Ordinary differential equations

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Today's outline

Overview

Ordinary differential equations

An equation containing a function of one independent variable and its derivatives, in contrast to a *partial differential equation*, which contains derivatives with respect to more independent variables.

Main question

How to solve

$$\frac{d\mathbf{y}}{dx} = f(\mathbf{y}(x), x) \quad \text{with} \quad \mathbf{y}(x=0) = \mathbf{y}_0$$

accurately and efficiently?

What is an ODE?

- Algebraic equation:

$$f(y(x), x) = 0 \qquad \text{e.g.} \ -\ln(K_{eq}) = (1-\zeta)$$

- First order ODE:

$$f\left(\frac{dy}{dx}(x), y(x), x\right) = 0 \quad \text{e.g.} \ \frac{dc}{dt} = -kc^n$$

- Second order ODE:

$$f\left(\frac{d^2y}{dx^2}(x), \frac{dy}{dx}(x), y(x), x\right) = 0 \quad \text{e.g.} \ \mathcal{D}\frac{d^2c}{dx^2} = -\frac{kc}{1+Kc}$$

About second order ODEs

Very often a second order ODE can be rewritten into a system of first order ODEs (whether it is handy depends on the boundary conditions!)

More general

Consider the second order ODE:

$$\frac{d^2y}{dx^2} + q(x)\frac{dy}{dx} = r(x)$$

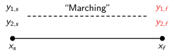
Now define and solve using z as a new variable:

$$\frac{dy}{dx} = z(x)$$
$$\frac{dz}{dx} = r(x) - q(x)z(x)$$

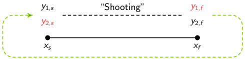
Importance of boundary conditions

The nature of boundary conditions determines the appropriate numerical method. Classification into 2 main categories:

- *Initial value problems (IVP)*
  We know the values of all y_i at some starting position x_s, and it is desired to find the values of y_i at some final point x_f.



- *Boundary value problems (BVP)*
  Boundary conditions are specified at more than one x. Typically, some of the BC are specified at x_s and the remainder at x_f.



Overview

Initial value problems:

- Explicit methods
  - First order: forward Euler
  - Second order: improved Euler (RK2)
  - Fourth order: Runge-Kutta 4 (RK4)
  - Step size control
- Implicit methods
  - First order: backward Euler
  - Second order: midpoint rule

Boundary value problems

- Shooting method

Today's outline

Euler's method

Consider the following single initial value problem:

$$\frac{dc}{dt} = f(c(t), t) \quad \text{with} \quad c(t=0) = c_0 \quad \text{(initial value problem)}$$

Easiest solution algorithm: Euler's method, derived here via Taylor series expansion:

$$c(t_0 + \Delta t) \approx c(t_0) + \left.\frac{dc}{dt}\right|_{t_0} \Delta t + \frac{1}{2} \left.\frac{d^2c}{dt^2}\right|_{t_0} (\Delta t)^2 + \mathcal{O}(\Delta t^3)$$

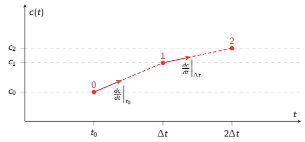
Neglect terms with higher order than two: $\left.\frac{dc}{dt}\right|_{t_0} = \frac{c(t_0+\Delta t)-c(t_0)}{\Delta t}$

Substitution:

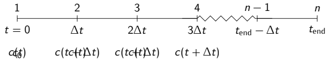
$$\frac{c(t_0 + \Delta t) - c(t_0)}{\Delta t} = f(c_0, t_0) \Rightarrow c(t_0 + \Delta t) = c(t_0) + \Delta t f(c_0, t_0)$$

Euler's method: graphical example

$$\frac{c(t_0 + \Delta t) - c(t_0)}{\Delta t} = f(c_0, t_0) \Rightarrow c(t_0 + \Delta t) = c(t_0) + \Delta t f(c_0, t_0)$$



Euler's method - solution method



Start with $t = t_0$, $c = c_0$, then calculate at discrete points in time: $c(t_1 = t_0 + \Delta t) = c(t_0) + \Delta t f(c_0, t_0)$.

> Pseudo-code Euler's method: $\frac{dy}{dx} = f(x, y)$ and $y(x_0) = y_0$.
>
> 1. Initialize variables, functions; set $h = \frac{x_1 - x_0}{N}$
> 2. Set $x = x_0$, $y = y_0$
> 3. While $x < x_{\text{end}}$ do
> $x_{i+1} = x_i + h; \quad y_{i+1} = y_i + hf(x_i, y_i)$

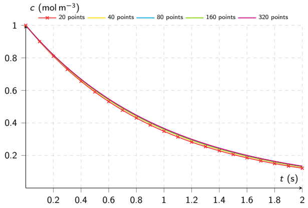
Euler's method - example

First order reaction in a batch reactor:

$$\frac{dc}{dt} = -kc \quad \text{with} \quad c(t=0) = 1\,\text{mol}\,\text{m}^{-3}, \quad k = 1\,\text{s}^{-1}, \quad t_{\text{end}} = 2\,\text{s}$$

Time [s]	Concentration [mol m^{-3}]
$t_0 = 0$	$c_0 = 1.00$
$t_1 = t_0 + \Delta t$	$c_1 = c_0 + \Delta t \cdot (-kc_0)$
$= 0 + 0.1 = 0.1$	$= 1 + 0.1 \cdot (-1 \cdot 1) = 0.9$
$t_2 = t_1 + \Delta t$	$c_2 = c_1 + \Delta t \cdot (-kc_1)$
$= 0.1 + 0.1 = 0.2$	$= 0.9 + 0.1 \cdot (-1 \cdot 0.9) = 0.81$
$t_3 = t_2 + \Delta t$	$c_3 = c_2 + \Delta t \cdot (-kc_2)$
$= 0.2 + 0.1 = 0.3$	$= 0.81 + 0.1 \cdot (-1 \cdot 0.81) = 0.729$
...	...
$t_{i+1} = t_i + \Delta t$	$c_{i+1} = c_i + \Delta t \cdot (-kc_i)$
...	...
$t_{20} = 2.0$	$c_{20} = c_{19} + \Delta t \cdot (-kc_{19}) = 0.1211577$

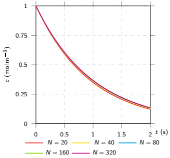
Euler's method - example



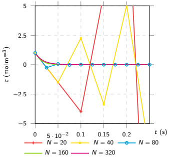
Problems with Euler's method

The question is: What step size, or how many steps to use?

1. *Accuracy* $\Rightarrow$ need information on numerical error!
2. *Stability* $\Rightarrow$ need information on stability limits!



Reaction rate: $k = 1\ \mathrm{s}^{-1}$



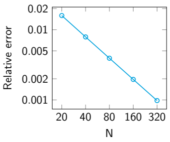
Reaction rate: $k = 50\ \mathrm{s}^{-1}$

Accuracy

Comparison with analytical solution for $k = 1\ \mathrm{s}^{-1}$:

$$c(t) = c_0 \exp(-kt) \Rightarrow \zeta = 1 - \exp(-kt) \Rightarrow \zeta_{\text{analytical}} = 0.864665$$

N	ζ	$\frac{\zeta_{\text{numerical}} - \zeta_{\text{analytical}}}{\zeta_{\text{analytical}}}$
20	0.878423	0.015912
40	0.871488	0.007891
80	0.868062	0.003929
160	0.866360	0.001961
320	0.865511	0.000979



Accuracy

For Euler's method: Error halves when the number of grid points is doubled, i.e. error is proportional to Δt: first order method.

Error estimate:

$$\left.\frac{dx}{dt}\right|_{t_0} = \frac{x(t_0+\Delta t) - x(t_0)}{\Delta t} + \frac{1}{2}\left.\frac{d^2x}{dt^2}\right|_{t_0}(\Delta t) + \mathcal{O}(\Delta t)^2$$

$$\frac{x(t_0+\Delta t) - x(t_0)}{\Delta t} = f(x_0, t_0) - \frac{1}{2}\left.\frac{d^2x}{dt^2}\right|_{t_0}(\Delta t) + \mathcal{O}(\Delta t)^2$$

Errors and convergence rate

L_2 norm (Euclidean norm)

$$\|\mathbf{v}\|_2 = \sqrt{v_1^2 + v_2^2 + \ldots + v_n^2} = \sqrt{\sum_{i=1}^{n} v_i^2}$$

L_∞ norm (maximum norm)

$$\|\mathbf{v}\|_\infty = \max\left(|v_1|, \ldots, |v_n|\right)$$

Absolute difference

$$\epsilon_{\text{abs}} = \left\|\mathbf{y}_{\text{numerical}} - \mathbf{y}_{\text{analytical}}\right\|_{2,\infty}$$

Relative difference

$$\epsilon_{\text{rel}} = \frac{\left\|\mathbf{y}_{\text{numerical}} - \mathbf{y}_{\text{analytical}}\right\|_{2,\infty}}{\left\|\mathbf{y}_{\text{analytical}}\right\|_{2,\infty}}$$

Errors and convergence rate

Convergence rate (or: order of convergence) r

$$\epsilon = \lim_{\Delta t \to 0} c(\Delta x)^r$$

- A first order method reduces the error by a factor 2 when increasing the number of steps by a factor 2
- A second order method reduces the error by a factor 4 when increasing the number of steps by a factor 2

What to do when there is no analytical solution available? Compare to calculations with different number of steps: $\epsilon_1 = c(\Delta x_1)^r$ and $\epsilon_2 = c(\Delta x_2)^r$ and solve for r:

$$\frac{\epsilon_2}{\epsilon_1} = \frac{c(\Delta x_2)^r}{c(\Delta x_1)^r} = \left(\frac{\Delta x_2}{\Delta x_1}\right)^r \Rightarrow \log\left(\frac{\epsilon_2}{\epsilon_1}\right) = \log\left(\frac{\Delta x_2}{\Delta x_1}\right)^r$$

$$\Rightarrow r = \frac{\log\left(\frac{\epsilon_2}{\epsilon_1}\right)}{\log\left(\frac{\Delta x_2}{\Delta x_1}\right)} = \frac{\log\left(\frac{\epsilon_2}{\epsilon_1}\right)}{\log\left(\frac{N_1}{N_2}\right)} \quad \text{in the limit of} \quad \Delta x \to 0 \quad \text{or} \quad N \to \infty$$

Example: Euler's method — order of convergence

N	ζ	$\frac{\zeta_{\text{numerical}} - \zeta_{\text{analytical}}}{\zeta_{\text{analytical}}}$	$r = \frac{\log\left(\frac{\epsilon_i}{\epsilon_{i-1}}\right)}{\log\left(\frac{N_{i-1}}{N_i}\right)}$
20	0.878423	0.015912	—
40	0.871488	0.007891	1.011832
80	0.868062	0.003929	1.005969
160	0.866360	0.001961	1.002996
320	0.865511	0.000979	1.001500

$\Rightarrow$ Euler's method is a first order method (as we already knew from the truncation error analysis)

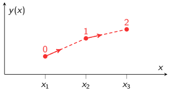
Wouldn't it be great to have a method that can give the answer using much less steps? $\Rightarrow$ Higher order methods

Runge-Kutta methods

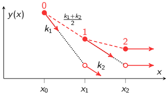
Propagate a solution by combining the information of several Euler-style steps (each involving one function evaluation) to match a Taylor series expansion up to some higher order.

Euler: $y_{i+1} = y_i + hf(x_i, y_i)$ with $h = \Delta x$, i.e.
slope $= k_1 = f(x_i, y_i)$.

Euler's method



RK2 method



Classical second order Runge-Kutta (RK2) method

This method is also called Heun's method, or improved Euler method:

1. Approximate the slope at x_i: $k_1 = f(x_i, y_i)$
2. Approximate the slope at x_{i+1}: $k_2 = f(x_{i+1}, y_{i+1})$ where we use Euler's method to approximate $y_{i+1} = y_i + hf(x_i, y_i) = y_i + hk_1$
3. Perform an Euler step with the average of the slopes: $y_{i+1} = y_i + h\frac{1}{2}(k_1 + k_2)$

In pseudocode:

```
x = x_0, y = y_0
while x < x_end do
    x_{i+1} = x_i + h
    k_1 = f(x_i, y_i)
    k_2 = f(x_i + h, y_i + h k_1)
    y_{i+1} = y_i + h (1/2)(k_1 + k_2)
end while
```


Runge-Kutta methods — derivation

$$\frac{dy}{dx} = f(x, y(x))$$

Using Taylor series expansion: $y_{i+1} = y_i + h\left.\frac{dy}{dx}\right|_i + \frac{h^2}{2}\left.\frac{d^2y}{dx^2}\right|_i + \mathcal{O}(h^3)$

$$\left.\frac{dy}{dx}\right|_i = f(x_i, y_i) \equiv f_i$$

$$\left.\frac{d^2y}{dx^2}\right|_i = \left.\frac{d}{dx}f(x, y(x))\right|_i = \left.\frac{\partial f}{\partial x}\right|_i + \left.\frac{\partial f}{\partial y}\right|_i \left.\frac{\partial y}{\partial x}\right|_i = \left.\frac{\partial f}{\partial x}\right|_i + \left.\frac{\partial f}{\partial y}\right|_i f_i \quad \text{(chain rule)}$$

Substitution gives:

$$y_{i+1} = y_i + hf_i + \frac{h^2}{2}\left(\left.\frac{\partial f}{\partial x}\right|_i + \left.\frac{\partial f}{\partial y}\right|_i f_i\right) + \mathcal{O}(h^3)$$

$$y_{i+1} = y_i + \frac{h}{2}f_i + \frac{h}{2}\left(f_i + h\left.\frac{\partial f}{\partial x}\right|_i + hf_i\left.\frac{\partial f}{\partial y}\right|_i\right) + \mathcal{O}(h^3)$$

Runge-Kutta methods — derivation

Note multivariate Taylor expansion:

$$f(x_i + h, y_i + k) = f_i + h\left.\frac{\partial f}{\partial x}\right|_i + k\left.\frac{\partial f}{\partial y}\right|_i + \mathcal{O}(h^2)$$

$$\Rightarrow \frac{h}{2}\left(f_i + h\left.\frac{\partial f}{\partial x}\right|_i + hf_i\left.\frac{\partial f}{\partial y}\right|_i\right) = \frac{h}{2}f(x_i + h, y_i + kf_i) + \mathcal{O}(h^3)$$

Concluding:

$$y_{i+1} = y_i + \frac{h}{2}f_i + \frac{h}{2}f(x_i + h, y_i + kf_i) + \mathcal{O}(h^3)$$

Rewriting:

$$k_1 = f(x_i, y_i)$$
$$k_2 = f(x_i + h, y_i + hk_1)$$
$$\Rightarrow y_{i+1} = y_i + \frac{h}{2}(k_1 + k_2)$$

Runge-Kutta methods — derivation

Generalization: $y_{i+1} = y_i + h(b_1k_1 + b_2k_2) + \mathcal{O}(h^3)$
with $k_1 = f_i$, $k_2 = f(x_i + c_2h, y_1 + a_{2,1}hk_1)$
(Note that classical RK2: $b_1 = b_2 = \frac{1}{2}$ and $c_2 = a_{2,1} = 1$.)

Bivariate Taylor expansion:

$$f(x_i + c_2h, y_i + a_{2,1}hk_1) = f_i + c_2h\left.\frac{\partial f}{\partial x}\right|_i + a_{2,1}hk_1\left.\frac{\partial f}{\partial y}\right|_i + \mathcal{O}(h^2)$$

$$\begin{aligned} y_{i+1} &= y_i + h(b_1k_1 + b_2k_2) + \mathcal{O}(h^3) \\ &= y_i + h\left[b_1f_i + b_2f(x_i + c_2h, y_1 + a_{2,1}hk_1)\right] + \mathcal{O}(h^3) \\ &= y_i + h\left[b_1f_i + b_2\left\{f_i + c_2h\left.\frac{\partial f}{\partial x}\right|_i + a_{2,1}hk_1\left.\frac{\partial f}{\partial y}\right|_i + \mathcal{O}(h^2)\right\}\right] + \mathcal{O}(h^3) \\ &= y_i + h(b_1 + b_2)f_i + h^2b_2\left(c_2\left.\frac{\partial f}{\partial x}\right|_i + a_{2,1}f_i\left.\frac{\partial f}{\partial y}\right|_i\right) + \mathcal{O}(h^3) \end{aligned}$$

Comparison with Taylor:

$$y_{i+1} = y_i + hf_i + \frac{h^2}{2}\left(\left.\frac{\partial f}{\partial x}\right|_i + \left.\frac{\partial f}{\partial y}\right|_i f_i\right) + \mathcal{O}(h^3)$$

Using $b_1 + b_2 = 1$, $c_2b_2 = \frac{1}{2}$, $a_{2,1}b_2 = \frac{1}{2}$ $\Rightarrow$ 3 eqns and 4 unknowns $\Rightarrow$ multiple possibilities!

Runge-Kutta methods — derivation

$$y_{i+1} = y_i + h(b_1 + b_2)f_i + h^2 b_2 \left(c_2 \left.\frac{\partial f}{\partial x}\right|_i + a_{2,1} f_i \left.\frac{\partial f}{\partial y}\right|_i \right) + \mathcal{O}(h^3)$$

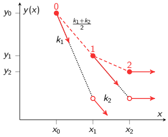
$$y_{i+1} = y_i + hf_i + \frac{h^2}{2} \left(\left.\frac{\partial f}{\partial x}\right|_i + \left.\frac{\partial f}{\partial y}\right|_i f_i \right) + \mathcal{O}(h^3)$$

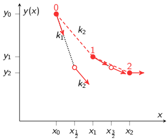
$\Rightarrow$ 3 eqns and 4 unknowns $\Rightarrow$ multiple possibilities!

1. Classical RK2:
   $b_1 = b_2 = \frac{1}{2}$ and $c_2 = a_{2,1} = 1$
2. Midpoint rule (modified Euler):
   $b_1 = 0,\ b_2 = 1,\ c_2 = a_{2,1} = \frac{1}{2}$

Second order Runge-Kutta methods

Classical RK2 method (= Heun's method, improved Euler method)	Explicit midpoint rule (modified Euler method)
$k_1 = f_i$	$k_1 = f_i$
$k_2 = f(x_i + h, y_i + hk_1)$	$k_2 = f(x_i + \frac{1}{2}h, y_i + \frac{1}{2}hk_1)$
$y_{i+1} = y_i + \frac{1}{2}h(k_1 + k_2)$	$y_{i+1} = y_i + hk_2$

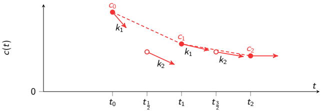




Second order Runge-Kutta method — Example

First order reaction in a batch reactor: $\frac{dc}{dt} = -kc$ with $c(t = 0) = 1\ \mathrm{mol\,m^{-3}}$, $k = 1\ \mathrm{s^{-1}}$, $t_{\mathrm{end}} = 2$ s.

Time [s]	C [$\mathrm{mol\,m^{-3}}$]	$k_1 = hf(x_i, y_i)$	$k_2 = hf(x_i + \frac{1}{2}h, y_n + \frac{1}{2}k_1)$
0	1.00	$0.1 \cdot (-1 \cdot 1) = -0.1$	$0.1 \cdot (-1 \cdot (1 - 0.5 \cdot 0.1)) = -0.095$
0.1	$1 - 0.095 = 0.905$	$0.1 \cdot (-1 \cdot 0.0905) = -0.0905$	$0.1 \cdot (-1 \cdot (0.905 - 0.5 \cdot 0.0905)) = 0.085975$
...	...	...	...
2	0.1358225	−0.0135822	−0.0129031



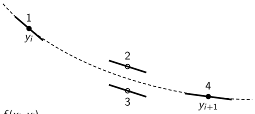
RK2 method — order of convergence

N	ζ	$\frac{\zeta_{\mathrm{numerical}} - \zeta_{\mathrm{analytical}}}{\zeta_{\mathrm{analytical}}}$	$r = \frac{\log\left(\frac{\epsilon_i}{\epsilon_{i-1}}\right)}{\log\left(\frac{N_{i-1}}{N_i}\right)}$
20	0.864178	5.634×10^{-4}	—
40	0.864548	1.355×10^{-4}	2.056
80	0.864636	3.323×10^{-5}	2.028
160	0.864658	8.229×10^{-6}	2.014
320	0.864663	2.048×10^{-6}	2.007

$\Rightarrow$ RK2 is a second order method. Doubling the number of cells reduces the error by a factor 4!

Can we do even better?

RK4 method (classical fourth order Runge-Kutta method)



$$k_1 = f(x_i, y_i)$$
$$k_2 = f(x_i + \frac{1}{2}h, y_i + \frac{1}{2}hk_1)$$
$$k_3 = f(x_i + \frac{1}{2}h, y_i + \frac{1}{2}hk_2)$$
$$k_4 = f(x_i + h, y_i + hk_3)$$
$$y_{i+1} = y_i + h\left(\frac{1}{6}k_1 + \frac{1}{3}(k_2 + k_3) + \frac{1}{6}k_4\right)$$

RK4 method — order of convergence

N	ζ	$\frac{\zeta_{\text{numerical}} - \zeta_{\text{analytical}}}{\zeta_{\text{analytical}}}$	$r = \frac{\log\left(\frac{\epsilon_i}{\epsilon_{i-1}}\right)}{\log\left(\frac{N_{i-1}}{N_i}\right)}$
20	0.864664472	2.836×10^{-7}	—
40	0.864664702	1.700×10^{-8}	4.060
80	0.864664716	1.040×10^{-9}	4.030
160	0.864664717	6.435×10^{-11}	4.015
320	0.864664717	4.001×10^{-12}	4.007

⇒ RK4 is a fourth order method: Doubling the number of cells reduces the error by a factor 16!

Can we do even better?

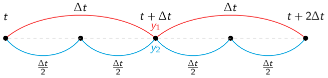
Adaptive step size control

The step size (be it either position, time or both (PDEs)) cannot be decreased indefinitely to favour a higher accuracy, since each additional grid point causes additional computation time. It may be wise to adapt the step size according to the computation requirements.

Globally two different approaches can be used:

1. Step doubling: compare solutions when taking one full step or two consecutive halve steps
2. Embedded methods: Compare solutions when using two approximations of different order

Adaptive step size control: step doubling



- RK4 with one large step of h: $y_{i+1} = y_1 + ch^5 + \mathcal{O}(h^6)$
- RK4 with two steps of $\frac{1}{2}h$: $y_{i+1} = y_2 + 2c(\frac{1}{2}h)^5 + \mathcal{O}(h^6)$

Adaptive step size control: step doubling

- Estimation of truncation error by comparing y_1 and y_2: $\Delta = y_2 - y_1$
- If Δ too large, reduce step size for accuracy
- If Δ too small, increase step size for efficiency.
- Ignoring higher order terms and solving for c: $\Delta = \frac{15}{16}ch^5 \Rightarrow ch^5 = \frac{16}{15}\Delta \Rightarrow y_{i+1} = y_2 + \frac{\Delta}{15} + \mathcal{O}(h^6)$ (local Richardson extrapolation)

Note that when we specify a tolerance *tol*, we can estimate the maximum allowable step size as: $h_{\text{new}} = \alpha h_{\text{old}} \left|\frac{\text{tol}}{\Delta}\right|^{\frac{1}{5}}$ with α a safety factor (typically $\alpha = 0.9$).

Adaptive step size control: embedded methods

Use a special fourth and a fifth order Runge Kutta method to approximate y_{i+1}

- The fourth order method is special because we want to use the same positions for the evaluation for computational efficiency.
- RK45 is there preferred method (minimum number of function evaluations) (this is built in Matlab as `ode45`).

Today's outline

Problems with Euler's method: instability

Consider the ODE:

$$\frac{dy}{dx} = f(x, y(x)) \qquad \text{with} \qquad y(x=0) = y_0$$

First order approximation of derivative: $\frac{dy}{dx} = \frac{y_{i+1} - y_i}{\Delta x}$.

Where to evaluate the function f?

1. Evaluation at x_i: Explicit Euler method (forward Euler)
2. Evaluation at x_{i+1}: Implicit Euler method (backward Euler)

Problems with Euler's method: instability – forward Euler

Explicit Euler method (forward Euler):

- Use values at x_i: $\frac{y_{i+1}-y_i}{\Delta x} = f(x_i, y_i) \Rightarrow y_{i+1} = y_i + hf(x_i, y_i)$.
- This is an explicit equation for y_{i+1} in terms of y_i.
- It can give instabilities with large function values.

Consider the first order batch reactor:

$$\frac{dc}{dt} = -kc \Rightarrow c_{i+1} = c_i - kc_i\Delta t \Rightarrow \frac{c_{i+1}}{c_i} = 1 - k\Delta t$$

It follows that unphysical results are obtained for $k\Delta t \geq 1$!!

Stability requirement

$k\Delta t < 1$
(but probably accuracy requirements are more stringent here!)

Problems with Euler's method: instability – backward Euler

Implicit Euler method (backward Euler):

- Use values at x_{i+1}: $\frac{y_{i+1}-y_i}{\Delta x} = f(x_{i+1}, y_{i+1}) \Rightarrow y_{i+1} = y_i + hf(x_{i+1}, y_{i+1})$.
- This is an implicit equation for y_{i+1}, because it also depends on terms of y_{i+1}.

Consider the first order batch reactor:

$$\frac{dc}{dt} = -kc \Rightarrow c_{i+1} = c_i - kc_{i+1}\Delta t \Rightarrow \frac{c_{i+1}}{c_i} = \frac{1}{1 + k\Delta t}$$

This equation does never give unphysical results!
The implicit Euler method is *unconditionally stable*
(but maybe not very accurate or efficient).

Semi-implicit Euler method

Usually f is a non-linear function of y, so that linearization is required (recall Newton's method).

$$\frac{dy}{dx} = f(y) \Rightarrow y_{i+1} = y_i + hf(y_{i+1}) \quad \text{using} \quad f(y_{i+1}) = f(y_i) + \left.\frac{df}{dy}\right|_i (y_{i+1} - y_i) + \dots$$

$$\Rightarrow y_{i+1} = y_i + h\left[f(y_i) + \left.\frac{df}{dy}\right|_i (y_{i+1} - y_i)\right]$$

$$\Rightarrow \left(1 - h\left.\frac{df}{dy}\right|_i\right) y_{i+1} = \left(1 - h\left.\frac{df}{dy}\right|_i\right) y_i + hf(y_i)$$

$$\boxed{\Rightarrow \quad y_{i+1} = y_i + h\left(1 - h\left.\frac{df}{dy}\right|_i\right)^{-1} f(y_i)}$$

For the case that $f(x, y(x))$ we could add the variable x as an additional variable $y_{n+1} = x$. Or add one fully implicit Euler step (which avoids the computation of $\frac{\partial f}{\partial x}$):

$$y_{i+1} = y_i + hf(x_{i+1}, y_{i+1}) \Rightarrow y_{i+1} = y_i + h\left(1 - h\left.\frac{df}{dy}\right|_i\right)^{-1} f(x_{i+1}, y_i)$$

Semi-implicit Euler method - example

Second order reaction in a batch reactor:
$\frac{dc}{dt} = -kc^2$ with $c_0 = 1$ mol m^{-3}, $k = 1$ m^3 mol^{-1} s^{-1}, $t_{\text{end}} = 2$ s
Analytical solution: $c(t) = \frac{c_0}{1+kc_0 t}$

Define $f = -kc^2$, then $\frac{df}{dc} = -2kc \Rightarrow c_{i+1} = c_i - \frac{hkc_i^2}{1+2hkc_i}$.

N	ζ	$\frac{\zeta_{\text{numerical}} - \zeta_{\text{analytical}}}{\zeta_{\text{analytical}}}$	$r = \frac{\log\left(\frac{\epsilon_i}{\epsilon_{i-1}}\right)}{\log\left(\frac{N_{i-1}}{N_i}\right)}$
20	0.654066262	1.89×10^{-2}	—
40	0.660462687	9.31×10^{-3}	1.02220
80	0.663589561	4.62×10^{-3}	1.01162
160	0.665134433	2.30×10^{-3}	1.00594
320	0.665902142	1.15×10^{-3}	1.00300

Second order implicit method: Implicit midpoint method

Implicit midpoint rule (second order)	Explicit midpoint rule (modified Euler method)
$y_{i+1} = y_i + hf\left(x_i + \frac{1}{2}h, \frac{1}{2}(y_i + y_{i+1})\right)$	$y_{i+1} = y_i + hf(x_i + \frac{1}{2}h, y_i + \frac{1}{2}hk_1)$

in case $f(y)$ then:

$$f\left(\frac{1}{2}(y_i + y_{i+1})\right) = f_i + \left.\frac{df}{dy}\right|_i \left(\frac{1}{2}(y_i + y_{i+1}) - y_i\right) = f_i + \frac{1}{2}\left.\frac{df}{dy}\right|_i (y_{i+1} - y_i)$$

Implicit midpoint rule reduces to:

$$y_{i+1} = y_i + hf_i + \frac{h}{2}\left.\frac{df}{dy}\right|_i (y_{i+1} - y_i)$$

$$\Rightarrow \left(1 - \frac{h}{2}\left.\frac{df}{dy}\right|_i\right) y_{i+1} = \left(1 - \frac{h}{2}\left.\frac{df}{dy}\right|_i\right) y_i + hf_i$$

$$\boxed{\Rightarrow \quad y_{i+1} = y_i + h\left(1 - \frac{h}{2}\left.\frac{df}{dy}\right|_i\right)^{-1} f_i}$$

Implicit midpoint method — example

Second order reaction in a batch reactor:
$\frac{dc}{dt} = -kc^2$ with $c_0 = 1\ \mathrm{mol\,m^{-3}}$, $k = 1\ \mathrm{m^3\,mol^{-1}\,s^{-1}}$, $t_{\mathrm{end}} = 2$ s
(Analytical solution: $c(t) = \frac{c_0}{1+kc_0t}$).

Define $f = -kc^2$, then $\frac{df}{dc} = -2kc$.

Substitution:

$$c_{i+1} = c_i + h\left(1 - \frac{h}{2}\cdot(-2kc_i)\right)^{-1} \cdot (-kc_i^2)$$

$$= c_i - \frac{hkc_i^2}{1 + hkc_i} = \frac{c_i + hkc_i^2 - hkc_i^2}{1 + hkc_i} \Rightarrow c_{i+1} = \frac{c_i}{1 + hkc_i}$$

You will find that this method is exact for all step sizes h because of the quadratic source term!

Implicit midpoint method — example

Second order reaction in a batch reactor:
$\frac{dc}{dt} = -kc^2$ with $c_0 = 1\ \mathrm{mol\,m^{-3}}$, $k = 1\ \mathrm{m^3\,mol^{-1}\,s^{-1}}$, $t_{\mathrm{end}} = 2$ s
Analytical solution: $c(t) = \frac{c_0}{1+kc_0t}$

$$c_{i+1} = \frac{c_i}{1 + hkc_i}$$

N	ζ	$\frac{\zeta_{\mathrm{numerical}} - \zeta_{\mathrm{analytical}}}{\zeta_{\mathrm{analytical}}}$	$r = \frac{\log\left(\frac{\epsilon_i}{\epsilon_{i-1}}\right)}{\log\left(\frac{N_{i-1}}{N_i}\right)}$
20	0.6666666667	1.665×10^{-16}	—
40	0.6666666667	0	—
80	0.6666666667	0	—
160	0.6666666667	0	—
320	0.6666666667	0	—

Implicit midpoint method — example

Third order reaction in a batch reactor
Analytical solution: $c(t) = \frac{c_0}{\sqrt{1+2kc_0^2t}}$

$$c_{i+1} = c_i - \frac{hkc_i^3}{1 + \frac{3}{2}hkc_i^2}$$

N	ζ	$\frac{\zeta_{\mathrm{numerical}} - \zeta_{\mathrm{analytical}}}{\zeta_{\mathrm{analytical}}}$	$r = \frac{\log\left(\frac{\epsilon_i}{\epsilon_{i-1}}\right)}{\log\left(\frac{N_{i-1}}{N_i}\right)}$
20	0.5526916174	1.71×10^{-4}	—
40	0.5527633731	4.17×10^{-5}	2.041
80	0.5527807304	1.03×10^{-5}	2.021
160	0.5527849965	2.55×10^{-6}	2.011
320	0.5527860538	6.34×10^{-7}	2.005

Today's outline

Systems of ODEs

A system of ODEs is specified using vector notation:

$$\frac{d\mathbf{y}}{dx} = \mathbf{f}(x, \mathbf{y}(x))$$

for

$$\frac{dy_1}{dx} = f_1(x, y_1(x), y_2(x)) \quad \text{or} \quad f_1(x, y_1, y_2)$$

$$\frac{dy_2}{dx} = f_2(x, y_1(x), y_2(x)) \quad \text{or} \quad f_2(x, y_1, y_2)$$

The solution techniques discussed before can also be used to solve systems of equations.

Systems of ODEs: Explicit methods

Forward Euler method

$$\mathbf{y}_{i+1} = \mathbf{y}_i + h\mathbf{f}(x_i, \mathbf{y}_i)$$

Improved Euler method (classical RK2)

$$\mathbf{y}_{i+1} = \mathbf{y}_i + \frac{h}{2}(\mathbf{k}_1 + \mathbf{k}_2) \quad \text{using} \quad \begin{aligned} \mathbf{k}_1 &= \mathbf{f}(x_i, \mathbf{y}_i) \\ \mathbf{k}_2 &= \mathbf{f}(x_i + h, \mathbf{y}_i + h\mathbf{k}_1) \end{aligned}$$

Modified Euler method (midpoint rule)

$$\mathbf{y}_{i+1} = \mathbf{y}_i + h\mathbf{k}_2 \quad \text{using} \quad \begin{aligned} \mathbf{k}_1 &= \mathbf{f}(x_i, \mathbf{y}_i) \\ \mathbf{k}_2 &= \mathbf{f}(x_i + \frac{h}{2}, \mathbf{y}_i + \frac{h}{2}\mathbf{k}_1) \end{aligned}$$

Systems of ODEs: Explicit methods

Classical fourth order Runge-Kutta method (RK4)

$$\mathbf{y}_{i+1} = \mathbf{y}_i + h\left(\frac{\mathbf{k}_1}{6} + \frac{1}{3}(\mathbf{k}_2 + \mathbf{k}_3) + \frac{\mathbf{k}_4}{6}\right)$$

using

$$\begin{aligned} \mathbf{k}_1 &= \mathbf{f}(x_i, \mathbf{y}_i) \\ \mathbf{k}_2 &= \mathbf{f}(x_i + \frac{h}{2}, \mathbf{y}_i + \frac{h}{2}\mathbf{k}_1) \\ \mathbf{k}_3 &= \mathbf{f}(x_i + \frac{h}{2}, \mathbf{y}_i + \frac{h}{2}\mathbf{k}_2) \\ \mathbf{k}_4 &= \mathbf{f}(x_i + h, \mathbf{y}_i + h\mathbf{k}_3) \end{aligned}$$

Systems of ODEs: Implicit methods

Backward Euler method

$$\mathbf{y}_{i+1} = \mathbf{y}_i + h\left(1 - h\left.\frac{d\mathbf{f}}{d\mathbf{y}}\right|_i\right)^{-1}\mathbf{f}(\mathbf{y}_i)$$

Implicit midpoint method

$$\mathbf{y}_{i+1} = \mathbf{y}_i + h\left(1 - \frac{h}{2}\left.\frac{d\mathbf{f}}{d\mathbf{y}}\right|_i\right)^{-1}\mathbf{f}(\mathbf{y}_i)$$

Stiff systems of ODEs

A system of ODEs can be stiff and require a different solution method. For example:

$$\frac{dc_1}{dt} = 998c_1 + 1998c_2 \qquad \frac{dc_2}{dt} = -999c_1 - 1999c_2$$

with boundary conditions $c_1(t=0) = 1$ and $c_2(t=0) = 0$.
The analytical solution is:

$$c_1 = 2e^{-t} - e^{-1000t} \qquad c_2 = -e^{-t} + e^{-1000t}$$

For the explicit method we require $\Delta t < 10^{-3}$ despite the fact that the term is completely negligible, but essential to keep stability.

The "disease" of stiff equations: we need to follow the solution on the shortest length scale to maintain stability of the integration, although accuracy requirements would allow a much larger time step.

Demonstration with example

Forward Euler (explicit)

$$\frac{dc_{1,i+1} - c_{1,i}}{dt} = 998c_{1,i} + 1998c_{2,i}$$
$$\frac{dc_{2,i+1} - c_{2,i}}{dt} = -999c_{1,i} - 1999c_{2,i}$$

$$\Rightarrow \begin{aligned} c_{1,i+1} &= (1 + 998\Delta t)\, c_{1,i} + 1998\Delta t c_{2,i} \\ c_{2,i+1} &= -999\Delta t c_{1,i} + (1 - 1999\Delta t)\, c_{2,i} \end{aligned}$$

Demonstration with example

Backward Euler (implicit)

$$\frac{dc_{1,i+1} - c_{1,i+1}}{dt} = 998c_{1,i+1} + 1998c_{2,i+1}$$
$$\frac{dc_{2,i+1} - c_{2,i+1}}{dt} = -999c_{1,i+1} - 1999c_{2,i+1}$$

$$\Rightarrow \begin{aligned} (1 - 998\Delta t)\, c_{1,i+1} - 1998\Delta t c_{2,i} &= c_{1,i} \\ 999\Delta t c_{1,i+1} + (1 + 999\Delta t)\, c_{2,i+1} &= c_{2,i} \end{aligned}$$

$$A\mathbf{c}_{i+1} = \mathbf{c}_i \text{ with } A = \begin{pmatrix} 1 - 998\Delta t & -1998\Delta t \\ 999\Delta t & 1 + 1999\Delta t \end{pmatrix} \text{ and } \mathbf{b} = \begin{pmatrix} c_{1,i} \\ c_{2,i} \end{pmatrix}$$

Demonstration with example

Backward Euler (implicit) $A\mathbf{c}_{i+1} = \mathbf{c}_i$ with

$$A = \begin{pmatrix} 1 - 998\Delta t & -1998\Delta t \\ 999\Delta t & 1 + 1999\Delta t \end{pmatrix} \quad \text{and} \quad \mathbf{b} = \begin{pmatrix} c_{1,i} \\ c_{2,i} \end{pmatrix}$$

Cramers rule:

$$c_{1,i+1} = \frac{\begin{vmatrix} c_{1,i} & -1998\Delta t \\ c_{2,i} & 1+1999\Delta t \end{vmatrix}}{\det(A)} = \frac{(1+1999\Delta t)c_{1,i} + 1998\Delta t c_{2,i}}{(1-998\Delta t)(1+1999\Delta t) + 1998 \cdot 999\Delta t^2}$$

$$c_{2,i+1} = \frac{\begin{vmatrix} 1-998\Delta t & c_{1,i} \\ 999\Delta t & c_{2,i} \end{vmatrix}}{\det(A)} = \frac{-999\Delta t c_{1,i} + (1-998\Delta t)c_{2,i}}{(1-998\Delta t)(1+1999\Delta t) + 1998 \cdot 999\Delta t^2}$$

Forward Euler: $\Delta t \leq 0.001$ for stability
Backward Euler: always stable, even for $\Delta t > 100$ (but then not very accurate!)

Demonstration with example

Cure for stiff problems: use implicit methods! To find out whether your system is stiff: check whether one of the eigenvalues have an imaginary part

Solving systems of ODEs in Matlab

Matlab provides convenient procedures to solve (systems of) ODEs automatically.

The procedure is as follows:

1. Create a function that specifies the ODEs. Specifically, this function returns the $\frac{dy}{dx}$ vector.
2. Initialise solver variables and settings (e.g. step size, initial conditions, tolerance), in a separate script
3. Call the ODE solver function, using a *function handle* to the ODE function described in point 1.
   - The ODE solver will return the vector for the independent variable, and a solution vector (matrix for systems of ODEs).

Solving systems of ODEs in Matlab: example

We solve the system: $\frac{dx_1}{dt} = -x_1 - x_2, \quad \frac{dx_2}{dt} = x_1 - 2x_2$

Create an ODE function

```
function [dxdt] = myODEFunction(t,x)
dxdt(1) = -x(1) - x(2);
dxdt(2) =  x(1) - 2*x(2);
dxdt=dxdt'; % Transpose to column vector
return
```

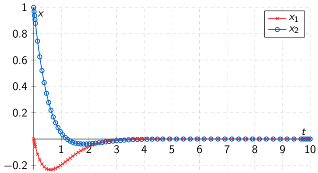
Create a solution script

```
x_init = [0 1];          % Initial conditions
tspan = [0 10];          % Time span
options = odeset('RelTol',1e-4,'AbsTol',[1e-4 1e-4]);
[t,x] = ode45(@myODEfunction,tspan,x_init,options);
```

Solving systems of ODEs in Matlab: example

Plot the solution:

```
plot(t,x(:,1),'r-x',t,x(:,2),'b-o')
```



Solving systems of ODEs in Matlab: example

A few notes on working with `ode45` and other solvers. If we want to give additional arguments (e.g. `a`, `b` and `c`) to our ODE function, we can list them in the function line:

```
function [dxdt] = myODE(t,x,a,b,c)
```

The additional arguments can now be set in the solver script by *adding them after the options*:

```
[t,x] = ode45(@myODE,tspan,x_0,options,a,b,c);
```

- Of course, in the solver script, the variables do not need to be called `a`, `b` and `c`:

  ```
  [t,x] = ode45(@myODE,tspan,x_0,options,k1,phi,V);
  ```

- These variables may be of any type (vectors, matrix, struct). Especially a struct is useful to carry many values in 1 variable.

Solving systems of ODEs in Matlab: example

You may have noticed that the step size in t varied. This is because we have given the begin and end times of our time span:

```
tspan = [0 10];
```

You can also solve at specific steps, by supplying all steps explicitly, e.g.:

```
tspan = linspace(0,10,101);
```

This example provides 101 explicit time steps between 0 and 10 seconds.

Note that you may affect the efficiency and accuracy of the solver algorithm by doing this!

Today's outline

Other methods

Other explicit methods:

- Burlisch-Stoer method (Richardson extrapolation + modified midpoint method)

Other implicit methods:

- Rosenbrock methods (higher order implicit Runge-Kutta methods)
- Predictor-corrector methods

Summary

- Several solution methods and their derivation were discussed:
  - Explicit solution methods: Euler, Improved Euler, Midpoint method, RK45
  - Implicit methods: Implicit Euler and Implicit midpoint method
  - A few examples of their spreadsheet implementation were shown
- We have paid attention to accuracy and instability, rate of convergence and step size
- Systems of ODEs can be solved by the same algorithms. Stiff problems should be treated with care.
- An example of solving ODEs with Matlab was demonstrated.