$h \equiv \frac{t_f - t_0}{n}, \quad t_k = t_0 + k h, \quad k \in [0, 1, \dots, n]$$

- Start with the **initial condition** x_0 at t_0
- Apply $x_{k+1} = x_k + h f(x_k, t_k)$ **once** to get x_1 from x_0
- Now iterate (repeat) ...

Convergence

- With a rule for finding x_{k+1} from x_k , t_k and the step size h (only) ...
- ... we can generate a sequence $[x_0^{(h)}, x_1^{(h)}, \dots, x_n^{(h)}]$ where each $x_k^{(h)}$ is only an approximation to the 'true' solution $\bar{x}(t_k)$ of the ODE.

- The **error** is defined to be

$$\epsilon_k^{(h)} \equiv x_k^{(h)} - \bar{x}(t_k)$$

- The method should **converge**: $\epsilon_k^{(h)} \rightarrow 0$ as $h \rightarrow 0$.
- The **rate of convergence** with step size h is important to understand.
- An n th-order method has local truncation error $\epsilon_1 = O(h^{n+1})$ and global truncation error $\epsilon_n = O(h^n)$.
- For example, Euler's method is a first-order method.

The ratio test

- **Q.** How can we check, in practice, that our implementation of a method has the correct rate of convergence ?
- **A.** Apply the **ratio test**.
- Let $x^{(h)}(t)$ be a numerical solution with step size h .
- Now find **three** numerical solutions and form the following ratio

$$r(t) = \frac{x^{(4h)}(t) - x^{(2h)}(t)}{x^{(2h)}(t) - x^{(h)}(t)}$$

- We want to compare at the same time t .
Since $t_k = t_0 + k h$, we actually do this:

$$r_k = \frac{x_k^{(4h)} - x_{2k}^{(2h)}}{x_{2k}^{(2h)} - x_{4k}^{(h)}}$$

The ratio test

- **Proposition:** A correctly-implemented s -th order method should generate ratios r_k approximately equal to $\sim 2^s$.
- **Proof:** If the method is order s , then

$$\epsilon(t) = \alpha_0(t)h^s + \alpha_1(t)h^{s+1} + \dots$$

where $\alpha_j(t)$ are numerical coefficients. So

$$\begin{aligned}x^{(h)}(t) &= \bar{x}(t) + \epsilon(t), \\ &= \bar{x}(t) + \alpha_0(t)h^s + O(h^{s+1}).\end{aligned}$$

- Thus:

$$\begin{aligned}x^{(4h)}(t) &= \bar{x}(t) + \alpha_0(t)(4h)^s + O(h^{s+1}), \\ x^{(2h)}(t) &= \bar{x}(t) + \alpha_0(t)(2h)^s + O(h^{s+1}), \\ x^{(h)}(t) &= \bar{x}(t) + \alpha_0(t)(1h)^s + O(h^{s+1}).\end{aligned}$$

(1)

The ratio test

- **Proof:** (continued)

$$x^{(4h)} - x^{(2h)} = (4^s - 2^s)\alpha_0 h^s + O(h^{s+1}),$$

$$x^{(2h)} - x^{(h)} = (2^s - 1)\alpha_0 h^s + O(h^{s+1}).$$

- Therefore the ratio $r(t) = \frac{x^{(4h)}(t) - x^{(2h)}(t)}{x^{(2h)}(t) - x^{(h)}(t)}$ is

$$\begin{aligned} r(t) &= \frac{2^{2s} - 2^s}{2^s - 1} + O(h) \\ &= 2^s + O(h). \end{aligned}$$

- (N.B. if the denominator passes close to zero this argument breaks down).

Example:

(a) Numerically solve the ODE

$$\frac{dx}{dt} = e^{-t/10} \sin(t) \sin(x), \quad x(0) = 1,$$

in the range $t \in [0, 20]$ using a **3rd order Runge-Kutta method**.

(b) Apply the ratio test to show that your method is 3rd-order accurate.

Runge-Kutta methods

Runge-Kutta methods

$$x_{j+1} = x_j + \sum_{i=1}^s b_i k_i$$

where s is the order of the method, and

$$k_1 = hf(x_j, t_j)$$

$$k_2 = hf(x_j + a_{21}k_1, t_j + c_2h)$$

$$k_3 = hf(x_j + a_{31}k_1 + a_{32}k_2, t_j + c_3h)$$

...

$$k_s = hf(x_j + a_{s1}k_1 + a_{s2}k_2 + \dots + a_{s,s-1}k_{s-1}, t_j + c_s h)$$

- A method is specified by the coefficients b_i , c_i and a_{ij} .
- Euler's method and the midpoint method are members of the **Runge-Kutta family of methods** that use intermediate estimates in a systematic way.

Runge-Kutta methods

- A method is specified by the coefficients b_i , c_i and a_{ij} .
- Butcher tableau are used to give these coefficients:

0						
c_2		a_{21}				
c_3		a_{31}	a_{32}			
...			
c_s		a_{s1}	a_{s2}	...	$a_{s,s-1}$	
		b_1	b_2	...	b_{s-1}	b_s

- **Example:** Midpoint method

$$k_1 = hf(x_j, t_j)$$

$$k_2 = hf(x_j + \frac{1}{2}k_1, t_j + \frac{1}{2}h)$$

$$x_{j+1} = x_j + k_2.$$

0			
1/2		1/2	
		0	1

Runge-Kutta methods

- The most well-used version is the **classical Runge-Kutta method** or **RK4 method** :

0				
1/2	1/2			
1/2	0	1/2		
1	0	0	1	
<hr/>				
	1/6	1/3	1/3	1/6

- This is a fourth-order accurate method. `odeint` uses this method.
- In this example we will implement a third-order RK method with:

0			
1/2	1/2		
1	-1	2	
<hr/>			
	1/6	4/6	1/6

Solution: part (a)

- Import modules:

```
import numpy as np
import matplotlib.pyplot as plt
```

- A function to calculate the derivative, i.e. the RHS of $\frac{dx}{dt} = f(x, t)$:

```
def dx_dt(x, t):
    return np.sin(t)*np.sin(x)*np.exp(-0.1*t)
```

- A function to implement **one step** of the RK3 method:

```
def rk3_step(x, t, h):
    """See Butcher tableau for RK3 method"""
    k1 = h*dx_dt(x, t)
    k2 = h*dx_dt(x+k1/2.0, t+h/2.0)
    k3 = h*dx_dt(x-k1+2*k2, t+h)
    x_next = x + (k1 + 4*k2 + k3)/6.0
    return x_next
```

Solution: part (a)

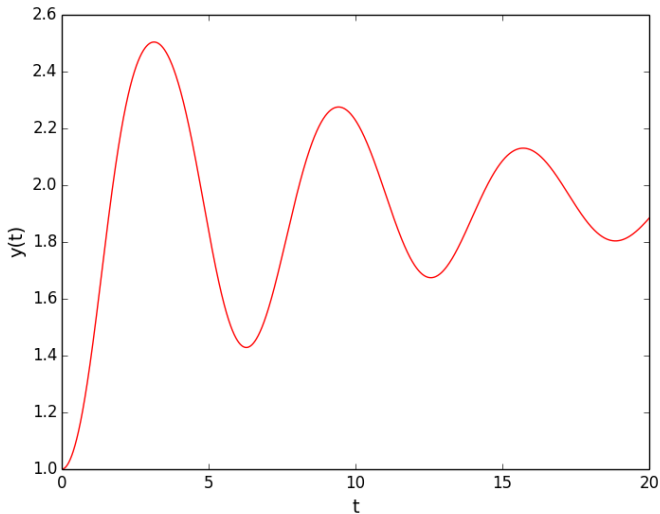
- A function to solve over the range $0 \leq t \leq 20$:

```
def rk3_solve(x0, h, tmin, tmax):  
    n = int((tmax - tmin)/h) # number of steps  
    ts = np.zeros(n+1); xs = np.zeros(n+1) # arrays  
    xs[0] = x0; ts[0] = tmin # set initial conditions  
    for k in range(n):  
        ts[k+1] = ts[k] + h  
        xs[k+1] = rk3_step(xs[k], ts[k], h)  
    return ts, xs
```

- Now test with step size $h = 0.01$:

```
x0 = 1.0; h = 0.01; tmin = 0.0; tmax = 20.0;  
ts, xs = rk3_solve(x0, h, tmin, tmax)  
plt.plot(ts, xs, 'r-')  
plt.xlim(tmin, tmax)  
plt.xlabel("t"); plt.ylabel("x(t)")  
plt.show()
```

Solution: part (a)



Solution: part (b)

- **Q.** How do we know the implementation of the method is truly **third-order accurate**? (i.e. that the **global truncation error** scales with h^3).
- **A.** Apply the **ratio test**.
- Let $x^{(h)}(t)$ be a numerical solution with time step h .
- Now form the ratio

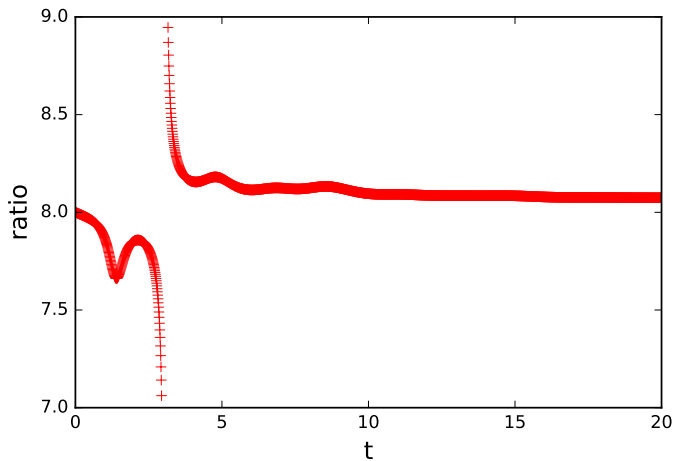
$$r(t) = \frac{x^{(4h)}(t) - x^{(2h)}(t)}{x^{(2h)}(t) - x^{(h)}(t)}$$

- As $h \rightarrow 0$, we expect $r \rightarrow 2^s$, where s is the order of the method.
- As the RK3 method is third order accurate we expect $r \rightarrow 8$.

Solution: part (b)

```
x0 = 1.0; h = 0.0025; tmin = 0.0; tmax = 20.0;
# call the function 3 times for 3 different intervals h
ts0, xs0 = rk3_solve(x0, 4*h, tmin, tmax) # crude resolution
ts1, xs1 = rk3_solve(x0, 2*h, tmin, tmax) # medium
ts2, xs2 = rk3_solve(x0, 1*h, tmin, tmax) # fine resolution
rs = (xs0 - xs1[:,2]) / (xs1[:,2] - xs2[:,4])
plt.plot(ts0, rs, 'ro')
plt.xlim(tmin, tmax); plt.ylim(0, 12)
plt.xlabel('t', fontsize=14); plt.ylabel('ratio', fontsize=14)
plt.show()
```


Solution: part (b)



Multi-step methods

- Runge-Kutta methods take one step forward by combining several intermediate steps:
- The intermediate steps are **thrown away** ... seems wasteful & inefficient
- Multi-step methods **re-use** information from earlier times
- **Linear** multi-step methods get x_{n+1} from a linear combination of $\{x_n, x_{n-1}, \dots\}$.

Linear multi-step methods

$$\frac{dx}{dt} = f(x, t), \quad x(t_0) = x_0$$

- **Example: The two-step method:**

$$x_{n+1} = x_n + h \left(\frac{3}{2} f(x_n, t_n) - \frac{1}{2} f(x_{n-1}, t_{n-1}) \right)$$

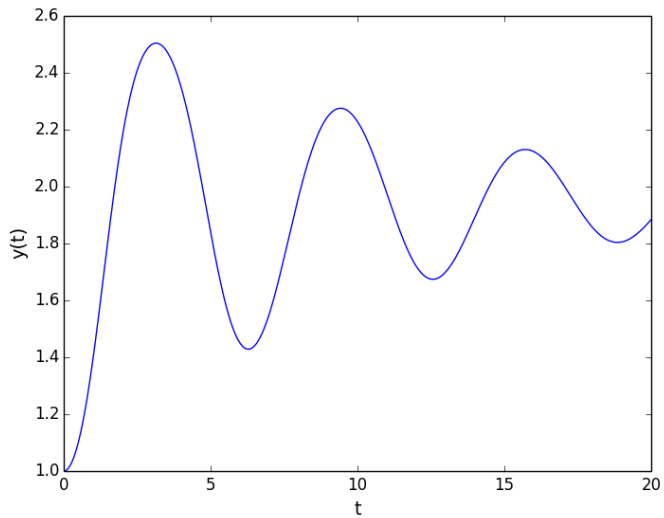
- The method uses both x_n and x_{n-1} .
- It is second order accurate (*Exercise: show this*).
- **Q:** How do we take the very first step?
- **A:** Use an alternative method of same order.

Implementation of the two-step method

$$x_{n+1} = x_n + h \left(\frac{3}{2} f(x_n, t_n) - \frac{1}{2} f(x_{n-1}, t_{n-1}) \right)$$

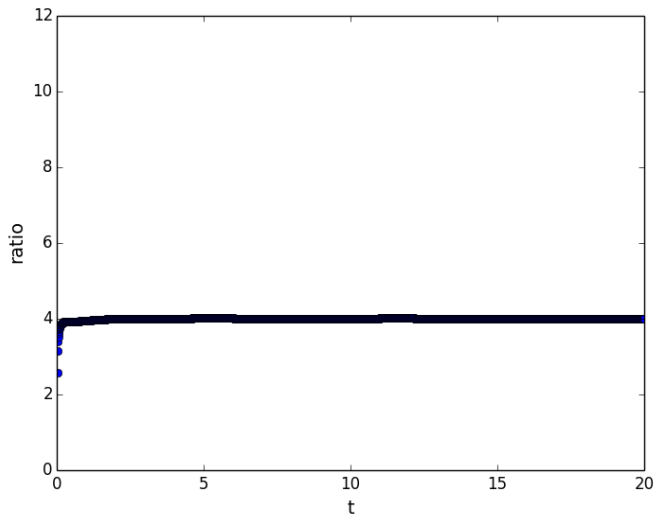
```
def twostep_solve(x0, h, tmin, tmax):
    n = int((tmax - tmin)/h) + 1
    ts = np.zeros(n)
    ts[0] = tmin
    xs = np.zeros(n)
    xs[0] = x0 # Use midpoint method for first step.
    xhalf = xs[0] + 0.5*h*dx_dt(xs[0], ts[0])
    xs[1] = xs[0] + h*dx_dt(xhalf, ts[0]+h/2.0)
    # Now apply the two-step method.
    for k in range(1,n-1):
        ts[k+1] = ts[k] + h
        xs[k+1] = xs[k] + (h/2.0)*(3*dx_dt(xs[k], ts[k])
                                - dx_dt(xs[k-1], ts[k-1]))
    return ts, xs
```

Plot



(as before)

Ratio test



(demonstrating the two-step method is 2nd order accurate)

Adams-Bashforth methods

- The two-step method is an example of a linear multi-step method
- **Explicit** linear multi-step methods go by the name of Adams-Bashforth methods:

$$y_{n+1} = y_n + h f_n \quad (\text{Euler method})$$

$$y_{n+1} = y_n + h \left(\frac{3}{2} f_n - \frac{1}{2} f_{n-1} \right) \quad (\text{2-step method})$$

$$y_{n+1} = y_n + h \left(\frac{23}{12} f_n - \frac{4}{3} f_{n-1} + \frac{5}{12} f_{n-2} \right)$$

$$y_{n+1} = y_n + h \left(\frac{55}{24} f_n - \frac{59}{24} f_{n-1} + \frac{37}{24} f_{n-2} - \frac{3}{8} f_{n-3} \right)$$

$$y_{n+1} = \dots$$

where

$$f_k = f(y_k, t_k)$$

Implicit Methods

Stiff sets of equations

- **Stiffness** occurs when there are two or more **very different scales** in t over which the dependent variables \mathbf{x} are changing.
- Consider this innocent-looking 2D linear system:

$$\begin{aligned}\dot{x} &= 998x + 1998y, & x(0) &= 1, \\ \dot{y} &= -999x - 1999y, & y(0) &= 0.\end{aligned}$$

- It has a simple exact solution,

$$x(t) = 2e^{-t} - e^{-1000t}, \quad y(t) = -e^{-t} + e^{-1000t}.$$

- But . . . **all** our explicit methods become **unstable** when applied to this system, if the step size is $h \gtrsim 1/1000$ (!).

Implicit methods

- Methods are only useful if they are **stable**, i.e. not subject to spurious divergences
- **Explicit** methods lead to instabilities for stiff equations. Stability issues get worse for **partial** differential equations, such as $\frac{\partial^2 u}{\partial t^2} - \frac{\partial^2 u}{\partial x^2} = 0$.
- **Implicit** methods have different (often better) stability properties, but are harder to implement
- **Example:** The **backwards Euler method**

$$x_{k+1} = x_k + h f(x_{k+1}, t_{k+1})$$

- Implicit, because we cannot write x_{k+1} as an explicit function of x_k (unless f is linear).

Stability: forward Euler method

- Consider a set of linear equations with constant coefficients,

$$\frac{d\mathbf{x}}{dt} = -\mathbf{C}\mathbf{x},$$

where \mathbf{C} is a **matrix** that is positive-definite
 \Rightarrow all the eigenvalues λ_i of \mathbf{C} are positive.

- The **forward** Euler method gives

$$\mathbf{x}_{k+1} = \mathbf{x}_k + h(-\mathbf{C}\mathbf{x}_k) = (\mathbf{I} - h\mathbf{C})\mathbf{x}_k$$

- \mathbf{C} positive-definite $\Rightarrow \mathbf{C} = \mathbf{A}^{-1}\mathbf{\Lambda}\mathbf{A}$ with $\mathbf{\Lambda}$ a diagonal matrix consisting of the positive eigenvalues λ_i .

$$\begin{aligned}\mathbf{x}_k &= (\mathbf{I} - h\mathbf{C})^k \mathbf{x}_0 \\ &= \mathbf{A}^{-1}(\mathbf{I} - h\mathbf{\Lambda})^k \mathbf{A} \mathbf{x}_0.\end{aligned}$$

- As $k \rightarrow \infty$, the solution **converges** iff $1 - h\lambda_{\max} > -1$,

$$\Rightarrow h < \frac{2}{\lambda_{\max}}.$$

Stability: backward Euler method

- **Implicit differencing** (**backward** method) gives

$$\begin{aligned}\mathbf{x}_{k+1} &= \mathbf{x}_k + h(-\mathbf{C}\mathbf{x}_{k+1}) \\ (\mathbf{I} + h\mathbf{C})\mathbf{x}_{k+1} &= \mathbf{x}_k \\ \Rightarrow \mathbf{x}_{k+1} &= (\mathbf{I} + h\mathbf{C})^{-1} \mathbf{x}_k\end{aligned}$$

- It follows that

$$\Rightarrow \mathbf{x}_k = \mathbf{A}^{-1} (1 + h\Lambda)^{-k} \mathbf{A} \mathbf{x}_0.$$

- This converges for **any** $h > 0$, since

$$(1 + h\lambda_i)^{-1} < 1$$

(\mathbf{C} is positive-definite $\Leftrightarrow \lambda_i > 0$).

- Backward differencing is **robust** for **stiff** problems

The backwards Euler method

$$x_{k+1} = x_k + hf(x_{k+1}, t_{k+1})$$

- **Q.** How do we actually find x_{k+1} ?
- **A1.** If ODE is linear, then find the matrix inverse.
- **A2.** If ODE is non-linear, apply an iterative method such as fixed-point iteration or the Newton-Raphson method at each step.
- **Fixed-point iteration:**

$$x_{k+1}^{[0]} = x_k, \quad x_{k+1}^{[i+1]} = x_k + hf(x_{k+1}^{[i]}, t_{k+1})$$

- Iterate until some convergence criterion is met:

$$\left| x_{k+1}^{[i+1]} - x_{k+1}^{[i]} \right| \leq \epsilon$$

The backwards Euler method: example

Example:

Use the backwards Euler method to solve the equations:

$$\begin{aligned}\dot{x} &= 998x + 1998y, & x(0) &= 1, \\ \dot{y} &= -999x - 1999y, & y(0) &= 0.\end{aligned}$$

on the domain $0 \leq t \leq 1$.

The backwards Euler method: solution

- The ODEs can be rewritten as

$$\frac{d\mathbf{x}}{dt} = \mathbf{B} \mathbf{x},$$

where

$$\mathbf{x} = \begin{pmatrix} x \\ y \end{pmatrix}, \quad \mathbf{B} = \begin{pmatrix} 998 & 1998 \\ -999 & -1999 \end{pmatrix}.$$

- The backwards Euler method:

$$\begin{aligned} \mathbf{x}_{k+1} &= \mathbf{x}_k + h \mathbf{B} \mathbf{x}_{k+1} \\ \Rightarrow (\mathbf{I} - h \mathbf{B}) \mathbf{x}_{k+1} &= \mathbf{x}_k \\ \Rightarrow \mathbf{x}_{k+1} &= (\mathbf{I} - h \mathbf{B})^{-1} \mathbf{x}_k. \end{aligned}$$

The backwards Euler method: solution

```
def backEuler(h=0.01, tmin=0.0, tmax=1.0):
    n = round((tmax - tmin)/h)
    ts = tmin + h*np.arange(0,n+1)
    xs = np.zeros(n+1); ys = np.zeros(n+1)
    xs[0] = 1; ys[0] = 0;
    #  $A = I - h B$ 
    Amat = np.matrix([[1-998*h, -1998*h], [999*h, 1+1999*h]])
    Ainv = np.linalg.inv(Amat) # inverse matrix
    for k in range(n):
        x, y = xs[k], ys[k]
        xs[k+1] = Ainv[0,0]*x + Ainv[0,1]*y
        ys[k+1] = Ainv[1,0]*x + Ainv[1,1]*y
    return ts, xs, ys

ts, xs, ys = backEuler()
plt.plot(ts, xs, 'r+', ts, ys, 'bs')
```


The backwards Euler method: solution

