Note Title 2020-03-27

$f(x)=x^2 \qquad f(X)=X^2$

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

$\|E^2\|\le\|E\|^2$

Fréchet derivative
(linear operator $\mathbb{R}^{n\times n}\to\mathbb{R}^{n\times n}$)

$\iff \hat{L}\in\mathbb{R}^{n^2\times n^2}: X^T\otimes I+I\otimes X$ (Jacobian of the map $\mathbb{R}^{n^2}\to\mathbb{R}^{n^2}$ $\operatorname{vec}X\mapsto\operatorname{vec}f(X)$)

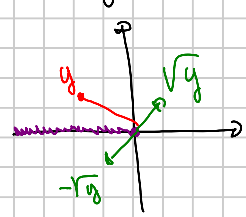
$L_{f+g,X}=L_{f,X}+L_{g,X}$

$L_{f\circ g,X}=L_{f,g(X)}\circ L_{g,X}$ $\quad \hat{L}_{f,g(X)}\cdot\hat{L}_{g,X}$ (matrix product)

$L_{f^{-1},f(X)}=L_{f,X}^{-1}$ $\quad (\hat{L}_{f,X})^{-1}$ (matrix inverse)

(because $I=L_{f^{-1}\circ f,X}=L_{f^{-1},f(X)}\circ L_{f,X}$)

Ex: Let us take $g(y)=\sqrt{y}$ (principal square root, $y\notin\mathbb{R}^-$, $\operatorname{Re}(\sqrt{y})>0$)



$g(Y)$ for Y without eigenvalues in $\mathbb{R}^-=(-\infty,0]$

$L_{g,Y}$ $\qquad$ g is the inverse of $f(X)=X^2$

$L_{g,Y}=(L_{f,X})^{-1}$ $\qquad Y=X^2=f(X) \qquad X=\sqrt{Y}=g(Y)$

$F=L_{g,Y}(E) \qquad L_{f,X}(F)=E$

$$\underbrace{X}_{A}F+F\underbrace{X}_{-B}=E \qquad (*)$$

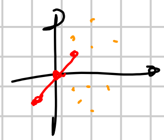
F is the solution of the Sylvester equation $XF+FX=E$

$\sqrt{Y}F+F\sqrt{Y}=E$

Condition for solvability of (*): $\Lambda(X) \cap \Lambda(-X) = \phi$

$\Leftrightarrow$ X does not have two eigenvalues that are one the opposite of the other.

The eigenvalues of X are $g(\lambda)$, λ eigenvalues of Y, and our definition of g ensures that $\operatorname{Re} g(\lambda) > 0$ so there are no opposites.



$\sqrt{Y} = X$

$$\hat{L} = \left((\sqrt{Y})^T \otimes I + I \otimes \sqrt{Y} \right)^{-1} \quad \left(\text{consistent with scalar case: } \frac{d}{dy}\sqrt{y} = \left(2\sqrt{y}\right)^{-1} \right)$$

More complicated: Fréchet derivative of $\exp(X)$

$$\exp(X) = 1 + X + \frac{1}{2}X^2 + \frac{1}{3!}X^3 + \dots$$

$$\exp(X+E) = 1 + (X+E) + \frac{1}{2}(X+E)^3 + \frac{1}{3!}(X+E)^3 + \dots$$

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

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

$(X+E)^4$

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

$\operatorname{vec}(AEB) = (B^T \otimes A)\operatorname{vec} E$

$$\hat{L} = I_{n^2 \times n^2} + \frac{1}{2}\left(1 \otimes X + X^T \otimes 1\right) + \frac{1}{3!}\left(1 \otimes X^2 + X^T \otimes X + (X^2)^T \otimes 1\right) + \dots$$

<u>Theorem</u>: Suppose $L_{f,X}$ exists. Then

$$f\left(\underbrace{\begin{bmatrix} X & E \\ 0 & X \end{bmatrix}}_{\in \mathbb{R}^{2n \times 2n}}\right) = \begin{bmatrix} f(X) & L_{f,X}(E) \\ 0 & f(X) \end{bmatrix}. \qquad \hat{L} \cdot \operatorname{vec}(E)$$

(cfr. with automatic differentiation: $f\left(\begin{bmatrix} x & 1 \\ 0 & x \end{bmatrix}\right) = \begin{bmatrix} f(x) & f'(x) \\ 0 & f(x) \end{bmatrix}$)

Proof: let us evaluate $f\left(\begin{bmatrix} X+\varepsilon E & E \\ 0 & X \end{bmatrix}\right)$, then let $\varepsilon \to 0$

Let us find Z s.t.

$$\begin{bmatrix} I & -Z \\ 0 & I \end{bmatrix}\begin{bmatrix} X+\varepsilon E & E \\ 0 & X \end{bmatrix}\begin{bmatrix} I & Z \\ 0 & I \end{bmatrix} \overset{!}{=} \begin{bmatrix} X+\varepsilon E & 0 \\ 0 & X \end{bmatrix}$$

$$LHS = \begin{bmatrix} X+\varepsilon E & E-ZX \\ 0 & X \end{bmatrix}\begin{bmatrix} I & Z \\ 0 & I \end{bmatrix} = \begin{bmatrix} X+\varepsilon E & \underbrace{(X+\varepsilon E)Z+E-ZX}_{\overset{!}{=}0} \\ 0 & X \end{bmatrix}$$

holds iff Z solves Sylv. equation $(X+\varepsilon E)Z - ZX + E = 0$

One can check that $Z = -\frac{1}{\varepsilon}I$ works: $-(\cancel{X}+\cancel{\varepsilon E})\frac{1}{\varepsilon} + \frac{1}{\varepsilon}\cancel{X} + \cancel{E} = 0$ ✓

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

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

$$= \begin{bmatrix} I & -\frac{1}{\varepsilon}I \\ 0 & I \end{bmatrix}\begin{bmatrix} f(X+\varepsilon E) & 0 \\ 0 & f(X) \end{bmatrix}\begin{bmatrix} I & \frac{1}{\varepsilon}I \\ 0 & I \end{bmatrix} = \begin{bmatrix} f(X+\varepsilon E) & -\frac{1}{\varepsilon}f(X) \\ 0 & f(X) \end{bmatrix}\begin{bmatrix} I & \frac{1}{\varepsilon}I \\ 0 & I \end{bmatrix}$$

$$= \begin{bmatrix} \underset{\to f(X)}{f(X+\varepsilon E)} & \underbrace{\tfrac{1}{\varepsilon}f(X+\varepsilon E) - \tfrac{1}{\varepsilon}X}_{\to L_{f,X}(E)} \\ 0 & f(X) \end{bmatrix}$$

let $\varepsilon \to 0$ ✓

□

Theorem: if $f \in C^{2n-1}(U)$, then $L_{f,X}$ exists for all $X \in \mathbb{R}^{n\times n}$ with eigenvalues in U

Proof: If f is $2n-1$-times diff'le, then we can evaluate $f\left(\begin{bmatrix} X & E \\ 0 & X \end{bmatrix}\right)$ for all matrices X with eigenvalues in U. $\Rightarrow$ the directional derivative

$$\frac{1}{\varepsilon}\left(f(X+\varepsilon E) - f(X)\right) \text{ exists } \forall E \text{ and is continuous in } E$$

(matrix functions are continuous!)

$\Rightarrow f$ is differentiable as a function $\mathbb{R}^{n^2} \to \mathbb{R}^{n^2}$ (from analysis II).

Relation between Jacobians and cond. number:

$K_{abs,f,x} = \| J_{f,x} \|$ (induced matrix norm of Jacobian)

$$K_{rel,f,x} = \frac{\| J_{f,x} \| \cdot \| x \|}{\| f(x) \|}$$

In particular, for matrix functions.

$K_{abs,f,x} = \| \hat{L}_{f,x} \|$ what norm though?

When we vectorize, $\| X \|_F = \| vec(X) \|_2$

$\| X \|_2 = ??$

$\| X \|_\infty = ??$ (They are norms in $\mathbb{R}^{n^2}$, but not "classical" ones)

$\| X \|_1 = ??$

With $\| X \|_F = \| vec X \|_2$,

$K_{abs,f,x} = \| \hat{L}_{f,x} \|_2$ (induced Euclidean norm of an $n^2 \times n^2$ matrix)

$$= \sigma_{max}(\hat{L}_{f,x}) = \rho(\hat{L}_{f,x}^T \hat{L}_{f,x})^{1/2}$$

(tells you the change in $\| f(X+E) - f(X) \|_F$ w.r.t. $\| E \|$

$$\frac{\| f(X+E) - f(X) \|_F}{\| E \|_F} \leq \| \hat{L}_{f,x} \|_2 + o(1) \quad (\text{when } \| E \|_F \to 0)$$

$n^2 \times n^2$ (computing it costs $O(n^6)$, unless one uses approximated methods)

Eigenvalues of Fréchet derivatives:

Let us assume f is a polynomial (interpolation!)

When we compute $f(X)$, we can replace $f(X)$ with $p(X)$ where p is an interpolating polynomial in the eigenvalues of X.

Is it still true that $L_{f,x} = L_{p,x}$?

In general no, but

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

if p $\to$ $\|$

interpolates f in the eigenvalues of X with twice multiplicities

$$\overset{\shortparallel}{p}\left(\begin{bmatrix} X & E \\ 0 & X \end{bmatrix}\right) = \begin{bmatrix} p(X) & L_{p,X}(E) \\ 0 & p(X) \end{bmatrix} \text{ f-d}$$

As long as p, f coincide with enough derivatives, $L_{f,X} = L_{p,X}$

But let us assume that $p(x) = p_0 + x p_1 + x^2 p_2 + \dots + x^d p_d$

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

$$= \underbrace{\left(p_0 I + p_1 X + \dots + p_d X^d\right)}_{p(X)} + \underbrace{p_1 E + p_2 (EX + XE) + \dots + p_d \left(X^{d-1}E + X^{d-2}EX + \dots + X^{d-1}E\right)}_{L_{p,X}(E)} + o(\|E\|)$$

$$\hat{L} = p_1 I + p_2 \left(X^T \otimes I + I \otimes X\right) + p_3 \left(X^{2^T} \otimes I + X^T \otimes X + I \otimes X^2\right) + \dots$$

$$\dots + p_d \left(I \otimes X^{d-1} + X^T \otimes X^{d-2} + X^{2^T} \otimes X^{d-3} + \dots + (X^{d-1})^T \otimes I\right)$$

$$\hat{L} = \sum_{k=1}^{d} p_k \sum_{h=1}^{k} (X^{k-h})^T \otimes X^{h-1}$$

$$\boxed{\begin{aligned} X^T &= Q_1 T_1 Q_1^* \\ X &= Q_2 T_2 Q_2^* \end{aligned}}$$

Schur forms

$$= \sum_k p_k \sum_h \underline{Q_1 T_1^{k-h} Q_1^*} \otimes \underline{Q_2 T_2^{h-1} Q_2^*} =$$

$$= \left(Q_1 \otimes Q_2\right) \left(\sum_k p_k \sum_h T_1^{k-h} \otimes T_2^{h-1}\right) \left(Q_1 \otimes Q_2\right)^*$$

is a Schur form of $\hat{L}_{f,X}$

unitary   triangular   unitary*

$$T_1^{k-h} \otimes T_2^{h-1} = \begin{bmatrix} t_{11}^{k-h} T_2^{h-1} & - & - & - \\ & t_{22}^{k-h} T_2^{h-1} & & \vdots \\ & & \ddots & \vdots \\ 0 & & & t_{nn}^{k-h} T_2^{h-1} \end{bmatrix}$$

$\operatorname{diag}(T_1) =$
$= \operatorname{diag}(T_2) =$
$= \lambda_1, \lambda_2, \dots \lambda_n$
$=$ eigenvalues of X)

The diagonal contains

$$\sum_{k=0}^{d} p_k \sum_{h=1}^{k} t_{ii}^{k-h} \cdot t_{jj}^{h-1} = \sum_{k=0}^{d} p_k \sum_{h=1}^{k} \lambda_i^{k-h} \lambda_j^{h-1} \qquad \text{for all } i,j = 1, \dots n$$

$$= \sum_{k=0}^{d} p_k \frac{\lambda_i^k - \lambda_j^k}{\lambda_i - \lambda_j} = \frac{1}{\lambda_i - \lambda_j}\Big(p(\lambda_i) - p(\lambda_j)\Big)$$

$$= \boxed{\frac{f(\lambda_i) - f(\lambda_j)}{\lambda_i - \lambda_j}}$$

Th: if X has eigenvalues $\lambda_1, \lambda_2, \dots \lambda_n$, the eigenvalues of $L_{f,X}$ are

$$f[\lambda_i, \lambda_j] = \begin{cases} \dfrac{f(\lambda_i) - f(\lambda_j)}{\lambda_i - \lambda_j} & \text{if } \lambda_i \neq \lambda_j \\ f'(\lambda_i) & \text{if } \lambda_i = \lambda_j \end{cases} \quad \text{for all } i,j = 1,2,\dots n$$

(Proved above)

By proceeding analogously with an eigendecomposition:

If $X = V \cdot \Lambda \cdot V^{-1}$ is diagonalizable, then

$$\hat{L}_{f,X} = (V^T \otimes V)\, \mathrm{diag}\Big(f[\lambda_i, \lambda_j] \quad i,j = 1..n\Big)\, (V^T \otimes V)^{-1}$$

$$\|\hat{L}_{f,X}\| = \|V^T\| \cdot \|V\| \cdot \max_{i,j} \big|f[\lambda_i, \lambda_j]\big| \cdot \|V^{-T}\| \cdot \|V^{-1}\|$$

$$= \underset{①}{K(V)^2} \cdot \max_{i,j} \big|f[\lambda_i, \lambda_j]\big|$$

Computing a matrix function may be ill-conditioned because either

① diagonalizing X is ill-conditioned, or

② $\big|f[\lambda_i, \lambda_j]\big|$ is large for some eigenvalues

When does ② happen for
A. $f(x) = \exp(x)$?
B. $f(x) = \sqrt{x}$?