

Numerical Methods - Initial Value Problems for ODEs

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Definition (Ordinary Differential Equation (ODE))

An **ordinary differential equation** is an equation that involves one or more derivatives of an univariate function.

- The solutions for an ODE are differ from each other by a constant.

Definition (Initial Value Problem)

A **solution** to the **initial value problem (IVP)**

$$\frac{dy}{dt} = f(t, y), \quad \text{with } y(t_0) = y_0$$

on an interval $[t_0, b]$ is a differential function $y = \phi(t)$ such that $\phi(t_0) = y_0$ and $\phi'(t) = f(t, \phi(t))$ for all $t \in [t_0, b]$

- The solution of IVP is unique.

Well-posed Problem

Theorem (Well-posed problem)

Suppose that $D = \{(t, y) | a \leq t \leq b \text{ and } -\infty < y < \infty\}$ and that $f(t, y)$ is continuous on D . If f satisfies a **Lipschitz** condition on D , then the initial value problem

$$y(t) = f(t, y), \quad a \leq t \leq b, \quad y(a) = y_0,$$

has a unique solution.

Definition (Lipschitz condition)

A function $f(t, y)$ is said to satisfy a **Lipschitz condition** in the variable y on a set $D \subset \mathbb{R}^2$ if there exist a constant $L > 0$ such that

$$|f(t, y_1) - f(t, y_2)| < L|y_1 - y_2|,$$

whenever (t, y_1) and (t, y_2) are in D . The constant L is called a **Lipschitz constant** for f .

Theorem

Suppose $f(t, y)$ is defined on a convex set $D \subset \mathbb{R}^2$. If there exists a constant $L > 0$, such that

$$\left| \frac{\partial f}{\partial y}(t, y) \right| \leq L, \quad \text{for all } (t, y) \in D,$$

then f satisfies a Lipschitz condition on D in the variable y with Lipschitz constant L .

Example

Show that there is a unique solution to the initial value problem

$$y'(t) = 1 + t \sin(yt), \quad 0 \leq t \leq 2, y(0) = 0.$$

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Euler's Method

- Euler's method is the simplest numerical method for solving well-posed IVP:

$$\frac{dy}{dt} = f(t, y), \quad a \leq t \leq b, \quad y(a) = \alpha.$$

- First partition / discretise the interval into $N + 1$ equally spaced mesh points: $a = t_0 < t_1 < t_2 < \dots < t_N = b, t_i = t_0 + ih, i \leq N$ and $h = (b - a)/N$.
- Consider the two adjacent mesh points $[t_i, t_{i+1}]$, from the Taylor's series,

$$y(t_{i+1}) = y(t_i + h) = y(t_i) + hy'(t_i) + \frac{h^2}{2}y''(\xi), \quad \xi \in [t_i, t_{i+1}].$$

- Write y_i as the approximation to the actual solution $y(t_i)$ and substitute $y'(t_i) = f(t_i, y(t_i))$, we have the Euler's method iteration rule:

$$y_{i+1} = y_i + hf(t_i, y_i).$$

- The initial starting point of the Euler's method is given by the initial condition $y_0 = y(a) = \alpha$.



Euler's Method

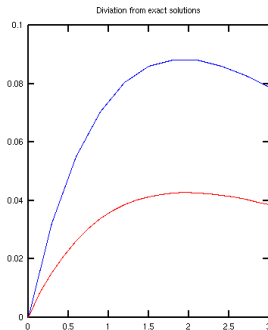
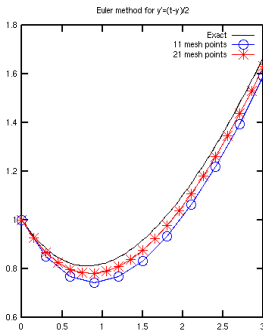
- The **local discretisation error** $\epsilon_i = |y(t_i + h) - y(t_i) - hf(t_i, y(t_i))|$ is $O(h^2)$.
- However, the **global discretisation error** $E_i = |y(t_i) - y_i|$ is $O(h)$.

Example

Solve the IVP $y' = (t - y)/2$ with $y(0) = 1$ over $0 \leq t \leq 3$ with Euler method.

ANSWER: MATLAB code : nm06_euler_driver.m

(Analytic solution is $3e^{-t/2} - 2 + t$)



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Taylor Series Method of Order n

Theorem

Suppose $f(t, y)$ is continuous and satisfies a Lipschitz condition in variable y , and consider the IVP

$$y' = f(t, y), \quad a \leq t \leq b, \quad y(a) = \alpha.$$

For the mesh points $t_{i+1} = t_i + h$, the Taylor series method approximate the solution $y(t_{i+1})$ with the formula:

$$y_{i+1} = y_0 + d_1 h + \frac{d_2}{2!} h^2 + \dots + \frac{d_n}{n!} h^n, \quad \text{for } i = 0, 1, 2, \dots, N,$$

where $d_i = y^{(i)}(t)$ evaluated at t_i .

- Note that the global error for the Taylor series method is $O(h^n)$.

Example

Solve the IVP $y' = (t - y)/2$ with $y(0) = 1$ over $0 \leq t \leq 3$ with Taylor series method of order 2.

ANSWER: MATLAB code : nm06_taylor2.m

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Runge-Kutta Method of Order 2

- The methods tried to imitate the Taylor series method without requiring analytic differentiation of the ODE.
- In Euler method: $y_{i+1} = y_i + hf(t_i, y_i)$, the slope $f(t, y)$ is evaluated at the start of the interval t_i , ie a forward difference scheme.
- Intuitively, for better accuracy, we could evaluate $f(t, y)$ at the midpoint by using the Euler method first to obtain $y_{i+h/2}$, then evaluate $f(t_{i+h/2}, y_{i+h/2})$ to get a symmetrical scheme.
- Because of the symmetry, the local error is reduced by an order (in the step size) and the method is now a second-order method called Runge-Kutta Method of order 2 (RK2) or the midpoint method.
- The RK2 algorithm:

$$\begin{aligned}k_1 &= hf(t_i, y_i) \\y_{i+1/2} &= y_i + k_1/2 \\k_2 &= hf(t_{i+1/2}, y_{i+1/2}) \\y_{i+1} &= y_i + k_2\end{aligned}$$



Runge-Kutta Method

- In general the Runge-Kutta method could be written in the form of

$$\begin{aligned}y_{i+1} &= y_i + w_1k_1 + w_2k_2 + w_3k_3 + w_4k_4 \dots \\k_1 &= hf(t_i, y_i) \\k_2 &= hf(t_i + a_1h, y_i + b_1k_1) \\k_3 &= hf(t_i + a_2h, y_i + b_2k_1 + b_3k_2) \\k_4 &= hf(t_i + a_3h, y_i + b_4k_2 + b_5k_2 + b_6k_3) \\&\vdots = \vdots,\end{aligned}$$

where the constants a_i and b_i are determined by comparing with the corresponding order of Taylor series method.

- For example, the 2nd order Taylor series method gives:

$$y(t_{i+1}) = y(t_i) + hf(t_i, y(t_i)) + \frac{h^2}{2} f'(t_i, y(t_i)) + \frac{h^3}{3!} f''(\xi_i, y(\xi_i)),$$

and we wish to find the corresponding w_1, w_2, a_1 and b_1 for k_1, k_2 and $y_{i+1} = y_i + w_1k_1 + w_2k_2$.



Runge-Kutta Method

- From the 2nd order Taylor series method gives:

$$\begin{aligned}y_{i+1} &= y_i + hf(t_i, y_i) + \frac{h^2}{2}f'(t_i, y_i) + O(h^3) \\ &= y_i + hf(t_i, y_i) + \frac{h^2}{2}[f_t(t_i, y_i) + f(t_i, y_i)f_y(t_i, y_i)] + O(h^3).\end{aligned}$$

- Also, we know $k_1 = hf(t_i, y_i)$ and expand k_2 in term of Taylor series

$$\begin{aligned}k_2 &= hf(t_i + a_1h, y_i + b_1k_1) \\ &= h[f(t_i, y_i) + a_1hf_t(t_i, y_i) + b_1k_1f_y(t_i, y_i)] + O(h^3) \\ &= h[f(t_i, y_i) + a_1hf_t(t_i, y_i) + b_1hf(t_i, y_i)f_y(t_i, y_i)] + O(h^3)\end{aligned}$$

- Substituting k_1 and k_2 into $y_{i+1} = y_i + w_1k_1 + w_2k_2$ get

$$y_{i+1} = y_i + h(w_1 + w_2)f(t_i, y_i) + w_2h^2[a_1f_t(t_i, y_i) + b_1f(t_i, y_i)f_y(t_i, y_i)]$$

- Comparing the coefficients we get:

$$w_1 + w_2 = 1, \quad a_1w_2 = \frac{1}{2}, \quad b_1w_2 = \frac{1}{2}.$$



Runge-Kutta Method

- Note that there are 3 equations for the four unknown w_1, w_2, a_1 and b_1 , therefore we have one degree of freedom in solving the coefficients.
- Choose $w_1 = 0, w_2 = 1, a_1 = b_1 = \frac{1}{2}$ we have the mid-point method:

$$k_1 = hf(t_i, y_i)$$

$$k_2 = hf(t_i + h/2, y_i + k_1/2)$$

$$y_{i+1} = y_i + k_2$$

- It is possible to choose an optimal value for a_1 such that the error $O(h^3)$ is minimized. The value chosen is $a_1 = \frac{2}{3}$ and thus $w_1 = \frac{1}{4}, w_2 = \frac{3}{4}, b_1 = \frac{2}{3}$:

$$k_1 = hf(t_i, y_i)$$

$$k_2 = hf(t_i + \frac{2}{3}h, y_i + \frac{2}{3}k_1)$$

$$y_{i+1} = y_i + \frac{1}{4}k_1 + \frac{3}{4}k_2$$

Runge-Kutta Method of Order 4

- Similarly, the Runge-Kutta Method of Order 4 (RK4) algorithm:

$$k_1 = hf(t_i, y_i)$$

$$k_2 = hf\left(t_i + \frac{h}{2}, y_i + \frac{k_1}{2}\right)$$

$$k_3 = hf\left(t_i + \frac{h}{2}, y_i + \frac{k_2}{2}\right)$$

$$k_4 = hf(t_i + h, y_i + k_3)$$

$$y_{i+1} = y_i + \frac{1}{6}(k_1 + 2k_2 + 2k_3 + k_4)$$

- Note that RK2 has global truncation error of $O(h^2)$, while RK4 has a global truncation error of $O(h^4)$.
- RK4 is a common, optimal and reliable numerical integrator, especially if it is used together with an **adaptive step-size control**.

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Adaptive Runge-Kutta-Fehlberg (RKF45) Method

- The RKF45 algorithm:

$$k_1 = hf(t_i, y_i)$$

$$k_2 = hf\left(t_i + \frac{1}{4}h, y_i + \frac{1}{4}k_1\right)$$

$$k_3 = hf\left(t_i + \frac{3}{8}h, y_i + \frac{3}{32}k_1 + \frac{9}{32}k_2\right)$$

$$k_4 = hf\left(t_i + \frac{12}{13}h, y_i + \frac{1932}{2197}k_1 - \frac{7200}{2197}k_2 + \frac{7296}{2197}k_3\right)$$

$$k_5 = hf\left(t_i + h, y_i + \frac{439}{216}k_1 - 8k_2 + \frac{3680}{513}k_3 - \frac{845}{4104}k_4\right)$$

$$k_6 = hf\left(t_i + \frac{1}{2}h, y_i - \frac{8}{27}k_1 + 2k_2 - \frac{3544}{2565}k_3 + \frac{1859}{4104}k_4 - \frac{11}{40}k_5\right)$$

$$\tilde{y}_{i+1} = y_i + \frac{25}{216}k_1 + \frac{1408}{2565}k_3 + \frac{2197}{4104}k_4 - \frac{1}{5}k_5$$

$$y_{i+1} = y_i + \frac{16}{135}k_1 + \frac{6656}{12825}k_3 + \frac{28561}{56430}k_4 - \frac{9}{50}k_5 + \frac{2}{55}k_6$$



Adaptive Runge-Kutta-Fehlberg (RKF45) Method

- The RKF45 algorithm gives two estimates for $y(t_i)$, ie:
 - 4th order estimate : \tilde{y}_{i+1} ; and
 - 5th order estimate : y_{i+1} .
- The difference between the two estimates gives the local truncation error. ie.
 $\epsilon = |\tilde{y}_{i+1} - y_{i+1}| \sim O(h^5)$.
- A simple adaptive scheme:
 - Choose an acceptable error ϵ_0 .
 - Suppose we did a calculation with step size h_c and error ϵ_c , then a new step-size that will produce error ϵ_0 is $h_0 = h_c(\epsilon_0/\epsilon_c)^{1/5}$. Hence,
 - If $\epsilon_c \leq \epsilon_0$, accept the calculation with current step-size h_c , but change the next step size to h_0 .
 - If $\epsilon_c > \epsilon_0$, reject y_{i+1} and repeat the calculation with step-size h_0 .
- The Matlab command `ode45` implement a variant of RK45 with adaptive step control.

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Multistep Methods

- **Multistep** methods make use of the information from several previous mesh points to compute the value at the new mesh point.
- Consider $y'(t) = f(t, y)$, integrate over $[t_i, t_{i+1}]$ and we have:

$$y(t_{i+1}) = y(t_i) + \int_{t_i}^{t_{i+1}} f(t, y(t)) dt.$$

- As $y(t_{i+1})$ is unknown, we cannot evaluate the integral explicitly. Instead, we rely on interpolating the integrand with a polynomial.
- For example, let say we know the value of $(t_i, y(t_i))$ and we are approximating $f(t, y)$ with interpolating polynomial of degree 0 (ie a horizontal line), then $f(t, y) = f(t_i, y(t_i)) + (t - t_i)f'(\tau_i, y(\tau_i))$ where $\tau_i \in [t_i, t_{i+1}]$.
- Integrating over $[t_i, t_{i+1}]$ and let $h = t_{i+1} - t_i$, gives

$$y(t_{i+1}) = y(t_i) + hf(t_i, y(t_i)) + \frac{h^2}{2}f'(\xi_i, y(\xi_i)),$$

- Which is the **one-step** Euler method

$$y_{i+1} = y_i + hf(t_i, y_i).$$

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Adams-Bashforth Explicit Methods

- Continue along the idea, now we use interpolating polynomial through the two points $(t_i, y(t_i))$ and $(t_{i-1}, y(t_{i-1}))$ for $f(t, y)$:

$$\begin{aligned}y(t_{i+1}) &= y(t_i) + \int_{t_i}^{t_{i+1}} \left\{ f(t_i, y(t_i)) + (t - t_i) \frac{f(t_i, y(t_i)) - f(t_{i-1}, y(t_{i-1}))}{h} \right. \\ &\quad \left. + \frac{(t - t_i)(t - t_{i-1})}{2!} f''(\tau_i, y(\tau_i)) \right\} dt \\ &= y(t_i) + \frac{h}{2} \{3f(t_i, y(t_i)) - f(t_{i-1}, y(t_{i-1}))\} + \frac{5}{12} h^3 f'''(\xi_i, y(\xi_i))\end{aligned}$$

- Two-step Adams-Bashforth method:

$$y_{i+1} = y_i + \frac{h}{2} [3f(t_i, y_i) - f(t_{i-1}, y_{i-1})] + \frac{5}{12} h^3 f'''(\xi_i, y(\xi_i))$$

Adams-Bashforth Explicit Methods

- One-step Adams-Bashforth:

$$y_{i+1} = y_i + hf(t_i, y_i) + \frac{h^2}{2} f'(\xi_i, y(\xi_i))$$

- Two-step Adams-Bashforth:

$$y_{i+1} = y_i + \frac{h}{2} [3f(t_i, y_i) - f(t_{i-1}, y_{i-1})] + \frac{5}{12} h^3 f''(\xi_i, y(\xi_i))$$

- Three-step Adams-Bashforth:

$$y_{i+1} = y_i + \frac{h}{12} [23f(t_i, y_i) - 16f(t_{i-1}, y_{i-1}) + 5f(t_{i-2}, y_{i-2})] + \frac{3}{8} h^4 f'''(\xi_i, y(\xi_i))$$

- Four-step Adams-Bashforth:

$$y_{i+1} = y_i + \frac{h}{24} [55f(t_i, y_i) - 59f(t_{i-1}, y_{i-1}) + 37f(t_{i-2}, y_{i-2}) - 9f(t_{i-3}, y_{i-3})] + \frac{251}{720} h^5 f^{(4)}(\xi_i, y(\xi_i))$$

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Adams-Moulton Implicit Methods

- Now we also include $(t_{i+1}, y(t_{i+1}))$ as additional interpolation node, then we have the Implicit formula.
- For example, use $(t_{i+1}, y(t_{i+1}))$ and $(t_i, y(t_i))$

$$\begin{aligned}y(t_{i+1}) &= y(t_i) + \int_{t_i}^{t_{i+1}} \left\{ f(t_i, y(t_i)) \frac{t - t_{i+1}}{t_i - t_{i+1}} + f(t_{i+1}, y(t_{i+1})) \frac{t - t_i}{t_{i+1} - t_i} \right. \\ &\quad \left. + \frac{(t - t_i)(t - t_{i+1})}{2!} f''(\tau_i, y(\tau_i)) \right\} dt \\ &= y(t_i) + \frac{h}{2} \{f(t_i, y(t_i)) - f(t_{i+1}, y(t_{i+1}))\} - \frac{1}{12} h^3 f'''(\xi_i, y(\xi_i))\end{aligned}$$

- One-step Adams-Moulton implicit method:

$$y_{i+1} = y_i + \frac{h}{2} [f(t_i, y_i) - f(t_{i+1}, y_{i+1})] - \frac{1}{12} h^3 f'''(\xi_i, y(\xi_i))$$

Adams-Moulton Implicit Methods

- One-step Adams-Moulton:

$$y_{i+1} = y_i + \frac{h}{2} [f(t_{i+1}, y_{i+1}) + f(t_i, y_i)] - \frac{1}{12} h^3 f''(\xi_i, y(\xi_i))$$

- Two-step Adams-Moulton:

$$y_{i+1} = y_i + \frac{h}{12} [5f(t_{i+1}, y_{i+1}) + 8f(t_i, y_i) - f(t_{i-1}, y_{i-1})] - \frac{1}{24} h^4 f'''(\xi_i, y(\xi_i))$$

- Three-step Adams-Moulton:

$$y_{i+1} = y_i + \frac{h}{24} [9f(t_{i+1}, y_{i+1}) + 19f(t_i, y_i) - 5f(t_{i-1}, y_{i-1}) \\ + f(t_{i-2}, y_{i-2})] - \frac{19}{720} h^5 f^{(4)}(\xi_i, y(\xi_i))$$

- Four-step Adams-Moulton:

$$y_{i+1} = y_i + \frac{h}{720} [251f(t_{i+1}, y_{i+1}) + 646f(t_i, y_i) - 264f(t_{i-1}, y_{i-1}) \\ + 106f(t_{i-2}, y_{i-2}) - 19f(t_{i-3}, y_{i-3})] - \frac{3}{160} h^6 f^{(5)}(\xi_i, y(\xi_i))$$



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Predictor-Corrector Methods

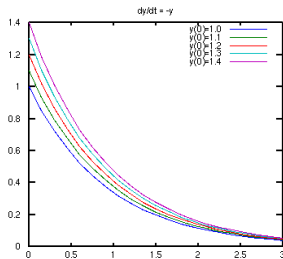
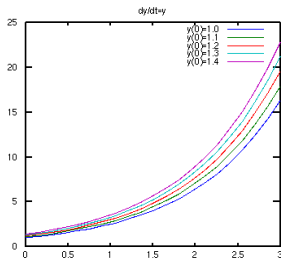
- One weakness the Adams-Moulton implicit formula is it not always possible to algebraically re-arrange the formula to make $y(t_{i+1})$ explicit.
- However, combine with Adams-Bashforth explicit formula to form a predictor-corrector pairs.
- The simplest example will be the so-called leapfrog algorithm:
 - Predictor (1-step AB) : $p_{i+1} = y_i + hf(t_i, y_i)$
 - Corrector (1-step AM) : $y_{i+1} = y_i + \frac{h}{2}[f(t_{i+1}, p_{i+1}) + f(t_i, y_i)]$
- Another commonly used method will be the 4th Order Adams-Bashforth-Moulton methods:
 - Predictor : $p_{i+1} = y_i + \frac{h}{24}[55f_i - 59f_{i-1} + 37f_{i-2} - 9f_{i-3}]$
 - Corrector : $y_{i+1} = y_i + \frac{h}{2}[9f_{i+1} + 19f_i - 5f_{i-1} + f_{i-2}]$, where $f_{i+1} = f(t_{i+1}, p_{i+1})$

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Convergence

- Stability of ODE scheme depends on the nature of IVP.
- Eg, Euler scheme diverges for $y' = \lambda y, y(0) = \alpha$, but converges for $y' = -\lambda y$.
- For convergent solution curves, the local errors at each step are reduced over t , and accumulative global error may be less than the sum of the local errors.



Theorem

For an initial value problem: $y' = f(t, y), \quad y(0) = \alpha$

- if $f_y > \delta$ for some positive δ , then the solution curve diverges.
- if $f_y < -\delta$, then the solution curve converges.

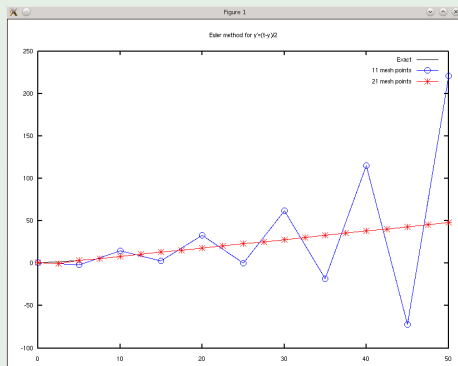
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Stability

- Even if the IVP is convergent, it could still be unstable due to large h .

Example

Consider IVP $y' = (t - y)/2, y(0) = 1$. We know that $f_y(t) = -1/2$ for all $t \in [0, 50]$, thus the Euler method should be convergent. However, the numerical solution $y(t)$ by using Euler method for $h = 2.5$ is convergent but diverge for $h = 5$.



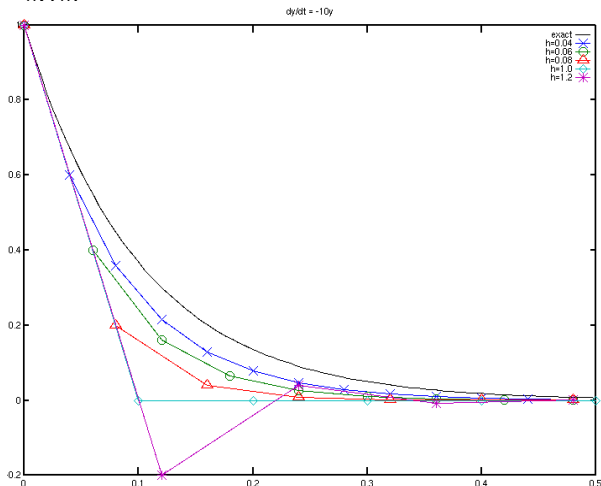
- Consider a linear (or linearized) ODE: $y' = -\lambda y$, and discretized, say by Euler method (of course could be other method).
- Then, we have $y_{i+1} = y_i - h\lambda y_i$.
- The **absolute stability function** is defined as

$$Q(h\lambda) = \left\| \frac{y_{i+1}}{y_i} \right\|.$$

- In the case for Euler method, we have $Q(h\lambda) = (1 - h\lambda)$.
- If the amplification factor $Q(h\lambda) < 1$, then we are guaranteed that the sequence $\{y_i\}$ will not grow without bound, and hence **stable**.
- Assuming that λ is real, then for the Euler method to be stable we need $-1 < 1 - \lambda h < 1$ or $0 < \lambda h < 2$, ie $h < 2/\lambda$ in order for the Euler method to be stable.

Stability

- The following figure shows an IVP ($y' = -10y, y(0) = 1$) solved by Euler method with different values of step size h .
- Note that the numerical solution curves become unstable when $h \geq 2/c = 0.10$.



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Higher Order ODE & System of ODEs

- Higher order ODE can be solved numerically by turning into a system of first order ODEs.
- Consider IVP of order n :

$$y^{(n)} = f(t, y, y', \dots, y^{(n-1)}), \quad y(0) = \alpha_0, y'(0) = \alpha_1, \dots, y^{(n-1)}(0) = \alpha_{n-1}.$$

- Define new variables x_1, x_2, \dots, x_n : $x_1 = y, x_2 = y', \dots, x_n = y^{(n-1)}$.
- Now the IVP is equivalent to

$$\begin{aligned}x_1' &= x_2, & x_1(0) &= \alpha_0 \\x_2' &= x_3, & x_2(0) &= \alpha_1 \\&\vdots \\x_n' &= f(t, x_1, x_2, \dots, x_n), & x_n(0) &= \alpha_{n-1}\end{aligned}$$

- In vector notation: $\mathbf{X}' = \mathbf{F}(t, \mathbf{X}), \quad \mathbf{X}(0) = \mathbf{A}$, where $\mathbf{X} = [x_1, x_2, \dots, x_n]^T$, $\mathbf{F} = [x_2, x_3, \dots, f]^T$ and $\mathbf{A} = [\alpha_0, \alpha_1, \dots, \alpha_{n-1}]$.



System of First Order ODEs

- Solve the system of first order ODEs numerically are very much like solving a single first order ODEs.
- For example, consider to solve $\mathbf{X}'(t) = \mathbf{F}(t, \mathbf{X})$, $\mathbf{X}(0) = \mathbf{A}$ with a Runge-Kutta method of order 4, we have
 - Discretise the time interval $[a, b]$ into n subdivisions with $h = (b - a)/n$.
 - RK4 iteration formula: $\mathbf{X}_{i+1} = \mathbf{X}_i + \frac{h}{6}[\mathbf{k}_1 + 2\mathbf{k}_2 + 2\mathbf{k}_3 + \mathbf{k}_4]$, where

$$\mathbf{k}_1 = h\mathbf{F}(t, \mathbf{X})$$

$$\mathbf{k}_2 = h\mathbf{F}\left(t + \frac{1}{2}h, \mathbf{X} + \frac{1}{2}\mathbf{k}_1\right)$$

$$\mathbf{k}_3 = h\mathbf{F}\left(t + \frac{1}{2}h, \mathbf{X} + \frac{1}{2}\mathbf{k}_2\right)$$

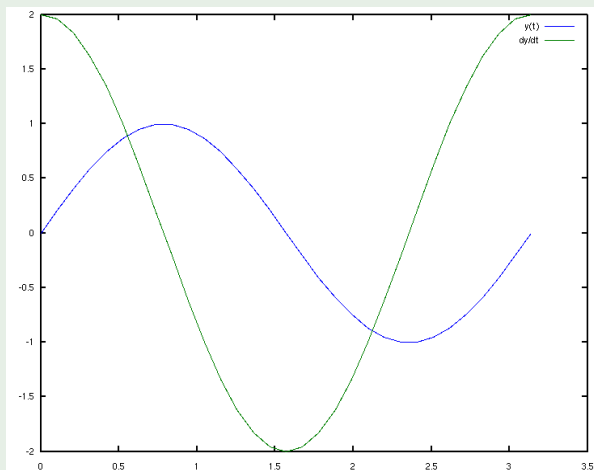
$$\mathbf{k}_4 = h\mathbf{F}(t + h, \mathbf{X} + \mathbf{k}_3)$$

System of ODEs (Example)

Example

Solve $y'' = -4y$, $y(0) = 0, y'(0) = 2$.

ANSWER: MATLAB code : nm06_system.m



System of ODEs (Example)

Example (Lorenz system)

Solve the Lorenz system:

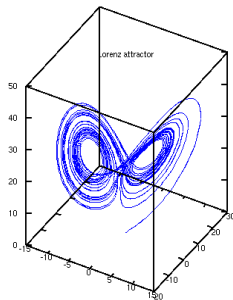
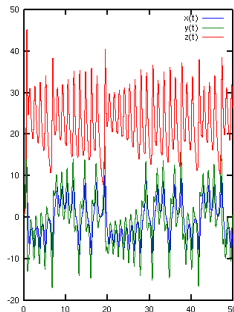
$$x' = \sigma(y - x)$$

$$y' = x(\rho - z) - y$$

$$z' = xy - \beta z$$

with the values $\sigma = 3$, $\rho = 26.5$ and $\beta = 1$.

ANSWER: MATLAB code : `nm06_lorenz.m`



THE END