Numerical methods for matrix functions

SF2524 - Matrix Computations for Large-scale Systems

Lecture 14: Specialized methods

Specialized methods

- Matrix exponential - scaling-and-squaring (`expm(A)`)
- Matrix square root (`sqrtm(A)`)
- Matrix sign function

From basic properties of matrix functions:

$$\exp(A) = \exp(A/2)\exp(A/2).$$

Repeat:

$$\exp(A) = \exp(A/4)\exp(A/4)\exp(A/4)\exp(A/4).$$

...

For any j

$$\exp(A) = \left(\exp(A/2^j)\right)^{2^j}$$

Repeated squaring

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

$$C_i = C_{i-1}^2, \quad i = 1, \ldots, j$$

We have $C_j = \exp(A)$.

* Matlab: squaring property *

Computing $\exp(A/m)$

How to compute $\exp(A/m)$, where $m = 2^j$ for large m?
Note: $\|\frac{1}{m}A\| \ll 1$ when m is large.
Use approximation of matrix exponential which is good close to origin.

Idea 0: Naive

Use Truncated Taylor with expansion $\mu = 0$

$$\exp(B) \approx I + \frac{1}{1!}B + \cdots + \frac{1}{N!}B^N$$

From Theorem 4.1.2:

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

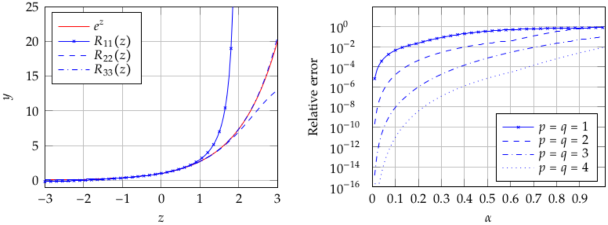
$\Rightarrow$ fast if when $m \gg \|A\|$

Idea 1: Better (rational approx)

Use a rational approximation of matrix expoential:

$$\exp(B) \approx N_{pq}(B)^{-1} D_{pq}(B)$$

where $N_{pq}, D_{pq} \in P_p$.One can show that this approximation better than truncated Taylor.More precisely,



(a) Error in Padé approximation (b) $\|R_{pq}(\alpha A) - \exp(\alpha A)\| / \|\exp(\alpha A)\|$

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

* Matlab demo with rational approx *

Matrix square root

PDF Lecture notes 4.3.2

Suppose

$$\lambda(A) \cap (-\infty, 0] = \emptyset$$

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

$$F = f(A)$$

is well-defined with the Jordan definition or Cauchy definition. Moreover,

$$F^2 = A$$

* Proof on black board. *

* MATLAB demo *

Newton's method for scalar-valued equation:

$$g(x) = x^2 - a = 0$$

Simplifies to

$$x_{k+1} = \ldots = \frac{1}{2}(x_k + a x_k^{-1})$$

Newton's method for matrix square root (Newton-SQRT)

$$\begin{aligned} X_0 &= A \\ X_{k+1} &= \frac{1}{2}(X_k + A X_k^{-1}) \end{aligned}$$

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

Unfortunately: Newton's method for matrix square root is numerically unstable

Better in terms of stability:

Denman-Beavers algorithm

$$\begin{aligned} Y_0 &= I \\ X_{k+1} &:= \frac{1}{2}(X_k + Y_k^{-1}) \\ Y_{k+1} &:= \frac{1}{2}(Y_k + X_k^{-1}) \end{aligned}$$

Properties of Denman-Beavers:

- Equivalent to Newton-SQRT in exact arithmetic, but very different in finite arithmetic

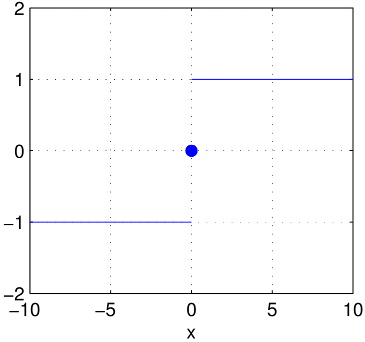
  proof on black board

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

Matrix sign function
PDF Lecture notes 4.3.3

Scalar-valued sign function

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



Now: Matrix version.

Applications

Quantum Chemistry (linear scaling DFT-code) and systems and control (Riccati equation)

For all cases except $x = 0$:

$$
\begin{aligned}
|x| &= \sqrt{x^2} \\
\mathrm{sign}(x) &= \frac{|x|}{x} = \frac{\sqrt{x^2}}{x}
\end{aligned}
$$

Definition matrix sign

$$\mathrm{sign}(A) = \sqrt{A^2} A^{-1}$$

Naive method

Compute directly

$$\operatorname{sign}(A) = \sqrt{A^2}A^{-1}$$

We can do better: Combine Newton-SQRT with A^2 and A^{-1}

* Derivation based on defining $S_k = A^{-1}X_k$ where X_k Newton-SQRT for $\sqrt{A^2}$* ...

Matrix sign iteration

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

Convergence

- Local quadratic convergence follows from Newton equivalence.
- We even have global convergence ...

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*
- $$\|S_{k+1} - S\| \le \frac{1}{2}\|S_k^{-1}\|\|S_k - S\|^2. \tag{2}$$