

RECAP

- $(E, \|\cdot\|_E)$, $(F, \|\cdot\|_F)$ finite-dimensional Hilbert spaces

• Def: The operator norm of

$$A \in \mathcal{L}(E, F) \text{ is } \|A\|_{E, F} := \sup_{x \neq 0} \frac{\|Ax\|_F}{\|x\|_E} \Rightarrow$$

$$\left[\begin{array}{l} \forall x \in E, \\ \|Ax\|_F \leq \|A\|_{E, F} \|x\|_E \end{array} \right.$$

RECAP

$$Ax = y$$

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- Def: The condition number of

$$A \in \mathcal{L}(E, F) \text{ is } \kappa(A) = \|A\|_{E, F} \|A^{-1}\|_{F, E}$$

Proof $\in \mathbb{R}^{m \times m}$

- 1) The matrix $A^T A$ is symmetric, hence diagonalisable in orthonormal basis of \mathbb{R}^m : $\left\{ \begin{array}{l} v_1, \dots, v_m \\ \lambda_1, \dots, \lambda_m \end{array} \right.$ eigenvectors
eigenvalues, $A^T A = V \begin{pmatrix} \lambda_1 & & \\ & \dots & \\ & & \lambda_m \end{pmatrix} V^T$

Proof

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- 2) The matrix $A^T A$ is semidefinite positive: $\forall x \in \mathbb{R}^m$, $x^T A^T A x = \|Ax\|^2 \geq 0$
 hence $\lambda_i \geq 0$, $i = 1, \dots, m$. We assume $\lambda_1 \geq \dots \geq \lambda_n \geq \lambda_{n+1} = 0 = \dots = \lambda_m$

$$\forall u \quad x^T \Pi x \geq 0$$

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- 3) let $\sigma_i = \sqrt{\lambda_i}$ and $u_i = \frac{Av_i}{\sigma_i}$ for all $i = 1, \dots, n$
- (u_i) o.m.b. of $\text{Im } A$: $\left\{ \begin{array}{l} \|u_i\|^2 = \frac{1}{\sigma_i^2} v_i^T A^T A v_i = \frac{\lambda_i}{\sigma_i^2} \|v_i\|^2 = 1 \\ \langle u_i, u_j \rangle = \frac{\lambda_j}{\sigma_i \sigma_j} v_i^T v_j = 0 \quad \text{if } i \neq j \end{array} \right.$

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- 3) let $\sigma_i = \sqrt{\lambda_i}$ and $u_i = \frac{A v_i}{\sigma_i}$ for all $i = 1, \dots, r$
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- 4) Hence $U_1 := (u_1, \dots, u_r) = A V_1 \Sigma_1^{-1}$, where $\Sigma_1 = \text{diag}(\sigma_1, \dots, \sigma_r)$
 i.e. $U_1 \Sigma_1 = A V_1$ $V_1 = (v_1, \dots, v_r)$

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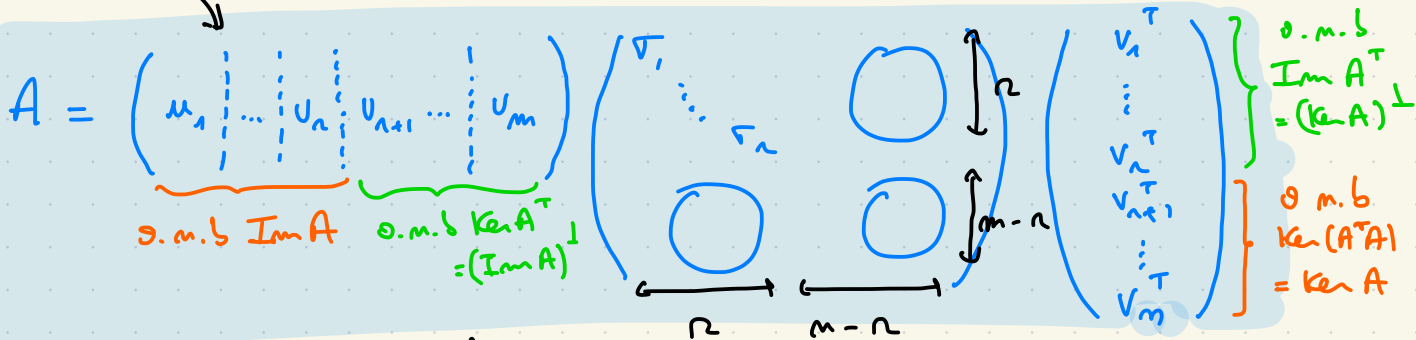
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 $\hookrightarrow U \begin{pmatrix} \Sigma & 0 \\ 0 & 0 \end{pmatrix} = A V$ where (u_1, \dots, u_m) o.m.b. of \mathbb{R}^m

SVD, RANGE, KERNEL

"left singular vectors"

"right singular vectors"

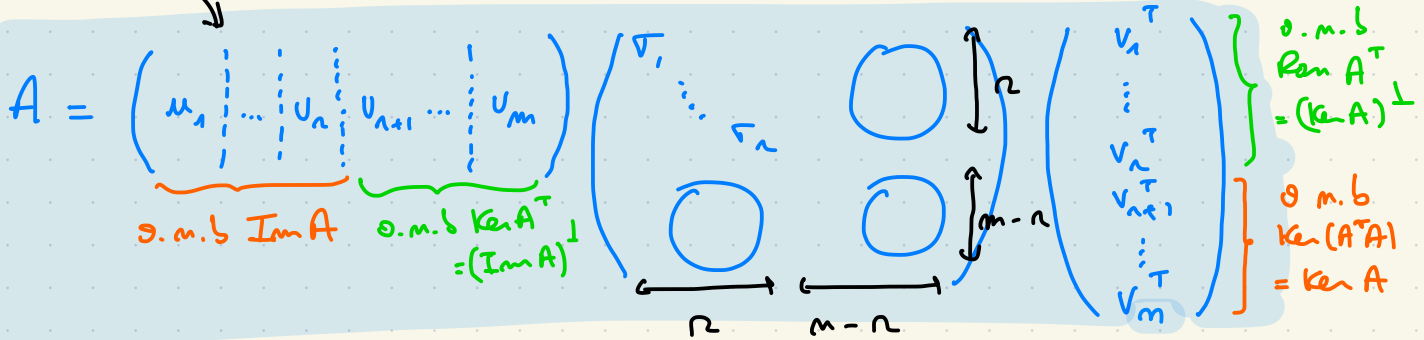


$$E = \text{Row } A + (\text{Row } A)^\perp$$

SVD, RANGE, KERNEL

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- Prop :
- $\text{Ker } A = \text{Span}(v_{n+1}, \dots, v_m)$
 - $\text{Ran } A = \text{Span}(u_1, \dots, u_n)$ (in particular $\text{rank } A = r$)
 - $\text{Ker } A^T = \text{Span}(u_{n+1}, \dots, u_m)$
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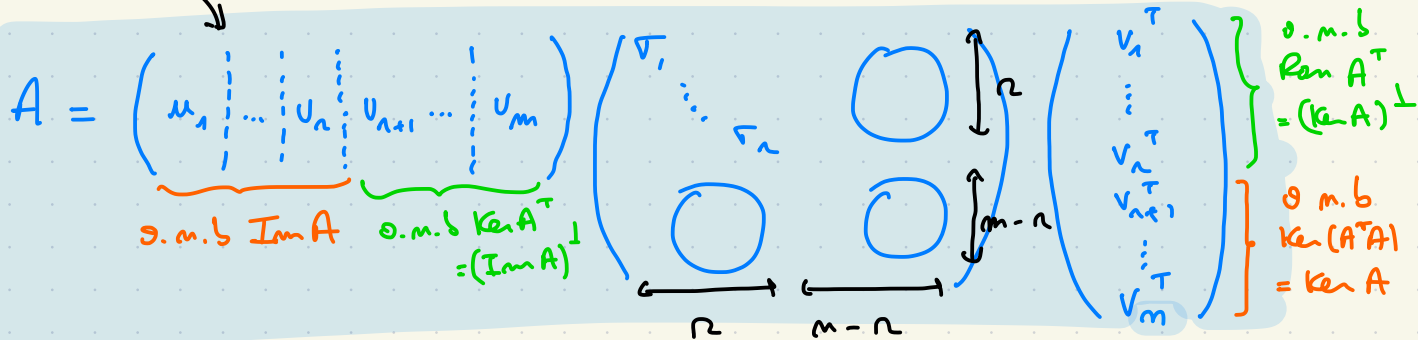
Rank : Singular values are unique (σ_i^2 eigenvalue of $A^T A$), singular vectors with multiplicity 1 are unique up to ± 1 factor

$$A = U \Sigma V^T = \underbrace{U_n \Sigma_n V_n^T}_{\text{reduced SVD}} = \sum_{i=1}^{\text{rank } A} \sigma_i u_i v_i^T$$

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generalizable to Hilbert bases of $\text{Ran } A$ and $(\text{Ker } A)^\perp$

CONDITION NUMBER

Prop: let $A = U \begin{pmatrix} \sigma_1 & & 0 \\ & \ddots & \\ & & \sigma_n & \\ 0 & & & 0 \end{pmatrix} V^T$, $\sigma_1 \geq \dots \geq \sigma_n > 0$. Then $\|A\|_{2,2} = \sigma_1$

Proof: let $x \in \{x \in \mathbb{R}^m / \|x\|_2 = 1\}$. Then

$$\|Ax\|_2^2 = \|U \Sigma V^T x\|_2^2 = \|\Sigma V^T x\|_2^2 \quad \text{since } U \text{ orthogonal}$$

$$= \sum_{i=1}^n \sigma_i^2 |v_i^T x|^2$$

$$\leq \sigma_1^2 \sum_{i=1}^n |v_i^T x|^2 \quad (= \text{if } x = v_1)$$

$$= \sigma_1^2 \|V^T x\|_2^2 = \sigma_1^2 \|x\|_2^2 = \sigma_1^2$$

$$\sup_{\|x\|_2=1} \|Ax\|_2 = \|A\|_{2,2}$$

Hence $\|A\|_{2,2} = \sup_{\|x\|_2=1} \|Ax\|_2 = \sigma_1$

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Hence $\|A\|_{2,2} = \sup_{\|x\|_2=1} \|Ax\|_2 = \sigma_1$

Prop: let $A \in \mathbb{R}^{m \times m}$ invertible. Then $\kappa_2(A) = \frac{\sigma_1}{\sigma_m}$

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 $A^{-1} = V \Sigma^{-1} U^T$

$$A = U \Sigma V^T \rightarrow A^{-1} = V \Sigma^{-1} U^T$$

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Remark: If $A \in \mathbb{R}^{m \times m}$, $\text{rank}(A) = r$, $\frac{\sigma_1}{\sigma_r} = \kappa \left(\begin{array}{c} P \\ \text{Rank } A \end{array} A \middle| \begin{array}{c} A \\ (\text{ker } A)^\perp \end{array} \right)$

INTERPRETATION OF $K(A)$

relative error on solution $\approx K(A) \cdot$ relative error on data

e.g. $\hookrightarrow 10^{-a} \approx K(A) \cdot 10^{-b}$

$$\hookrightarrow a \approx b - \log_{10}(K(A))$$

$\log_{10}(K(A))$ = number of significant digits one may lose when solving $Ax = y$.

SOLVING (LS) WITH SVD

$$\min_{x \in \mathbb{R}^m} \|Ax - y\|_2^2 \quad (\text{LS})$$

let (U, Σ, V) be the SVD of A . We have, for $x \in \mathbb{R}^m$:

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because $\Sigma = \begin{pmatrix} \sigma_1 & & 0 \\ & \ddots & \\ 0 & & \sigma_n \\ & & & 0 \end{pmatrix} \rightarrow = \sum_{i=1}^n |\sigma_i (v_i^T x) - (u_i^T y)|^2 + \sum_{i=n+1}^m |u_i^T y|^2$

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\Rightarrow The minimum is attained for $x_* = \sum_{i=1}^r \frac{u_i^T y}{\sigma_i} v_i + x_0$

$x_0 \in \text{Ker } A$
 $x_* \in (\text{Ker } A)^\perp$

SOLVING (LS) WITH SVD

$$\min_{x \in \mathbb{R}^m} \|Ax - y\|_2^2 \quad (LS)$$

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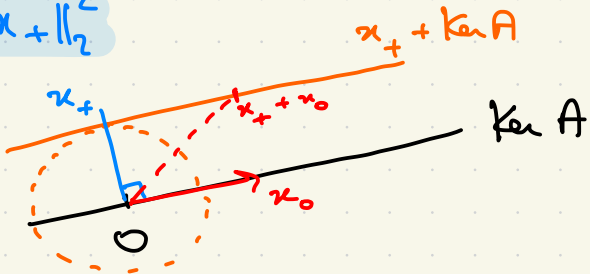
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and $\|x_*\|_2^2 = \|x_+\|_2^2 + \|x_0\|_2^2 \geq \|x_+\|_2^2$

ii $x_+ \in (\text{Ker } A)^\perp$



PSEUDO-INVERSE

- Solutions of $\min_{x \in \mathbb{R}^m} \|Ax - y\|_2^2$ are of the form

$$x_* = x_+ + x_0, \text{ where } x_+ = \sum \frac{u_i^T y}{\sigma_i} v_i \text{ and } x_0 \in \ker A$$

- In matrix form:

$$\mathbb{R}^m \ni x_+ = A^+ y, \text{ where } A^+ := V \begin{matrix} \xrightarrow{n} & \xrightarrow{m-n} \\ \left(\begin{array}{cc|cc} \underbrace{1/\sigma_1}_{\uparrow} & \dots & \underbrace{1/\sigma_n}_{\uparrow} & 0 \\ \hline 0 & & 0 & 0 \end{array} \right) U^T \in \mathbb{R}^{m \times m} \end{matrix}$$

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- Prop :
- If A is injective, then $A^+ y$ is the (unique) solution of the least-squares problem.
 - If A is not injective, then $A^+ y$ is the (unique) solution of minimal l^2 -norm.

Rem : $\frac{\sigma_1}{\sigma_n} = \|A\| \|A^+\| =: \kappa_2(A)$ for non-invertible matrix

PSEUDO - INVERSE (2)

- More generally

Def: let $A \in \mathcal{L}(E, F)$, and let $\tilde{A} : (\text{Ker } A)^\perp \rightarrow \text{Ran } A$ be its restriction. The Moore-Penrose pseudo-inverse A^+ (or generalized inverse) is the unique linear extension of \tilde{A}^{-1} to $\text{Ran } A \oplus (\text{Ran } A)^\perp$ with $\text{Ker } A^+ = (\text{Ran } A)^\perp$.

$= F$

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- Prop: A^+ is characterized by the equations

$$- AA^+A = A$$

$$- A^+A = P_{(\text{Ker } A)^\perp} (= I - P_{\text{Ker } A})$$

$$- A^+AA^+ = A^+$$

$$- AA^+ = P_{\text{Ran } A}$$

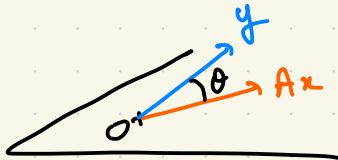
CONDITIONING OF LEAST-SQUARES

for $m \geq n$

Thm: let $A \in \mathbb{R}^{m \times n}$ with $\text{rank } A = n$. let x be the solution of $\min_z \|Az - y\|_2^2$, and let \tilde{x} be the solut^o of the perturbed problem $\min_z \|Az - (y + \delta y)\|_2^2$. Then

$$\frac{\|x - \tilde{x}\|_2}{\|x\|_2} \lesssim \frac{\kappa(A)}{\cos \theta} \frac{\|\delta y\|_2}{\|y\|_2}$$

where $\theta := \text{angle}(y, Ax)$



CONDITIONING OF LEAST-SQUARES

for $m \geq n$

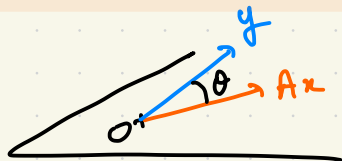
Thm: let $A \in \mathbb{R}^{m \times n}$ with $\text{rank } A = n$. let x be the solution of $\min_z \|Ax - y\|_2^2$, and let \tilde{x} be the solut^o of the perturbed problem $\min_z \|Az - (y + \delta y)\|_2^2$. Then

$$\frac{\|x - \tilde{x}\|_2}{\|x\|_2} \lesssim \frac{\kappa(A)}{\cos \theta} \frac{\|\delta y\|_2}{\|y\|_2} \quad \text{where } \theta := \text{angle}(y, Ax)$$

let \hat{x} be the solution of $\min_z \|(A + \delta A)z - (y + \delta y)\|_2^2$

Then

$$\frac{\|x - \hat{x}\|_2}{\|x\|_2} \lesssim \kappa(A) \left(\frac{\|\delta A\|_2}{\|A\|_2} + \frac{1}{\cos \theta} \frac{\|\delta y\|_2}{\|y\|_2} \right) + \kappa(A)^2 \tan \theta \frac{\|\delta A\|_2}{\|A\|_2}$$



$\tan \theta$

CONDITIONING OF LEAST-SQUARES

for $m \geq n$

Proof (of the 1st inequality): let $\delta x = \tilde{x} - x$

normal equations: $A^T A \tilde{x} = A^T (y + \delta y)$

$$A^T A x = A^T y$$

hence $A^T A \delta x = A^T \delta y$

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(*) in particular
 $A = U \begin{pmatrix} \Sigma_1 \\ 0 \end{pmatrix} V^T$

hence $A^T A \delta x = A^T \delta y$

Since A is full column-rank, $A^T A$ is invertible and

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$(\frac{1}{\sigma_1}, \dots, \frac{1}{\sigma_n}, 0)$

But $A^T A = V \Sigma_1^2 V^T$, $(A^T A)^{-1} A^T = V (\Sigma_1^{-1} \ 0) U^T$

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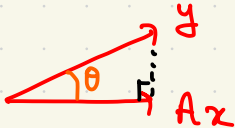
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$$\leq \kappa(A) \frac{\|\delta y\|_2}{\|y\|_2} \frac{\|y\|_2}{\|Ax\|_2} = \frac{\kappa(A)}{\cos \theta} \frac{\|\delta y\|_2}{\|y\|_2}$$

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If $A^T A > 0$ then $\exists!$ R upper triang. with $R_{ii} > 0$ s.t. $A^T A = R^T R$

\leadsto Solve $R^T z = y$ then $Rx = z$

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reasonable cost: $mn^2 + n^3/3$ operations

unstable: $\kappa_2(A^T A) = \kappa_2(A)^2$; require $A^T A$ non-singular ($\ker A = \{0\}$)

Example: $A = \begin{bmatrix} 1 & 1 & 1 \\ \varepsilon & 0 & 0 \\ 0 & \varepsilon & 0 \\ 0 & 0 & \varepsilon \end{bmatrix}$, $A^T A = \begin{bmatrix} 1+\varepsilon^2 & 1 & 1 \\ 1 & 1+\varepsilon^2 & 1 \\ 1 & 1 & 1+\varepsilon^2 \end{bmatrix}$

$$A \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix} = \begin{bmatrix} x_1 + x_2 + \varepsilon x_3 \\ \varepsilon x_1 \\ \varepsilon x_2 \\ \varepsilon x_3 \end{bmatrix}$$

NUMERICAL APPROACHES

For $m \geq n$

Solving $Ax = y$ in the least-squares sense with:

$A \setminus b$

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$$\|Ax - y\|^2 = \left\| Q \begin{bmatrix} R \\ 0 \end{bmatrix} x - y \right\|^2 = \left\| \begin{bmatrix} R \\ 0 \end{bmatrix} x - Q^T y \right\|^2$$

NUMERICAL APPROACHES

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reasonable cost: $2mn^2 - \frac{2}{3}n^3$ operations

reasonably stable

A GLANCE IN INFINITE DIMENSION

let $A \in \mathcal{L}(E, F)$ continuous

• Properties in finite dimension

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Proof: let $V \ni x_n \rightarrow x \in E \setminus V$

let (e_1, \dots, e_d) basis of V . Then

(e_1, \dots, e_d, x) lin. indep. in E , so

in $\text{Span}(e_1, \dots, e_d, x)$,

$x_n = (\alpha_1^{(n)}, \dots, \alpha_d^{(n)}, 0)$ and $x = (0, \dots, 0, 1)$

hence at the limit $0 = 1$

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Why does it matter?

1) maintain Hilbert structure

(completeness)

2) existence of projection

$$\|z - x_0\| = \inf_{x \in S} \|z - x\|$$

("projection theorem")

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$$\overline{\text{Ran } A} \perp \text{Ran } A^\perp \quad (\text{exercise})$$

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Remark: $\text{Ran } A \oplus (\text{Ran } A)^\perp$ is dense in F

COMPACT OPERATORS

- SVD can be generalized for a specific class of operators

Def: let $A \in \mathcal{L}(E, F)$. A is said to be compact if for any bounded set $B \subset E$, $\overline{A(B)}$ is compact.

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Examples: • $Af = \int_{\Omega} k(\cdot, y) f(y) dy$, with e.g. $k(x) = e^{-\frac{|x|^2}{\sigma^2}}$ (convolution)

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* ill-posedness \leftrightarrow "smoothness" of the kernel K

* in fact

Prop: If E, F are of infinite dimension, then $A \in \mathcal{L}(E, F)$ compact is never invertible.

SINGULAR VALUE EXPANSION

- SVD can be generalized to compact operators

Thm (Singular Value Expansion) Let $A \in \mathcal{L}(E, F)$ be compact.

Then $\exists (\sigma_j)_{j \in \mathbb{N}} \in \mathbb{R}_+$, and orthon. fam. $(e_j) \in E$ and $(f_j) \in F$ s.t. $\sigma_j \xrightarrow{j \rightarrow \infty} 0$ and

$$\begin{cases} \forall x \in E, Ax = \sum_{j=1}^{\infty} \sigma_j \langle x, e_j \rangle f_j \\ \forall y \in F, A^*y = \sum_{j=1}^{\infty} \sigma_j \langle y, f_j \rangle e_j \end{cases}$$

(f_j) Hilbert basis* of $\overline{\text{Ran } A}$

(e_j) Hilbert basis of $(\text{Ker } A)^\perp$

* 1) orthonormal

2) Span (e_i) dense

$$\left(\cos \sqrt{x} + \sqrt{x} \cos(2mx) \right) \cup \left(\sin \sqrt{x} + \sqrt{x} \sin(2mx) \right) \quad m \in \mathbb{N}$$

$$\notin L^2([0, \pi])$$

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Importantly, $\left\| \sum_1^N \sigma_j \langle x, e_j \rangle f_j \right\|^2 \leq \sum_1^N \sigma_j^2 \langle x, e_j \rangle^2 \leq \sigma_1^2 \sum_1^N \langle x, e_j \rangle^2 \leq \sigma_1^2 \|x\|^2$

\nearrow Bessel

so $\lim_{N \rightarrow \infty}$ is valid.

PICARD CRITERION

Thm: $A \in \mathcal{L}(E, F)$ compact, with SVE $\{\sigma_i, e_i, f_i\}$

The equation $Ax = y$ has a solution iff

1) $y \in \overline{\text{Ran } A}$

2) $\sum_{j=1}^{\infty} \frac{\langle y, f_j \rangle^2}{\sigma_j^2} < \infty$ (Picard's criterion)

Proof: • If $Ax = y$ then $y \in \text{Ran } A \subset \overline{\text{Ran } A}$. Furthermore

$$\langle x, e_i \rangle = \frac{1}{\sigma_i} \langle x, A^* f_i \rangle = \frac{1}{\sigma_i} \langle y, f_i \rangle$$

so $\sum_{i=1}^{\infty} \frac{1}{\sigma_i^2} \langle y, f_i \rangle^2 \leq \|x\|^2 < \infty$

• If $y \in \overline{\text{Ran } A}$ then $y = \sum_{i=1}^{\infty} \langle y, f_j \rangle f_j$, and

$$x = \sum \frac{1}{\sigma_j} \langle y, f_j \rangle e_j \text{ satisfies } Ax = y.$$

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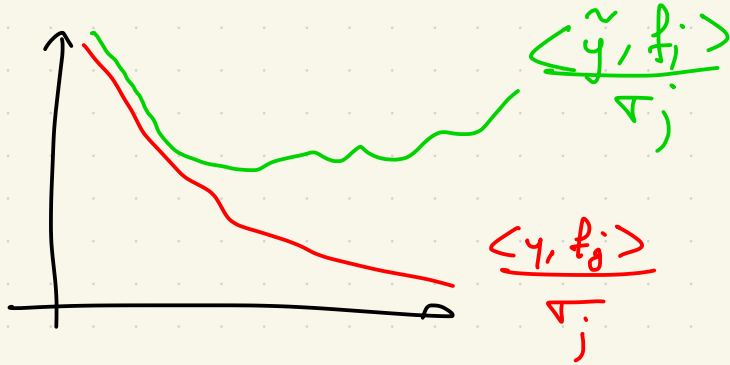
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Picard's criterion asks for some *regularity* in the data: the coefficients $\langle y, f_j \rangle$ must decrease faster than σ_j

Never holds in practice, since $\tilde{y} = y + \delta y$



paulcat@github.io/teaching.html