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M\crNA Manchester Numerical Analysis

How and Why to Estimate Condition Numbers for Matrix Functions

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Joint work with Sam Relton and Lijing Lin

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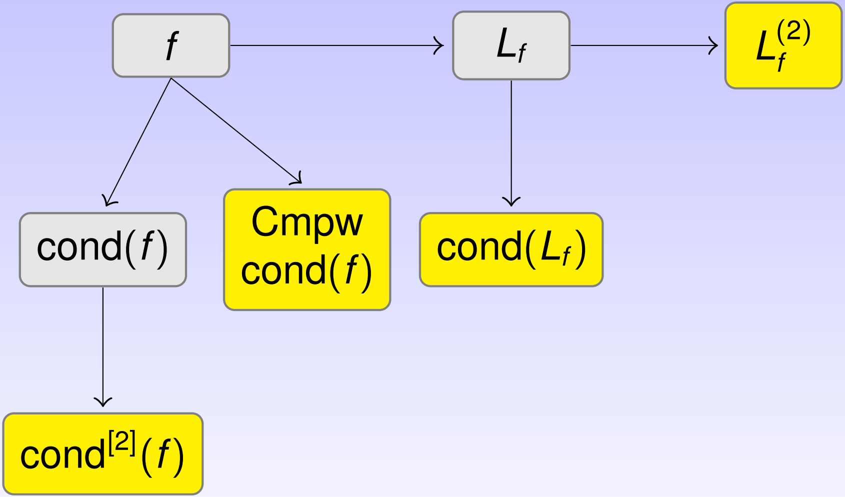
The Big Picture



Fréchet Derivative

Fréchet derivative of $f : \mathbb{C}^{n\times n} \to \mathbb{C}^{n\times n}$ at $X \in \mathbb{C}^{n\times n}$

A linear mapping $L_f : \mathbb{C}^{n\times n} \to \mathbb{C}^{n\times n}$ s.t. for all $E \in \mathbb{C}^{n\times n}$

$$f(A+E) - f(A) - L_f(A,E) = o(\|E\|).$$

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Examples:

$$(A+E)^2 - A^2 = AE + EA + E^2 \Rightarrow L_{x^2}(A,E) = AE + EA.$$

$$(A+E)^{-1} - A^{-1} = -A^{-1}EA^{-1} + O(E^2)$$
$$\Rightarrow L_{x^{-1}}(A,E) = -A^{-1}EA^{-1}.$$

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$$(A+E)^{-1} - A^{-1} = -A^{-1}EA^{-1} + O(E^2)$$

$$\Rightarrow L_{x^{-1}}(A,E) = -A^{-1}EA^{-1}.$$

Scalar case: $L_f(x,e) = f('x)e$.

Applications of Fréchet Derivative

- First *and second* Fréchet derivative in Halley's method on Banach space (2003).
- Matrix geometric mean computation (2012).
- Model reduction (2012).
- Computation of correlated choice probabilities (2013).
- Registration of MRI images (2013).
- Markov models applied to cancer data (2014).
- Computing linearized backward errors for matrix functions (2014).

Computing L_f: Methods for Specific f

- **exponential** Kenney & Laub (1998), Al-Mohy & H (2009).
- **logarithm** Al-Mohy, H & Relton (2013).
- **fractional power** H & Lin (2013).

Latter three methods obtained by differentiating alg for f.

Computing L_f: General Methods

Theorem (Mathias, 1996)

If f is $2n-1$ times ctsly diffble,

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

Complex step method .

Assume $f : \mathbb{R}^{n\times n} \to \mathbb{R}^{n\times n}$ and $A, E \in \mathbb{R}^{n\times n}$. Then (H & Al-Mohy, 2010):

$$L_f(A,E) \approx \operatorname{Im} \frac{f(A+ihE)}{h}.$$

Componentwise Sensitivity (1)

Let $E = e_i e_j^T$. Then

$$\lim_{\epsilon \to 0} \frac{f(A + \epsilon e_i e_j^T) - f(A)}{\epsilon} = L_f(A, e_i e_j^T).$$

$(L_f(A, e_i e_j^T))_{rs}$ measures the sensitivity of $f(A)_{rs}$ to perturbations in a_{ij}.

Componentwise Sensitivity (2)

Since L_f is a linear operator,

$$\mathrm{vec}(L_f(A, E)) = K_f(A)\mathrm{vec}(E)$$

where $K_f(A) \in \mathbb{C}^{n^2 \times n^2}$ is the **Kronecker form** of $L_f(A)$.

	a_{11}	a_{21}	a_{31}	$\dots$	a_{nn}
f_{11}					
f_{21}					
f_{31}			$K_f(A) \equiv$		
$\vdots$			$L_f(A, e_i e_j^T)$		
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f_{11}					
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f_{31}			$K_f(A) \equiv L_f(A, e_i e_j^T)$		
$\vdots$					
f_{nn}					

In progress: sensitivity of $y' = A(t)y$ (nuclear physics).

Absolute Condition Number

$$\text{cond}_{\text{abs}}(f, A) = \lim_{\epsilon \to 0} \sup_{\|E\| \le \epsilon} \frac{\|f(A+E) - f(A)\|}{\epsilon}.$$

$$\|L_f(A)\| := \max_{E \neq 0} \frac{\|L_f(A, E)\|}{\|E\|}.$$

Lemma

$$\text{cond}_{\text{abs}}(f, A) = \|L_f(A)\|.$$

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Lemma

$$\mathrm{cond}_{\mathrm{abs}}(f, A) = \|L_f(A)\|.$$

Scalar case: $\mathrm{cond}_{\mathrm{abs}}(f, x) = |f'(x)|$.

Relative Condition Number

$$\begin{aligned}\mathrm{cond}_{\mathrm{rel}}(f, A) &:= \lim_{\epsilon\to 0} \sup_{\|E\|\le\epsilon\|A\|} \frac{\|f(A+E) - f(A)\|}{\epsilon\|f(A)\|}\\ &= \mathrm{cond}_{\mathrm{abs}}(f, A)\frac{\|A\|}{\|f(A)\|}.\end{aligned}$$

The Setup

- Assume we have $O(n^3)$ algs for $f(A)$ and $L_f(A, E)$.
- $K_f(A)$ has n^4 entries.
- Computing $K_f(A)$ requires $O(n^5)$ flops.
- Wish to estimate norms and condition numbers in $O(n^3)$ flops.
- In practice we only ever work with $n \times n$ matrices.

Condition Estimation (1)

Can show

$$\frac{\|L_f(A)\|_1}{n} \le \|K_f(A)\|_1 \le n\|L_f(A)\|_1.$$

So problem reduces to **matrix norm estimation**.

Use the **block 1-norm estimator** of H & Tisseur (2000).
For $\|B\|_1$ it needs Bx and B^*y for several x and y. Here,

$$\begin{aligned} K_f(A)x &= \mathrm{vec}(L_f(A,X)), & \mathrm{vec}(X) &= x, \\ K_f(A)^*y &= \mathrm{vec}(L_f^\star(A,Y)), & \mathrm{vec}(Y) &= y. \end{aligned}$$

Condition Estimation (2)

Theorem (H & Lin, 2013)

Let $f \in C^{2n-1}$ and $\widetilde{f}(z) := \overline{f(\overline{z})}$.
If $\widetilde{f}(A)^* = \widetilde{f}(A^*)$ for all $A \in \mathbb{C}^{n\times n}$ then
$K_f(A)^* x = \mathrm{vec}(L_{\widetilde{f}}(A, X^*)^*)$*, where* $\mathrm{vec}(X) = x$.

For most functions of interest, $\widetilde{f} = f$, and we can deduce that

$$K_f(A)^* x = \mathrm{vec}(L_f(A, X^*)^*).$$

Higher Derivatives

Needed for

- level-2 condition number,
- understanding accuracy of algorithms for computing $L_f(A, E)$.

Second Fréchet derivative $L_f^{(2)}(A, E_1, E_2)$ is unique multilinear function of E_1, E_2 satisfying

$$L_f(A + \mathbf{E_2}, E_1) - L_f(A, E_1) - L_f^{(2)}(A, E_1, \mathbf{E_2}) = o(\|\mathbf{E_2}\|).$$

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***k*th** Fréchet derivative defined by

$$L_f^{(k-1)}(A+\mathbf{E_k}, E_1, \ldots, E_{k-1}) - L_f^{(k-1)}(A, E_1, \ldots, E_{k-1}) - L_f^{(k)}(A, E_1, \ldots, \mathbf{E_k}) = o(\|\mathbf{E_k}\|).$$

Existing Literature

- Large literature on Fréchet derivatives in Banach space.
- Need specialized results for matrix functions.

Existence & Continuity of Fréchet Derivatives

- $\mathcal{D}$ = open subset of $\mathbb{C}$.
- $\mathbb{C}^{n\times n}(\mathcal{D}, p)$ = matrices with spectrum in $\mathcal{D}$ and largest Jordan block of size p.

Theorem (H & Relton, 2013)

If $f \in C^{2^k p-1}(\mathcal{D})$ and $A \in \mathbb{C}^{n\times n}(\mathcal{D}, p)$ then the kth Fréchet derivative $L_f^{(k)}(A)$ exists and $L_f^{(k)}(A, E_1, \dots, E_k)$ is continuous in A and $E_1, \dots, E_k \in \mathbb{C}^{n\times n}$.

- Proof uses Gâteaux derivative.
- $k = 1$: Mathias (1996).
- *Open problem*: necessary conditions.

Properties

Assume from now on conditions of theorem satisfied.
Then the E_i are interchangeable:

$$L_f^{(2)}(A, E_1, E_2) = L_f^{(2)}(A, E_2, E_1).$$

Indeed

$$L_f^{(k)}(A, E_1, \ldots, E_k) = \frac{\partial}{\partial s_1 \cdots \partial s_k}\bigg|_{\mathbf{s}=0} f(A + s_1 E_1 + \cdots + s_k E_k).$$

How to Compute $L_f^{(2)}$

$X_1 = \left[\begin{smallmatrix} A & E_1 \\ 0 & A \end{smallmatrix}\right]$. Know $f(X_1) = \begin{bmatrix} f(A) & L_f(A,E) \\ 0 & f(A) \end{bmatrix}$.

Let

$$X_2 = \underbrace{I_2 \otimes X_1 + \begin{bmatrix} 0 & 1 \\ 0 & 0 \end{bmatrix} \otimes E_2}_{\text{“nivellateur”}} = \left[\begin{array}{cc|cc} A & E_1 & E_2 & 0 \\ 0 & A & 0 & E_2 \\ \hline 0 & 0 & A & E_1 \\ 0 & 0 & 0 & A \end{array}\right].$$

Then

$$f(X_2) = \left[\begin{array}{cc|cc} f(A) & L_f(A,E_1) & L_f(A,E_2) & L_f^{(2)}(A,E_1,E_2) \\ 0 & f(A) & 0 & L_f(A,E_2) \\ \hline 0 & 0 & f(A) & L_f(A,E_1) \\ 0 & 0 & 0 & f(A) \end{array}\right].$$

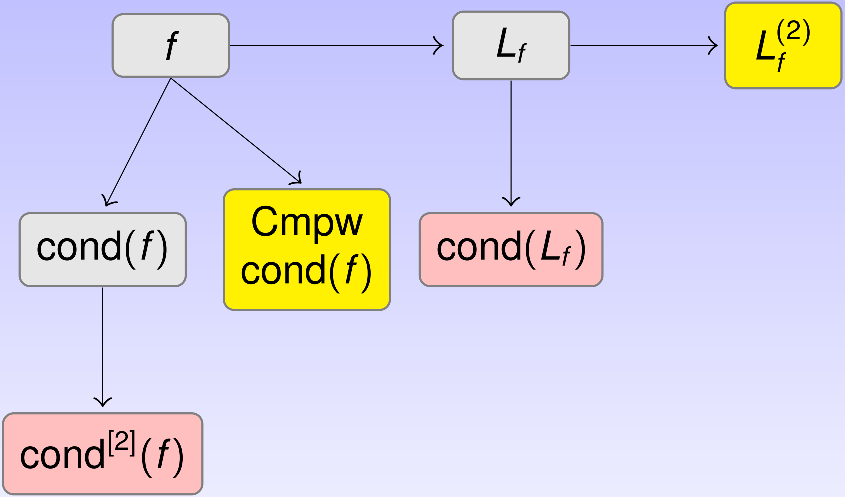
How to Compute $L_f^{(k)}$

Define $X_i \in \mathbb{C}^{2^i n \times 2^i n}$ by

$$X_i = I_2 \otimes X_{i-1} + \begin{bmatrix} 0 & 1 \\ 0 & 0 \end{bmatrix} \otimes I_{2^{i-1}} \otimes E_i, \qquad X_0 = A.$$

Theorem (H & Relton, 2013)

The $(1, n)$ block of $f(X_k)$ is $L_f^{(k)}(A, E_1, \ldots, E_k)$.


f
L_f
L_f^(2)
cond(f)
Cmpw
cond(f)
cond(L_f)
cond^[2](f)

Condition Number of the Fréchet Derivative

$$\mathrm{cond}_{\mathrm{rel}}(L_f, A, E) = \lim_{\epsilon\to 0} \sup_{\substack{\|\Delta A\|\le\epsilon\|A\| \\ \|\Delta E\|\le\epsilon\|E\|}} \frac{\|L_f(A+\Delta A, E+\Delta E) - L_f(A,E)\|}{\epsilon\|L_f(A,E)\|}$$

Theorem (H & Relton, 2013)

$$\begin{aligned} \max(\mathrm{cond}_{\mathrm{abs}}(f,A), sM)r &\le \mathrm{cond}_{\mathrm{rel}}(L_f, A, E) \\ &\le (\mathrm{cond}_{\mathrm{abs}}(f,A) + sM)r, \end{aligned}$$

$$s = \frac{\|A\|}{\|E\|}, \quad r = \frac{\|E\|}{\|L_f(A,E)\|}, \quad M = \max_{\|\Delta A\|=1} \|L_f^{(2)}(A, E, \Delta A)\|.$$

Hence we can compute $\mathrm{cond}_{\mathrm{rel}}(L_f, A, E)$ to within a factor 2.

Estimating $\text{cond}_{\text{rel}}(L_f, A, E)$

Need second Kronecker form satisfying $K_f^{(2)}(A) \in \mathbb{C}^{n^4 \times n^2}$

$$\text{vec}(L_f^{(2)}(A, E_1, E_2)) = (\text{vec}(E_1)^T \otimes I_{n^2})K_f^{(2)}(A)\text{vec}(E_2).$$

Can show M is within factor n of $\|(\text{vec}(E)^T \otimes I_{n^2})K_f^{(2)}(A)\|_1$.

Theorem (H & Relton 2013)

For most functions of interest,

$$\left[(\text{vec}(E)^T \otimes I_{n^2})K_f^{(2)}(A)\right]^* = (\text{vec}(E^*)^T \otimes I_{n^2})K_f^{(2)}(A^*).$$

Estimating $\text{cond}_{\text{rel}}(L_f, A, E)$

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Get $O(n^3)$ estimate of $\text{cond}_{\text{rel}}(L_f, A, E)$ within factor $\approx 6n$.

Level-2 Condition Number

"Condition number of the condition number".

Demmel (1987) showed that for

- matrix inversion (and **D. J. Higham**, 1995),
- the eigenproblem,
- polynomial zero-finding,
- pole assignment in linear control problems

(relative) level-1 and level-2 cond no's are equivalent.

Cheung & Cucker (2005) show same holds when "condition number = 1 / distance to nearest ill-posed problem".

Level-2 Condition Number

$$\mathrm{cond}^{[2]}_{\mathrm{abs}}(f,A) = \lim_{\epsilon\to 0} \sup_{\|Z\|\le\epsilon} \frac{|\mathrm{cond}_{\mathrm{abs}}(f,A+Z) - \mathrm{cond}_{\mathrm{abs}}(f,A)|}{\epsilon}.$$

Theorem (H & Relton, 2013)

In the Frobenius norm,

$$\mathrm{cond}^{[2]}_{\mathrm{abs}}(f,A) \le \|K^{(2)}_f(A)\|_2.$$

Level-2 Condition Number: Exponential

Theorem

Let $A \in \mathbb{C}^{n\times n}$ be normal. Then in the 2-norm

$$\mathrm{cond}_{\mathrm{abs}}^{[2]}(\exp, A) = \mathrm{cond}_{\mathrm{abs}}(\exp, A).$$

Level-2 Condition Number: Exponential

Theorem

Let $A \in \mathbb{C}^{n\times n}$ be normal. Then in the 2-norm

$$\mathrm{cond}^{[2]}_{\mathrm{abs}}(\exp, A) = \mathrm{cond}_{\mathrm{abs}}(\exp, A).$$

Theorem

Let $A \in \mathbb{C}^{n\times n}$ be normal. Then in the 2-norm

$$1 \le \mathrm{cond}^{[2]}_{\mathrm{rel}}(\exp, A) \le 2\mathrm{cond}_{\mathrm{rel}}(\exp, A) + 1.$$

Level-2 Condition Number: Hermitian A

Theorem (H & Relton, 2013)

Let $A \in \mathbb{C}^{n\times n}$ be Hermitian and let $f : \mathbb{R} \to \mathbb{R}$ have a strictly monotonic derivative. Then in the Frobenius norm,

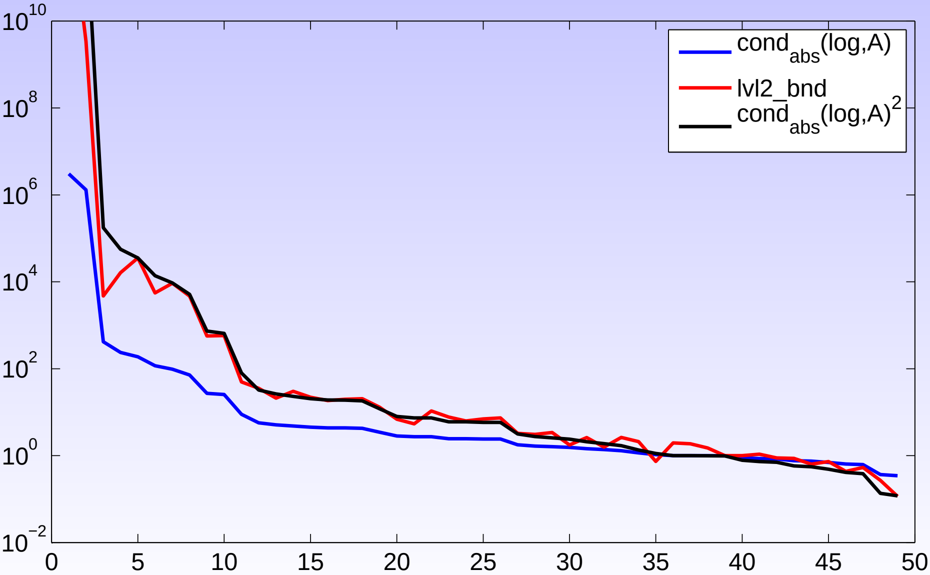
$$\mathrm{cond}_{\mathrm{abs}}(f, A) = \max_i |f'(\lambda_i)|.$$

Moreover, if the maximum is attained uniquely for $i = k$ then

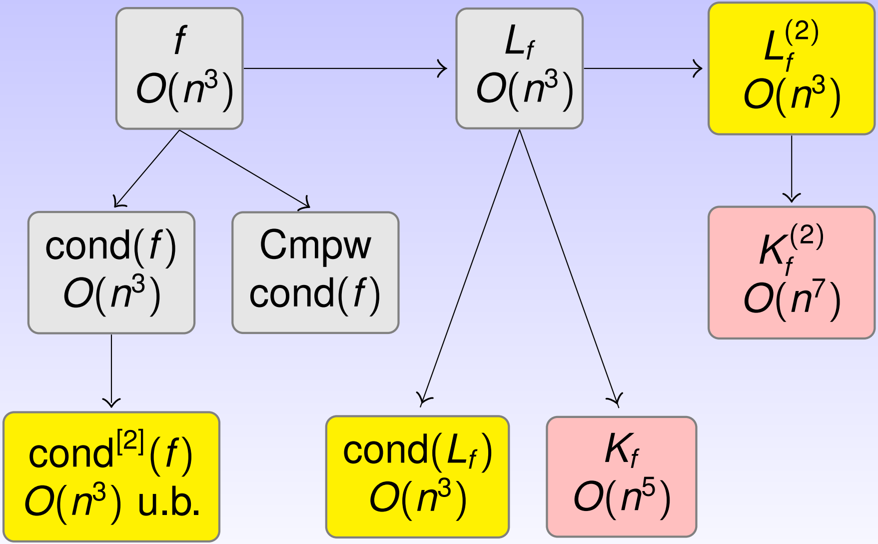
$$\mathrm{cond}^{[2]}_{\mathrm{abs}}(f, A) \geq |f''(\lambda_k)|.$$

- Applies to log, square root, inverse.
- For inverse the inequality is an equality.

Logarithm Experiment



Summary


f
$O(n^3)$
L_f
$O(n^3)$
$L_f^{(2)}$
$O(n^3)$
cond(f)
$O(n^3)$
Cmpw
cond(f)
$K_f^{(2)}$
$O(n^7)$
cond$^{[2]}$(f)
$O(n^3)$ u.b.
cond(L_f)
$O(n^3)$
K_f
$O(n^5)$

Open Questions

- Necessary conditions for existence of L_f?
- Quality of upper bound for $\mathrm{cond}^{[2]}(f)$?
- Relation between level-1 and level-2 condition numbers?
- How can we exploit the **symmetry** of $L_f^{(k)}(E_1, E_2, \ldots, E_k)$ in the E_i?

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Extra slides

Level-2 Condition Number: Matrix Inverse

Theorem

For nonsingular $A \in \mathbb{C}^{n\times n}$,

$$\mathrm{cond}_{\mathrm{abs}}^{[2]}(x^{-1}, A) = 2\,\mathrm{cond}_{\mathrm{abs}}(x^{-1}, A)^{3/2}.$$

- Latter is what is expected from the scalar case: $f(x) = x^{-1} \ \Rightarrow\ |f''| = |2(f')^{3/2}|$.
- Have experimental evidence that matrix case can be similar to scalar case.