Numerical methods for matrix functions

SF2524 - Matrix Computations for Large-scale Systems

Lecture 14: Specialized methods

Specialized methods

- Matrix exponential - scaling-and-squaring
  - Matlab: `expm(A)`
  - Julia: `exp(A)`
- Matrix square root
  - Matlab: `sqrtm(A)`
  - Julia: `sqrt(A)`
- Matrix sign function

Matrix exponential

PDF Lecture notes 4.3.1

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Repeated squaring

Given $C = \exp(A/2^j)$, we can compute $\exp(A)$ with j matrix-matrix multiplications: $C_0 = C$

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From Theorem 4.1.2:

$$\mathrm{Error} \sim \|B\|^N = \|A/m\|^N = \|A\|^N/m^N$$

$\Rightarrow$ fast if $m \gg \|A\|$

Idea 1: Better (rational approx)

Use a rational approximation of matrix expoential:

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where $N_{pq} \in P_p$ and $D_{pq} \in P_q$.

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More precisely, for *Padé approximation* of exponential we have

$$\begin{aligned} N_{pq}(z) &= \sum_{k=0}^{p} \frac{(p+q-k)!p!}{(p+q)!k!(p-k)!} z^k \\ D_{pq}(z) &= \sum_{k=0}^{q} \frac{(p+q-k)!q!}{(p+q)!k!(q-k)!} (-z)^k. \end{aligned}$$

Parameters p and q can be chosen such that a specific error can be guaranteed.

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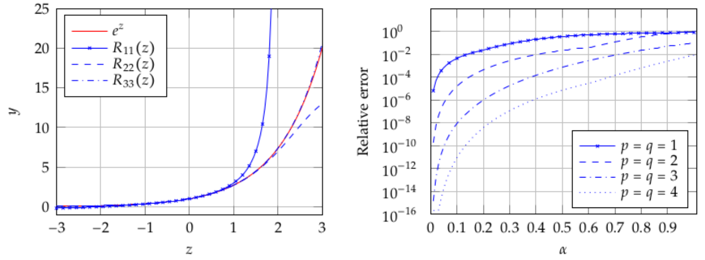
$$\sum^{p} \quad (p+q-k)!p!$$



(a) Error in Padé approximation

(b) $\|R_{pq}(\alpha A) - \exp(\alpha A)\| / \|\exp(\alpha A)\|$

Parame … e

guarant

Input: $\delta > 0$ and $A \in \mathbb{R}^{n \times n}$
Output: $F = \exp(A + E)$ where $\|E\|_\infty \leq \delta \|A\|_\infty$.

begin

$j = \max(0, 1 + \text{floor}(\log_2(\|A\|_\infty)))$

$A = A/2^j$

Let q be the smallest non-negative integer such that $\varepsilon(q, q) \leq \delta$.

$D = I; N = I; X = I; c = 1$

for $k = 1 : q$ **do**

$c = c(q - k + 1)/((2q - k + 1)k)$

$X = AX; N = N + cX; D = D + (-1)^k cX$

end

Solve $DF = N$ for F

for $k = 1 : j$ **do**

$F = F^2$

end

end

Algorithm 2: Scaling-and-squaring for the matrix exponential

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- Matrix-vector product: $\mathcal{O}(n^2)$ (Exploit in next lecture for $f(A)b$)
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$N_{pp}(B) = D_{pp}(-B)$ which gives that

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Result: High-degree approximation can be evaluated cheaper than Taylor.

Matrix square root

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Then, with $f(z) = \sqrt{z}$ the matrix function

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$$F^2 = A$$

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* Prove equivalence with Newton's method for $A = A^T$ *

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- Much less sensitive to round-off than Newton-SQRT
- One step requires two matrix inverses

Matrix sign function

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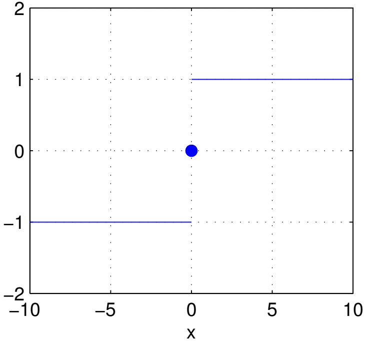
Scalar-valued sign function

$$\mathrm{sign}(x) = \begin{cases} -1 & \text{if } x < 0 \\ 0 & \text{if } x = 0 \\ 1 & \text{if } x > 0 \end{cases}$$



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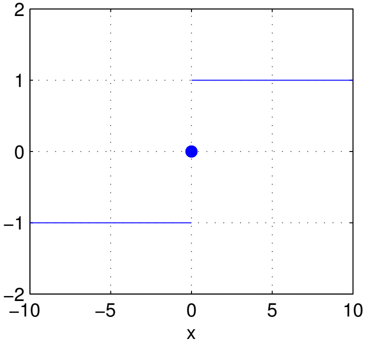

Now: Matrix version.

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Definition matrix sign

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Matrix sign iteration

$$\begin{aligned} S_0 &= A \\ S_{k+1} &= \frac{1}{2}(S_k + S_k^{-1}) \end{aligned}$$

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Theorem (Global quadratic convergence of sign iteration)

Suppose $A \in \mathbb{R}^{n\times n}$ has no eigenvalues on the imaginary axis. Let $S = \operatorname{sign}(A)$, and S_k be generated by Sign iteration. Let

$$G_k := (S_k - S)(S_k + S)^{-1}. \tag{1}$$

Then,

- $S_k = S(I + G_k)(I - G_k)^{-1}$ *for all* k,
- $G_k \to 0$ *as* $k \to \infty$,
- $S_k \to S$ *as* $k \to \infty$, *and*
- $$\|S_{k+1} - S\| \leq \frac{1}{2}\|S_k^{-1}\|\|S_k - S\|^2. \tag{2}$$