LECTURE 7

$AV = VD$

$f(A) = V f(D) V^{-1} \approx V \tilde{f}(D) V^{-1}$ (MATLAB ≥ 2024A)

\+ MATRICI SIMMETRICHE

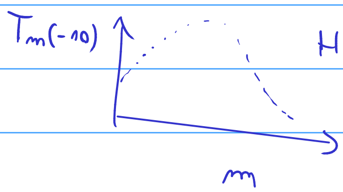
$\| V f(D) V^{-1} - V \tilde{f}(D) V^{-1} \| \leq$ expm.m

$\text{cond}(V) \; \| f(D) - \tilde{f}(D) \|$

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

$f(z) = e^z$

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



HUMP

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

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

ROUGH

SCALING AND SQUARING

$e^z = e^{z/2} \cdot e^{z/2} = \underbrace{(e^{z/4} e^{z/4})} \underbrace{(e^{z/4} e^{z/4})}$

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

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

for $i = 1:s$

$E = E * E$

end

s should not be too large OVERSCALING

$1 + \frac{z}{2^s} + \frac{\left(\frac{z}{2^s}\right)^2}{2} + \dots$

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

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

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

$$\begin{cases} 1 = a_1 \\ 1 + b_2 = a_2 \\ \frac{1}{2} + b_2 = 0 \end{cases} \qquad e^z \approx \frac{1 + \frac{z}{2}}{1 - \frac{z}{2}}$$

Padé approximation $(1,1)$

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

TRAPEZOIDAL RULE $y(1)$

$$y_{n+1} = y_n + \frac{z}{2} y_n + \frac{z}{2} y_{n+1} \Rightarrow y_{n+1} = \frac{1 + \frac{z}{2}}{1 - \frac{z}{2}} y_n$$

Higher Order $R_{p,p}(z)$

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

MATLAB
expm.m
Padé +
scaling and squaring

NICE SIDE EFFECT

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

$$\varphi_1(z) = \frac{e^z - 1}{z} \qquad \text{use it for } |z| > 1$$

$$\varphi_1(z) = 1 + \frac{z}{2} + \frac{z^2}{6} + \dots$$

MODIFIED SCALING AND SQUARING

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

PROOF

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

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

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

$\approx \varphi_1$

COMPUTE $P_1 = T_{m,1}\left(\frac{z}{2^s}\right)$

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

for $i = 1:s$

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

$E = E * E$ $\Rightarrow \approx e^z$

end

Padè for $\varphi_1(z)$

$$e^z - 1 \approx z \cdot \frac{a_1 + a_2 z}{1 + b_2 z}$$

$$\varphi_2(z) = \sum_{i=0}^{\infty} \frac{z^i}{(i+2)!} = \frac{1}{2} + \frac{z}{6} + \frac{z^2}{24} + \dots$$

$$= \frac{e^z - 1 - z}{z^2} = \frac{\frac{e^z-1}{z} - 1}{z} = \frac{\varphi_1(z) - 1}{z}$$

MODIFIED SCALING AND SQUARING

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

PROOF :

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

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

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

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

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

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

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

For $i = 1:s$

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

$\approx \varphi_1(z)$

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

$\approx e^{z}$

$E = E * E$

$\approx \varphi_2\left(\frac{z}{2}\right)$

end

$\varphi_2\left(\frac{z}{4}\right)$

MATRIX CASE : ALMOST THE SAME

TAYLOR T_6 FOR e^A : $I + A + \frac{A^2}{2} + \frac{A^3}{6} + \frac{A^4}{24} + \frac{A^5}{5!} + \frac{A^6}{6!}$

COST : $1 \quad A^2 * A \quad A^3 * A$

$1 \quad 1 \quad 1 \quad 1$

5 matrix-matrix products (DGEMM BLAS 3)

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

COST : 5 matrix-matrix products

PATERSON STOCKMEYER

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

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

$A^2 \quad 1$

$A^3 \quad 1 \qquad$ 3 matrix-matrix

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

PADÉ $\qquad e^A \approx (I + b_2 A)^{-1} (a_1 I + a_2 A)$

linear system solutions LAPACK

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

GOOD FOR cond (A) not too large

AND $\|A\| \to 1$

if $\|A\| < 1$ TAYLOR

PADÈ

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

GO BACK TO e^A: how to select s, m

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

$$T_m\left(\frac{A}{2^s}\right)^{2^s} - \exp(A) = E$$ FORWARD ERROR

$$\log(e^{-x} T_m(x)) = h_{m+1}(x)$$

$$e^{-x} T_m(x) = e^{h_{m+1}(x)}$$

$$T_m(x) = e^{x + h_{m+1}(x)}$$

$$T_m\left(\frac{A}{2^s}\right)^{2^s} = \left(e^{\frac{A}{2^s} + h_{m+1}\left(\frac{A}{2^s}\right)}\right)^{2^s} =$$

$$= e^{A + 2^s h_{m+1}\left(\frac{A}{2^s}\right)} = e^{A + \Delta A}$$

$$h_{m+1}(x) = \log\Big(e^{-x}\big(\underbrace{e^x - \frac{x^{m+1}}{(m+1)!} - \frac{x^{m+2}}{(m+2)!} - \dots}_{T_m(x)}\big)\Big) =$$

$$\log\left(1 + O(x^{m+1})\right) =$$

HINT:

$\log(1 + x^2) =$

$x^2 - \dots$

$$\log\left(1 + b_{m+1} x^{m+1} + b_{m+2} x^{m+2} + \dots\right) =$$

$$c_{m+1} x^{m+1} + c_{m+2} x^{m+2} + \dots$$

c_{m+1}, c_{m+2} can be compute with a software for high precision arithmetic

$$h_{m+1}(x) = \sum_{i=m+1}^{\infty} c_i x^i$$

We want

$$\frac{\|\Delta A\|}{\|A\|} = \frac{\|2^s h_{m+1}(2^{-s}A)\|}{\|A\|} =$$

$$\frac{\|h_{m+1}(2^{-s}A)\|}{\|2^{-s}A\|} \leq \frac{\tilde{h}_{m+1}(2^{-s}\|A\|)}{2^{-s}\|A\|} \leq tol$$

$$h_{m+1}(x) = \sum_{i=m+1}^{\infty} c_i x^i \qquad \tilde{h}_{m+1}(x) = \sum_{i=m+1}^{\infty} |c_i| x^i$$

$$\|h_{m+1}(x)\| \leq \|\tilde{h}_{m+1}(x)\| \leq \tilde{h}_{m+1}(\|x\|)$$

$$2^{-s}\|A\|_1 \leq \vartheta_m$$

$$\frac{\tilde{h}_{m+1}(\vartheta)}{\vartheta} \leq tol$$

increasing function

$$\tilde{h}_{m+1}(\vartheta_m) = \vartheta_m \cdot tol = \frac{\varepsilon}{2}$$

$$\mathrm{tol} = \frac{\varepsilon}{2} \approx 1.1 \cdot 10^{-16}$$

$\vartheta_{55} = 9.9$ $\qquad$ $\vartheta_{40} = 6$

$$\|A\|_1 = 19$$

$s = 1$ $\quad \frac{19}{2} = 9.5$ $\qquad$ $s=2$ $\quad \frac{19}{2^2} = 4.75$

T_{55} $\quad$ 54 matrix-matrix
+ 1 squaring
55

T_{40} $\quad$ 39 matrix-matrix
+ 2 squaring
41

BACKWARD ERROR ANALYSIS

+ EARLY TERMINATION