Ordinary Differential Equations (ODE)

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

- unkown is a function
- derivative appears in Eq.

ODE: function only depends on one vanable

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

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

2 Integration by separation of variables

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

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

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

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

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

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

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

initial value

Second example : time to reach terminal velocity

$\bar{F} = B\, v$ ← velocity

mechanical mobility

$v(t=0) = 0$

$\bar{F} = m\, g$

mass   gravity

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

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

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

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

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

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

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

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

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

$$\mathcal{L}(af + bg) = a\bar{F}(s) + bG(s)$$

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

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

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

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

$$\frac{1}{(s-2)(s-3)} = \frac{A}{(s-2)} + \frac{B}{(s+3)}$$ "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 $f = A \cdot \exp(\lambda x)$ $\rightarrow \lambda$ complex $\Rightarrow$ sinusoids

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

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

Solution approach for homogeneous case

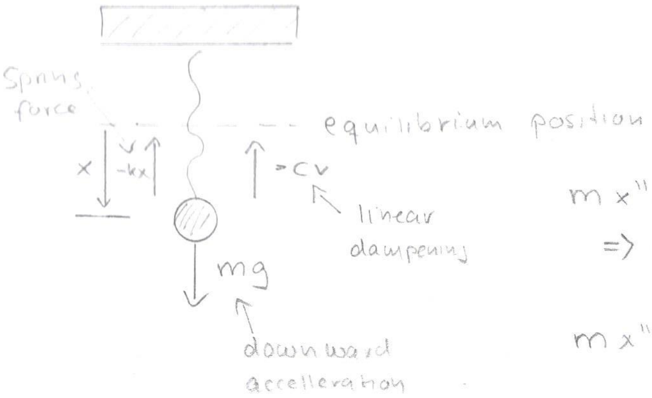
characteristic equation

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

$\rightarrow$ 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

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

$\Rightarrow$ evolution back to equilibrium

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

impuls / external forcing

Solve

$$m x''(t) + c x'(t) + k x(t) = 0 \qquad \text{IVP: } \underset{\text{intial position}}{\underset{\uparrow}{x(0) = -1}} \quad \underset{\text{initial velocity}}{\underset{\uparrow}{x'(0) = 0}}$$

charact Eq.

$$m \lambda^2 + c\lambda + k = 0 \qquad \text{Constants: } m = 10 \quad c = 1 \quad k = 1$$

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

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

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

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

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

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

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

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

Systems of ODEs

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

example

$$mx'' + cx' + kx = 0$$

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

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

$$q_1' = q_2$$

$$q_2' = \frac{1}{m}(-cq_2 - kq_1)$$

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

$\boxed{\vec{q}\,' = A\vec{q}}$ matrix form of homogeneus 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

$\lambda, v = eigen(A)$

Similarity with SVD:

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

diagonal matrix with λ_i as entries

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 $\vec{v}_i$

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

real λ : exp

complex λ : sinusoidals

use initial cond. to get c_i

Valid for homogeneous linear systems

Example: Reaction chains

$$\frac{dq_1}{dt} = -a q_1$$

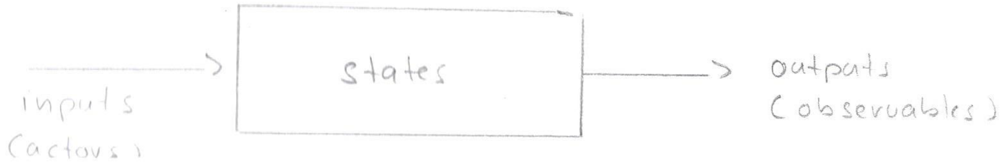
$$\frac{dq_2}{dt} = a q_1 - b q_2 \qquad A = \begin{bmatrix} -a & 0 & 0 \\ a & -b & 0 \\ 0 & b & 0 \end{bmatrix}$$

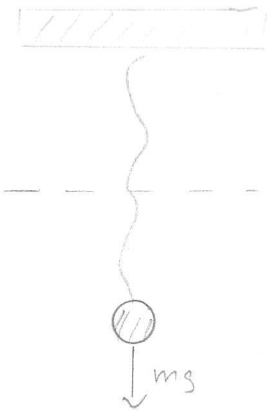
$$\frac{dq_3}{dt} = b q_2$$

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

Homework: find analytical solution and compare to notes

State Space Modeling





forced oscillator

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

inputs $f(t)$

outputs (observables)

- position
- velocity
- acceleration

$\}$ → derived properties

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

States:

variables needed to predict future of system

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

$$q_1 = x$$

$$q_2 = x'$$

$$q_1' = q_2$$

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

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

$$\boxed{q' = A q + B f}$$

Input Eq.

q: State vanables

outputs:

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

$$y_1 = f - c q_2 - k q_1$$

$$y_2 = q_2$$

$$y_3 = q_1$$

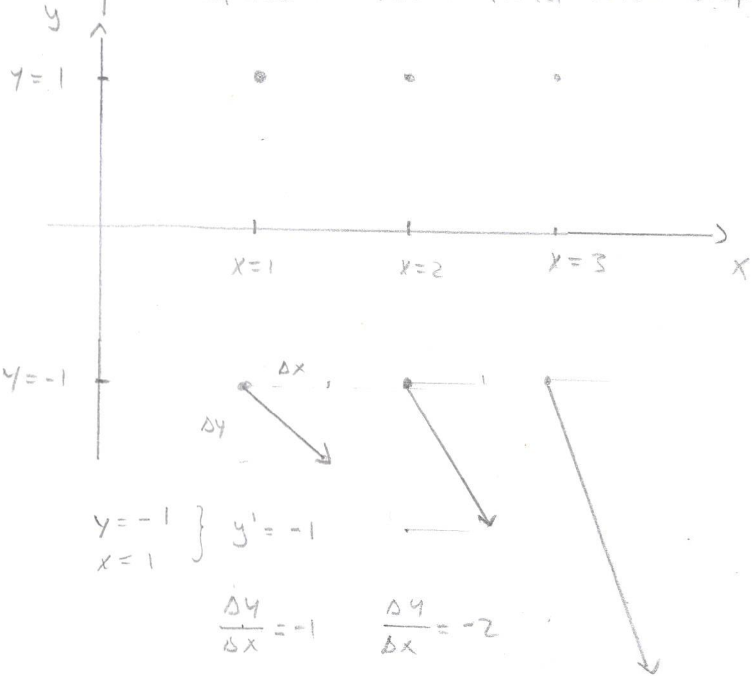
$$\begin{bmatrix} y_1 \\ y_2 \\ y_3 \end{bmatrix} = \begin{bmatrix} -k & -c \\ 0 & 1 \\ 1 & 0 \end{bmatrix} \begin{bmatrix} q_1 \\ q_2 \end{bmatrix} + \begin{bmatrix} 1 \\ 0 \\ 0 \end{bmatrix} f$$

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

Numerical Solutions

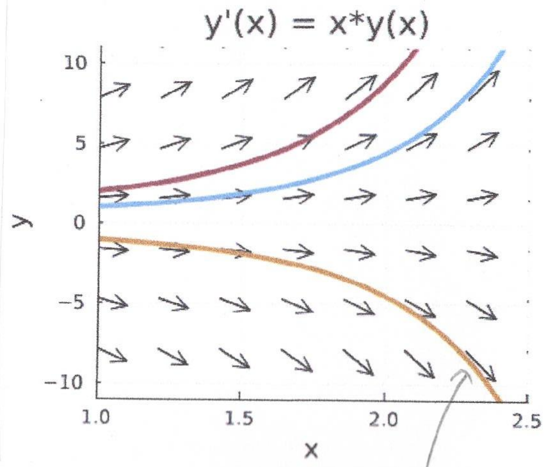
example: $\frac{dy}{dx} = y(x)\, x$ IVP: $y(x=1) = 1$

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



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

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



Integral curves

"slope field is tangent to function"

Numerical Integration: Euler's Method

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

e.g. $F(x, y) = x \cdot y(x)$ $\quad y_0 = a \quad x_0 = 1$

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

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 $\approx \frac{1}{2} h^2 f''(x)$

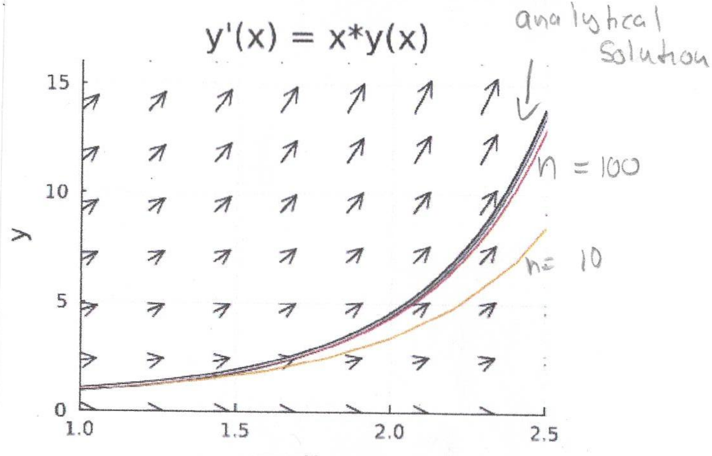
  (local truncation error)

- error at end: accumulated error $\propto h$

  (global truncation error)

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

-> solution converges

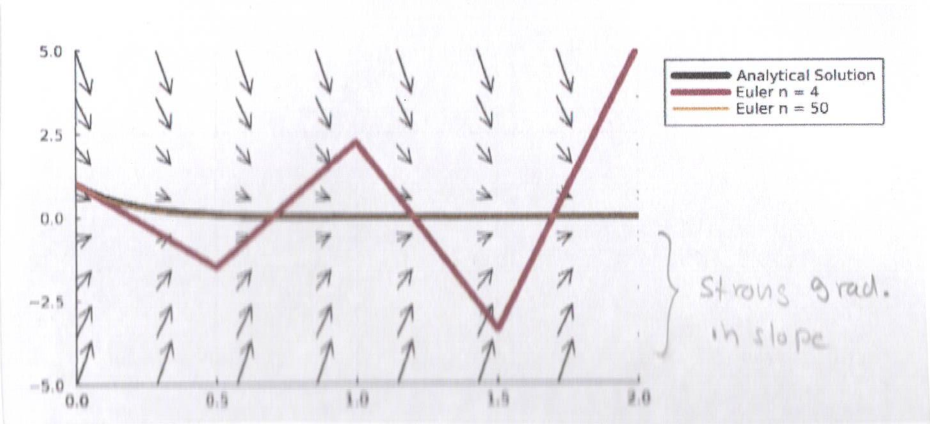


Stiff Equations

- 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)

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

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

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

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

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

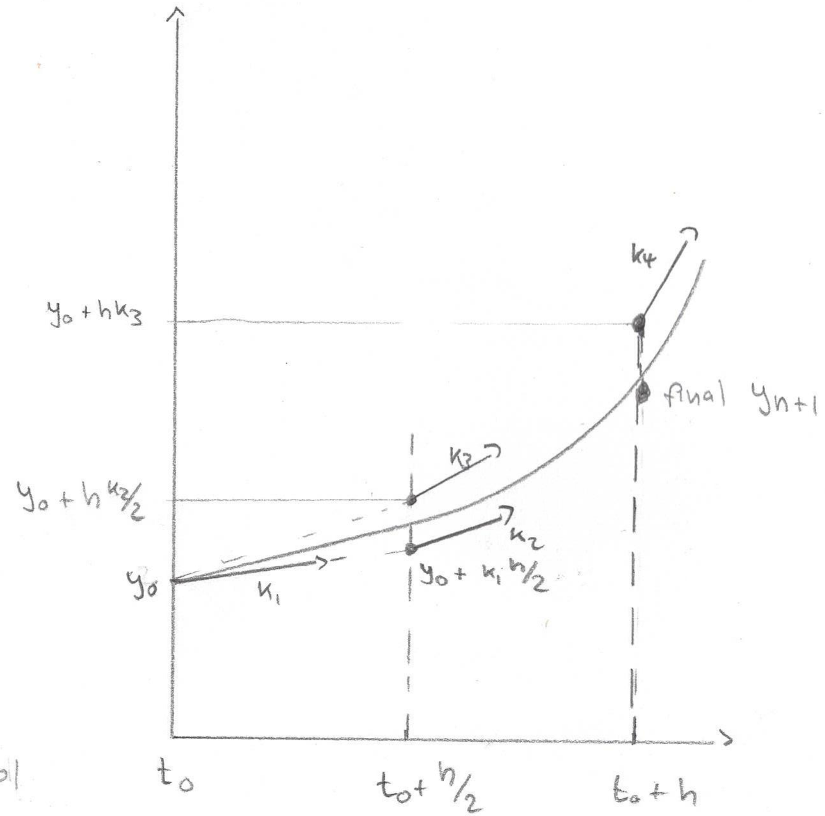
$$k_3 = f(t_n + h/2, y_n + h\frac{k_2}{2})$$

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

- 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

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