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The Structured Condition Number of a Differentiable Map Between Matrix Manifolds

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Motivating Example

Let $a > 0$ and consider the matrix logarithm of X,

$$X = \begin{bmatrix} e^a & 0 \\ 0 & e^{-a} \end{bmatrix}, \qquad \log X = \begin{bmatrix} a & 0 \\ 0 & -a \end{bmatrix}.$$

X symplectic $\Rightarrow$ $\log(X)$ is Hamiltonian.

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X symplectic $\Rightarrow$ $\log(X)$ is Hamiltonian.

Apply tiny perturbation to X (norm = $\epsilon\|X\|$),

$$\widetilde{X} = \begin{bmatrix} e^a & 0 \\ 0 & e^{-a} + \epsilon e^a \end{bmatrix} \Rightarrow \log \widetilde{X} = \begin{bmatrix} a & 0 \\ 0 & -a \end{bmatrix} + \epsilon \begin{bmatrix} 0 & 0 \\ 0 & e^{2a} \end{bmatrix} + o(\epsilon).$$

Worst case scenario, so the **relative conditioning** is

$$\frac{e^{2a}}{a}.$$

Motivating Example (Cont.)

Now consider a pertubation preserving the symplectic structure,

$$X = \begin{bmatrix} e^a & \epsilon e^a \\ 0 & e^{-a} \end{bmatrix} \Rightarrow \ln X = \begin{bmatrix} a & 0 \\ 0 & -a \end{bmatrix} + \epsilon \begin{bmatrix} 0 & \frac{ae^a}{\sinh(a)} \\ 0 & 0 \end{bmatrix} + o(\epsilon)$$

This is the worse we can do but the effect is much milder!

The **relative structured conditioning** is

$$\frac{e^a}{\sinh(a)} < \frac{e^{2a}}{a}$$

Structure conditioning $\ll$ unstructured conditioning for average or large values of a.

Condition Number of $f(X)$

Let $f : \mathbb{F}^{n\times n} \to \mathbb{F}^{n\times n}$ be $\mathbb{F}$-Fréchet differentiable, $\mathbb{F} = \mathbb{R}$ or $\mathbb{C}$.

Define absolute **condition number of $f(X)$**:

$$\mathrm{cond}(f, X) = \lim_{\epsilon\to 0} \sup_{\substack{\|Y-X\|\le\epsilon \\ Y\in\mathbb{F}^{n\times n}}} \frac{\|f(Y) - f(X)\|}{\epsilon}.$$

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The Fréchet derivative of f at X is a $\mathbb{F}$-linear map $L_f(X, \cdot)$ so

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

where $K_f(X) \in \mathbb{F}^{n^2\times n^2}$ is **Kronecker form of the Fréchet derivative**. Then, for the Frobenius norm,

$$\mathrm{cond}(f, X) = \max_{\substack{E\in\mathbb{F}^{n\times n} \\ E\neq 0}} \frac{\|L_f(X, E)\|_F}{\|E\|_F} = \|K_f(X)\|_2 .$$

Restricting the Perturbations

Suppose $f : \mathcal{M} \to \mathcal{N}$ is differentiable with $\mathcal{M}, \mathcal{N} \subseteq \mathbb{F}^{n\times n}$ **smooth matrix manifolds**. Let $X \in \mathcal{M}$ and enforce the perturbations $Y - X$ to be s.t. $Y \in \mathcal{M}$.

Define **structured condition number of f at X**:

$$\mathrm{cond}_{\mathsf{struc}}(f, X) = \lim_{\epsilon\to 0} \sup_{\substack{\|Y-X\|\le\epsilon \\ Y\in\mathcal{M}}} \frac{\|f(Y) - f(X)\|}{\epsilon}$$

$$\Rightarrow \|f(Y) - f(X)\| \le \mathrm{cond}_{\mathsf{struc}}(f, X)\|Y - X\| + o(\|Y - X\|).$$

Also, by the definition of supremum, we have

$$\mathrm{cond}_{\mathsf{struc}}(f, X) \le \mathrm{cond}(f, X).$$

Square Matrix Manifolds

Consider three classes:

1. real submanifolds of the n^2-dimensional real vector space $\mathbb{R}^{n\times n}$ (e.g., real symplectic matrices),
2. complex submanifolds of the n^2-dimensional complex vector space $\mathbb{C}^{n\times n}$ (e.g., complex orthogonal matrices),
3. real submanifolds of the $2n^2$-dimensional *real* vector space $\mathbb{C}^{n\times n}$ (e.g., Hermitian, unitary matrices).

Need to distinguish between

- **ambient field** $\mathbb{F}$: field in which the entries of X lie,
- **base field** $\mathbb{K}$: field the ambient vector space is built on.

$$X = X^* = \begin{bmatrix} a & b + \mathrm{i}c \\ b - \mathrm{i}c & d \end{bmatrix},\ a, b, c, d \in \mathbb{R} \text{ so } \mathbb{F} = \mathbb{C},\ \mathbb{K} = \mathbb{R}.$$

Theoretical Tools: Differential Geometry

Let $\mathcal{M}, \mathcal{N} \subseteq \mathbb{F}^{n\times n}$ with base field $\mathbb{K}$ and let $f : \mathcal{M} \to \mathcal{N}$ be $\mathbb{K}$-differentiable.

(*The differential plays the role of the derivative for maps f between manifolds: best (local)* $\mathbb{K}$*-linear approx. to f.*)

$$df_X : T_X\mathcal{M} \to T_{f(X)}\mathcal{N}, \quad df_X(\gamma'(0)) = (f \circ \gamma)'(0),$$

for a smooth curve $\gamma : \mathbb{K} \to \mathcal{U} \subset \mathcal{M}$ such that $\gamma(0) = X$,
$T_X\mathcal{M}$: **tangent space** of $\mathcal{M}$ at X.

Theorem (Arslan, Noferini, T.'17)

For the ***structured condition number of*** f ***at*** $X \in \mathcal{M}$ *we have*

$$\mathrm{cond}_{\text{struc}}(f, X) = \|df_X\|.$$

Structured Condition Number (Cont.)

Uniqueness of differential and Fréchet derivative imply $\Rightarrow$

$$df_X(E) = L_f(X, E), \quad E \in T_X\mathcal{M}.$$

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$T_X\mathcal{M}$ is a **$\mathbb{K}$-linear** subspace of $\mathbb{F}^{n\times n}$ so $\text{vec}(E) = By$,
$B \in \mathbb{F}^{n^2\times p}$ (basis for $T_X\mathcal{M}$), $y \in \mathbb{K}^p$ (vector of parameters),
$p = \dim_{\mathbb{K}} T_X\mathcal{M}$.

Structured Condition Number (Cont.)

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$p = \dim_{\mathbb{K}} T_X\mathcal{M}$. Now using

$$\text{vec}(df_X(E)) = \text{vec}(L_f(X, E)) = K_f(X)\text{vec}(E) = K_f(X)By,$$

we have

$$\text{cond}_{\text{struc}}(f, X) = \max_{\substack{E\in T_X\mathcal{M}\\ E\neq 0}} \frac{\|df_X(E)\|_F}{\|E\|_F} = \max_{\substack{y\in\mathbb{K}^p\\ y\neq 0}} \frac{\|K_f(X)By\|_2}{\|By\|_2}.$$

If $B^*B = I_p$ then $\text{cond}_{\text{struc}}(f, X) = \|K_f(X)B\|_2$.

From Theory to Computation

The theory is simple and elegant, but computing the (un)structured condition number is an issue, since the cost of a naive algorithm is

- $O(n^5)$ for $\mathrm{cond}(f, X) = \|K_f(X)\|_2$,
  $K_f(X)e_{i+(j-1)n} = \mathrm{vec}(L_f(X, e_i e_j^T))$, $i = 1\colon n$, $j = 1\colon n$,
- $O(n^6)$ for $\mathrm{cond}_{\mathrm{struc}}(f, X) = \|K_f(X)B\|_2$ when $B^*B = I_p$,
  $K_f(X)Be_i = \mathrm{vec}\big(L_f(X, \mathrm{unvec}(Be_i))\big)$, $i = 1\colon p$.

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When $B^*B \neq I_p$, can compute the lower/upper bounds

$$\|K_f(X)B\|_2 \|B\|_2^{-1} \leq \mathrm{cond}_{\mathrm{struc}}(f, X) \leq \|K_f(X)B\|_2 \|B^+\|_2.$$

Computational tool: the power method

This alg. applies the power method to $K_f(X)^* B^* B K_f(X)$ to compute a lower bound γ for $\|K_f(X)B\|_2$.

```
Start with z_0 ∈ F^p.
for k = 0: ∞
    vec(E_k) = B z_k
    W_{k+1} = L_f(X, E_k)
    E_{k+1} = L_f^⋆(X, W_{k+1})
    γ_{k+1} = ‖Z_{k+1}‖_F / ‖W_{k+1}‖_F
    z_{k+1} = B^* vec(Y_{k+1})
    if converged, γ = γ_{k+1}, quit, end
end
```

$$L_f^{\star}(X,E) = \begin{cases} L_f(X^T, E), & \mathbb{F} = \mathbb{R} \\ L_{\bar{f}}(X^*, E), & \mathbb{F} = \mathbb{C} \end{cases}$$

Cost: $O(n^2 p)$ per iteration but often the structure of B can be exploited to reduce the cost to $O(np)$. Typically, $p = O(n^2)$.

Structured Matrices

A scalar product $\langle \cdot, \cdot \rangle_M$ is a non degenerate (M nonsingular) bilinear or sesquilinear form on $\mathbb{F}^n$.

$$\langle x, y \rangle_M = \begin{cases} x^T M y & \text{real or complex } \textbf{bilinear} \text{ forms,} \\ x^* M y & \textbf{sesquilinear} \text{ forms.} \end{cases}$$

Any matrix A has a unique adjoint $A^\star$ given by

$$A^\star = \begin{cases} M^{-1} A^T M, & \text{real or complex } \textbf{bilinear} \text{ forms,} \\ M^{-1} A^* M, & \textbf{sesquilinear} \text{ forms.} \end{cases}$$

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Associated with $\langle \cdot, \cdot \rangle_M$ are three classes of structured matrices: a Jordan algebra $\mathbb{J}_M$, a Lie algebra $\mathbb{L}_M$, and an automorphism group $\mathbb{G}_M$.

Automorphism Groups

Having fixed the scalar product $\langle \cdot, \cdot \rangle_{\mathrm{M}}$, the associated **automorphism group** is

$$\begin{aligned} \mathbb{G}_{\mathrm{M}} &:= \{G \in \mathbb{F}^{n\times n} : \langle Gx, Gy \rangle_{\mathrm{M}} = \langle x, y \rangle_{\mathrm{M}} \} \\ &= \{G \in \mathbb{F}^{n\times n} : G^{\star} = G^{-1}\}. \end{aligned}$$

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Theorem (Arslan, Noferini, T.'17)

$\mathbb{G}_{M}$ is a real submanifold of $\mathbb{F}^{n\times n}$. When $\langle\cdot,\cdot\rangle_{M}$ is a complex bilinear form, $\mathbb{G}_{M}$ is also a complex submanifold of $\mathbb{C}^{n\times n}$.

Tangent Spaces and Lie Algebras

Having fixed $\langle\cdot,\cdot\rangle_{\mathrm{M}}$, the associated **Lie algebra** is

$$\begin{aligned}\mathbb{L}_{\mathrm{M}} &:= \{F \in \mathbb{K}^{n\times n} : \langle Fx, y\rangle_{\mathrm{M}} = -\langle x, Fy\rangle_{\mathrm{M}}\} \\ &= \{G \in \mathbb{K}^{n\times n} : G^{\star} = -G\}.\end{aligned}$$

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Theorem

Let $X \in \mathbb{G}_M$, then

$$T_X\mathbb{G}_M = \{E \in \mathbb{F}^{n\times n} : E = XF, F \in \mathbb{L}_M.\}.$$

A basis for $T_X\mathbb{G}_M$ is $B = (I_n \otimes XM^{-1})D$, where D has orthonormal columns and does not depend on X.

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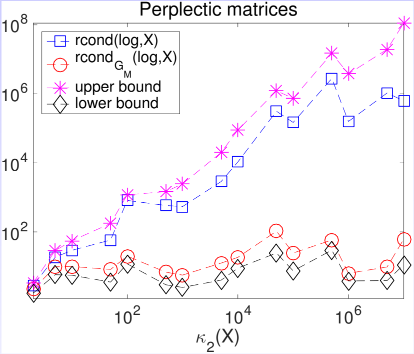
$$\frac{\|K_f(X)B\|_2}{\|M^{-1}\|_2\|X\|_2} \le \mathrm{cond}_{\mathrm{s}}(f, X) \le \|K_f(X)B\|_2\|X\|_2\|M\|_2.$$

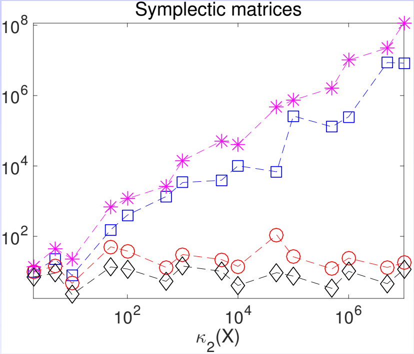
Commonly Used M

M	Structure of M	Name of $\mathbb{G}_M$	Where they appear
I	I_n	orthogonal cplx orthogonal unitary	everywhere
J	$\begin{bmatrix} 0 & I_{n/2} \\ -I_{n/2} & 0 \end{bmatrix}$	symplectic cplx symplectic conjugate sympl.	physics engineering
R	$\begin{bmatrix} & & 1 \\ & ⋰ & \\ 1 & & \end{bmatrix}$	perplectic	maths, chemistry
S_{pq}	$\begin{bmatrix} I_p & 0 \\ 0 & -I_q \end{bmatrix}$ $p+q=n$	pseudo-orthogonal pseudo-unitary	physics

Principal Logarithm

$\log(X) : \mathbb{G}_M \to \mathbb{L}_M$. Generate random $X \in \mathbb{G}_M \subset \mathbb{R}^{10\times 10}$, $M = R, J$ with increasing $\kappa_2(X) = \|X\|_2 \|X^{-1}\|_2$.





$$X^{-1} = RX^T R$$

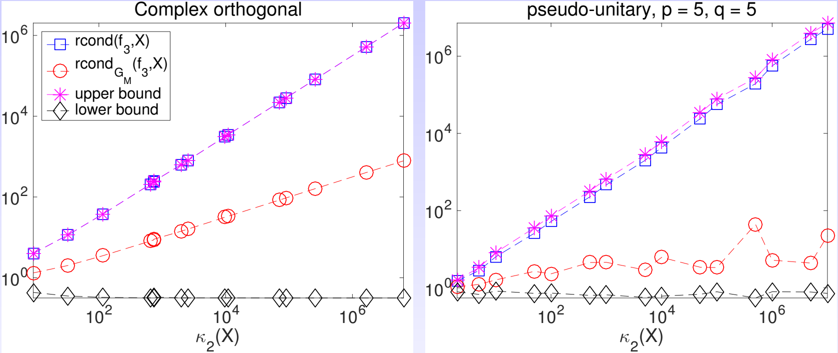
$$R = \begin{bmatrix} & & 1 \\ & \cdot^{\cdot^{\cdot}} & \\ 1 & & \end{bmatrix}$$

$$X^{-1} = -JX^T J$$

$$J = \begin{bmatrix} 0 & I_{n/2} \\ -I_{n/2} & 0 \end{bmatrix}$$

Unitary Polar Factor

$f_3 : \mathbb{G}_M \to \mathbb{G}_M \cap \mathbb{G}_I$, $f_3(X) = U$, where $X = UH$ (polar decomposition). f_3 is only $\mathbb{R}$-differentiable.



$$X^{-1} = X^T, \qquad X^{-1} = \begin{bmatrix} I_p & 0 \\ 0 & -I_q \end{bmatrix} X^* \begin{bmatrix} I_p & 0 \\ 0 & -I_q \end{bmatrix}.$$

For complex orthogonal, must choose base field $\mathbb{K} = \mathbb{R}$.

Principal Square Root $X^{1/2} : \mathbb{G}_M \to \mathbb{G}_M$

Let $A = X^{1/2}$ and $\widehat{A}$ be the computed square root of X.
Relative error bound:

$$\frac{\|\widehat{A} - X^{1/2}\|_F}{\|X^{1/2}\|_F} \lesssim \mathrm{cond}(\mathrm{sqrt}, X) \frac{\|\widehat{A}^2 - X\|_F}{\|X^{1/2}\|_F}. \tag{1}$$

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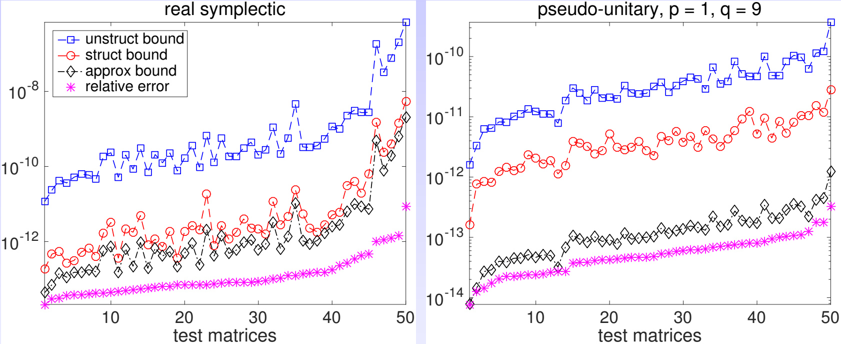
Use structure preserving and cubically converging iteration

$$Y_{k+1} = \frac{1}{3} Y_k \left[I + 8\left(I + 3Z_k Y_k\right)^{-1} \right], \qquad Y_0 = X,$$
$$Z_{k+1} = \frac{1}{3} \left[I + 8\left(I + 3Z_k Y_k\right)^{-1} \right] Z_k, \qquad Z_0 = I,$$

where $Y_k, Z_k \in \mathbb{G}_M$ and $Y_k \to X^{1/2}$ (see Higham, Mackey, Mackey, T., SIMAX'05). Can replace $\mathrm{cond}(\mathrm{sqrt}, X)$ by $\mathrm{cond}_{\mathbb{G}_M}(\mathrm{sqrt}, X)$ in (1).

Relative Error Bounds

Bounds on $\|\widehat{A} - X^{1/2}\|_F / \|X^{1/2}\|_F$, $\kappa_2(X) = 10^5$, $N = 10$.



$$X^{-1} = -JX^TJ \qquad X^{-1} = S_{pq}X^*S_{pq}$$

$$J = \begin{bmatrix} 0 & I_{n/2} \\ -I_{n/2} & 0 \end{bmatrix} \qquad S_{pq} = \begin{bmatrix} I_p & 0 \\ 0 & -I_q \end{bmatrix}.$$

Concluding Remarks

- Framework to define and compute structured condition numbers of maps between matrix manifolds
- Structured condition number expensive to compute but lower/upper bounds are cheap. The lower bound is often a good approximation.
- Gave numerical evidence that often s.c.n. $\ll$ u.c.n. This suggests that using a structure preserving alg to compute $f(X)$ might be advantageous.
- MIMS EPrint available (soon) on my web page.