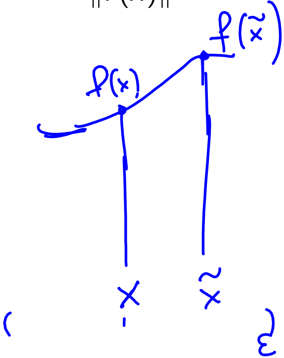
Conditioning of computing matrix functions

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

Jacobian

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

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



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

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

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

Example

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

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

$L_{f,X}$ 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,

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

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

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: $\Lambda(X) \cap \Lambda(-X) = \emptyset$.

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.

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

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

Let f be Fréchet differentiable. Then,

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

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 $\begin{bmatrix} f(A+\varepsilon E) & \frac{f(A+\varepsilon E)-f(A)}{\varepsilon} \\ 0 & f(A) \end{bmatrix}$.

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.

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 $\kappa_{abs}(f, X) = \|\widehat{L}_{f,X}\|_2$.

$$\|\tilde{X} - X\|_F = \|\operatorname{vec}(\tilde{X} - X)\|_2$$

condizionamento in norma-Frobenius di $f(X) = \|K_{f,X}\|_2$

$\|\tilde{X} - X\|_2 =$ (norma complicata su $\mathbb{R}^{n^2}$) di vec $\tilde{X} - X$

cond. in norma-2 di $f(X) =$ (norma complicata su $\mathbb{R}^{n^2 \times n^2}$) di $K_{f,X}$

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 replace $f(x)$ with its interpolating polynomial $p(x)$ on the spectrum of A (and twice the multiplicities, to make sure the 'trick' with $\left[\begin{smallmatrix} X & E \\ 0 & X \end{smallmatrix}\right]$ works).

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

Not simple to express.

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

Eigenvalues of Fréchet derivatives

More formally,

$$K(X) = \sum_{k=0}^{d} p_k \sum_{h=1}^{k} (X^{k-h})^T \otimes X^{h-1}$$

We can reduce it to a triangular matrix if we take Schur forms
$X = Q_1 T_1 Q_1^T$, $X^T = Q_2 T_2 Q_2^T$.
Its eigenvalues are

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

TL;DR: theorems

Theorem

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

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

Theorem

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

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

Captures at least one of the two factors for ill-conditioning, i.e., eigenvalues. The other factor, non-normality, is trickier to account for properly.