Ordinary Differential Equations (ODE)

$$\frac{df(t)}{dt} = -kf(t)$$

- unkown is a function
- derivative appears in Eq.

ODE: function only depends on one variable

PDE: two or more variables (e.g. t, x, y, z)

order: highest derivative

$$\frac{d^2f}{dt^2} + \frac{df}{dt} = \exp(f)$$

- second order

Initial Value Problem (IVP)

ODE + initial condition specifies $f(t)$ in the domain

Analytical solutions to ODEs

$$\frac{df(t)}{dt} = -k\,f(t)$$

seek a function $f(t)$ that satisfies the equation

(1) brute force

$f(t) = \exp(-kt)$ guess

test solution

$$\frac{df}{dt} = -k\exp(-kt) = -k\,f(t) \quad \checkmark$$

2 Integration by Separation of variables

$$\frac{df}{dt} = -kf \qquad \text{initial value } f(0) = a$$

$$\frac{1}{f}\,df = -k\,dt$$

$$\int_a^x \frac{1}{f}\,df = \int_0^{\tilde{\tau}} -k\,dt \qquad f(t=0) = a$$

$$\Big[\ln f\Big]_a^x = \Big[-kt\Big]_0^{\tilde{\tau}}$$

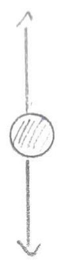
$$\ln(x) - \ln(a) = -k\tilde{\tau} - 0$$

$$\frac{x}{a} = \exp(-k\tilde{\tau})$$

$$x = a\exp(-k\tilde{\tau})$$

initial value

Second example : time to reach terminal velocity



mechanical mobility

$F = B v$ velocity

$v(t=0) = 0$

$F = m g$

mass gravity

$$\sum F = m \frac{dv}{dt} = mg - Bv$$

Newton's Law

$$\frac{dv}{dt} + \frac{B}{m} v = g$$

$\tau = \frac{m}{B}$ "relaxation time"

$$\frac{dv}{dt} + \frac{1}{\tau} v = g$$

$$\int_0^v \frac{1}{g - \frac{1}{\tau} v'} dv' = \int_0^t dt$$

$$\frac{d(\ln(a+bx))}{dx} = \frac{b}{a+bx}$$

$$\left[\tau \ln \left(g - \frac{1}{\tau} v'\right) \right]_0^v = t \quad \Rightarrow \quad v = g\tau\left(1 - \exp\left(t/\tau\right)\right)$$

Similar to RC circuit

3. Solution using the Laplace Transform

$$f' + 3f = \exp(2t) \qquad f(0) = 1$$

$$\mathcal{L}(f' + 3f) = \mathcal{L}\exp(2t)$$

$$sF - 1 + 3F = \frac{1}{s-2}$$

$$F = \frac{1}{(s-2)(s+3)} + \frac{1}{s+3}$$

$$\mathcal{L}^{-1}(F) = \mathcal{L}^{-1}\frac{1}{(s-2)(s+3)} + \mathcal{L}^{-1}\frac{1}{s+3}$$

$$f = \frac{1}{5}(\exp(2t) - \exp(-3t) + \exp(-3t)$$

$$f(t) = \frac{1}{5}\exp(2t) + \frac{4}{5}\exp(-3t)$$

$$\mathcal{L}(af + bg) = aF(s) + bG(s)$$

$$\mathcal{L}f' = F(s) - f(0)$$

$$\mathcal{L}f'' = s^2F(s) - sf(0) - f'(0)$$

$$
\begin{aligned}
1 &= \mathcal{L}^{-1}\left\{\tfrac{1}{s}\right\} \\
t^n &= \mathcal{L}^{-1}\left\{\tfrac{n!}{s^{n+1}}\right\}, \quad n = 1, 2, 3, \cdots \\
e^{at} &= \mathcal{L}^{-1}\left\{\tfrac{1}{s-a}\right\} \\
\sin kt &= \mathcal{L}^{-1}\left\{\tfrac{k}{s^2+k^2}\right\} \\
\cos kt &= \mathcal{L}^{-1}\left\{\tfrac{s}{s^2+k^2}\right\} \\
\sinh kt &= \mathcal{L}^{-1}\left\{\tfrac{k}{s^2-k^2}\right\} \\
\cosh kt &= \mathcal{L}^{-1}\left\{\tfrac{s}{s^2-k^2}\right\}
\end{aligned}
$$

what is $\mathcal{L}^{-1} \dfrac{1}{(s-2)(s+3)}$?

$$\frac{1}{(s-2)(s-3)} = \frac{A}{(s-2)} + \frac{B}{(s+3)}$$ "partial fraction" decomposition

assume $s=2$ and multiply by $(s-2)$

$\Rightarrow A = \frac{1}{5}$

assume $s=-3$ and multiply by $(s+3)$

$\Rightarrow B = -\frac{1}{5}$

$$= \frac{1}{5} \frac{1}{s-2} - \frac{1}{5} \underbrace{\frac{1}{s+3}}$$ $\mathcal{L}^{-1}$

$$\frac{1}{5} \exp(2t) - \frac{1}{5} \exp(-3t)$$

Higher Order ODEs

$$a f''' + b f'' + c f' + d = g(t)$$

homogeneous : $g(t) = 0$

inhomogeneous : $g(t) \neq 0$

IVP : $f(0), f'(0), f''(0), \ldots$

typical solution $\quad f = A \cdot \exp(\lambda x) \quad \rightarrow \lambda$ complex $\Rightarrow$ sinusoids

$$f' = A\lambda \exp(\lambda x)$$

$$f'' = A\lambda^2 \exp(2\lambda x)$$

Solution approach for homogeneous case

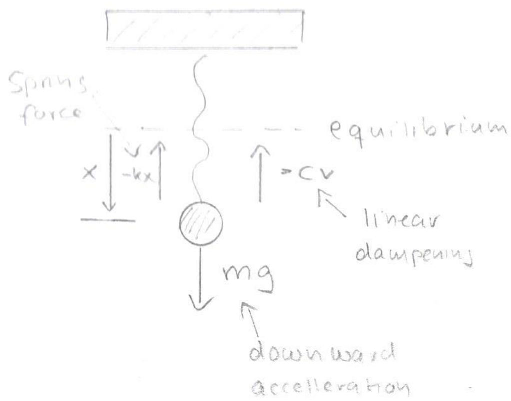
characteristic equation

$$a\lambda^3 + b\lambda^2 + c\lambda + d = 0$$

$\rightarrow$ find roots

$$f(t) = c_1 \exp(\lambda_1 x) + c_2 \exp(\lambda_2 x) + \ldots$$

example : harmonic oscillator



x : position

v : velocity

Newton's Second law

$$m x''(t) + c x'(t) + k x = 0$$

=> evolution back to equilibrium

$$m x''(t) + c x'(t) + k x = f(t)$$

impuls / external forcing

Solve

$m x''(t) + c x'(t) + k x(t) = 0$ IVP: $x(0) = -1$ (initial position) $x'(0) = 0$ (initial velocity)

charact Eq.

$m \lambda^2 + c\lambda + k = 0$ Constants: $m = 10$ $c = 1$ $k = 1$

$\Rightarrow \lambda_1 = \frac{1}{2} + \frac{1}{2}\sqrt{39}\, i$ $\lambda_2 = \frac{1}{2} - \frac{1}{2}\sqrt{39}\, i$

$x(t) = c_1 \exp(\lambda_1 t) + c_2 \exp(\lambda_2 t)$

$x(t) = c_1 \exp((a+bi)t) + c_2 \exp((a-bi)t)$

$x(t) = \exp(at)\left[d_1 \cos(bt) + d_2 \sin(bt)\right]$

$x'(t) = a\exp(at)\left[d_1 \cos(bt) + d_2 \sin(bt)\right] + \exp(at)\left[-d_1 b \sin(bt) + d_2 b \cos(bt)\right]$

$a = \frac{1}{2}$ $b = \frac{\sqrt{39}}{2}$

use $x(0) = -1$ and $x'(0) = 0$ to find

$d_1 = -\frac{1}{\sqrt{39}}$ $d_2 = -1$

Systems of ODEs

"A differential equation of order n can be written as a system of ODEs of order 1"

example

$$m x'' + c x' + k x = 0$$

$$q_1 = x \quad \Rightarrow \quad q_1' = x'$$

$$q_2 = x' \quad \Rightarrow \quad q_2' = x''$$

$$q_1' = q_2$$

$$q_2' = \frac{1}{m} \left(-c q_2 - k q_1 \right)$$

$$\begin{bmatrix} q_1' \\ q_2' \end{bmatrix} = \begin{bmatrix} 0 & 1 \\ -k/m & -c/m \end{bmatrix} \begin{bmatrix} q_1 \\ q_2 \end{bmatrix}$$

$\boxed{\vec{q}\,' = A \vec{q}}$ matrix form of homogeneous eq.

Solution to systems => Eigenvalues

A nonzero vector v of dimension N is an eigenvector of a square matrix A if it satisfies

$$Av = \lambda v$$

eigenvalue

eigenvector

example

$$A = \begin{bmatrix} -2 & 2 \\ -2 & 1 \end{bmatrix} \qquad \lambda_1 = -3 \quad v_1 = \begin{bmatrix} -0.894 \\ -0.447 \end{bmatrix}$$

$$\lambda_2 = 2 \quad v_2 = \begin{bmatrix} 0.447 \\ -0.894 \end{bmatrix}$$

- N eigenvalue / eigenvector pairs
- eigenvectors are the principle axes of the system
  - ↳ can use to orthogonalize system

How to find λ?

(1) solve $\det(A - \lambda I)\lambda_i = 0$.

(2) use Eigendecomposition from Linear Algebra package

$\lambda, v = \text{eigen}(A)$

similarity with SVD:

$$A^{-1} = Q \Lambda^{-1} Q^{-1}$$

Λ: diagonal matrix with λ_i as entries

Q: matrix of eigenvectors

$$\Lambda^{-1}_{ii} = \frac{1}{\lambda_i}$$

zero λ_i - matrix is rank deficient
- not invertible

near zero λ_i = ill posed inversion

Solving

$$\vec{q}' = A\vec{q}$$

(1) obtain λ_i throug eigen(A) or $\det(A - \lambda I) = 0$

(2) obtain eigenvectors $\vec{v}_i$

$$\vec{q}(t) = \left[\vec{v}_1 \exp(\lambda_1 t) \quad \vec{v}_2 \exp(\lambda_2 t) \ldots \quad \vec{v}_n \exp(\lambda_n t)\right] \begin{bmatrix} c_1 \\ \vdots \\ c_n \end{bmatrix}$$ ← constants

real λ : exp

complex λ : sinusoidals

use initial cond. to get c_i

Valid for homogeneous linear systems

Example: Reaction chains

$$\frac{dq_1}{dt} = -aq_1$$

$$\frac{dq_2}{dt} = aq_1 - bq_2 \qquad A = \begin{bmatrix} -a & 0 & 0 \\ a & -b & 0 \\ 0 & b & 0 \end{bmatrix}$$

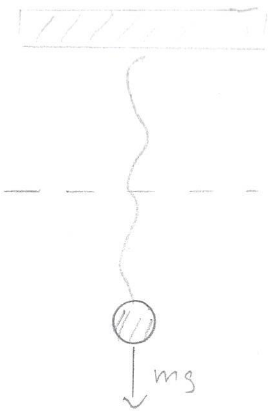
$$\frac{dq_3}{dt} = bq_2$$

$a = 1$ $\quad b = \frac{1}{2}$ $\quad q_1(0) = 2$ $\quad q_2(0) = 0$ $\quad q_3(0) = 0$

Homework: find analytical solution and compare to notes

State Space Modeling

inputs (actors) $\longrightarrow$ $\boxed{\text{states}}$ $\longrightarrow$ outputs (observables)



forced oscillator

$$m x''(t) + c x'(t) + kx = f(t)$$

inputs $f(t)$

outputs (observables)

- position
- velocity
- acceleration

$\rightarrow$ derived properties

- force $m x''$
- frequency of oscillation

States:

variables needed to predict future of system

$$m x'' + c x' + k x = f$$

$$q_1 = x$$

$$q_2 = x'$$

$$q_1' = q_2$$

$$q_2' = \frac{1}{m}(f - c q_2 - k q_1)$$

$$\begin{bmatrix} q_1' \\ q_2' \end{bmatrix} = \begin{bmatrix} 0 & 1 \\ -k/m & -c/m \end{bmatrix} \begin{bmatrix} q_1 \\ q_2 \end{bmatrix} + \begin{bmatrix} 0 \\ 1/m \end{bmatrix} f$$

$$\boxed{q' = Aq + Bf}$$

Input Eq.

q: state variables

outputs:

$$\left.\begin{aligned} y_1 &= m x'' \quad &&(\text{force}) \\ y_2 &= x' \quad &&(\text{velocity}) \\ y_3 &= x \quad &&(\text{position}) \end{aligned}\right\}\ \text{not limited by number}$$

$y_1 = f - c q_2 - k q_1$

$y_2 = q_2$

$y_3 = q_1$

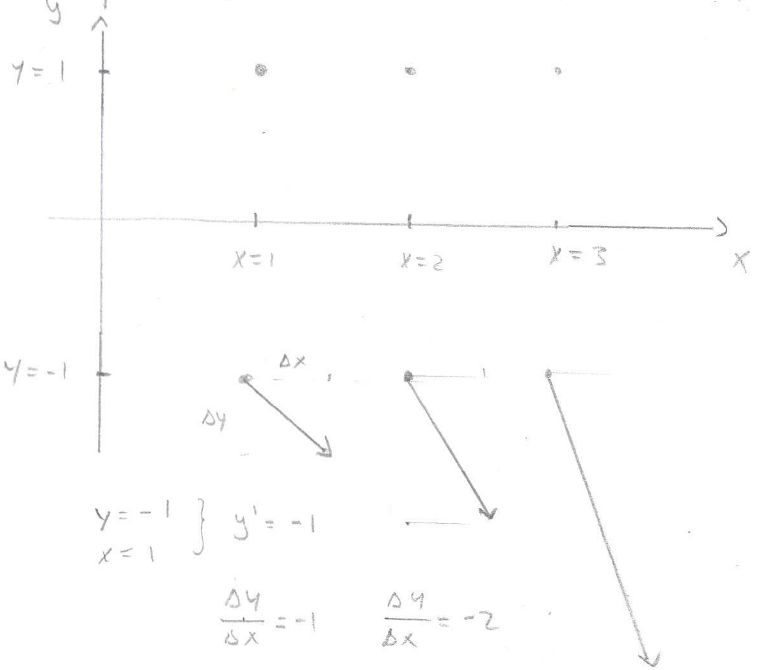
$$\begin{bmatrix} y_1 \\ y_2 \\ y_3 \end{bmatrix} = \begin{bmatrix} -k & -c \\ 0 & 1 \\ 1 & 0 \end{bmatrix} \begin{bmatrix} q_1 \\ q_2 \end{bmatrix} + \begin{bmatrix} 1 \\ 0 \\ 0 \end{bmatrix} f$$

$$\boxed{\vec{y} = C\vec{q} + D\vec{f}}$$ output equations

Numerical Solutions

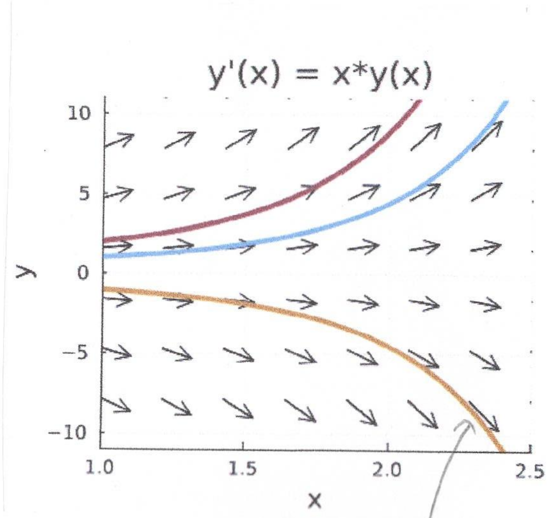
example: $\frac{dy}{dx} = y(x)\,x$ IVP: $y(x=1) = 1$

phase space: vector field with slopes given by $y'(x)$



$\left.\begin{array}{l} y=-1 \\ x=1 \end{array}\right\}$ $y' = -1$

$\frac{\Delta y}{\Delta x} = -1$ $\frac{\Delta y}{\Delta x} = -2$



Integral curves

"slope field is tangent to function"

Numerical Integration: Euler's Method

$\frac{dy}{dx} = F(x, y)$ e.g. $F(x,y) = x \cdot y(x)$ $y_0 = a$ $x_0 = 1$

$\frac{y(x_0+h) - y(x_0)}{h} = F(x_0, y_0)$ forward finite difference

$y_1 = y(x_0 + h) = F(x_0, y_0)h + y(x_0)$

$x_1 = x_0 + h$

$y_2 = y_1(x_1 + h) = hF(x_1, y_1) + y(x_1)$

$\vdots$

$y_{n+1} = y(x_n + h) = hF(x_n, y_n) + y(x_n)$

$x_{n+1} = x_n + h$

Euler example

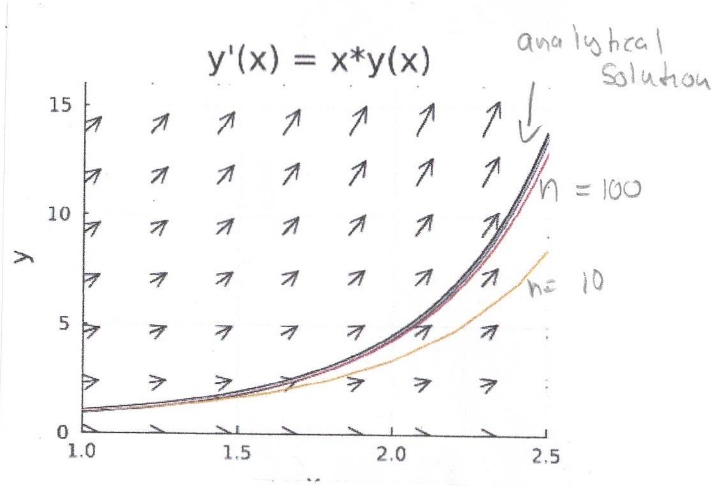
- need to set h (timestep)
- error per step $\approx \frac{1}{2} h^2 f''(x)$

  (local truncation error)
- error at end: accumulated error $\propto h$

  (global truncation error)

$\lim_{h \to 0}$ -> error approaches zero

-> solution converges

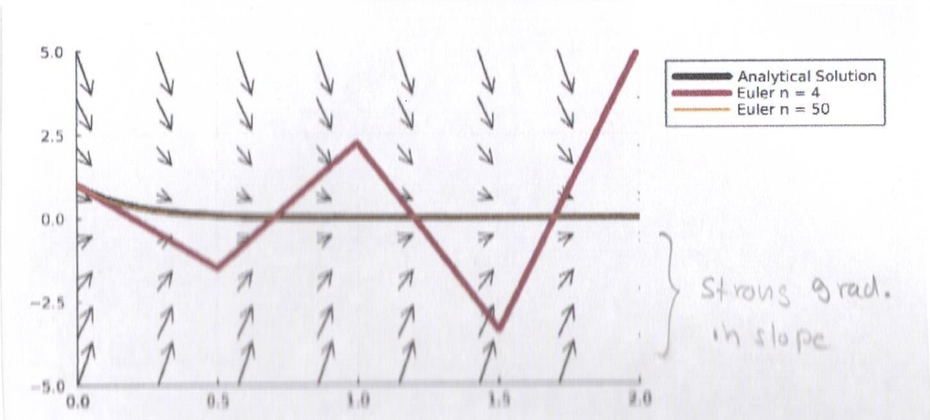


Stiff Equations

- const step causes overshoot
- can lead to oscillation
- requires adaptive h or small h
- many physical systems are stiff

$$y' = -5y$$

$$y = y_0 \exp(-5x)$$



Strong grad. in slope

Runge Kutta Method (RK4)

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

$$y_{n+1} = y_n + \frac{h}{6}(k_1 + 2k_2 + 2k_3 + k_4)$$

$$t_{n+1} = t_0 + h$$

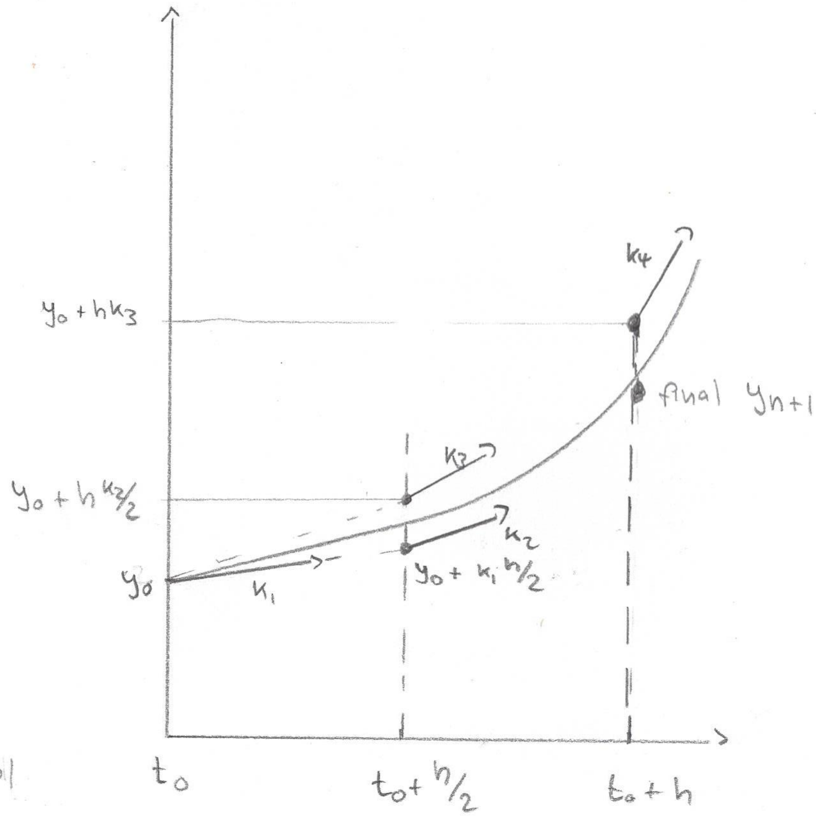
$$k_1 = f(t_n, y_n)$$

$$k_2 = f(t_n + h/2, y_n + h\frac{k_1}{2})$$

$$k_3 = f(t_n + h/2, y_n + h\frac{k_2}{2})$$

$$k_4 = f(t_n + h, y_n + h k_3)$$

- local truncation error $O(h^5)$
- global truncation error $O(h^4)$



Adaptive RK4

- vary h such that local error < rtol and global error < atol

ODE Solvers

(1) define function that returns derivative

generally works for arrays

```
function f(u, p, t)
    du = -3u
    return du
end
```

u : current value

t : current time

p : parameters

(t, p) may not be used

(2) define initial conditions and range to integrate

$u_0 = 10$

$t = [0, 10]$

(3) define solver method

e.g. Euler, RK4, ...

set truncation error limit or timestep

(4) call ode solver

(5) evaluate the solution