LECTURE 10

$$e^A \;\begin{cases} \{\text{Taylor, Padé}\} + \text{scaling and squaring} \\ e^{\mu} e^{A-\mu I} = e^A \\ \text{BACKWARD ERROR ANALYSIS : } \dfrac{\|\Delta A\|}{\|A\|} \leq tol \end{cases}$$

$$T_m\left(\frac{A}{2^s}\right)^{2^s} = \exp(A + \Delta A)$$

$$\varphi_\ell(A) \;\begin{cases} \{\text{Taylor, Padé}\} + \text{modified scaling and squaring} \\ \varphi_\ell(A - \mu I) \overset{?}{\longrightarrow} \varphi_\ell(A) \\ \text{QUASI BACKWARD ERROR ANALYSIS} \end{cases}$$

- $\varphi_\ell(A) = \displaystyle\int_0^1 e^{(1-s)A} \frac{s^{\ell-1}}{(\ell-1)!} \, ds \approx$ formule di quadrature

- $$\exp\left(\begin{bmatrix} A & v \\ 0 & 0 \end{bmatrix}\right) = \begin{bmatrix} I & 0 \\ 0 & 1 \end{bmatrix} + \begin{bmatrix} A & v \\ 0 & 0 \end{bmatrix} + \frac{1}{2}\begin{bmatrix} A^2 & Av \\ 0 & 0 \end{bmatrix} + \frac{1}{6}\begin{bmatrix} A^3 & A^2v \\ 0 & 0 \end{bmatrix} + \frac{1}{24} \cdots$$

AUGMENTED MATRIX

$\hat{A}$

$$\begin{bmatrix} e^A & \varphi_1(A)v \\ 0 & 1 \end{bmatrix}$$

$$\exp\left(\begin{bmatrix} A & v \\ 0 & 0 \end{bmatrix}\right)\begin{bmatrix} u_0 \\ 1 \end{bmatrix} = \begin{bmatrix} e^A u_0 + \varphi_1(A)v \\ * \end{bmatrix}$$

BEA, shifting μ for $\exp(\hat{A})$

Identity of size $p-1$

$$\hat{A} = \begin{bmatrix} A & u_p & u_{p-1} & \dots & u_1 \\ 0 & & J & & \end{bmatrix} \qquad J = \begin{bmatrix} 0 & I_{p-1} \\ 0 & 0 \end{bmatrix}$$

τ time step

$$\exp(\tau \hat{A}) \begin{bmatrix} u_0 \\ e_p \end{bmatrix} = \begin{bmatrix} e^{\tau A} u_0 + \tau \varphi_1(\tau A) u_1 + \overset{\tau}{\tau^2} \varphi_2(\tau A) \overset{\tau u_2}{u_2} + \dots + \tau^p \varphi_p(\tau A) u_p \\ * \end{bmatrix}$$

$$e_p = \begin{bmatrix} 0 \\ \vdots \\ 0 \\ 1 \end{bmatrix} \Big\} p-1$$

sc $A \approx \partial_{xx}$ + Neumann b.c.

$$n = \begin{bmatrix} 1 \\ 1 \\ 1 \\ 1 \end{bmatrix}$$

- Krylov

$AV = VD \qquad V^{-1}AV = D$

$$e^A = V e^D V^{-1} \qquad e^D = \begin{pmatrix} e^{\lambda_1} & & \\ & \ddots & \\ & & e^{\lambda_N} \end{pmatrix}$$

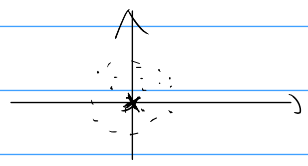
A with minimal polynomial $\mu(t)$ of degree ν ($\mu(A) = 0$, it divides the characteristic of A)

Let $p_{\nu-1}(t)$ the interpolation polynomial of $f(x)$ in the Hermite sense at the roots of $\mu(t)$

Then $f(A) = p_{\nu-1}(A)$

Truncated Taylor series is an interpolation of e^x at repeated nodes $= 0$

$$A \to A - \mu I \qquad \mu = \frac{\mathrm{trace}(A)}{N}$$



$K_m(A, v)$ Krylov space $= \langle \{ v, Av, A^2 v, \ldots, A^{m-1} v \} \rangle$

$A \in \mathbb{R}^{N \times N}$

$m \ll N$

$K_m(A, v) = \langle \{ v_1, v_2, \ldots, v_m \} \rangle$ $\qquad v_1 = \frac{v}{\|v\|_2}$

orthonormal basis

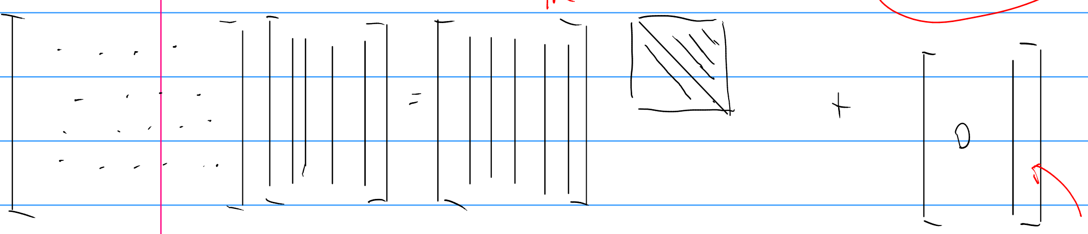
$V_m = [v_1, v_2, \ldots, v_m] \in \mathbb{R}^{N \times m}$

$V_m^T V_m = I_m \qquad V_m V_m^T = ???$

Arnoldi factorization

$$A V_m = V_m \underbrace{H_m}_{\substack{\text{Hessenberg} \\ \mathbb{R}^{m \times m}}} + \underbrace{h_{m+1,m}}_{\in \mathbb{R}} \underbrace{v_{m+1}}_{\in \mathbb{R}^N} \underbrace{e_m^T}_{\in \mathbb{R}^m}$$

different from zero



$= V_{m+1} \bar{H}_m \qquad \bar{H}_m = \begin{bmatrix} H_m \\ 0 \ldots 0 \; h_{m+1,m} \end{bmatrix} \in \mathbb{R}^{m+1 \times m}$

$$V_m^T A V_m = H_m$$

Arnoldi costs $\underbrace{\mathcal{O}(m^2)}_{\text{orthogonalization}} + \underbrace{\mathcal{O}(mN)}_{m \text{ matrix-vector}}$

number of nonzeros of A is $\mathcal{O}(N)$ A is sparse

- Arnoldi factorization is used for iterative methods for linear systems (GMRES)

- Arnoldi incomplete orthogonalization: costs $\mathcal{O}(m) + \mathcal{O}(mN)$

$$A V_m \approx V_m H_m$$

$$(\lambda I_N - A) V_m \approx V_m (\lambda I_m - H_m) \qquad \lambda \in \mathbb{C}$$

$$\|v\|_2 V_m (\lambda I_m - H_m)^{-1} e_1 \approx \|v\|_2 (\lambda I_N - A)^{-1} V_m e_1 =$$

$$v_1 = \frac{v}{\|v\|_2} \qquad \|v\|_2 (\lambda I_N - A)^{-1} v_1 = (\lambda I_N - A)^{-1} v$$

$$\lambda \notin \mathcal{F}(A) = \{ x^* A x : x \in \mathbb{C}^N, \|x\|_2 = 1 \} \supseteq \sigma(A)$$

Field of values

if $Av = \lambda v$

$v^* A v = \lambda$

$$\mathcal{F}(A) \supseteq \mathcal{F}(H_m)$$

$$V_m^T A V_m = H_m \qquad x^* H_m x \in \mathcal{F}(H_m)$$

$$\quad = \underbrace{x^* V_m^T}\, A\, \underbrace{V_m x}$$

$$e^{A} v = \frac{1}{2\pi i} \int_{\Gamma} e^{\lambda} (\lambda I_n - A)^{-1} v \, d\lambda$$

Γ exterior to $\sigma(A)$

Cauchy contour integral representation

$$\approx \frac{1}{2\pi i} \int_{\Gamma} e^{\lambda} \|v\|_2 V_m (\lambda I_m - H_m)^{-1} e_1 \, d\lambda =$$

$$\|v\|_2 V_m \frac{1}{2\pi i} \int_{\Gamma} e^{\lambda} (\lambda I_m - H_m)^{-1} e_1 \, d\lambda =$$

$$\|v\|_2 V_m e^{H_m} e_1 \approx e^{A} v$$

Krylov approximation to $e^{A} v$

$h_{j+1,j} \neq 0 \Rightarrow$ the geometric multiplicity of each eigenvalue of H_m is 1.

minimal polynomial $\equiv$ characteristic polynomial

$$e^{H_m} = p_{m-1}(H_m)$$

$p_{m-1}(x)$ interpolates e^{x} at the eigenvalues of H_m

Lemma: $p_j(A) v_1 = V_m p_j(H_m) e_1$

for every polynomial p_j of degree $j \leq m-1$

proof: By induction

$j=0$ $\quad v_1 = V_m e_1$ $\quad$ TRUE

Suppose true for $j \leq m-2$.

$V_m V_m^T w = w \qquad w \in K_m(A, v)$

$w = \alpha_1 v_1 + \dots + \alpha_m v_m$

$$V_m^T w = \begin{pmatrix} \alpha_1 \\ \alpha_2 \\ \vdots \\ \alpha_m \end{pmatrix} \qquad V_m \begin{pmatrix} \alpha_1 \\ \vdots \\ \alpha_m \end{pmatrix} = w$$

$$\underset{\substack{\cap \\ K_m}}{A^{j+1} v_1} = V_m V_m^T A^{j+1} v_1 = V_m V_m^T A \underbrace{A^j v_1}_{\in K_m}$$

$$= V_m \underbrace{V_m^T A V_m}_{H_m} V_m^T A^j v_1$$

$$= V_m H_m V_m^T A^j v_1$$

by induction hypotesis $\quad A^j v_1 = V_m H_m^j e_1$

$$V_m^T A^j v_1 = H_m^j e_1$$

$$= V_m H_m H_m^j e_1 = V_m H_m^{j+1} e_1$$

$\square$

Theorem

$$e^A v \approx \|v\| V_m e^{H_m} e_1 = p_{m-1}(A) v$$

$p_{m-1}(x)$ interpolates e^x at the eigenvalues of H_m

Proof

$$\|v\| V_m e^{H_m} e_1 = \|v\| V_m p_{m-1}(H_m) e_1 =$$

$$\|v\| p_{m-1}(A) v_1 =$$

$$p_{m-1}(A) v$$

$\square$

Rational Krylov

$$K_m := \{ v, (\eta A - I)^{-1} v, (\eta A - I)^{-2} v, \dots, (\eta A - I)^{1-m} v \}$$

$$(\eta A - I)^{-1} V_m \approx V_m H_m$$

$$f\left((\eta A - I)^{-1} \right) v \approx \|v\| V_m f(H_m) e_1$$

$$f(z) = e^{\frac{z^{-1}+1}{\eta}}$$

m for rational Krylov < m for (polynomial) Krylov

it requires linear systems to be solved