LECTURE 07

$AV = VD$ (eig in MATLAB size(A) ≈ 1000)

$f(A) = V f(D) V^{-1}$

DIAGONALIZATION is cond(V) is small

$A \approx D_{xx}$ A was symmetric

For normal matrices $\mathrm{cond}_2(V) = 1$

For general boundary, A is not symmetric

In some exponential integrator

$f_1(A) = V f_1(D) V^{-1}$ $\varphi_1(\tau A)$

$f_2(A) = V f_2(D) V^{-1}$ $\varphi_1(c_2 \tau A)$ $c_2 \neq 1$

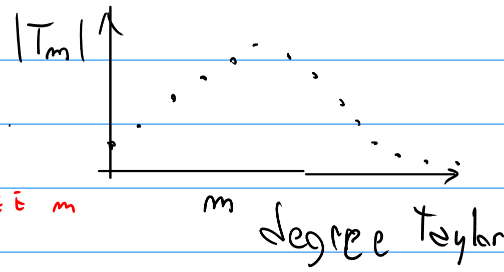
$A \approx d D_{xx} + c D_x$ DIFFUSION - ADVECTION

$d \frac{1}{h^2}[1,-2,1] + c \frac{1}{2h}[-1,0,1]$

$f(z) = e^z$ $z \in \mathbb{C}$ TAYLOR + SCALING AND SQUARING

$e^z = 1 + z + \frac{z^2}{2} + \dots$

$e^{-10} = 1 + (-10) + \frac{100}{2} + \frac{-1000}{6} + \dots$



TAYLOR SUM OF DEGREE m

$\shortparallel$

If $|z| < 1$ $e^z \approx T_m(z)$ is good

if $\left| \frac{z^{m+1}}{(m+1)!} \right| < \left(\sum_{k=0}^{m} \frac{z^k}{k!} \right) \cdot tol$ STOP

EARLY TERMINATION

SCALING AND SQUARING TECHNIQUE

$$e^{z} = e^{z/2} e^{z/2} = \left(e^{z/4} e^{z/4}\right) \underbrace{\left(e^{z/4} e^{z/4}\right)}_{e^{z/2}}$$

if $z = -s$

Find the smallest scaling $s \in \mathbb{N}$ such that $\frac{|z|}{2^s} < 1$

compute $E = T_m\left(\frac{z}{2^s}\right)$

for $i = 1:s$
  $E = E \cdot E$
end

ATTENTION

s should not be too large

$$T_m\left(\frac{z}{2^s}\right) = \underbrace{1 + \frac{z}{2^s}}_{\text{could be 1 in finite arithmetic}} + \frac{\left(\frac{z}{2^s}\right)^2}{2} + \frac{\left(\frac{z}{2^s}\right)^3}{6} + \dots$$

s too large produces overscaling

$$e^{z} = \lim_{m \to \infty} \left(1 + \frac{z}{m}\right)^m$$

$$e^{z} \approx \left(\underbrace{1 + \frac{z}{m}}_{\text{overscaling for } m \text{ large}}\right)^m$$

PADÉ AND SCALING AND SQUARING

if $|z| < 1$ $\qquad e^{z} \approx \frac{a_1 + a_2 z}{1 + b_2 z} = R_{1,1}(z)$

$$\left(1+b_2 z\right)\left(1+z+\frac{z^2}{2}+\dots\right)=a_1+a_2 z$$

degree 0 $\quad 1 = a_1$

degree 1 $\quad 1+b_2 = a_2$

degree 2 $\quad \frac{1}{2}+b_2 = 0$

$$e^z \approx \frac{1+\frac{z}{2}}{1-\frac{z}{2}}$$

$$\begin{cases} y'(t) = z\,y(t) \\ y(0) = 1 \end{cases} \qquad y(t) = e^{tz}$$

APPLY THE TRAPEZOIDAL RULE FOR $y(1)$

$$y_{m+1} = y_m + \frac{1}{2} z\, y_m + \frac{1}{2} z\, y_{m+1}$$

$$y_{m+1} = \frac{1+\frac{z}{2}}{1-\frac{z}{2}}\, y_m$$

Higher order $R_{p-1,p-1}(z)$

$$e^z \approx \frac{1+\frac{z}{2}+a_3 z^2+\dots+a_p z^{p-1}}{1-\frac{z}{2}+a_3 z^2-a_4 z^3+\dots+(-1)^{p-1} a_p z^{p-1}}$$

All the coefficients are explicitly known for any degree

$$R_{p-1,p-1}(-z) = \frac{1}{R_{p-1,p-1}(z)}$$

property preserving

$$e^{-z} = \frac{1}{e^z}$$

FALSE FOR TAYLOR

$$1-z+\frac{z^2}{2}-\frac{z^3}{6}+\dots \neq \frac{1}{1+z+\frac{z^2}{2}+\dots}$$

$\varphi_1(z) \qquad z \in \mathbb{C}$

$$\varphi_1(z) = \frac{e^z-1}{z}$$

can be used for $|z| \geq 1$

phi1.m

$\varphi_1(z) = 1 + \frac{z}{2} + \frac{z^2}{6} + \dots$ for $|z| < 1$ phi1.m

$|z| < 2$ it is also fine

MODIFIED SCALING AND SQUARING

$$\varphi_1(z) = \frac{1}{2}\left(e^{z/2} + 1\right)\varphi_1\left(\frac{z}{2}\right) \qquad \varphi_1\left(\frac{z}{2}\right) = \frac{e^{\frac{z}{2}} - 1}{\frac{z}{2}}$$

Proof

$$\varphi_1(z) = \frac{e^z - 1}{z} = \frac{1}{z}\left[e^{\frac{z}{2}}\left(\frac{z}{2}\varphi_1\left(\frac{z}{2}\right) + 1\right) - 1\right] =$$

$$\frac{1}{\cancel{z}}\left[\frac{\cancel{z}}{2} e^{\frac{z}{2}} \varphi_1\left(\frac{z}{2}\right) + \frac{\cancel{z}}{2}\varphi_1\left(\frac{z}{2}\right) \cancel{+1} \cancel{-1}\right] = \frac{1}{2}\left(e^{\frac{z}{2}} + 1\right)\varphi_1\left(\frac{z}{2}\right)$$

Find $s \in \mathbb{N}$ such that $\frac{|z|}{2^s} < 1$

TAYLOR SUM OF DEGREE m FOR φ_1 $= T_{m,1}\left(\frac{z}{2^s}\right) = P_1$

$$\frac{z}{2^s} P_1 + 1 = E$$

for $i = 1 : s$

$P_1 = \frac{1}{2}(E + 1) \cdot P_1$

$E = E \cdot E$

end

EXAMPLE : suppose $S = 2$

$$\left.\begin{aligned} P_1 &= \varphi_1\left(\frac{z}{4}\right) \\ E &= e^{z/4} \\ P_1 &= \varphi_1\left(\frac{z}{2}\right) \\ E &= e^{z/2} \\ P_1 &= \varphi_1(z) \\ E &= e^{z} \end{aligned}\right\}$$

FOR SOME ERK2

$C_2 = \frac{1}{2}$

$\varphi_1(\tau A) \qquad \varphi_1\left(\frac{\tau}{2} A\right)$

$\exp(\tau A)$

$$\varphi_2(z) = \frac{1}{2} + \frac{z}{6} + \frac{z^2}{24} + \dots$$ CAN BE USED FOR $|z|<1$

$$\varphi_2(z) = \frac{\varphi_1(z)-1}{z} \qquad |z|>1$$

MODIFIED SCALING AND SQUARING

Find $s \in \mathbb{N}$ such that $\frac{|z|}{2^s} < 1$

$$T_{m,2}\left(\frac{z}{2^s}\right)$$

$$\varphi_2(z) = \frac{1}{4}\left[\left(e^{\frac{z}{2}}+1\right)\varphi_2\left(\frac{z}{2}\right) + \varphi_1\left(\frac{z}{2}\right)\right]$$

PROOF:

$$\varphi_2(z) = \frac{\varphi_1(z)-1}{z} = \frac{1}{z}\,\frac{1}{2}\left[\left(e^{\frac{z}{2}}+1\right)\varphi_1\left(\frac{z}{2}\right) - 2\right] =$$

$$\frac{1}{2z}\left[e^{\frac{z}{2}}\left(\frac{z}{2}\varphi_2\left(\frac{z}{2}\right)+1\right) + \left(\frac{z}{2}\varphi_2\left(\frac{z}{2}\right)+1\right) - 2\right] =$$

... EXERCISE FOR YOU

COMPUTE $P_2 = T_{m,2}\left(\frac{z}{2^s}\right)$

$$P_1 = \frac{z}{2^s} P_2 + 1$$

$$E = \frac{z}{2^s} P_1 + 1$$

$$\begin{array}{c|ccc} 0 & & & \\ c_2 & a_{2,1} & & \\ c_3 & a_{3,1} & a_{3,2} & \\ \vdots & & & \\ c_\nu & & & \\ \hline & b_1 & b_2 & b_3 \end{array}$$

for $i = 1 : s$

$$P_2 = \frac{1}{4}\left[(E+1)P_2 + P_1\right]$$

$$P_1 = \frac{1}{2}(E+1)P_1$$

$$E = E \cdot E$$

end

we get also $\varphi_2\left(\frac{z}{2^s}\right), \varphi_2\left(\frac{z}{2^{s-1}}\right), \dots, \varphi_1\left(\frac{z}{2^s}\right), \dots, e^{\frac{z}{2^s}}$

TAYLOR EXPANSION FOR $\exp(A)$

GOOD WHEN $\|A\| < 1$

$\|A\|_1$ is much easier $\|A\|_2 = \sqrt{\rho(A^T A)}$

$\|A\|_\infty$

$\|A\|_F$

$$\exp(A) \approx I + A + \frac{A^2}{2} + \frac{A^3}{6} + \frac{A^4}{24} + \frac{A^5}{5!} + \frac{A^6}{6!} = T_6(A)$$

$$\frac{\|A^{m+1}\|}{(m+1)!} < \left\| \sum_{k=0}^{m} \frac{A^k}{k!} \right\| \cdot tol$$

$A_2 = A \cdot A$ $\underbrace{A_2 \cdot A}_{= A_3}$ $A_2 \cdot A_2$ $A_3 A_2$ $A_3 A_3$

1   2   3   4   5

MAIN COST IS 5 matrix - matrix

GEMM BLAS

Horner scheme
$$\left(\left(\left(\left(\left(\frac{A}{6!} + \frac{I}{5!}\right) A + \frac{I}{24}\right) A + \frac{I}{6}\right) A + \frac{I}{2}\right) A + I\right) A + I$$

1   2   3   4   5

PATERSON - STOCKMEYER

$$\underbrace{\frac{1}{6!}}_{B_2} (A^3)^2 + \underbrace{\left(\frac{1}{5!} A^2 + \frac{A}{24} + \frac{I}{6}\right)}_{B_1} A^3 + \underbrace{\left(\frac{A^2}{2} + A + I\right)}_{B_0} =$$

$$(B_2 A^3 + B_1) A^3 + B_0$$

$A_2 = A^2 = A \cdot A$ 1

$A^3 = A_2 \cdot A$ 1   3 GEMM

$(B_2 A^3 + B_1) \cdot A^3$ 1

P.S. requires in advance the degree m

PADÉ : $\exp(A) \approx (I + \underset{= -\frac{1}{2}}{b_2} A)^{-1} (\underset{= 1}{a_1} I + \underset{= \frac{1}{2}}{a_2} A)$

$= R_{1,1}(A)$

requires solution of linear systems LAPACK

$$\varphi_1(A) = (\exp(A) - I)\, A^{-1}$$ only for A non-singular

GOOD FOR 1) cond(A) not too large
AND 2) $\|A\| > 1$

if $\|A\| < 1 \Rightarrow T_{m,1}(A)$ or $R_{p-1,p-1}(A)$
if $\|A\| > 1$ and $\mathrm{cond}(A) \gg 1$ then
MODIFIED SCALING AND SQUARING

$$\varphi_2(A) = (\varphi_1(A) - I)\, A^{-1}$$

expm. in MATLAB :
- DIAGONALIZATION IF A is Hermitian (edit expm)
- PADÉ APPROX. WITH SCALING AND SQUARING

phipade.m : always padé approximation

phi_funm.m : " " "

OPEN PROBLEM : HOW TO CHOOSE m in T_m ?
WE WOULD LIKE TO ESTIMATE m
DEPENDING ON A GIVEN TOLERANCE.
IF YOU KNOW m, YOU TRANSFOR AN ITERATIVE
METHOD INTO A DIRECT METHOD.