(1) Finite precision accuracy

n - digit accuracy $\Rightarrow$ store number as

$$\underbrace{x.xxx}_{\text{4 digit accuracy}} \times 10^{y}$$

and round after every operation

i.e if had: add two numbers then divide, you would round after adding and then divide.

(2) Matrix basics

- $A = A^T \Rightarrow$ Symmetric $\Rightarrow a_{ij} = a_{ji}$

- Diagonal: $a_{ij} = \alpha_i \delta_{ij}$

- $(AB)_{ij} = \sum_{k=1}^{n} a_{ik} B_{kj}$

- $\operatorname{Det} A \neq 0 \Rightarrow A\underline{x} = \underline{b}$ has unique solution

- $\operatorname{Det} A = 0 \Rightarrow A\underline{x} = \underline{b}$ has either no or many solution

③ Gaussian Elimination

For $A\underline{x} = \underline{b}$ use $\underline{\tilde{A}} = [A\,\underline{b}]$

Augmented matrix

- row operations and backward substitution
- pivoting strategies ← 3 of them

④ LU Decomposition

l_{i1}

- first step $\quad a_{ij}^{(1)} = a_{ij} - \dfrac{a_{i1}}{a_{11}} a_{1j} \qquad i \geq 2$
- k^{th} step $\quad a_{ij}^{(k+1)} = a_{ij}^{(k)} - \dfrac{a_{ik}^{(k)}}{a_{kk}^{(k)}} a_{kj}^{(k)} \qquad i \geq k$

l_{ik}

at k^{th} step

$$A = \begin{pmatrix} 1 & & & \\ l_{21} & 1 & & 0 \\ \vdots & l_{32} & \ddots & \\ l_{n1} & 0 & \cdots & 1 \end{pmatrix} \begin{pmatrix} a_{11} & \cdots & \cdots & \cdots \\ 0 & 0 & \ddots & \\ \vdots & \vdots & & a_{kk}^{(k+1)} \\ 0 & 0 & & \end{pmatrix} \quad (*)$$

⑤ some general results :

Sheet 1 → Q4, 5, 7, 9

Sheet 2 → Q4, 5, 6(a)

⑥ Permutation matricies

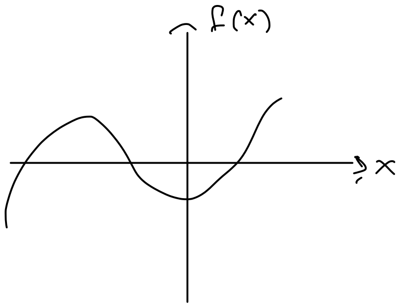
$$PP^T = I \Rightarrow P^{-1} = P^T \quad (\text{often } P^2 = I)$$

- pre multiply by P_{ij} $\Rightarrow$ swap i and j rows
- postmultiply by P_{ij}^T $\Rightarrow$ swap i and j collumns
- at k^{th} step $P_{ij} A = P_{ij} L_k^{-1} P_{ij}^T P_{ij} A^{(k)}$ ✱

  follows from $A = L_k^{-1} A^{(k)}$

⑦ Bisection method for $f(x)=0$

- Draw graph



- find (a,b) pairs s.t $f(a)f(b) < 0$

- $x_n = \frac{1}{2}(a+b) \rightarrow \begin{cases} f(x_n) = 0 & \checkmark \text{ Done} \\ f(a)f(x_n) < 0 \Rightarrow b = x_n \\ f(b)f(x_n) < 0 \Rightarrow a = x_n \end{cases}$

$n = n+1$

- max error after n steps is

① $\dfrac{|b-a|}{2^n}$ or if ε = tolerance

then $n > \dfrac{\log\left(\frac{|b-a|}{\varepsilon}\right)}{\log(2)}$ ②

prove from ① to ②

⑧ Fixed point iteration

- $f(x^*) = 0 \Rightarrow g(x^*) - x^* = 0$

and

$x_{n+1} = g(x_n)$ s.t. $x_n \longrightarrow x^*$

— Need fixed point theorem

for $x \in [a,b]$ need

$$\begin{cases} g(x) \in [a,b] \\ |g'(x)| < 1 \end{cases}$$

implies exists unique $x^* \in [a,b]$ and

$\forall x_0 \in [a,b]$, $x_n \longrightarrow x^*$

9. order of convergence

$$\lim_{n\to\infty} \frac{|x_{n+1} - x^*|}{|x_n - x^*|^\alpha} = \lambda$$ where α = order of convergence

and λ = asymptotic error constant

- Note: error $= e_n = x_n - x^*$
- $\alpha = 1$ requires $\lambda < 1$ to converge, linear
- $\alpha = 2, 3, \ldots$ any λ works, but x_0 needs to be close to x^*
- $g'(x^*) = g''(x^*) = \cdots = g^{(p-1)}(x^*) = 0$

  and $g^{(p)}(x^*) \neq 0$ $\Rightarrow$ implies order of convergence $\alpha = p$

  and $$\lambda = \frac{|g^{(p)}(x^*)|}{p!}$$

(10) Newton - Raphson

$$x_{n+1} = x_n - \frac{f(x_n)}{f'(x_n)} \qquad g = x - \frac{f}{f'}$$

- need to be able to show

$$g'(x^*) = 0 \quad \text{and} \quad g''(x^*) = \frac{f''(x^*)}{f'(x^*)}$$

- if $|x_0 - x^*| < \frac{2}{M}$, where $M = \max |g''(\xi)|$

$\xi \in (x_0, x^*)$ Then N-R converges

- if $f'(x^*) = f'' = \cdots = f^{(m-1)}(x^*) = 0$

and $f^{(m)}(x^*) \neq 0$ then x^* is root of multiplicity m

- if $m > 1$ then N-R $\rightarrow$ linear

then define $F = \frac{f}{f'}$, let

$$g = x - \frac{F}{F'}$$ and go again

11 Aitken Δ^2

$$\frac{x_{n+1} - x^*}{x_n - x^*} \simeq \frac{x_{n+2} - x^*}{x_{n+1} - x^*}$$

starting point

if x_n is linearly convergent

$$\Rightarrow \hat{x}_n = x_n - \frac{(\Delta x_n)^2}{\Delta^2 x_n}$$ where

faster than linear

$$\Delta x_n = x_{n+1} - x_n$$

$$\Delta^2 x_n = x_{n+2} - 2x_{n+1} + x_n$$

12 Multidimensional N-R Fast

$$\underline{f}(\underline{x}^*) = \underline{0}$$

method: $\underline{x}^{(m+1)} = \underline{x}^{(m)} - J^{-1} \underline{f}(\underline{x}^{(m)})$

and $J_{ij} = \dfrac{\partial f_i}{\partial x_j}$

- need $\underline{x}^{(0)} - \underline{x}^*$ to be "small"
- if $\det(J)\big|_{\underline{x} = \underline{x}^{(0)}} = 0$ then poor choice of $\underline{x}^{(0)}$

(13) Steepest descent slow

for $\underline{f}(\underline{x}^*) = \underline{0}$

- let $g(\underline{x}) = \sum_{i=1}^{n} f_i^2$

and do $\underline{x}^{(m+1)} = \underline{x}^{(m)} - \alpha_m \nabla g$

gradient of g

$\left(\frac{\partial g}{\partial x_i}\right)$

s.t $h'(\alpha_m) = 0$ where

$$h(\alpha_m) = g\left[\underline{x}^{(m)} - \alpha_m \nabla g(\underline{x}^{(m)})\right]$$

"h is a height of new iterate"

(14) Differentiation

- FD, BD, CD are three schemes to remember

- $\left.\begin{matrix} f'(x_0) \\ \text{or} \\ f''(x_0) \end{matrix}\right\} = \alpha_1 f(x_0 + h_1) + \alpha_2 f(x_0 + h_2)$

e.g $\alpha f(x_0 - h) + \beta f(x_0) + \gamma f(x_0 + h)$

- method :

  Taylor expand about x_0 and match coefficients of $f(x_0)$ $f'(x_0)$ $f''(x_0)$ ... to determine $\alpha, \beta, \gamma, \ldots$ and to determine error $E(h)$

- Rounding error : write $f(x) = \hat{f}(x) + e(x)$ where $|e| < \varepsilon$ = tolerance.

(15) Richardson Extrapolation

if $N_1(h) \simeq N$ & error is a series in h

Then compute $N_1(h)$ & $N_1(\frac{h}{2})$ & eliminate leading order error in h

(+ repeat by half and half ...)

(16) Lagrange Polynomials

$$P_n(x) = \sum_{j=0}^{n} f(x_j) \prod_{\substack{i=0 \\ \neq j}}^{n} \frac{(x-x_i)}{(x_j-x_i)}$$

↑

degree n polynomial through $\left((x_0, f(x_0)), \dots, (x_n, f(x_n)) \right)$

(17) Trapezoidal rule

$$\int_a^b f(x)\,dx = T_n - \underbrace{\frac{h^2}{12}(b-a) f''(\xi)}_{\text{error term}}$$

where

$$T_n = \frac{h}{2}\left[f(x_0) + 2\left(f(x_1) + \cdots + f(x_{n-1})\right) + f(x_n)\right]$$

& $h = \frac{b-a}{n}$ $\qquad x_i = a + ih$

(18) <u>Simpsons rule</u>

$$\int_a^b f(x)\,dx = S_n - \underbrace{\frac{h^4}{180}(b-a) f^{(iv)}(\xi)}_{\text{error}}$$

where

$$S_n = \frac{h}{3}\left[f_0 + 4f_1 + 2f_2 + \cdots + 4f_{n-1} + f_n\right]$$

(n even)

(19) Romberg

Trapezoidal rule: $$\int_a^b f(x)\,dx = T_n + \underbrace{a_2 h^2 + a_4 h^4 + \cdots}_{\text{error}}$$

↳ Compute T_n and $T_{\frac{n}{2}}$

equivalent to h

equivalent to $2h$

so eliminate $O(h^2)$ error

and repeat

(20) Problems with quadrature

e.g.:

- Singularities
- rapid oscillations

} irregularities which make function non smooth, so remove problem by hand.

- infinite ranges } map to finite range

(21) orthogonal polynomials

For given $w(x)$ and (a,b) define ϕ_i a polynomial of degree i, s.t

$$\langle \phi_i , \phi_j \rangle = \int_a^b w(x)\, \phi_i\, \phi_j \, dx = 0 \qquad i \neq j$$

and standardisation condition

Note: CRAM-SCHMIDT

$\therefore \langle x\phi_i , \phi_j \rangle = \langle \phi_i , x\phi_j \rangle$ is useful

(22) Gauss Quadrature

$$\int_a^b w(x) f(x)\, dx \simeq \underbrace{\sum_{j=1}^{n} w_j f(x_j)}$$

exact if f is polynomial of degree $(2n-1)$ or less

Sampling points x_j are solutions of $\phi_j(x) = 0$

weighrs ω_j are given by

$$\omega_j = \int_a^b \omega(x) \prod_{\substack{i=1 \\ \neq j}}^{n} \frac{(x - x_i)}{(x_j - x_i)} \, dx$$

Also mapping intervals

23 Euler's Method

$y' = f, \quad y(a) = \alpha$

$y_0 = \alpha, \quad y_{i+1} = y_i + h f(t_i, y_i) \qquad i = 0, \ldots, N-1$

where $t_i = a + ih$ and $h = \frac{b-a}{N}$

has local error $O(h^2)$

24 Error

i) local error : $\tau_{i+1} = \underbrace{y(t_i + h)}_{\text{exact and taylor expand about } t_i} - \underbrace{y_{i+1}}_{\text{Approximate Solution assuming solution at previous step is exact.}}$

Dahlquist theorem if $\tau_{i+1} = O(h^{p+1})$ and $p > 0$ (consistent) and stable then convergent.

if convergent then the global error is $O(h^p)$ and p is the order of accuracy.

(25) Difference equations

of the form $a_1 y_{i+1} + a_2 y_i + a_3 y_{i-1} + \dots = f(i)$

solution: $y_i = y_i^h + y_i^p$

particular solution, need to guess

RHS $= 0$ and solve with $y_i = Az^i$ giving characteristic equation for z.

(26) Euler for higher order ODEs

e.g $y'' = f(t, y, y')$, $y(a) = \alpha$, $y'(a) = \beta$

1) 1st order : let $y' = v$

$$v' = y'' = f(t, y, y')$$

2) Euler step:

$$\left.\begin{aligned} y_{i+1} &= y_i + h v_i \\ v_{i+1} &= v_i + h f(t_i, y_i, v_i) \end{aligned}\right\} \quad \begin{aligned} y_0 &= \alpha \\ v_0 &= \beta \end{aligned}$$

3) Eliminate to get second order difference equation.

(27) Higher order Taylor method:

$$y(t_i + h) = y(t_i) + h \underbrace{y'(t_i)}_{=f} + \frac{h^2}{2} \underbrace{y''(t_i)}_{\frac{d}{dt} f = f_t + f f_y}$$

Error $\tau_{i+1} = O(h^3)$

28 RK2

$$y_{i+1} = y_i + a f(t_i, y_i) + b f(t_i + c, y_i + d)$$

- Impose one constraint on a, b, c, d and use Taylor to determine 3 others

29 Multistep methods

$$y_{i+1} = \alpha_1 y_i + \alpha_2 y_{i-1} + \dots + h\beta_0 f_{i+1} + h\beta_1 f_i + \dots$$

(to α_k) (to β_k)

Find α_j, β_j by eliminating τ_{i+1} error

30 Stability $h \to 0$

- solve $y' = 0$ with $y(0) = 1$
for $h\beta_j \to 0$

use the scheme to get a linear difference equation $y_i = Az^i$ and then a characteristic equation for z

giving root condition theorem:

If roots satisfy $|z_j| \leq 1$ $\forall j$ and any z_j s.t. $|z_j|$ must be simple, then method is stable

(31) Time Stability

Solve $y' = \lambda y$, $y(0) = c$, $\lambda \in \mathbb{C}$, $Re\{\lambda\} < 0$

The scheme:

→ $y_i = A z^i$

→ Difference equation

→ time stability polynomial

→ Time Stability $|z_j| < 1$ for $\forall j$ in LH plane

→ Boundary $z = e^{i\theta}$, $0 \le \theta \le 2\pi$

Inside given λ sets values of h s.t the scheme is time stable

(32) Stiff ODEs

Suffers from time - instability

↳ Need small h or implicit schemes