Conditioning of computing matrix functions

Recall: the condition number of a differentiable $f : \mathbb{R}^m \to \mathbb{R}^n$ is the norm of its Jacobian.

$\nabla f(\xi)$

$$\kappa_{abs}(f,x) = \lim_{\varepsilon\to 0} \sup_{\|\tilde{x}-x\|\le\varepsilon} \frac{\|f(\tilde{x})-f(x)\|}{\|\tilde{x}-x\|} = \boxed{\|\nabla f\|}$$

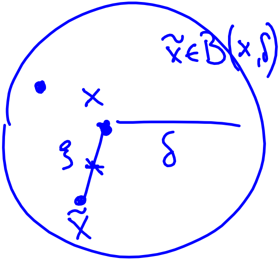
$$\frac{|f'_x|\cdot|x|}{|f(x)|}$$

$$\underline{\kappa_{rel}(f,x)} = \lim_{\varepsilon\to 0} \sup_{\frac{\|\tilde{x}-x\|}{\|x\|}\le\varepsilon} \frac{\frac{\|f(\tilde{x})-f(x)\|}{\|f(x)\|}}{\frac{\|\tilde{x}-x\|}{\|x\|}} = \kappa_{abs}(f,x)\frac{\|x\|}{\|f(x)\|}.$$

(Taylor univariato):

$$\boxed{f(\tilde{x})-f(x)=\nabla f(\xi)\cdot(\tilde{x}-x)}$$

$$\|f(\tilde{x})-f(x)\| \le \|\nabla f(\xi)\|\cdot\|\tilde{x}-x\|$$



funzione di matrice: mappa da $A \in \mathbb{R}^{n \times n}$ a

$f(A) \in \mathbb{R}^{n \times n}$

Fréchet derivative

Direct generalization of the Jacobian to matrix functions:

Definition

The Fréchet derivative of a matrix function f is the linear operator $L_{f,X} : \mathbb{R}^{m\times m} \to \mathbb{R}^{m\times m}$ (when it exists) such that

$$f(X+E) = f(X) + \boxed{L_{f,X}(E)} + o(\|E\|).$$

I.e., in a neighbourhood of X, f behaves like a linear function.

Example

$L_{f,X}: \mathbb{R}^{n\times n} \to \mathbb{R}^{n\times n}$

$f(x) = x^2$, $f(X) = X^2$.

$o(\|E\|)$

$$\underbrace{(X+E)^2}_{f(X+E)} = \underbrace{X^2}_{f(X)} + XE + EX + E^2 = X^2 + \boxed{\underbrace{XE + EX}_{L_{f,X}(E)}} + o(\|E\|).$$

$L_{f,X}$ is a linear operator that maps matrices to matrices — we can consider its vectorized version:

$$\widehat{L} : \operatorname{vec} E \mapsto \operatorname{vec} L_{f,X}(E).$$

In this case,

$$\boxed{\widehat{L} = X^T \otimes I + I \otimes X.}$$

$\widehat{L}$ is the "usual" Jacobian of the map $\operatorname{vec} X \mapsto \operatorname{vec} f(X)$.

$$\mathrm{vec}\,E = \mathrm{vec}\left(\left[E_1 \middle| E_2 \middle| \cdots \middle| E_n\right]\right) = \begin{bmatrix} E_1 \\ E_2 \\ \vdots \\ E_n \end{bmatrix}$$

prodotti di Kronecker:

$$A \otimes B = \begin{bmatrix} a_{11}B & a_{12}B & \cdots \\ a_{21}B & & \vdots \\ \vdots & & \\ a_{n1}B & \cdots & a_{nn}B \end{bmatrix}$$

$\hat{L} : \mathbb{R}^{n^2} \to \mathbb{R}^{n^2}$ mappa associata

$$\hat{L}\,\mathrm{vec}(E) = \mathrm{vec}\,L_{f,X}(E)$$

$$\mathrm{vec}(AXB) = (B^T \otimes A)\,\mathrm{vec}X$$

$$\mathrm{vec}(XE) = (I \otimes X)\,\mathrm{vec}\,E$$

$$\mathrm{vec}(EX) = (X^T \otimes I)\,\mathrm{vec}\,E$$

$$\mathrm{vec}(XE + EX) = (I \otimes X + X^T \otimes I)\,\mathrm{vec}\,E$$

$$\hat{L} = \underbrace{\boxed{\underline{I \otimes X + X^T \otimes I}}}_{}\ \ n^2 \times n^2$$

Properties

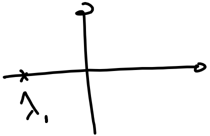
Follow from those of Jacobians:

- $L_{f+g,X} = L_{f,X} + L_{g,X}$.
- $L_{f\circ g,X} = L_{f,g(X)} \circ L_{g,X}$.
- $L_{f^{-1},f(X)} = L_{f,X}^{-1}$.

Example Let $g(y) = \sqrt{y}$ (principal branch: we take the root in the right half-plane), Y with no real nonpositive eigenvalue. Then $g(y)$ is the inverse of $f(x) = x^2$, and its Fréchet derivative $F = L_{g,Y}(E)$ is the matrix such that $L_{f,X}(F) = E$, i.e.,

$$XF + FX = E, \quad X = f(Y) = Y^{1/2}.$$

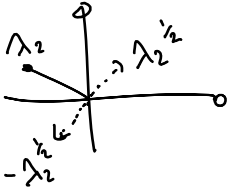
(solution of a Sylvester equation). X has eigenvalues in the right half-plane, so the Sylvester equation is always solvable: $\Lambda(X) \cap \Lambda(-X) = \emptyset$.



radici di λ_1: $\pm\sqrt{|\lambda_1|}\, i$

nessuna nel RHP

Y senza autoval. reali negativi



$$Y = f(X) = X^2$$

$$X = g(Y) = Y^{1/2}$$ ha autoval. nel RHP

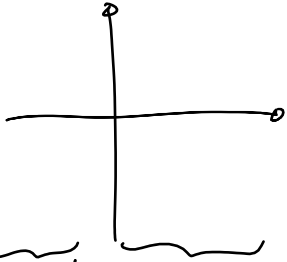
$$L_{f,X}(E) = XE + EX \qquad L = L_{g,Y}(F) = \left[L_{f(X)}\right]^{-1}(F)$$

$$L_{f,X}(L) = F \qquad XL + LX = F \qquad \boxed{Y^{1/2}L + LY^{1/2} = F}$$

La der. di Fréchet di $\sqrt{Y}$ nel punto Y è la soluzione →

dell'equazione di Sylvester $Y^{1/2}L + LY^{1/2} = F$

L'equaz. è risolubile se $Y^{1/2}$ e $-Y^{1/2}$ non hanno autoval. comuni



autoval. di $-Y^{1/2}$ stanno tutti nel LHP

autoval. di $Y^{1/2}$ stanno tutti nel RHP

Derivative of the exponential

Derivative of the matrix exponential:

$$\begin{aligned}
\exp(X+E) &= I + (X+E) + \frac{1}{2}(X+E)^2 + \frac{1}{3!}(X+E)^3 + \dots \\
&= I + (X+E) + \frac{1}{2}(X^2 + EX + XE + E^2) + \frac{1}{3!}(X^3 + \dots) \\
&= \exp(X) + E + \frac{1}{2}(EX + XE) + \frac{1}{3!}(X^2E + XEX + X^2E) \\
&\qquad + \dots + O(\|E\|^2)
\end{aligned}$$

Not simple to express.

$$\widehat{L} = I + \frac{1}{2}(I \otimes X + X^T \otimes I) + \frac{1}{3!}(I \otimes X^2 + X^T \otimes X + (X^2)^T \otimes I) + \dots$$

$$\exp(X+E) = I + X + E + \frac{1}{2}\left(X^2 + XE + EX + E^2\right) + \frac{1}{3!}\left(X^3 + X^2E + XEX + EX^2 + E^2X + EXE + XE^2 + E^3\right) + \dots$$

$$= \exp(X) + E + \frac{1}{2}(XE + EX) + \frac{1}{3!}\left(X^2E + XEX + EX^2 + \dots\right) + O\left(\|E\|^2\right)$$

$$L_{\exp,X}(E) = E + \frac{1}{2}(XE + EX) + \frac{1}{3!}\left(X^2E + XEX + EX^2\right) + \frac{1}{4!}\left(X^3E + X^2EX + \dots\right) \dots$$

$$\operatorname{vec} I \cdot E \cdot I = (I \otimes I) \operatorname{vec} E$$

$$\operatorname{vec}\left(X^2 E \cdot I\right) = \left(I \otimes X^2\right) \operatorname{vec} E$$

$$\operatorname{vec}(XEX) = \left(X^T \otimes X\right) \operatorname{vec} E$$

$f: \mathbb{R}^{n^2} \to \mathbb{R}^{n^2}$

$L_{f,X}: \mathbb{R}^{n\times n} \to \mathbb{R}^{n\times n}$

$\hat{L}: \mathbb{R}^{n^2} \to \mathbb{R}^{n^2}$ $\sim$ $\quad X, E \in \mathbb{R}^{n\times n}$

Possiamo calcolare $L_{f,X}(E)$ calcolando una $f(\ )$ di una matrice $2n \times 2n$:

$$f\left(\begin{bmatrix} X & E \\ 0 & X \end{bmatrix}\right) = \begin{bmatrix} f(X) & L_{f,X}(E) \\ 0 & f(X) \end{bmatrix}$$

$f: U \to \mathbb{R}^n \quad f \in C^{2n-1} \quad f(J) = \begin{bmatrix} f(\lambda) & \cdots & f^{(2n-1)}(\lambda) \\ & \ddots & \vdots \\ 0 & & f(\lambda) \end{bmatrix}$

Trick to compute $L_{f,X}(E)$

$\in C^{2n-1}(U)$. Then, for all $X \in \mathbb{R}^n$ with eigenvalues in U

Let f ~~be Fréchet differentiable~~. Then,

permette di valutare l'azione di $\hat{L}$

$$f\left(\begin{bmatrix} X & E \\ 0 & X \end{bmatrix}\right) = \begin{bmatrix} f(X) & L_{f,X}(E) \\ 0 & f(X) \end{bmatrix}.$$

Proof (sketch) Evaluate $f\left(\begin{bmatrix} A+\varepsilon E & E \\ 0 & A \end{bmatrix}\right)$ by block-diagonalizing.

We need $\begin{bmatrix} I & X \\ 0 & I \end{bmatrix}$, where X solves $(A+\varepsilon E)X - XA = E$, which has solution $X = \frac{1}{\varepsilon} I$ (to block-diagonalize it, it is sufficient to find one solution, even if the Sylvester equation is singular). The evaluation gives $\begin{bmatrix} f(A+\varepsilon E) & \frac{f(A+\varepsilon E)-f(A)}{\varepsilon} \\ 0 & f(A) \end{bmatrix}$.

$$f\left(\begin{bmatrix} X+\varepsilon E & E \\ 0 & X \end{bmatrix}\right) =$$

$A = V\Lambda V^{-1}$ $\quad V^{-1}AV = \Lambda$

Colonne di V = autovettori

$$\begin{bmatrix} I & -Z \\ 0 & I \end{bmatrix}\begin{bmatrix} X+\varepsilon E & E \\ 0 & X \end{bmatrix}\begin{bmatrix} I & Z \\ 0 & I \end{bmatrix} = \begin{bmatrix} X+\varepsilon I & 0 \\ 0 & X \end{bmatrix} \quad (**)$$

se Z risolve l'eq. di Sylvester

$$(X+\varepsilon E)Z - ZX + E = 0 \qquad (*)$$

$$\boxed{Z = -\frac{1}{\varepsilon} I}$$

$$(X+\varepsilon E)\left(-\frac{1}{\varepsilon}I\right) - \left(-\frac{1}{\varepsilon}I\right)\cdot X + E = -\frac{1}{\varepsilon}X - E + \frac{1}{\varepsilon}X + E = 0$$

Remark: $X+\varepsilon E$, X potrebbero avere autoval. in comune $\Rightarrow$ questa eq. di Sylvester non avrebbe soluzione unica.

Ma tanto $(**)$ è verificata per ogni sol. di $(*)$

$$f\left(\begin{bmatrix} X+\varepsilon E & E \\ 0 & X \end{bmatrix}\right) = \begin{bmatrix} 1 & Z \\ 0 & 1 \end{bmatrix} \cdot f\left(\begin{bmatrix} 1 & -Z \\ 0 & 1 \end{bmatrix}\begin{bmatrix} X+\varepsilon E & E \\ 0 & X \end{bmatrix}\begin{bmatrix} 1 & Z \\ 0 & 1 \end{bmatrix}\right) \cdot \begin{bmatrix} 1 & -Z \\ 0 & 1 \end{bmatrix} =$$

[Perché $f(A) = S^{-1} f(SAS^{-1}) S$ per ogni S invertibile]

$$= \begin{bmatrix} 1 & Z \\ 0 & 1 \end{bmatrix} f\left(\begin{bmatrix} X+\varepsilon E & 0 \\ 0 & X \end{bmatrix}\right)\begin{bmatrix} 1 & -Z \\ 0 & 1 \end{bmatrix} = \begin{bmatrix} 1 & Z \\ 0 & 1 \end{bmatrix}\begin{bmatrix} f(X+\varepsilon E) & 0 \\ 0 & f(X) \end{bmatrix}\begin{bmatrix} 1 & -Z \\ 0 & 1 \end{bmatrix} =$$

$$= \begin{bmatrix} f(X+\varepsilon E) & f(X+\varepsilon E)\cdot(-Z) + Z f(X) \\ 0 & f(X) \end{bmatrix} = \begin{bmatrix} f(X+\varepsilon E) & \dfrac{f(X+\varepsilon E) - f(X)}{\varepsilon} \\ 0 & f(X) \end{bmatrix}.$$

(versione matriciale di

$$f\left(\begin{bmatrix} x & e \\ 0 & y \end{bmatrix}\right) = \begin{bmatrix} f(x) & e\dfrac{f(x)-f(y)}{x-y} \\ 0 & f(y) \end{bmatrix}$$
)

Per $\varepsilon \to 0$, se f è Fréchet-derivabile, allora

$$\lim_{\varepsilon \to 0} \frac{f(X+\varepsilon E) - f(X)}{\varepsilon} = L_{f,X}(E)$$

Perché $f(X+\varepsilon E) = f(X) + L_{f,X}(\varepsilon E) + o(\|\varepsilon E\|) =$

$$= f(X) + \varepsilon L_{f,X}(E) + o(\|\varepsilon E\|)$$

$$\Rightarrow \frac{f(X+\varepsilon E) - f(X)}{\varepsilon} = L_{f,X}(E) + \boxed{\frac{o(\varepsilon \|E\|)}{\varepsilon}} \to 0$$

se $\varepsilon \to 0$

Quindi $f\left(\begin{bmatrix} X & E \\ 0 & X \end{bmatrix}\right) = \begin{bmatrix} f(X) & L_{f,X}(E) \\ 0 & f(X) \end{bmatrix}$

Existence of the Fréchet derivative

Theorem

If $f \in \mathcal{C}^{2m-1}(U)$, then $L_{f,X}$ exists for each $X \in \mathbb{R}^{m \times m}$ with eigenvalues in U.

Proof (sketch) The proof of the previous theorem shows that the directional derivatives of f (seen as a map $\mathbb{R}^{m^2} \to \mathbb{R}^{m^2}$) exist and are continuous (since matrix functions are continuous). It is a classical result in multivariate calculus that then f is continuously differentiable.

Abbiamo dimostrato che

$$f\left(\begin{bmatrix} X+\varepsilon E & E \\ 0 & X \end{bmatrix}\right) = \begin{bmatrix} f(X+\varepsilon E) & \dfrac{f(X+\varepsilon E)-f(X)}{\varepsilon} \\ 0 & f(X) \end{bmatrix}$$

A sinistra, abbiamo una f. di matrice (che esiste perché $f \in C^{2n-1}$). f di matrici sono continue, quindi

$$A_\varepsilon \to A \quad f(A_\varepsilon) \to f(A)$$

$\Rightarrow$ estraendo il blocco (1,2), $\dfrac{f(X+\varepsilon E)-f(X)}{\varepsilon}$ converge

e il limite è una funzione continua.

$\Rightarrow$ esistono le derivate direzionali lungo ogni direzione E della nostra mappa $\mathbb{R}^{n^2} \to \mathbb{R}^{n^2}$ e sono continue.

Per un teo. standard di analisi 2, se esistono continue tutte le derivate direzionali, allora la funzione è differenziabile

$\Rightarrow$ esiste $L_{f,X}$

In particolare, polinomi, esponenziali (logaritmi, radici)... sono tutte funzioni di matrici Fréchet-diff.bili

Fréchet derivative and condition number

Hence, $\kappa_{abs}(f, X) = \|L_{f,X}\|$.

...with some attention to what 'norm' means here.

The norm used for $\|\widetilde{X} - X\|$ is any matrix norm on $n \times n$ matrices, and $\|L_{f,X}\|$ is the 'operator norm' (on $n^2 \times n^2$ matrices) induced by it.

Easy case If we take $\|\widetilde{X} - X\|_F$, it corresponds to $\|\operatorname{vec} X\|_2$, so $\kappa_{abs}(f, X) = \|\widehat{L}_{f,X}\|_2$.

$$\|X\|_F \Leftrightarrow \|\operatorname{vec} X\|_2$$

$\underbrace{\text{norma indotta su } \|\widehat{L}_{f,X}\| : \text{norma-2 di matrici } n^2 \times n^2}$

Se invece prendessi $\|X\|_2$, la norma indotta è un oggetto meno usuale.

Eigenvalues of Fréchet derivatives [Higham book '08, Ch. 3]

How to compute the eigenvalues of a Fréchet derivative $L_{f,X}$? (sketched only)
We may assume $f(x) = p(x)$ is a polynomial. Like for the exponential,

$$\begin{aligned} p(X+E) &= p_0 + (X+E) + p_1(X+E)^2 + p_2(X+E)^3 + \dots \\ &= p_0 + p_1(X+E) + p_2(X^2 + EX + XE + E^2) + p_3(X^3 + \dots) \\ &= p(X) + p_1 E + p_2(EX + XE) + p_3(X^2 E + XEX + X^2 E) \\ &\qquad + \dots + O(\|E\|^2) \end{aligned}$$

Not simple to express.

$$\widehat{L} = p_0 + p_1(I \otimes X + X^T \otimes I) + p_2(I \otimes X^2 + X^T \otimes X + (X^2)^T \otimes I) + \dots$$

Triangular if we take Schur forms $X = Q_1 T_1 Q_1^T$, $X^T = Q_2 T_2 Q_2^T$.

Se $f(X) = \varphi(X) = p_0 + p_1 X + p_2 X^2 + p_3 X^3 + \dots$

$$p(X+E) = p_0 I + p_1 (X+E) + p_2 (X+E)^2 + p_3 (X+E)^3 + \dots$$

$$= \underline{p_0 I} + \underline{p_1 X} + \underline{p_1 E} + p_2 \left(\underline{X^2} + \underline{EX + XE} + o(\|E\|) \right)$$

$$+ p_3 \left(\underline{X^3} + \underline{EX^2 + XEX + X^2 E} + o(\|E\|) \right)$$

$$+ p_4 \left(\underline{X^4} + \underline{EX^3 + XEX^2 + X^2 EX + X^3 E} + o(\|E\|) \right)$$

$$+ \dots$$

Termini in blu: $f(X)$

Termini in rosso: $L_{f,X}(E) = p_1 E + p_2 (EX + XE) + p_3 (EX^2 + XEX + X^2 E)$

$$+ p_4 (EX^3 + XEX^2 + X^2 EX + X^3 E) + \dots$$

Posso usare prodotti di Kronecker per costruire la matrice associata:
$$\underbrace{\mathrm{vec}(AEB)}_{\in\mathbb{R}^{n^2}} = \underbrace{(B^T \otimes A)}_{\in\mathbb{R}^{n^2\times n^2}} \cdot \underbrace{\mathrm{vec}\,E}_{\in\mathbb{R}^{n^2}}$$

$$\mathrm{vec}(X^i E X^j) = \left((X^T)^j \otimes X^i\right)\cdot \mathrm{vec}\,E$$

$$\hat{L}_{f,X} = P_1(I\otimes I) + P_2(I\otimes X + X^T\otimes I) + P_3(I\otimes X^2 + X^T\otimes X + (X^T)^2\otimes I) + \dots$$

Faccio un cambio di base che rende triang. superiori contemporaneamente tutte queste matrici:

$$A \otimes B = \begin{bmatrix} a_{11}B & a_{12}B & \cdots & a_{1n}B \\ \vdots & & & \\ a_{n1}B & \cdots & & a_{nn}B \end{bmatrix}$$

triang. sup. se A, B sono triang. sup.

Siano $Q_1^T X Q_1 = T_1$, $Q_2^T X^T Q_2 = T_2$ fattorizz. di Schur.

$\mathrm{diag}(T_1) = \mathrm{diag}(T_2) = (\lambda_1, \lambda_2, \dots \lambda_n)$

ortogonale, perché $(Q_2 \otimes Q_1)^T Q_2 \otimes Q_1 = I \otimes I$

$$(Q_2^T \otimes Q_1^T)\left((X^T)^j \otimes X^i\right)(Q_2 \otimes Q_1) =$$

$$= Q_2^T (X^T)^j Q_2 \otimes Q_1^T X^i Q_1 =$$

$= T_2^j \otimes T_1^i =$ triangolare con $\lambda_h^j \lambda_k^i$ (al variare di h, k) sulla diagonale

ES:
$$\begin{bmatrix} \lambda_1^2 & * \\ 0 & \lambda_2^2 \end{bmatrix} \otimes \begin{bmatrix} \lambda_1^3 & * \\ 0 & \lambda_2^3 \end{bmatrix} = \left[\begin{array}{cc|cc} \lambda_1^2\lambda_1^3 & \lambda_1^2 * & \multicolumn{2}{c}{*} \\ & \lambda_1^2\lambda_2^3 & & \\ \hline \multicolumn{2}{c|}{\multirow{2}{*}{0}} & \lambda_2^2\lambda_1^3 & \lambda_2^2 * \\ & & 0 & \lambda_2^2\lambda_1^3 \end{array}\right]$$

Con un po' di lavoro, si può vedere cosa finisce sulla diagonale di $(Q_2^T \otimes Q_1^T)(\hat{L}_{f,X})(Q_2 \otimes Q_1)$

Se X diagonalizzabile, $X = V_1 \Lambda V_1^{-1}$, uno potrebbe rifare lo stesso conto con $(V_2^{-1} \otimes V_1^{-1})\hat{L}_{f,X}(V_2 \otimes V_1)$, che produce una matrice diagonale $(\Lambda^j \otimes \Lambda^i)$

Produce una fattorizzazione

$V_1^{-1} X V_1 = \Lambda \overset{\text{trasponendo}}{\rightsquigarrow} \underbrace{V_1^T}_{V_2^{-1}} X^T \underbrace{V_1^{-T}}_{V_2} = \Lambda$

$$\hat{L}_{f,X} = \left(V_2 \otimes V_1\right) D \left(V_2^{-1} \otimes V_1^{-1}\right), \text{ dove}$$

D diagonale con elementi $f[\lambda_i, \lambda_j]$ $\begin{matrix} i = 1, \dots, n \\ j = 1, \dots, n \end{matrix}$

$$\|\hat{L}_{f,X}\| \leq \|V_2 \otimes V_1\| \cdot \|D\| \cdot \|V_2^{-1} \otimes V_1^{-1}\| =$$

$$= \|V_2\| \cdot \|V_1\| \cdot \max |f[\lambda_i, \lambda_j]| \cdot \|V_2^{-1}\| \cdot \|V_1^{-1}\| = K(V)^2 \cdot \max f[\lambda_i, \lambda_j]$$

TL;DR: theorems

Theorem

Let X have eigenvalues $\lambda_1, \dots, \lambda_n$. The eigenvalues of $L_{f,X}$ are

for all $i = 1, 2, \dots n$
$j = 1, 2, \dots n$

$$f[\lambda_i, \lambda_j] := \begin{cases} \frac{f(\lambda_i) - f(\lambda_j)}{\lambda_i - \lambda_j} & i \neq j, \quad = f'(\xi) \\ f'(\lambda_i) & i = j. \end{cases}$$

Theorem

Let $X = V \Lambda V^{-1}$ be diagonalizable. Then, for the Frobenius norm,

$$\kappa_{abs}(\underset{L_{f,X}}{\cancel{f, X}}) \leq \kappa_2^2(V) \max_{i,j} |f[\lambda_i, \lambda_j]|.$$

$f(X)$ mal condizionata se:

- $\kappa(V)$ alto (cioè eig(X) mal cond.)
- f' grande nel dominio

$g(x)=\sqrt{x}$

$L_{g,X}(E)$ soluzione dell'equazione di Sylv. $\boxed{X^{\frac{1}{2}}L+LX^{\frac{1}{2}}=E}$

$\Rightarrow$ a volte possiamo usare funzioni di matrici per risolvere equazioni matriciali

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- segno (Newton)
- radice quadrata
- $XCX+AX+XB+D=0$ — Iterazioni fun., Newton, doubling
- $AX+XA^T=B$ — denso; sparso (A larga sparsa)