Sci Comp I: Study Guide

(I) Root-Finding

1) **Newton:** $x_{n+1} = x_n - \frac{f(x_n)}{f'(x_n)}$

- 2^{nd} order $\longrightarrow$ $e_{n+1} = x_{n+1} - \alpha$
$= g(x_n) - \alpha$
$= g(\alpha + e_n) - \alpha$
$= e_n g'(\alpha) + \frac{1}{2} e_n^2 g''(\alpha) + \ldots$; $g'(\alpha) = 0$ for Newton's
- comes from eq of a line

$\frac{y - f(x_n)}{x - x_n} = f'(x_n)$

2) **Secant:**

- come from equation of a line: $x_{n+1} = x_n - \frac{f(x_n)}{\left[\frac{f(x_n) - f(x_{n-1})}{x_n - x_{n-1}}\right]}$ $\qquad y = 0 = \frac{f(x_n) - f(x_{n-1})}{x_n - x_{n-1}}(x - x_{n-1}) + f(x_{n-1})$, $x \uparrow x_{n+1}$
- ≈ 1.7 order conv.

3) **Fixed Point:** $x_{n+1} = g(x_n)$

- $|g'(x)| < 1$ for some neighborhood of α

4) **Aitken's:**

- Assume constant in error remains the same: $e_{n+1} \approx g'(\alpha) e_n = C e_n$
- Takes first order scheme and makes a 2^{nd} order

$\longrightarrow e_{n+1} = Ce_n$ or $x_{n+1} - \alpha = C(x_n - \alpha)$
$x_{n+2} - \alpha = C(x_{n+1} - \alpha)$

$\therefore C = \frac{x_{n+2} - x_{n+1}}{x_{n+1} - x_n}$

Now solve for α: $\alpha = x_{n+2} - \frac{(x_{n+2} - x_{n+1})^2}{x_{n+2} - 2x_{n+1} - x_n}$

- **Algorithm:** x_0 = initial guess
for $n = 0, 1, \ldots$
$y_1 = g(x_n)$
$y_2 = g(y_1)$
$x_{n+1} = y_2 - \frac{(y_2 - y_1)^2}{y_2 - 2y_1 + x_n}$

still an iterative scheme (fixed pt)

$x_{n+1} = h(x_n) = g(g(x_n)) - \frac{\left(g(g(x_n)) - g(x)\right)^2}{g(g(x)) - 2g(x) + x}$

where $g(x)$ is your original method

- if $g(\alpha) = \alpha \longrightarrow h(\alpha) = \alpha$ and $h'(\alpha) = 0$

$x - \frac{f(x)}{f'(x)}$ $\quad 1 - \frac{f(x)}{f'(x)}$ $\quad - \frac{f(x)f''(x)}{f'(x)^2}$

(II) Interpolation:

(I) if N+1 data pts, need N+1 eqs, $\Rightarrow \exists$ unique $p(x) \in \Pi_n$ w/ this property : Proof: $p, q \in \Pi_n$ $(p-q)(x_i) = p(x_i) - q(x_i) = 0$

$(p-q)(x) = (x-x_0)\cdots(x-x_n)\, h(x)$

$h(x) = 0$

(II) Existence $\rightarrow$ via Newton interpolation

(III) Methods: ① Standard :

$$\begin{bmatrix} 1 & x_0 & x_0^2 & x_0^3 & \cdots & x_0^n \\ 1 & x_1 & \cdots & & & \\ \vdots & \vdots & & & & \vdots \\ 1 & x_n & \cdots & & & x_n^n \end{bmatrix} \begin{pmatrix} a_0 \\ \vdots \\ a_n \end{pmatrix} = \begin{pmatrix} y_0 \\ \vdots \\ y_n \end{pmatrix}$$

- ill conditioned as $n \to \infty$ ($\because n > 4$)

② Newton :

$$\begin{bmatrix} 1 & 0 & 0 & \cdots \\ 1 & x_1 - x_0 & 0 & \\ 1 & x_2 - x_0 & (x_2-x_0)(x_2-x_1) & \\ 1 & x_3 - x_0 & (x_3-x_0)(x_3-x_1) & \\ \vdots & \vdots & & \\ 1 & x_n - x_0 & (x_n-x_0)(x_n-x_1) & \cdots \end{bmatrix} \begin{pmatrix} a_0 \\ \vdots \\ a_n \end{pmatrix} = \begin{pmatrix} y_0 \\ \vdots \\ y_n \end{pmatrix}$$

- lower triangular matrix
- sweep method $\rightarrow \Theta(n^2)$
- Note: divided diff is $\Theta(n^2)$ operation

$$p(x) = f(x_0) + (x-x_0) f[x_0,x_1] + (x-x_0)(x-x_1) f[x_0,x_1,x_2]$$

③ Lagrange :

$$\begin{bmatrix} L_0(x_0) & & & \\ & L_1(x_1) & & \\ & & \ddots & \\ & & & L_n(x_n) \end{bmatrix} \begin{pmatrix} a_0 \\ \vdots \\ a_n \end{pmatrix} = \begin{pmatrix} y_0 \\ \vdots \\ y_n \end{pmatrix}$$

- diagonal matrix

$$p(x) = y_0 L_0(x) + \ldots y_n L_n(x) \quad ; \quad L_i = \prod_{j \neq i} \frac{(x-x_j)}{(x_i - x_j)} \qquad L_i(x_k) = \delta_{ik} = \begin{cases} 1 & i = k \\ 0 & i \neq k \end{cases}$$

(IV) Error Analysis: $e(t) = \underbrace{f(t)}_{\text{true}} - \underbrace{p(t)}_{\text{interp}}$

Define $q(t)$ = interp of f at $x_0, \ldots, x_n$ and t $\quad q \in \Pi_{n+1}$

ie: $q(t) = p(x) + f[x_0, \ldots, x_n, t]\, (x-x_0)\cdots(x-x_n)$

$d(t) = f(x) - q(x)$ ← has at least $n+2$ roots

$\therefore$ $d^{(n+1)}(t)$ has ≥ 1 roots, call one ξ

$$= f^{(n+1)}(\xi) = q^{(n+1)}(\xi)$$

$$= \underbrace{p^{(n+1)}(\xi)}_{0} + f[x_0, \ldots, x_n, t] \underbrace{\frac{d^{(n+1)}}{dx^{n+1}} \prod_{i=0}^{n}}_{(n+1)!}$$

$$\therefore f[x_0, \ldots, x_n, t] = \frac{f^{(n+1)}(\xi)}{(n+1)!}$$

$\longrightarrow e(t) = f(t) - p(t)$

$\approx q(t) - p(t)$

$$\boxed{e(t) = p(t) + f[x_0, \ldots, x_n, t](x-x_0)\cdots(x-x_n) - p(t) = \frac{f^{(n+1)}(\xi)}{(n+1)!}(x-x_0)\cdots(x-x_n)}$$

(V) <u>Weierstrass Thm</u>: If f is continuous on $[a,b]$, then $\lim\limits_{n\to\infty} \min\limits_{p\in\Pi_n} \|f-p\|_\infty = 0$ or $\forall \varepsilon > 0$, $\exists\, p(x)$ such that $\|f-p\|_\infty \le \varepsilon$

<u>Note</u>: ① uniform pts is bad for "normal" f's $\rightarrow$ ie: error on boundaries

② pick Chebyshev! $\quad T_n(x) = \cos(n\cos^{-1}x) \quad x\in[-1,1]$

$$T_{n+1} = 2xT_n - T_{n-1}$$

<u>Roots</u>: $\cos(n\cos^{-1}x) = 0 \rightarrow n\cos^{-1}x = \frac{\pi}{2} + k\pi$

$$\cos^{-1}x = \frac{\frac{\pi}{2}+k\pi}{n}$$

$$x = \cos\left[\frac{\pi/2 + k\pi}{n}\right] \quad ; k\in\mathbb{Z}$$

③ <u>error w/ Cheby on $[-1,1]$</u>:
$$e(x) = \frac{f^{(n+1)}(\xi)}{(n+1)!} \underbrace{(x-x_0)\cdots(x-x_n)}_{\text{factors of } \frac{T_{n+1}(x)}{\text{coeff of } x^{n+1}}}$$
$$= \frac{f^{(n+1)}(\xi)}{(n+1)!} \frac{T_{n+1}(x)}{2^n}$$

(VI) <u>Interpolation w/ more info about derivatives</u>

① Divided difference: $f(x_0), f'(x_0), f(x_1), f(x_2)$:

x_0	$f(x_0)$			
x_0	$f(x_0)$	$f'(x_0)$		
x_1	$f(x_1)$	$f[x_0,x_1]$	$f[x_0,x_0,x_1]$	
x_2	$f(x_2)$	$f[x_1,x_2]$	$f[x_0,x_1,x_2]$	$f[x_0,x_0,x_1,x_2]$

② <u>Hermite Interpolation</u>: • using info from $f(x_k)$, $f'(x_k)$ for $k=0,1,\ldots,n$

• If $P_n^H(x) \in \Pi_{2n+1}$, then $e(x) = 0$ if $f(x)\in\Pi_{2n+1}$

• $e(x) = \frac{f^{(2n+2)}(\xi)}{(2n+2)!}(x-x_0)^2(x-x_1)^2\cdots(x-x_n)^2$

(III) <u>Stencils</u>: (I) • can interpolate from $[a,b]$; what if break interval into N subintervals, ie: $h = 1/N$, $x_i = x_{ref} + hy_i$

• usually let $x_{ref} = 0$

• <u>error @ ref</u>: $e(x_{ref}) = \frac{f^{(n+1)}(\xi)}{(n+1)!}(x_{ref}-x_0)\cdots(x_{ref}-x_n) = \frac{f^{(n+1)}(\xi)}{(n+1)!}(-1)^n h^n (y_0\cdots y_n)$

• <u>Steps</u>: (1) compute $P_n(x)$ via Newton-Interpolation

(2) Evaluate $P_n(x_{ref})$ to get stencil

(3) Error given above

<u>or</u>

$$\begin{bmatrix} 1 & 1 & 1 & \cdots & 1 \\ y_0 & y_1 & y_2 & \cdots & y_n \\ \vdots & & & & \vdots \\ y_0^n & \cdots & & & y_n^n \end{bmatrix}\begin{pmatrix} a_0 \\ a_1 \\ \vdots \\ a_n\end{pmatrix} = \begin{pmatrix} 1 \\ 0 \\ \vdots \\ 0 \end{pmatrix}$$

ie: for k^{th} eq: $\sum_{j=0}^{n} a_j y_j^k = x^k\Big|_{x_{ref}}$

(II) <u>Derivatives</u>: Use same steps as before except on RHS vector is $\frac{d}{dx}\begin{pmatrix} 1 \\ x \\ x^2 \\ \vdots \\ x^n \end{pmatrix}\Bigg|_{x=x_{ref}=0} = \begin{pmatrix} 0 \\ 1 \\ 0 \\ \vdots \end{pmatrix}$

<u>**Error**</u>: $e(x) = f'(x) - p'(x) = \frac{d}{dx}\left[\overbrace{f[x_0,\ldots,x_n,x]}^{g(x)}\overbrace{(x-x_0)\cdots(x-x_n)}^{w(x)}\right]$

$$= g'(x)w(x) + g(x)w'(x) \approx Ch^{n+1} + \tilde{C}h^n$$

$$\text{error} = \begin{cases} O(h^{n+1}) & 0 \notin \text{interp pt} \\ O(h^n) & 0 \in \text{interp pt}\end{cases}$$

Error in general: if $p \in \Pi_{n+1}$, then error of k^{th} derivative is at most $\Theta(h^{n-k})$

Proof: keep using product rule like we did for 1^{st} derivative

(III) Richardson Extrapolation:

Say $F(h)$ = approximate value w/ h steps

$F(h/q)$ = approximate value w/ h/q steps ; $q \in \mathbb{Z}^+$

$$F(h) = y + ch^p + \Theta(h^{p+1})$$
$$F(h/q) = y + c\left(\frac{h}{q}\right)^p + \Theta(h^{p+1})$$

y is true value, c is error constant

Solve for
$$\boxed{y = F_h - \frac{F_h - F_{h/q}}{q^{-p} - 1} + \Theta(h^{p+1})}$$
now is order $p+1$

(IV) Integration

(I) Error $= \int_a^b (f - P_n(x))\,dx = \int_a^b \underset{\Theta(1)}{g(x)}\, \underset{\Theta(h^{n+1})}{w(x)}\,dx \approx \Theta(h^{n+2})$; $h \sim (b-a)$

(II) Composite Methods:

① Trapezoid: 0 — h

$$\begin{bmatrix} 1 & 1 \\ 0 & h \end{bmatrix}\begin{pmatrix} c_1 \\ c_2 \end{pmatrix} = \begin{pmatrix} \int_0^h 1\,dx \\ \int_0^h h\,dx \end{pmatrix} \Longrightarrow \text{pick } h=1$$

$$\boxed{\int_0^h f(x)\,dx \approx \frac{h}{2}[f(0) + f(h)]}$$

② Simpson's: $-h$ — 0 — h stencil $= (2h)(c_0 f_0 + c_1 f_1 + c_2 f_2)$

$$\begin{bmatrix} 1 & 1 & 1 \\ -1 & 0 & 1 \\ (-1)^2 & 0 & 1^2 \end{bmatrix}\begin{pmatrix} c_0 \\ c_1 \\ c_2 \end{pmatrix} = \begin{pmatrix} \int_{-1}^1 1\,dx \\ \int_{-1}^1 x\,dx \\ \int_{-1}^1 x^2\,dx \end{pmatrix}$$

$$\boxed{\int_{-h}^h f(x)\,dx \approx 2h\left(\frac{1}{6}f_0 + \frac{4}{6}f_1 + \frac{1}{6}f_2\right)}$$

(III) Error Analysis:

Note: if error on $[0,h]$ is h^k, in general error on $[a,b]$ is h^{k-1}

~~[illegible]~~ h^k ie: $\frac{N}{(b-a)}h^k = h^{k-1}$

ex) Trap Error:

$\frac{h}{2} f(0) = \frac{h}{2} f(0)$

$\frac{h}{2} f(h) = \frac{h}{2}\left(f(0) + hf'(0) + \frac{1}{2}h^2 f''(0) + \dots\right)$

$hf(0) + \frac{h^2}{2}f'(0) + \frac{h^3}{4}f''(0) + \dots$

$$\int_0^h f(x)\,dx \approx \int_0^h (f(0) + xf'(0) + \dots)\,dx = hf(0) + \frac{h^2}{2}f'(0) + \frac{h^3}{6}f''(0) + \dots$$

$$\therefore \text{error} = \int_0^h f(x)\,dx - \frac{h}{2}[f(0) + f(h)] = h^3 f''(0)\left(\frac{1}{6} - \frac{1}{4}\right) \therefore \Theta(h^3) \text{ locally} \therefore \Theta(h^2) \text{ globally}$$

(IV) Gauss Quadrature : pick both interpolation pts and weights to minimize the error

- Gram-Schmidt :

$$P_0 = 1$$
$$P_1 = xP_0 - \frac{\langle xP_0, P_0\rangle}{\langle P_0, P_0\rangle} P_0$$
$$P_2 = xP_1 - \sum_{k=0}^{1} \frac{\langle xP_1, P_k\rangle}{\langle P_k, P_k\rangle} P_k$$
$$\vdots$$

Note: $P_{n+1} = \frac{2n+1}{n+1} x P_n - \frac{n}{n+1} P_{n-1}(x)$

- Error : locally h^{2n+3} globally h^{2n+2} Exact for polys up to: x^{2N+1}

- Steps : for $(2n+1)^{th}$ order , need n-pts

(1) compute : $P_0, P_1, \ldots, P_n$ * Zeros of P_n are gauss quad pts *

(2) Find Weights :
$$\begin{bmatrix} 1 & 1 & 1 & \cdots \\ x_0 & x_1 & x_2 & \\ \vdots & \vdots & \vdots & \\ x_0^n & x_1^n & & \cdots \end{bmatrix} \begin{pmatrix} w_0 \\ w_1 \\ \vdots \\ w_n \end{pmatrix} = \begin{pmatrix} \int 1\,dx \\ \int x\,dx \\ \int x^2\,dx \\ \vdots \end{pmatrix}$$
; Note: if $\langle \cdot , \cdot \rangle = \int_a^b w \cdot \cdot \, dx$ RHS is $\int_a^b w \cdot 1\, dx$, etc

(3) $\int_a^b f(x)dx \approx w_0 f(x_0) + w_1 f(x_1) + \ldots + w_n f(x_n)$

(V) Romberg Integration : similar to Richardson Extrapolate (actually the same)

- call I_h = integration method of $[0,h]$
  $I_{h/2}$ = integration method of $[0,h/2] + [h/2, h]$
  error $\sim \theta(h^k)$
  (Note : in general could use $I_{h/q}$)

$$I_h = I + ch^k + \theta(h^{k+1})$$
$$I_{h/q} = I + c\left(\frac{h}{q}\right)^k + \theta(h^{k+1})$$

$$\Longrightarrow \boxed{I = I_h - \frac{I_h - I_{h/q}}{q^{-k} - 1} + \theta(h^{k+1})}$$

*** can bootstrap this method ***

(VI) Adaptive Integration :

1) ε = error tolerance

2) integrate $\int_A^B f\, dx$:
$$I_{fine} = I\left(A, \frac{A+B}{2}\right) + I\left(\frac{A+B}{2}, B\right)$$
$$I_{coarse} = I(A,B)$$

3) if $\varepsilon > \left| \frac{I_{fine} - I_{coarse}}{2^{k-1} - 1} \right|$, return I_{fine}

else Integrate$\left(A, \frac{A+B}{2}, \frac{\varepsilon}{2}\right)$ + Integrate$\left(\frac{A+B}{2}, B, \frac{\varepsilon}{2}\right)$

(VII) Singularities :

1) Tell # of pts

2) if f is singular like x^r , make smooth function $g(x) = \frac{f(x)}{x^r}$, weighted inner product is : $\langle \cdot , \cdot \rangle = \int x^r \cdot \cdot \, dx$

3) Compute P_{n+1} using Gram-Schmidt and find the zeros

4) Now w/ interpolation pts, find the weights

(V) ODEs:

(I) Existence/Uniqueness: $\frac{dy}{dt} = f(y,t)$ if f is Lipschitz continuous, ie: in $\mathbb{R}$ $\exists L$ s.t. $|f(y_1,t) - f(y_2,t)| \le L\,|y_1 - y_2|$

then solution exists and is unique.

(II) Methods:

① Euler: $y_{n+1} = y_n + hf(t, y_n)$

② Taylor Methods: $y_{n+1} = y_n + hf(t_n, y_n) + \frac{h^2}{2} f''(t_n, y_n) + \dots$; Note: $\frac{d}{dt} f = f_t + f_y f$

K^{th} order

③ RK2: $y_{n+1} = y_n + \frac{h}{2}\left[f(y_n) + f(y_n + f(y_n)h)\right]$ ← 2^{nd} order

④ RK4: $y_{n+1} = y_n + \frac{1}{6}\left(K_1 + 2K_2 + 2K_3 + K_4\right)$

$K_1 = hf(t_n, y_n)$

$K_2 = hf(t_n + h/2,\ y_n + \frac{1}{2}K_1)$

$K_3 = hf(t_n + h/2,\ y_n + \frac{1}{2}K_2)$

$K_4 = hf(t_n + h,\ y_n + K_3)$

Runge Kutta Notation:

coefficient of h

$$\begin{array}{c|cccc} 0 & & & & \\ 1/2 & 1/2 & & & \\ 1/2 & 0 & 1/2 & & \\ 1 & 0 & 0 & 1 & \\ \hline & 1/6 & 2/6 & 2/6 & 1/6 \end{array}$$

*rows add to LHS

ie:

$$\begin{array}{c|ccccc} c_1 & & & & & \\ c_2 & a_{21} & & & & \\ \vdots & a_{31} & a_{32} & & & \\ c_n & a_{n1} & a_{n2} & \cdots & a_{n,n-1} & \\ \hline & a_1 & a_2 & \cdots & a_{n-1} & a_n \end{array} \quad \leftarrow K_n$$

$K_n = hf\left(t_n + c_n h,\ y_n + \sum_{j=1}^{n-1} a_{nj} K_j\right)$

$y_{n+1} = y_n + \sum_{j=1}^{n} a_j K_j$

⑤ Trapezoid: $y_{n+1} = y_n + \frac{h}{2}\left[f(t_n, y_n) + f(t_{n+1}, y_{n+1})\right]$

⑥ Implicit Euler: $y_{n+1} = y_n + hf(t_{n+1}, y_{n+1})$

III) Stability: $y_{n+1} \le \lambda y_n$ need $|\lambda| \le 1$

IV) Consistency: Taylor Series!

ex) $y_{n+1} = y_n + hf(t, y_n)$

$y_{n+1} = y_n + hy_n' + \frac{1}{2}h^2 y_n'' + \dots$

$y_n + hy_n' + \frac{1}{2}h^2 y_n'' = y_n + h\overset{f(t_n,y_n)}{y_n'}$

$\rightarrow O(h^2)$

Convergence: Stability + Consistency

(VI) DFT : Given $y_0, \dots, y_N$, $x_0, \dots, x_N$, DFT is : $\hat{y}_k = \frac{1}{N} \sum_{j=0}^{N-1} y_j e^{-2\pi i k x_j}$

- Interpolating polynomial : $P(x) = \sum_{k=0}^{N-1} \overset{\hat{y}_k}{\overset{\shortparallel}{\hat{f}_k}} e^{i2\pi k x} dx = \sum_{k=0}^{N-1} \left[\frac{1}{N} \sum_{j=0}^{N-1} y_j e^{-2\pi i k x_j} \right] e^{2\pi i k x}$

- Approximate $\int_0^1 f\,dx$ by taking FFT of data and then summing each component

  - $\int_0^1 f\,dx \approx \int_0^1 P(x)\,dx$

$$= \frac{1}{N} \sum_{k=0}^{N-1} \sum_{j=0}^{N-1} y_j e^{-2\pi i k x_j} \int_0^1 e^{i2\pi k x} dx$$

$$= \frac{1}{N} \sum_{j=0}^{N-1} y_j e^{-2\pi i (0) x_j} \int_0^1 e^0 dx + \frac{1}{N} \sum_{k=1}^{N-1} \sum_{j=0}^{N-1} y_j e^{-2\pi i k x_j} \underbrace{\int_0^1 e^{i2\pi k x} dx}_{0 \text{ for } k \geq 1}$$

$$= \frac{1}{N} \sum_{j=0}^{N-1} y_j \leftarrow \text{LHR}$$

- Error : $\int_{x_j}^{x_j+h} f(x)dx - \frac{1}{N} f(x_j)$ $\quad h = 1/N$, $j = 0, 1, \dots, N$

$$= \int_{x_j}^{x_j+h} \left(f(x_j) + h f'(x_j) + \dots \right) dx - \frac{1}{N} f(x_j)$$

$$= h f(x_j) + \frac{1}{2} h^2 f'(x_j) + \dots - \frac{1}{N} f(x_j)$$

$$= \theta(h^2) \quad \underline{\text{locally}}$$

Globally

$$\int_0^1 f(x)dx - \int_0^1 P(x)dx$$

$$= \sum_{j=0}^{N-1} \left[\int_{x_j}^{x_j+h} f(x)dx - h f(x_j) \right]$$

$$= N\,\theta(h^2)$$

$$= \theta(h) \quad \underline{\text{globally}}$$