The matrix square root

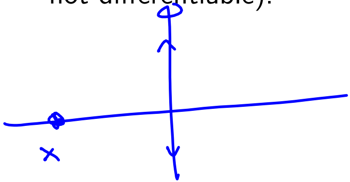
$f(x) = \sqrt{x} \in RHP$

Next (and last, for us) matrix function: $A^{1/2}$, principal square root.

$A^{1/2}$ is well defined unless A has:

- Real eigenvalues $\lambda_i < 0$, or
- Non-trivial Jordan blocks at $\lambda_i = 0$ (because $g(x) = x^{1/2}$ is not differentiable).

$f'(x) = \frac{1}{2\sqrt{x}}$ non esiste in 0



Non esiste $\begin{bmatrix} 0 & 1 \\ 0 & 0 \end{bmatrix}^{1/2}$

(non esistono matrici $Y \in \mathbb{C}^{2\times 2}$ tali che $Y^2 = \begin{bmatrix} 0 & 1 \\ 0 & 0 \end{bmatrix}$)

Condition number / sensitivity

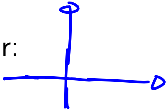
The Fréchet derivative of $f(X) = X^2$ is

$$L_{f,X}(E) = XE + EX, \quad \widehat{L} = I \otimes X + X^T \otimes I.$$

The Fréchet derivative of $g(Y) = Y^{1/2}$ is its inverse,

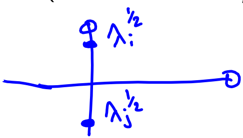
$$\widehat{L}_{g,Y} = (I \otimes Y^{1/2} + (Y^{1/2})^T \otimes I)^{-1}$$

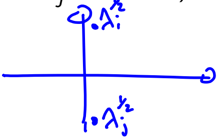
with eigenvalues $\frac{1}{\lambda_i^{1/2}+\lambda_j^{1/2}}$, $i, j = 1, \ldots, n$.

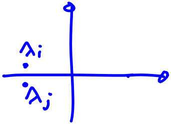


In particular, g is ill-conditioned for matrices that either:

- have a small eigenvalue (taking $i = j$), or
- have two complex conjugate eigenvalues close to the negative real axis (because then $\lambda_i^{1/2} \approx ai$, $\lambda_j^{1/2} \approx -ai$).







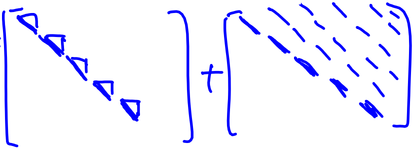
Teo: gli autovalori di $I\otimes A + B\otimes I$ sono dati da $\lambda_i+\mu_j$, dove λ_i sono gli autoval. di A e μ_j sono quelli di B

dim: $A = Q_A T_A Q_A^T$, $B = Q_B T_B Q_B^T$,

$$\overbrace{(Q_B\otimes Q_A)^T}^{\text{ortogonale}}\left(I\otimes A + B\otimes I\right)\left(\overbrace{Q_B\otimes Q_A}^{\text{ortogonale}}\right)=$$

$$= Q_B^TQ_B\otimes Q_A^TAQ_A + Q_B^TBQ_B\otimes Q_A^TQ_A =$$

$$= I\otimes T_A + T_B\otimes I =$$



matrice triang. sup. che ha $\lambda_i + \mu_j$ $i,j = 1, \dots n$, sulla diagonale.

Schur method

Recall: Schur method:

1. Reduce to a triangular T using a Schur form;
2. Compute diagonal of $S = f(T)$;
3. Compute off-diagonal entries from $ST = TS$
   Involves a denominator $t_{ii} - t_{jj}$: if it is 0, we must work on blocks.

In the case of $A^{1/2}$, we can use $S^2 = T$ to get the off-diagonal entries instead:

$$s_{ii}s_{ij} + s_{i,i+1}s_{i+1,j} + \cdots + s_{ij}s_{jj} = t_{ij}.$$

Involves a denominator $s_{ii} + s_{jj}$: always invertible because $s_{ii} + s_{jj} \in RHP$.

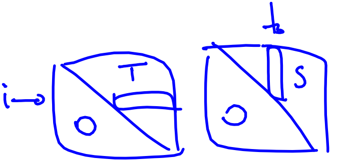
(This is what Matlab uses, by the way.)

Schur in generale:

$$s_{ii} = f(t_{ii})$$

$f(T)$

$\boxed{s_{ij} \text{ calcolato usando } TS = ST}$



$$(TS)_{ij} = t_{ii}s_{ij} + t_{i,i+1}s_{i+1,j} + \dots t_{ij}s_{jj}$$

$$\shortparallel$$

$$(ST)_{ij} = s_{ii}t_{ij} + s_{i,i+1}t_{i+1,j} + \dots + s_{ij}t_{jj}$$

Calcolando diagonale per diagonale, posso risolvere per

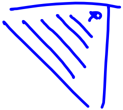
$$s_{ij} = \frac{\text{"..."}}{t_{ii} - t_{jj}} \quad \to \text{ funziona se } t_{ii} \neq t_{jj}$$

Se $f(x) = x^{1/2}$: posso calcolare S_{ij} usando

$$S^2 = T$$

$$(S^2)_{ij} = S_{ii}S_{ij} + S_{i,i+1}S_{i+1,j} + \dots + S_{ij}S_{jj} \overset{!}{=} t_{ij}$$

$$S_{ij} = \frac{t_{ij} - S_{i,i+1}S_{i+1,j} - \dots - S_{i,j-1}S_{j-1,j}}{S_{ii} + S_{jj}}$$



$S_{ii} + S_{jj}$ non è mai zero, se $T^{1/2}$ è definita:

difatti: $\underset{\text{RHP}}{\underset{\cap}{S_{ii} = t_{ii}^{1/2}}}$ $\quad$ $\underset{\text{RHP}}{\underset{\cap}{S_{jj} = t_{jj}^{1/2}}}$ $\Rightarrow S_{ii} + S_{jj} \in \text{RHP}$

(RHP = semipiano dx aperto)

Newton method

Newton method on $\boxed{X^2 - A}$:

$$\boxed{X_{k+1} = X_k - E, \quad \text{where } E \text{ solves } EX_k + X_k E = X_k^2 - A.}$$

Much more expensive than the Schur method: we solve a Sylvster equation at each step (and this requires a Schur form).

Trick: If X_0 commutes with A (for instance, taking $X_0 = \alpha I$), then $\boxed{E = (2X_0)^{-1}(X_0^2 - A)}$ and E, X_1 commute with A, too, ...

Resulting iteration:

(Modified) Newton iteration

$$\boxed{X_{k+1} = \frac{1}{2}(X_k + X_k^{-1}A),} \quad X_0 = \alpha I.$$

At each step, $X_k A = AX_k$.

Newton per una funzione multivariata $h(x)$:

$$X_{k+1} = X_k - \left(\mathrm{Jac}\, h_{X_k}\right)^{-1} h(X_k) \qquad h(X) = X^2 - A$$

$$X_{k+1} = X_k - L_{h,X_k}^{-1}\left(X_k^2 - A\right)$$

$$L_{h,X_k}(E) = EX_k + X_kE$$

(perché $\underbrace{(X_k+E)^2 - A}_{h(X+E)} = \underbrace{X_k^2 - A}_{h(X)} + \underbrace{EX_k + X_kE}_{L_{h,X_k}(E)} + o\left(\|E\|^2\right)$)

$X_{k+1} = X_k - E$, dove E risolve

$$\underbrace{EX_k + X_kE}_{\mathcal{L}_{h,X_k}(E)} = X_k^2 - A$$

$$\mathcal{L}_{h,X_k}(E) = h(X_k) \iff E = \mathcal{L}_{h,X_k}^{-1}(h(X_k))$$

$$EX_0 + X_0E = X_0^2 - A \qquad (*)$$

se X_0, A commutano, ha soluzione $(2X_0)^{-1}(X_0^2 - A) = E$

E commuta con X_0, A, quindi basta verificare $(*)$

$X_1 = X_0 - E$ commuta con A $\Rightarrow$ posso applicare lo stesso trucco anche a $X_1, X_2, X_3, \dots$

Square root and sign

(Modified) Newton iteration

$$\boxed{X_{k+1} = \frac{1}{2}(X_k + X_k^{-1}A), \quad X_0 = \alpha I.}$$

Pre-multiply by $A^{-1/2}$, and use commutativity:

$X_0 = \alpha I \quad \alpha > 0$

$$A^{-1/2}X_{k+1} = \frac{1}{2}\left(A^{-1/2}X_k + (A^{-1/2}X_k)^{-1}\right), \quad A^{-1/2}X_0 = \alpha A^{-1/2}.$$

$Z_{k+1} = \frac{1}{2}(Z_k + Z_k^{-1})$

$Z_0 = \alpha A^{-\frac{1}{2}}$

This is the sign iteration! $A^{-1/2}X_k \to \operatorname{sign}(A^{-1/2}) = I$.

Hence,

$Z_k = A^{-\frac{1}{2}} X_k \to \operatorname{sign}(Z_0) = \operatorname{sign}(\alpha A^{-\frac{1}{2}}) = I$

$\boxed{X_k \to A^{1/2}}$, i.e., the modified Newton iteration converges (for each starting point $X_0 = \alpha I$ with $\alpha > 0$).

Local convergence

True Newton

$$X_{k+1} = X_k - E, \quad \text{where } E \text{ solves } EX_k + X_k E = X_k^2 - A.$$

This is a Newton method, so it converges quadratically (locally).

Modified Newton

$$X_{k+1} = \frac{1}{2}(X_k + X_k^{-1}A).$$

The two iterations coincide, if $\boxed{X_0 A = AX_0.}$ ...in exact arithmetic! In practice, this property is lost numerically. We need to study the convergence of MN separately.

MN is the fixed-point iteration associated to $h(X) = \frac{1}{2}(X + X^{-1}A)$.

$$h(X) = \frac{1}{2}\left(X + X^{-1}A\right)$$

$$\left(B^{-1} - C^{-1} = C^{-1}(C-B)B^{-1}\right)$$

$$L_{h,X}(E) = \frac{1}{2}\left(E - X^{-1}EX^{-1}A\right)$$

Derivata di $g(X) = X^{-1}$

$$\underbrace{(X+E)^{-1} - X^{-1}}_{g(X+E)-g(X)} = -(X+E)^{-1}\left((X+E) - \cancel{X}\right)X^{-1} =$$

$$= -(X+E)^{-1}EX^{-1} = -X^{-1}EX^{-1} + o(\|E\|)$$

$$L_{h,A^{1/2}} = \frac{1}{2}\left(E - X^{-1}EX^{-1}A\right)\Big|_{X=A^{1/2}} = \frac{1}{2}\left(1\cdot E\cdot 1 - A^{-1/2}EA^{1/2}\right)$$

$$\hat{L}_{h,A^{1/2}} = \frac{1}{2}\left(1\otimes 1 - \left(A^{1/2}\right)^T \otimes A^{-1/2}\right) \quad \in \mathbb{C}^{n^2\times n^2}$$

È vero che $\hat{L}_{h,A^{1/2}}$ ha tutti autovalori con modulo < 1?

Se λ_i sono gli autoval. di A, $\hat{L}$ ha autoval.

$$\frac{1}{2}\left(1 - \lambda_i^{1/2}\cdot\lambda_j^{-1/2}\right) \quad i,j = 1,\dots n$$

Local convergence

Local convergence of a fixed-point iteration depends on the eigenvalues of the Jacobian in the fixed-point.

The Jacobian / Fréchet derivative of $h(X) = \frac{1}{2}(X + X^{-1}A)$ is

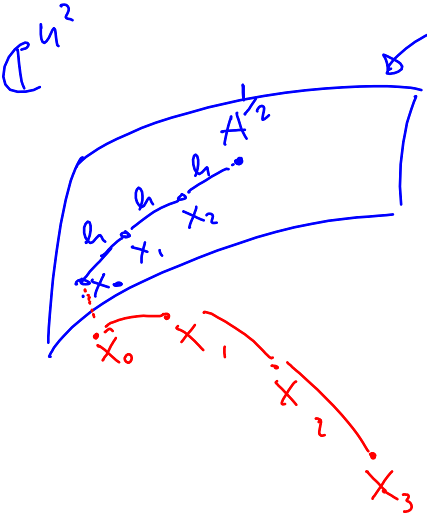
$$L_{h,X}(E) = \frac{1}{2}(E + X^{-1}EX^{-1}A),$$

using $(X+E)^{-1} - X^{-1} = (X+E)^{-1}EX^{-1} = X^{-1}EX^{-1} + o(\|E\|)$.

Hence $L_{h,A^{1/2}} = \frac{1}{2}(E + A^{-1/2}EA^{1/2})$, or
$\widehat{L}_{h,A^{1/2}} = \frac{1}{2}\left(I + (A^{1/2})^T \otimes A^{-1/2}\right)$.

It has eigenvalues $\frac{1}{2} + \frac{1}{2}\lambda_i^{1/2}\lambda_j^{-1/2}$, where λ_i are the eigenvalues of A.

It's easy to construct cases in which $L_{h,A^{1/2}}$ has eigenvalues with modulus > 1, hence $A^{1/2}$ is an unstable fixed point of $h(X)$.



sottovarietà di metriche che commutano con A

← converge (stabilmente) se resto all'interno della sottovar.

← diverge se sono fuori