Summer School on Applied Harmonic Analysis and Machine Learning

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Minicourse on ill-posed problems

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Lecture 1 What's an inverse problem?

What's an ill-posed problem?

Inverse to what?

$$\begin{tikzcd} \boxed{\text{Problem 1}} \arrow[r, bend left] & \boxed{\text{Problem 2}} \arrow[l, bend left] \end{tikzcd}$$

If problem formulation of one involves the other

$\rightsquigarrow$ "Problem 1 & 2 are inverse to each other"

A <u>direct</u> & an <u>inverse</u> problem

How to decide which one is direct / inverse?

Can be

- historical reasons (older problem is direct problem)
- physical meaning

  direct: given: present state of a physical system & underlying physical laws,
  predict: future states

inverse: • determine present state from future observations

• identify physical parameters from observations

• difficulty

declare the "harder" problem as the inverse problem

to be discussed...

Example 1: Differentiation & integration

Which one is the inverse problem?

A more interesting (& clear) property: <u>ill-posedness</u>

Consider $f \in C^1[0,1]$ and a slightly perturbed version $f_n^\delta(x) := f(x) + \delta \sin\frac{nx}{\delta}$ [$\delta \in (0,1)$, $n \in \mathbb{N}$ arbitrary]

Then $\|f - f_n^\delta\|_\infty = \delta$

$$\|f' - (f_n^\delta)'\|_\infty = n$$

$\Rightarrow$ data error δ can be arbitrarily small & still create an arbitrarily large error in the result (of the differentiation)

The derivative does not depend continuously on the data (w.r.t. sup norm) $\rightsquigarrow$ INSTABILITY

In contrast: integration of a $C[0,1]$ function is a <u>stable</u> problem

General phenomenon:

$$\boxed{\text{Direct problem: smoothing process}}$$

$$\Downarrow$$

$$\boxed{\text{Inverse problem: small data error of high frequency creates large oscillations in solution}}$$

Possible remedy?

Differentiation revisited: Numerical computation via difference quotients

f true function, f^δ its noisy version, where

$$\|f - f^\delta\|_\infty \le \delta$$

Suppose $f \in C^2[0,1]$
Taylor expansion: $$\frac{f(x+h)-f(x-h)}{2h} = f'(x) + O(h)$$

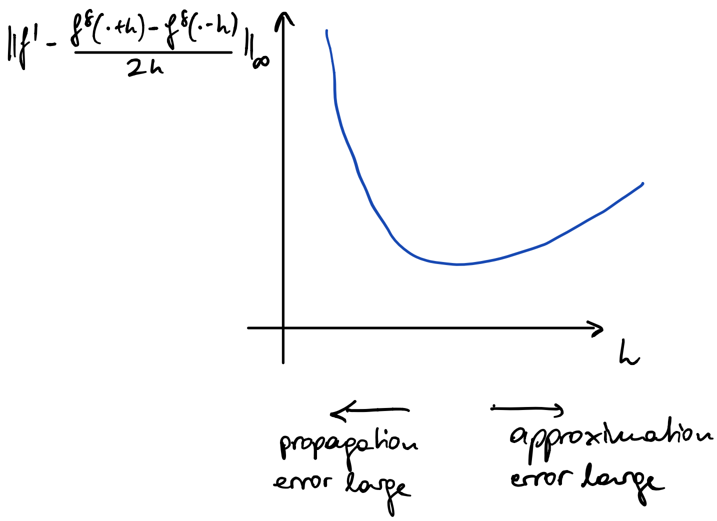
Only f^δ is available:

$$\frac{f^\delta(x+h)-f^\delta(x-h)}{2h} \sim \frac{f(x+h)-f(x-h)}{2h} + \frac{\delta}{h}$$

Two error terms: $\mathcal{O}(h)$ approximation error

$\mathcal{O}(\frac{\delta}{h})$ propagated data error

For fixed δ:



How to choose the discretization parameter h in an optimal way?

Choice will depend on δ (asymptotically)

$\rightsquigarrow$ <u>regularization theory</u>

E.g. choose h as $h \sim \delta^\mu$ and search for μ that minimizes total error.

$\Rightarrow$ total error is $\mathcal{O}(\delta^{1/2})$ for $f \in C^2[0,1]$

Best possible: $f \in C^l[0,1]$ $\Rightarrow$ total error is $\Theta(\delta^{2/3})$

$l \geq 3$

this rate cannot be improved!

diff. quotient: $f'(x) + \Theta(h^2)$

Typical properties of ill-posed problems:

- Amplification of high frequency errors
- Restoration of stability by using prior information (here: smoothness of true function)
- two conflicting error terms
- Choice of optimal parameters depends on a-priori information
- Loss of information even under perfect circumstances

Lecture 2 Ill-posed linear operator eqns

$T: X \to Y$ BLT X, Y Hilbert spaces

$Tx = y$

Hadamard's criteria of well-posedness:

Existence: For all $y \in Y$, there exists $x \in X$ s.t. $Tx = y$

$$\mathcal{R}(T) = Y$$

Uniqueness: For all $y \in Y$, the solution is unique:

$$\mathcal{N}(T) = \{0\}$$

Stability: The solution depends continuously on the data:

$$T^{-1} \in \mathcal{L}(Y, X)$$

Lack of stability: recall example of differentiation

$\hookrightarrow$ creates serious numerical issues

Relaxed notion of solution: the generalized solution

If $Tx = y$ is not solvable, i.e. $y \notin \mathcal{R}(T)$,
then: search for

$\bar{x} \in X \quad$ s.t. $\quad \|T\bar{x}-y\| \leq \|Tz-y\| \;\; \forall z \in X.$

such $\bar{x}$ is called <u>least-squares solution</u>
[not necessarily unique!]

Let Q be the orth. projection of Y on $\overline{\mathcal{R}(T)}$
i.e. $\forall y \in Y, \forall u \in \overline{\mathcal{R}(T)}$: $\langle Qy, u\rangle_Y = \langle y, u\rangle_Y$

Known facts: minimality property

$$\|Qy-y\| \leq \|u-y\| \quad \forall u \in \overline{\mathcal{R}(T)}$$

and

$$Qy-y \in \mathcal{R}(T)^\perp \qquad (1)$$

Also recall:

$$\mathcal{N}(T) = \mathcal{R}(T^*)^\perp, \qquad \overline{\mathcal{R}(T)} = \mathcal{N}(T^*)^\perp$$

<u>Theorem 1</u>: Let $y \in Y$ and $x \in X$. The following are equivalent:

1.) $Tx = Qy$
2.) $\|Tx-y\| \leq \|Tz-y\| \;\; \forall z \in X$
3.) $T^*Tx = T^*y$.

Proof: 1.) $\Rightarrow$ 2.)

$$\|Tz-y\|^2 \overset{(1)}{=} \|Tz-Qy\|^2 + \|Qy-y\|^2$$
$$\overset{\text{ass.}}{=} \|Tz-Qy\|^2 + \|Tx-y\|^2$$
$$\geq \|Tx-y\|^2$$

2.) $\Rightarrow$ 3.) $\quad Qy \in \overline{\mathcal{R}(T)}$

$$\Rightarrow \exists\, (x_n)_{n\in\mathbb{N}} \subset X \text{ s.t.}$$

$$Tx_n \xrightarrow{n\to\infty} Qy$$

$$\Rightarrow \|Qy-y\|^2 = \lim_{n\to\infty} \|Tx_n - y\|^2 \underset{\text{ass.}}{\geq} \|Tx-y\|^2$$

Furthermore,

$$\|Tx-y\|^2 \overset{(1)}{=} \|Tx-Qy\|^2 + \|Qy-y\|^2$$

$$\geq \underbrace{\|Tx-Qy\|^2}_{=0} + \|Tx-y\|^2$$

$$\Rightarrow Tx = Qy \qquad \Rightarrow Tx-y = Qy-y \in \mathcal{R}(T)^\perp = \mathcal{N}(T^*)$$

$$\Rightarrow T^*(Tx-y) = 0.$$

3.) $\Rightarrow$ 1.) $\quad Tx-y \in \mathcal{N}(T^*) = \mathcal{R}(T)^\perp$

$$\Rightarrow 0 = Q(Tx-y) = QTx - Qy = Tx - Qy$$

$$\Rightarrow Tx = Qy. \qquad \square$$

<u>Corollary 1:</u> 1.) The set of least-squares solutions

$$L(y) := \{x \in X : T^*Tx = T^*y\}$$

is non-empty iff $y \in \mathcal{R}(T) \oplus \mathcal{R}(T)^\perp$.

2.) If $y \in \mathcal{R}(T) \oplus \mathcal{R}(T)^\perp$, then $L(y)$ is a non-empty, closed & convex subset of X.

Proof of 1.): "$\Rightarrow$" $x \in L(y) \Rightarrow Tx - y \in N(T^*) = R(T)^\perp$

$$\Rightarrow \quad y = \underset{\substack{\cap \\ R(T)}}{Tx} + \underset{\substack{\cap \\ R(T)^\perp}}{(y - Tx)} \quad \Rightarrow y \in R(T) \oplus R(T)^\perp$$

"$\Leftarrow$" $y = y_1 + y_2$, $y_1 \in R(T)$, $y_2 \in R(T)^\perp$.

This splitting is unique: $Qy = y_2$ and $\exists\, x \in X$ s.t. $y_1 = Tx$.

$$\Rightarrow \quad Qy = Tx \underset{\text{Thm 1}}{\Rightarrow} x \in L(y).$$

Proof of 2.): <u>convexity</u>:

Let $x, x' \in L(y)$:

By Thm 1: $T^*Tx = T^*y$

$T^*Tx' = T^*y$

Let $z := tx' + (1-t)x$, $t \in [0,1]$ arbitrary

$$T^*Tz = t\,T^*Tx' + (1-t)\,T^*Tx$$
$$= t\,T^*y + (1-t)\,T^*y = T^*y.$$

$\Rightarrow z \in L(y)$.

<u>closedness</u>:

Let $(x_n) \subseteq L(y)$ with $x_n \xrightarrow{n\to\infty} x$, $x \in X$.

Then, $\|Tx - y\| = \lim_{n\to\infty} \|Tx_n - y\| \le \|Tz - y\| \quad \forall z \in X$.

$\Rightarrow x \in L(y)$. □

Least-sq. solution : not (necessarily) unique

Possible approach: Pick the one with minimal norm

Q: Why is this unique?

$\hookrightarrow$ convexity of $L(y)$ (if $y \in \mathcal{R}(T) \oplus \mathcal{R}(T)^\perp$)

Definition [Moore-Penrose generalized inverse]:

The generalized inverse T^+ is the operator with domain $\mathcal{D}(T^+) = \mathcal{R}(T) \oplus \mathcal{R}(T)^\perp$ that maps each $y \in \mathcal{D}(T^+)$ to $x \in L(y)$ with minimal norm ($x := T^+ y$).

Corollary 2:

1.) $\mathcal{D}(T^+)$ is dense in Y
    If $\mathcal{R}(T)$ is closed, then $\mathcal{D}(T^+) = Y$.

2.) If $\mathcal{R}(T)$ is closed and T^{-1} exists, then
$$T^+\big|_{\mathcal{R}(T)} = T^{-1}.$$

3.) $\mathcal{R}(T^+) = \mathcal{N}(T)^\perp \quad \left(= \overline{\mathcal{R}(T^*)}\right)$

4.) T^+ is linear

5.) T^+ is bounded iff $\mathcal{R}(T)$ is closed

6.) For $y \in \mathcal{D}(T^+)$, $T^+ y$ is the unique element that is a least-sq. solution in $\mathcal{N}(T)^\perp$.

Ad 1.) One can show that if $y \notin \mathcal{D}(T^+)$, then no least-sq. solution of $Tx = y$ exists!

What does 5.) mean in terms of Hadamard's criteria?

In the generalized solution sense:

$$\text{Existence} \Leftrightarrow \text{stability}$$

Generalized inverse restores uniqueness (not necessarily existence nor stability)

Compact operators

special case of BLTs $\rightsquigarrow$ representable by SVD

$K: X \to Y$ compact

$$K = \sum_{n=1}^{\infty} \sigma_n \langle \cdot, u_n \rangle_X v_n \qquad \text{SVD: } (\overset{\mathbb{R}}{\sigma_n}; \overset{X}{u_n}, \overset{Y}{v_n})$$

Basic property? $\sigma_n \xrightarrow{n \to \infty} 0$

i.e. either the operator has finite rank or the singular values accumulate (only!) at zero.

$$\boxed{R(K) \text{ closed} \iff R(K) \text{ finite-dim.}}$$

Recall Corollary 2: $R(K)$ closed $\iff K^+$ bounded

so that $\dim R(K) = \infty \Rightarrow K^+$ is a densely defined <u>unbounded</u> operator

i.e. compact operator equations are inherently <u>unstable</u>.

Equation for K^+? Straightforward if SVD is known:

$$\boxed{K^+ = \sum_{n=1}^{\infty} \frac{\langle \cdot , v_n \rangle}{\sigma_n} u_n} \qquad (2)$$

Proof: It is based on Picard's criterion:

$$\boxed{y \in \mathcal{D}(K^+) \iff \sum_{n=1}^{\infty} \frac{|\langle y, v_n \rangle|^2}{\sigma_n^2} < \infty} \qquad (3)$$

$$y \in \mathcal{D}(K^+) \quad \Rightarrow \quad \left(\frac{|\langle y, v_n \rangle|}{\sigma_n} \right)_{n \in \mathbb{N}} \in \ell^2$$

$$\underset{\text{(Riesz-Fischer)}}{\Rightarrow} \quad x := \sum_{n=1}^{\infty} \frac{\langle y, v_n \rangle}{\sigma_n} u_n \in X \qquad [X \text{ complete, } \{u_n\} \text{ ONS } \Rightarrow x \in X]$$

$$\Rightarrow \quad \underline{Kx} = \sum_{n=1}^{\infty} \frac{\langle y, v_n \rangle}{\sigma_n} K u_n = \sum_{n=1}^{\infty} \langle y, v_n \rangle v_n$$

$$\underline{= Qy}$$

where Q : orth. proj. onto $\overline{\mathcal{R}(K)}$

$$Q := \sum_{n=1}^{\infty} \langle \cdot , v_n \rangle v_n$$

$\Rightarrow$ x is least-sq. solution

Since $\{u_n\}_{n \in \mathbb{N}}$ spans $\mathcal{N}(K)^\perp$ $\Rightarrow$ $x \in \mathcal{N}(K)^\perp$

$$\underset{\text{Corollary 2}}{\Rightarrow} \quad x = K^+ y.$$

D

<u>Note</u>:

- Earlier comment: generalized solution does not always exist

For compact operators, this is characterized by Picard's criterion:

only if $\left\{ \frac{\langle y, v_n \rangle}{\sigma_n} \right\}_{n \in \mathbb{N}}$ decays fast enough

(note: while $\sigma_n \xrightarrow{n \to \infty} 0$!)

- Error components corresponding to σ_n large
  $\rightsquigarrow$ harmless

  Error components corresponding to σ_n small
  $\rightsquigarrow$ get amplified!

- Ill-posedness of compact operator equations is characterized by decay rate of σ_n

  mild ill-posedness: $\sigma_n = \mathcal{O}(n^{-\alpha})$, $\alpha > 0$

  otherwise severe ill-posedness: e.g. $\sigma_n = \mathcal{O}(q^{-n})$, $q > 1$.

<u>Example 2</u>: Backwards heat equation

$$\frac{\partial u}{\partial t}(x,t) = \frac{\partial^2 u}{\partial x^2}(x,t) \qquad x \in [0,\pi],\ t \geq 0$$

$$u(0,t) = u(\pi,t) = 0, \quad t \geq 0 \qquad \text{(homog. Dirichlet BCs)}$$

"Backwards": assuming a final temperature

$$f(x) := u(x,1), \quad x \in [0,\pi]$$

with $f(0) = f(\pi) = 0$

determine initial temperature

$$v_0(x) := u(x,0), \quad x \in [0,\pi]$$

Note: $\varphi_n(x) := \sqrt{\frac{2}{\pi}} \sin(nx)$ is a complete ONS in $L^2[0,\pi]$

also $\varphi_n'' = -n^2 \varphi_n \Rightarrow \{\varphi_n\}_{n\in\mathbb{N}}$ eigensystem of $\frac{d^2}{dx^2}$ on $[0,\pi]$ with homog. Dirichlet BCs

Expansion for v_0:

$$v_0(x) = \sum_{n=1}^{\infty} c_n \varphi_n(x), \quad x \in [0,\pi]$$

with $$c_n = \sqrt{\frac{2}{\pi}} \int_0^{\pi} v_0(\tau) \sin(n\tau)\, d\tau$$

$\Rightarrow$ ansatz for $u(x,t)$:

$$u(x,t) := \sum_{n=1}^{\infty} a_n(t) \varphi_n(x), \quad x \in [0,\pi],\ t \geq 0.$$

One can find that $a_n(t) = c_n e^{-n^2 t}, \quad t \geq 0$

$$\Rightarrow f(x) = u(x,1) = \sum_{n=1}^{\infty} c_n e^{-n^2} \varphi_n(x)$$

$$= \frac{2}{\pi} \sum_{n=1}^{\infty} \int_0^{\pi} v_0(\tau) \sin(n\tau)\, d\tau\, e^{-n^2} \sin(nx).$$

$\rightsquigarrow$ integral operator of the 1st kind with kernel

$$k(x,\tau) := \frac{2}{\pi} \sum_{n=1}^{\infty} e^{-n^2} \sin(n\tau) \sin(nx)$$

SVD: $\left(e^{-n^2}; \sqrt{\frac{2}{\pi}} \sin(nx), \sqrt{\frac{2}{\pi}} \sin(nx)\right)$

$\downarrow$

<u>severely</u> ill-posed

Note: Sing. fcts are complete ONS

$$\Rightarrow \mathcal{R}(K) \text{ is dense in } L^2[0,\pi]$$
$$= \mathcal{D}(K^+)$$

$\underset{(3)}{\Rightarrow}$ backwards heat eqn is (uniquely) solvable iff

$$\sum_{n=1}^{\infty} e^{2n^2} |f_n|^2 < \infty$$

where $f_n := \sqrt{\frac{2}{\pi}} \int_0^\pi f(\tau) \sin(n\tau) d\tau$

i.e. if Fourier coeff. of f decay rapidly (much faster than e^{-n^2})!

More generally: For BLT $T: X \to Y$, the spectrum of T^*T reveals stability properties of the inverse problem.

$$T^*T = \int \lambda \, dP_\lambda$$

projection valued measure

[recall: for self-adjoint BLT $A: X \to X$

$\rightsquigarrow$ functional calculus for cont. functions

$$f \mapsto f(A)$$

$\rightarrow$ For $\psi \in X$:

$\langle \psi, f(A)\psi \rangle$ is cont. lin. functional on $C(\sigma(A))$

$\Rightarrow$ there is unique measure μ_ψ on $\sigma(A)$ s.t.
Riesz-Markov
comp. set

$$\langle \psi, f(A)\psi \rangle = \int_{\sigma(A)} f(\lambda)\, d\mu_\psi$$

spectral measure associated with ψ

$\rightsquigarrow$ extend functional calculus to bounded Borel functions [via polarization identity & Riesz lemma]

$\rightsquigarrow$ can take characteristic functions

$$P_\Omega = \chi_\Omega(A) \qquad \text{spectral projection of } A$$

characteristic function

Theorem 2 [Spectral theorem – p.v.m. form]

There is a 1-to-1 correspondence between (bdd) self-adj. operators and (bdd) projection-valued measures $\{P_\Omega\}$:

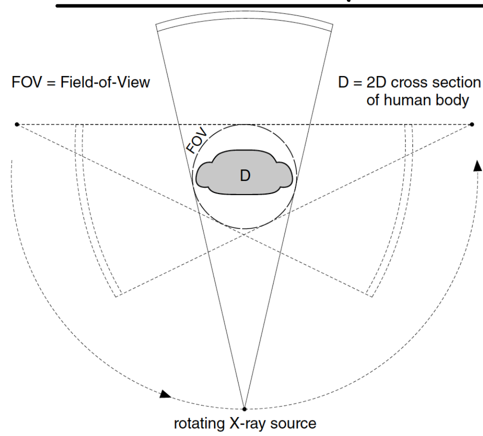
$$A \mapsto \{P_\Omega\} = \{\chi_\Omega(A)\}$$

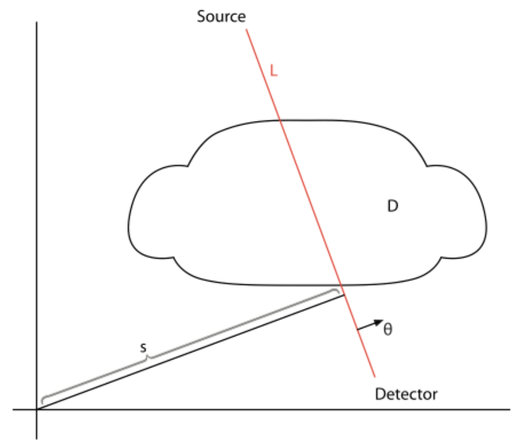
$$\{P_\Omega\} \mapsto A = \int \lambda \, dP_\lambda$$

Lecture 3: Limited data CT & regularization

Problem 1: Limited data CT (2D)

Classical CT (full data):





Measurements modelled as Radon transform of object density:

$$(Rf_D)(\theta, s) = \int_{\mathbb{R}} f_D(s\theta + t\theta^\perp)\, dt$$

CT reconstruction : inversion of Radon transform

$\rightsquigarrow$ singular values ?

$$R: L^2(B_2) \longrightarrow L^2\left([-1,1] \times S^1, (1-s^2)^{-1/2}\right)$$

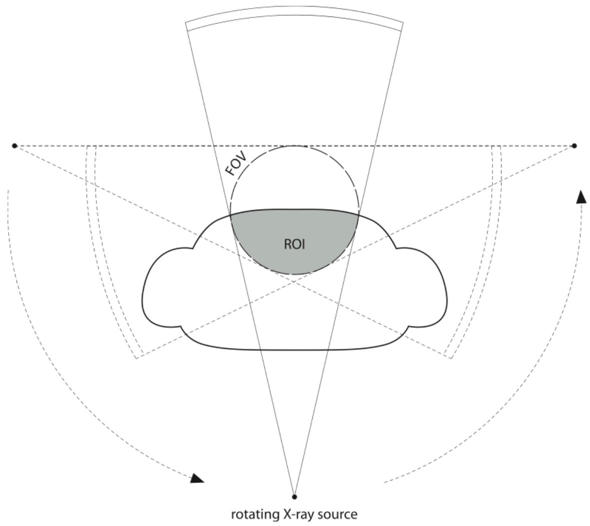
unit disk

singular values $\quad \sigma_{m\ell} = \dfrac{2\sqrt{\pi}}{\sqrt{m+1}}$ $\quad$ (see book by Natterer, 2001)

As $m \to \infty \quad \sigma_{m\ell} \sim \dfrac{1}{\sqrt{m}}$

$\rightsquigarrow$ mild ill-posedness $\rightsquigarrow$ CT reconstruction can be easily regularized

A limited data problem:



Inversion of Radon transform in 3 steps:

1. Differentiation

$$r_D(\phi, s) = \frac{\partial}{\partial s} (Rf_D)(\theta, s)$$

$$\theta^\perp = (\cos\phi, \sin\phi)$$

2. Back-projection

$$b_{\phi_1,\phi_2}(x) = \frac{1}{\pi} \int_{\phi_1}^{\phi_2} r_D(\phi, s)\Big|_{s = x\cdot\theta} d\phi$$

$$= \dots$$

$$= (H_{\theta_2^\perp} f_D)(x) - (H_{\theta_1^\perp} f_D)(x)$$

3. Hilbert transform inversion:

Choice $\phi_2 = \phi_1 + \pi \Rightarrow \theta_2^\perp = -\theta_1^\perp$

$$\Rightarrow \quad b_{\phi_1, \phi_1+\pi}(x) = 2\,(H_{\theta_2^\perp} f_D)(x)$$

Inversion of $H_{\theta_2^\perp}$ recovers f_D on a line

$\rightsquigarrow$ family of 1D problems

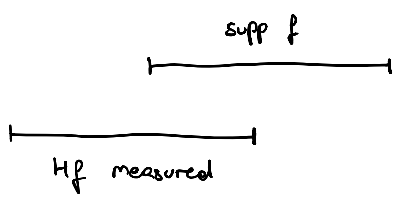
Limited data:

$f \in L^2([a_2, a_4])$: 1D slice of f_D

Hf only known on $[a_1, a_3]$

one possible scenario:

$$a_1 < a_2 < a_3 < a_4$$



Define $H_T := P_{[a_1, a_3]} H P_{[a_2, a_4]}$

recall $$(Hf)(x) = \frac{1}{\pi}\, \text{p.v.} \int_{\mathbb{R}} \frac{f(y)}{y-x}\, dy$$

$$H : L^2(\mathbb{R}) \to L^2(\mathbb{R})$$

$$H_T^* = -P_{[a_2, a_4]} H P_{[a_1, a_3]}$$

What is the spectrum $\sigma(H_T^* H_T)$?

Problem of Landau-Pollak-Slepian

$$\mathcal{F}_{TW} := P_{[-W,W]} \underset{\substack{\uparrow \\ \text{Fourier transform}}}{\tilde{\mathcal{F}}} P_{[-T,T]}$$

Find largest eigenvalue of $\underbrace{\mathcal{F}_{TW}^* \mathcal{F}_{TW}}$

commutes with 2^{nd} order differential operator
$\rightsquigarrow$ its eigenfunctions are the eigenfunctions of $\mathcal{F}_{TW}^* \mathcal{F}_{TW}$

$\rightsquigarrow$ well-studied problem $\rightsquigarrow$ exploit Sturm-Liouville theory

Similarly: diff. operators $L_S, \tilde{L}_S$ exist s.t.

$$H_T L_S = \tilde{L}_S H_T$$

search for $L_S, \tilde{L}_S$:

based on work by Katsevich (inspired by work by Maass on interior Radon transform) + intuition + luck / magic

crucial property: $L_S, \tilde{L}_S$ <u>self-adjoint</u>

Theorem 3 [Hellinger-Toeplitz]:

Let A be a linear everywhere-defined operator on a Hilbert space X with

$$\langle u_1, Au_2 \rangle = \langle Au_1, u_2 \rangle \quad \forall u_1, u_2 \in X$$

Then, A is bounded.

([1] Michael Reed & Barry Simon
[2] Barbara MacCluer: Elementary functional analysis)

Definition: A densely defined operator A on X is symmetric iff

$$\langle u_1, Au_2 \rangle = \langle Au_1, u_2 \rangle \quad \forall u_1, u_2 \in D(A).$$

Note: A self-adj. iff A is symmetric and $D(A) = D(A^*)$.

$\Rightarrow$ Unbounded self-adj. operators: $D(A) \subsetneq X$.

Note: Spectrum of A unbdd.: very sensitive to choice of $D(A)$!

Search for L_s, Σ_s: start with differential form $L(x, d_x)$

$$L(x, d_x)\,\psi(x) := \big(P(x)\psi'(x)\big)' + 2\Big(x - \frac{1}{4}\sum_{i=1}^{4} a_i\Big)^2 \psi(x)$$

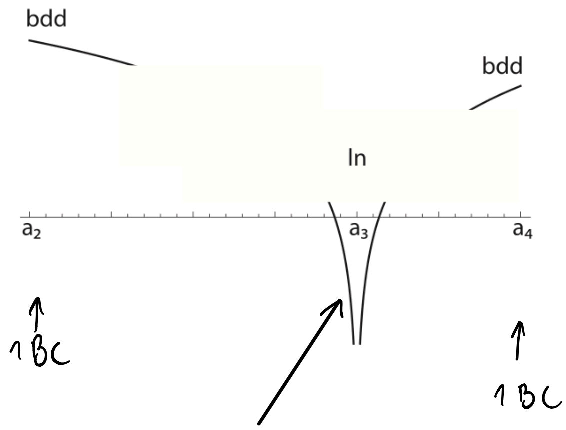
where $P(x) = \prod_{i=1}^{4}(x - a_i)$

a_i are reg. sing. points

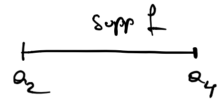
$\rightsquigarrow$ add boundary & transmission $\underbrace{\text{conditions}}$ to obtain self-adj. realizations

$\downarrow$

use intuition on singular functions of H_1



2TCs to connect
(a_2,a_3) & (a_3,a_4)



$$H_T u_n = \sigma_n v_n$$
$$H_T^* v_n = \sigma_n u_n$$

$$\phi_{11}(x) + \phi_{12}(x) \ln|x-a_3|$$
$$\phi_{21}(x) + \phi_{22}(x) \ln|x-a_3|$$

in terms of SL theory:

a_3 is an <u>interior</u> singular point

$\rightsquigarrow$ not a standard singular SL problem
↓
sing. points only at boundary

"two interval problem"

Next steps: Prove that

- $\sigma(L_S)$ is purely discrete
- eigenfunctions u_n of L_S are complete in $L^2([a_2,a_4])$
- $\sigma(L_S)$ is simple (each eigenvalue has multiplicity 1)
- $(H_T L(y,d_y) u_n)(x) = L(x,d_x)(H_T u_n)(x)$

$$\boxed{H_T L_S = \tilde{L}_S H_T}$$

Theorem 4. The eigenfunctions u_n of L_S, together with

$$\sigma_n := H_T u_n / \| H_T u_n \|_{L^2([a_1,a_3])} \quad \text{and}$$

$$\tilde{\sigma}_n := \| H_T u_n \|_{L^2([a_1,a_3])}$$

form the SVD of H_T:

$$H_T u_n = \tilde{\sigma}_n \sigma_n$$
$$H_T^* \sigma_n = \tilde{\sigma}_n u_n .$$

One can show: $\mathcal{N}(H_T) = \{0\}$ $\rightsquigarrow$ uniqueness

$\mathcal{R}(H_T) \neq L^2([a_2,a_4])$, $\mathcal{R}(H_T)$ is dense

$\rightsquigarrow$ instability

Furthermore:

Theorem 5: The values 0 and 1 are (the only) accumulation points of the sing. values of H_T.

$\Rightarrow$ H_T is non-compact

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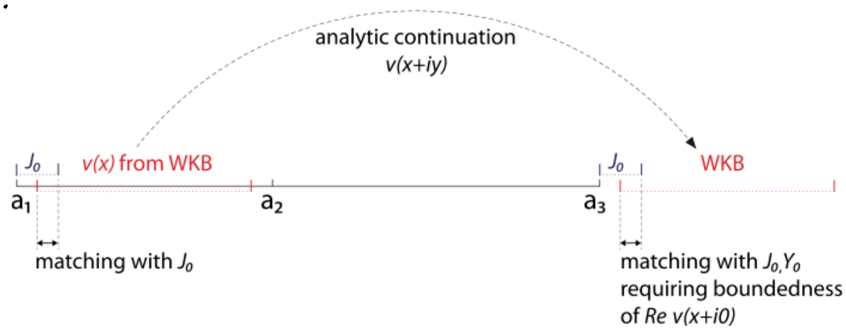
[3] Anton Zettl, Sturm-Liouville theory

How severe is the ill-posedness?

Asymptotic analysis of SVD (via L_S, $\tilde{L}_S$):

Find asymptotics of eigenfunctions of L_S as $\lambda_n \to \pm\infty$ in $L_S \varphi_n = \lambda_n \varphi_n$

Ingredients:



WKB (Wentzel-Kramers-Brillouin) approximation: global asympt.

Bessel solutions J_0, Y_0 : local asymptotics

Then: asymptotic matching

$\rightsquigarrow$ asymptotics of sing functions of H_T

$\rightsquigarrow$ use this to find asymptotics for

$$\sigma_n \xrightarrow{n\to\infty} 1$$

$$\sigma_{-n} \xrightarrow{n\to\infty} 0$$

Result:

$$\sigma_n = 2e^{-c_1 n} \cdot \left(1 + \mathcal{O}(n^{-1/2+\delta})\right), \quad n \to \infty$$

$$\sigma_{-n} = 1 - 2e^{-c_2 n} \left(1 + \mathcal{O}(n^{-1/2+\delta})\right)$$

for a small fixed $\delta > 0$.

$\leadsto$ Severe ill-posedness!
(typical for limited data problems in CT)

Regularization:

General task: Extract information stably from an unstable problem!

Recall Moore-Penrose inverse: best-approximate solution via

$$x^+ = T^+ y$$

In practice: y is not known exactly, but only measurement y^δ s.t. $\|y - y^\delta\| \leq \delta$
"noise level"

If Hadamard 3.) is violated: T^+ is not continuous!

$T^+ y^\delta$: (in general) not a good approximation of $T^+ y$.

Note: $T^+ y^\delta$ might not even exist ($\mathcal{D}(T^+) \subsetneq Y$)

Regularization: find approximation x^δ of x^+ s.t.

- x^δ depends cont. on y^δ
- $x^\delta \to x^+$ as $\delta \to 0$

How? Via family of continuous operators $\{R_\alpha\}$ that approximate T^+
unbounded

i.e. $\alpha = \alpha(\delta, y^\delta)$, $x_\alpha^\delta := R_\alpha y^\delta$

and $\quad x_\alpha^\delta \to x^+$ as $\delta \to 0$.

Definition. Let $T: X \to Y$ be a BLT between Hilbert spaces and $\alpha_0 \in (0,\infty]$. For every $\alpha \in (0,\alpha_0)$, let

$$R_\alpha : Y \to X$$

be a continuous operator. The family $\{R_\alpha\}$ is called a regularization for T^+ if for all $y \in D(T^+)$ there exists a parameter choice rule $\alpha = \alpha(\delta, y^\delta) : \mathbb{R}^+ \times Y \to (0,\alpha_0)$ satisfying

$$\lim_{\delta\to 0} \sup \left\{ \alpha(\delta, y^\delta) : y^\delta \in Y, \ \|y - y^\delta\| \le \delta \right\} = 0 \quad (4)$$

and s.t. the following holds:

$$\lim_{\delta\to 0} \sup \left\{ \| R_{\alpha(\delta,y^\delta)} y^\delta - T^+ y \| : y^\delta \in Y, \ \|y-y^\delta\| \le \delta \right\} = 0. \ (5)$$

For a specific $y \in D(T^+)$, a pair (R_α, α) is called a (convergent) regularization method for solving

$$Tx = y$$

if (4) and (5) hold.

$\rightsquigarrow$ 2 components of regularization:

- operators R_α
- parameter choice rule $\alpha(\delta, y^\delta)$

Theorem 6 [Bakushinskii]:

If $\alpha = \alpha(y^\delta)$ yields convergent regularization method, then $T^\dagger$ is bounded.

Possible choices: $\alpha = \alpha(\delta)$ "a-priori"

$\alpha = \alpha(\delta, y^\delta)$ "a-posteriori"

Theorem 7: If for all $\alpha > 0$, R_α is a continuous operator, then $\{R_\alpha\}$ is a regularization of $T^\dagger$ if

$$R_\alpha \xrightarrow{\alpha \to 0} T^\dagger \text{ pointwise on } \mathcal{D}(T^\dagger).$$

In this case, for all $y \in \mathcal{D}(T^\dagger)$:

a-priori rule $\alpha(\delta)$ exists for which (R_α, α) is a conv. reg. method for $Tx = y$.

<u>Linear</u> reg. methods: R_α linear operators

[One can also consider nonlinear R_α for $T^\dagger$ linear e.g. version of conjugate gradient method].

$\{P_\lambda\}$ spectral projections of T^*T

If T^*T continuously invertible:

$$(T^*T)^{-1} = \int \frac{1}{\lambda} \, dP_\lambda$$

and

$$x^\dagger \underset{\underset{a}{\uparrow}}{=} \int \frac{1}{\lambda} \, dP_\lambda \, T^* y \qquad (6)$$

If $\mathcal{R}(T)$ is not closed: instability

$\rightsquigarrow$ pole at zero in (6)

$\rightsquigarrow$ replace $\frac{1}{\lambda}$ by family $\{ s_\alpha(\lambda) \}$

$$x_\alpha := \int s_\alpha(\lambda)\, dP_\lambda T^* y$$

$$R_\alpha := \int s_\alpha(\lambda)\, dP_\lambda T^* \qquad (7)$$

+ continuity conditions of $s_\alpha(\lambda)$.

Theorem 8. For all $\alpha > 0$, let $s_\alpha : [0, \|T\|^2] \to \mathbb{R}$ be piecewise continuous and suppose there is a constant $C > 0$ s.t. for all $\lambda \in (0, \|T\|^2]$

$$|\lambda\, s_\alpha(\lambda)| \leq C \qquad (8)$$

and

$$\lim_{\alpha \to 0} s_\alpha(\lambda) = \frac{1}{\lambda}. \qquad (9)$$

Then, for all $y \in D(T^+)$

$$\lim_{\alpha \to 0} x_\alpha = x^+.$$

with $x^+ = T^+ y$.

$$x_\alpha^\delta := \int s_\alpha(\lambda)\, dP_\lambda T^* y^\delta$$

a-posteriori rule that yields convergence:

Morozov's discrepancy principle

$r_\alpha(\lambda) := 1 - \lambda s_\alpha(\lambda)$ $\qquad [\, x^+ - x_\alpha = r_\alpha(T^*T) x^+ \,]$

Theorem 9. Let s_α be as in Thm 8 and fulfill (8) & (9). Furthermore, let

$$S_\alpha := \sup \{ |s_\alpha(\lambda)| : \lambda \in [0, \|T\|^2] \} \text{ be s.t.}$$

$$S_\alpha \leq \frac{\tilde{c}}{\alpha} \quad , \alpha > 0$$

for some constant $\tilde{c} > 0$ and

$$\tau > \sup \{ |r_\alpha(\lambda)| : \alpha > 0, \lambda \in [0, \|T\|^2] \}$$

Note: if $y \in D(T^+)$, but $y \notin R(T)$: solve for $T^*Tx = T^*y$ which is solvable for $y \in D(T^+)$.

Then, the discrepancy principle defined by

$$\alpha(\delta, y^\delta) := \sup \{ \alpha > 0 : \|Tx_\alpha^\delta - y^\delta\| \leq \tau\delta \}$$

and R_α as in (7) form a convergent regularization method (R_α, α) for all $y \in R(T)$.

Philosophy of discrepancy principle: compare residual and error bound δ

2 examples of regularization methods:

a.) $$s_\alpha(\lambda) := \begin{cases} 1/\lambda & \lambda \geq \alpha \\ 0 & \lambda < \alpha \end{cases}$$

$\rightsquigarrow$ for operator with SVD $(\sigma_n; u_n, v_n)$:

truncated SVD $$x_\alpha^\delta = \sum_{\substack{n=1 \\ \sigma_n^2 \geq \alpha}}^{\infty} \frac{1}{\sigma_n} \langle y^\delta, u_n \rangle v_n$$

b.) $$s_\alpha(\lambda) := \frac{1}{\lambda + \alpha}$$

Note: $\{\lambda+\alpha : \lambda \in \sigma(T^*T)\}$ is the spectrum of

$$\overset{\nearrow}{Q} \quad T^*T+\alpha I$$

$$\Rightarrow \quad x_\alpha^\delta = \int s_\alpha(\lambda)\, dP_\lambda T^* y^\delta = (T^*T+\alpha I)^{-1} T^* y^\delta .$$

i.e. $\quad (T^*T+\alpha I)\, x_\alpha^\delta = T^* y^\delta \qquad (10)$

$\uparrow$ regularized normal eqn

$\rightsquigarrow$ for operator with SVD:

$$x_\alpha^\delta = \sum_{n=1}^{\infty} \frac{\sigma_n}{\sigma_n^2+\alpha} \langle y^\delta, u_n \rangle v_n .$$

$\uparrow$

$\frac{1}{\sigma_n}$ unbdd, replaced by bdd term

(10): Tikhonov regularization

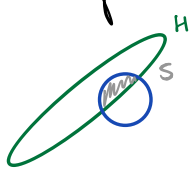
equivalent to minimization problem $\quad x \mapsto \|Tx-y^\delta\|^2 + \alpha \|x\|^2$

Different view on regularization: Theory by Miller

T^{-1} unbounded $\Rightarrow$ $H(\delta, y^\delta) := \{x \in X : \|Tx - y^\delta\| \le \delta\}$

is an unbounded set

regularization $\hat{=}$ restricting set of admissible solutions:



$S(\delta, y^\delta) \subset H(\delta, y^\delta)$

by assuming prior knowledge on solution

so that

$$\operatorname{diam} S(\delta, y^\delta) \to 0 \quad \text{as } \delta \to 0. \tag{11}$$

restriction typically as $\|Lx\|_X \le c$

where L is densely defined with bounded inverse

e.g. identity or diff. operator

If (11) holds, any method (R_α, α) that guarantees

$$R_{\alpha(\delta, y^\delta)}\, y^\delta \in S(\delta, y^\delta)$$

is a conv. regularization method.

truncated Hilbert trafo: knowledge on SVD + Miller's approach to prove convergence of reg. methods

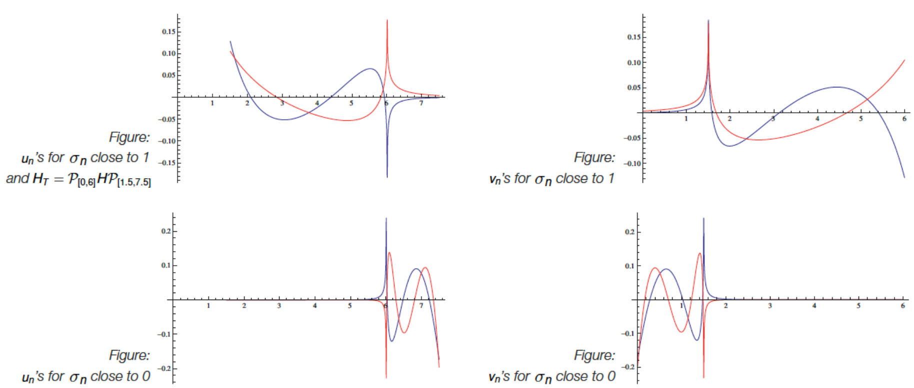
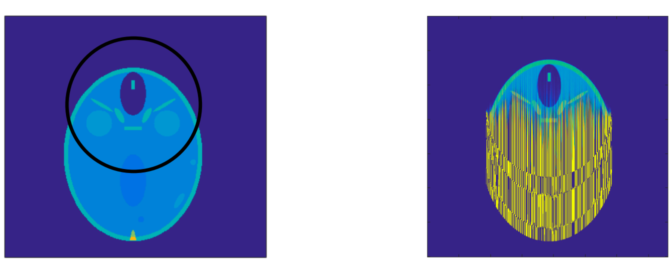


Figure: u_n's for σ_n close to 1 and $H_T = \mathcal{P}_{[0,6]} H \mathcal{P}_{[1.5,7.5]}$

Figure: v_n's for σ_n close to 1

Figure: u_n's for σ_n close to 0

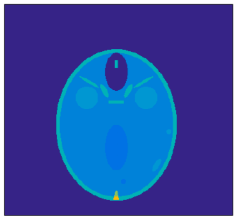
Figure: v_n's for σ_n close to 0



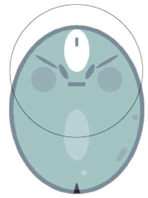
(a) Original phantom

(b) Reconstructed phantom

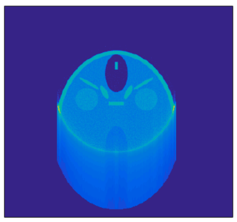
(no reg.)



(a) Original phantom



(b) Field of view



(c) Tikhonov reg.

(d) TV reg.

Lecture 4: Nonlinear problems & beyond

$$F(x) = y \quad , \quad F : \mathcal{D}(F) \subset X \to Y$$

ill-posedness now: lack of cont. dependence on data

Nonlinear operators: no spectral theory $\rightsquigarrow$ analysis of regularization challenging!

A class of nonlinear problems:

parameter estimation in PDEs

Example: heat conduction in material in $\Omega \subset \mathbb{R}^3$

temperature distribution u after suff. long time while keeping zero temp. at boundary:

$$-\nabla \cdot (\underbrace{q(x)}_{\text{heat conductivity}} \nabla u) = \underbrace{f(x)}_{\text{internal heat sources}} \quad , \quad x \in \Omega$$

$$u = 0 \quad \text{on } \partial\Omega$$

Inverse problem:

Determine q from internal measurements of u or from boundary measurements of heat flux $q \frac{\partial u}{\partial n}$?

$F : q \mapsto u_q$ not explicit but described through PDE.

General assumption:

- F is continuous
- F is weakly sequentially closed:

$$\left.\begin{array}{l} x_n \rightharpoonup x \text{ in } X \\ F(x_n) \rightharpoonup y \text{ in } Y \end{array}\right\} \Rightarrow x \in \mathcal{D}(F) \;\&\; F(x) = y$$

- for simplicity: $y \in \mathcal{R}(F)$

Linear problems: minimum-norm solution

Now: x^*-minimum-norm solution $x^\dagger$ (0 no longer plays special role)

minimizes $\|x - x^*\|$

should include a-priori info

Linear operators: closedness of range characterizes stability

What if we consider linearization of nonlinear operator?

In general: no guaranteed connection between ill-posedness of nonlinear problem & its linearization!

Linear operator: T compact + injective + X infinite-dim.

$\Rightarrow T^{-1}$ unbounded

Nonlinear case: F compact & locally injective:

Theorem 10. Let F be a nonlinear compact and continuous operator with $\mathcal{D}(F)$ weakly closed. Let $F(x^\dagger) = y$ and suppose there exists $\varepsilon > 0$ s.t. $F(x) = \hat{y}$ is uniquely solvable for all $\hat{y} \in \mathcal{R}(F) \cap B_\varepsilon(y)$.
If there exists a sequence $\{x_n\}_{n\in\mathbb{N}} \subset \mathcal{D}(F)$ with

$$x_n \rightharpoonup x^\dagger \quad \text{while} \quad x_n \not\to x^\dagger, \qquad (*)$$

then F^{-1} (defined on $\mathcal{R}(F) \cap B_\varepsilon(y)$) is <u>not</u> continuous in y.

Note: If $B_\varepsilon(x^\dagger) \subset \mathcal{D}(F)$: take $x_n = x^\dagger + \varepsilon \cdot e_n$
$\uparrow$ basis elements (X separable)

then $x_n \rightharpoonup x^\dagger$ $\quad (e_n \rightharpoonup 0)$

but $\|x_n - x^\dagger\| = \varepsilon$.

i.e. $(*)$ ~ infinite-dimensionality of $\mathcal{D}(F)$ around $x^\dagger$

$\Rightarrow$ roughly: compactness + local injectivity + "$\mathcal{D}(F)$ infinite dimensional around $x^\dagger$"

$\Rightarrow$ non-continuity

2 standard approaches:

Tikhonov regularization

Iterative methods (also for linear problems: take solver like conjugate gradient with appropriate stopping criterion $\to$ acts as parameter choice rule)

Tikhonov regularization

$$\|F(x)-y^\delta\|^2 + \alpha\|x-x^*\|^2 \longrightarrow \min, \quad x \in \mathcal{D}(F) \qquad (11)$$

[note: by our assumptions, (11) admits solution
but nonlinearity of F $\Rightarrow$ solution not unique in general]

$\rightsquigarrow$ just search for a solution, denote by x_α^δ

{In general non-convex $\rightsquigarrow$ get stuck in loc. minima]

Theorem 11. Let $y^\delta \in Y$, $\|y^\delta - y\| \leq \delta$ and let $\alpha(\delta)$ be s.t.

$\alpha(\delta) \to 0$ as $\delta \to 0$,

$\delta^2/\alpha(\delta) \to 0$ as $\delta \to 0$.

Then, every sequence $\{x_{\alpha_k}^{\delta_k}\}$ where $\delta_k \to 0$, $\alpha_k := \alpha(\delta_k)$ and $x_{\alpha_k}^{\delta_k}$ is a solution of (11), has a convergent subsequence.

The limit of every convergent subsequence is an x^*-minimum-norm solution.

If the x^*-minimum-norm solution $x^\dagger$ is unique, then

$$\lim_{\delta \to 0} x_{\alpha(\delta)}^\delta = x^\dagger.$$

Note on a-posteriori parameter choice rules:

Solving $\|F(x_\alpha^\delta) - y^\delta\| = C\delta$ is problematic
(only solvable under restrictive assumptions)

$\rightsquigarrow$ need complicated a-posteriori strategies

$\rightsquigarrow$ high computational effort

Iterative methods: stop at k_* where:

$$\|y^\delta - F(x^\delta_{k_*})\| \leq \tau\delta < \|y^\delta - F(x_k^\delta)\| \quad , \quad k < k_*$$

easy to implement

A nonlinear inverse problem: Phase retrieval

Hilbert space X

measurement system $(\varphi_\lambda)_{\lambda\in\Lambda} \subset X$

Task: reconstruct signal f from $\left(|\langle f, \varphi_\lambda\rangle_X|\right)_{\lambda\in\Lambda}$.

up to a global factor $\tau \in S^1$

$\operatorname{dist}(f_1,f_2) := \inf_{\tau\in S^1} \|f_1 - \tau f_2\|_X$

<u>Gabor phase retrieval:</u>

$X = L^2(\mathbb{R})$

$\varphi(t) = e^{-\pi t^2}$

$\varphi_\lambda = \underbrace{M_y T_x \varphi}_{\text{time-freq. shift of } \varphi} \qquad (x,y) = \lambda$

Consider best case scenario: $\Lambda = \mathbb{C}$

i.e. reconstruct f from $\left(|V_\varphi f(x,y)|\right)_{(x,y)\in\mathbb{C}}$.

$\left(V_\varphi f(x,y) = \langle f, \varphi_{(x,y)}\rangle \right)$.

Define $\mathcal{A}_\varphi : L^2(\mathbb{R})/S^1 \to L^2(\mathbb{R}^2, \mathbb{R}_0^+)$

$f \longmapsto |V_\varphi f|$

(forward operator)

Injectivity:

Fundamental formula:

$$\boxed{\mathcal{F}\left(|V_g f|^2\right)(x,y) = V_f f(-y,x)\cdot\overline{V_g g(-y,x)}}$$

For φ Gaussian: $V_\varphi \varphi$ has no zeroes
[simple computation: $V_\varphi\varphi$ is a 2D Gaussian]

$\Rightarrow$ Given $|V_\varphi f|$ one can recover $V_f f$ uniquely.

If
$$\mathcal{F}\left(|V_\varphi f_1|^2\right)(x,y) = V_{f_1} f_1(-y,x)\cdot\overline{V_\varphi \varphi(-y,x)}$$
$$\mathcal{F}\left(|V_\varphi f_2|^2\right)(x,y) = V_{f_2} f_2(-y,x)\cdot\overline{V_\varphi \varphi(-y,x)}$$

and $|V_\varphi f_1| = |V_\varphi f_2|$,
then:
$$\left(V_{f_1} f_1 - V_{f_2} f_2\right)\cdot\overline{V_\varphi \varphi} = 0$$

$$\Rightarrow \quad V_{f_1} f_1 = V_{f_2} f_2$$

One can show (take 1D FTs):

$$V_{f_1} f_2 = V_{f_2} f_2 \quad\Rightarrow\quad f_1 = \tau f_2 \quad \text{for some } \tau \in S^1.$$

[Note: formula not very useful in practice: exp. decay of $V_\varphi\varphi$]

Continuous inverse:

General property of phase retrieval when measurement system is frame:

$\mathcal{A}_\varphi$ injective $\Rightarrow$ $\mathcal{A}_\varphi^{-1}$ is continuous on $\mathcal{R}(\mathcal{A}_\varphi)$.
(see A., Grohs SIAM Math An. [1])

However: in practice instabilities <u>do</u> occur

Another general property of PR when <u>dim $X = \infty$</u>:
no uniform continuity of $\mathcal{A}_\varphi^{-1}$:

$$\alpha \operatorname{dist}(f_1,f_2) \overset{?}{\le} \|\mathcal{A}_\varphi(f_1) - \mathcal{A}_\varphi(f_2)\|_{L^2(\mathbb{R}^2)} \le \beta \operatorname{dist}(f_1,f_2)$$

fundamental difference to linear case!

no such $\alpha > 0$ exists! (see [1])

Quantification for Gabor case:

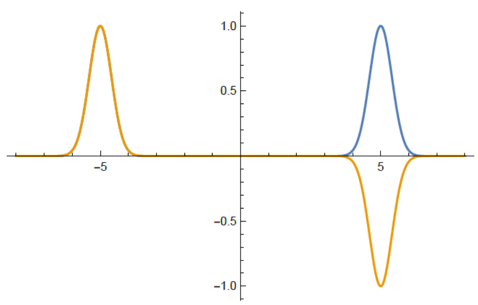
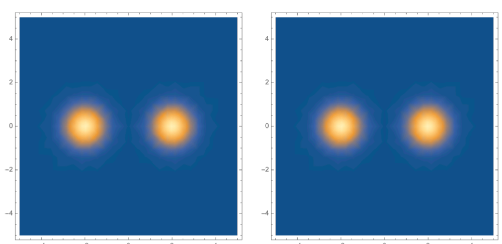


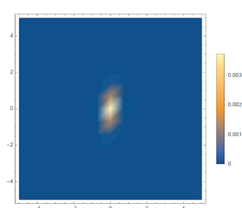
Figure 1: The functions f_a^+ (blue) and f_a^- (orange) for $a = 5$.



(a) $|V_\varphi f_a^+|$ (b) $|V_\varphi f_a^-|$

$$f_a^+ = T_a\varphi + T_{-a}\varphi$$

$$f_a^- = T_a\varphi - T_{-a}\varphi$$



$||V_\varphi f_a^+| - |V_\varphi f_a^-||$

Theorem [A., Grohs '19]: There is a uniform constant $C>0$ s.t.
$\forall a>0 \ \forall k\in(0,\pi/2)$:

$$\min_{\tau\in\{\pm1\}} \|f_a^+ - \tau f_a^-\|_{L^2(\mathbb{R})} \geq C e^{ka^2} \| |V_\varphi f_a^+| - |V_\varphi f_a^-| \|_{W^{1,2}(\mathbb{R})}$$

$\Rightarrow$ exponential degradation of stability!
"Severe" in some sense

<u>Regularization?</u>

Minimizer of $\| \mathcal{A}_\varphi(f) - u\|^2_{L^2(\mathbb{R}^2)} + \tau |||f|||$
measured data

Classical penalties [e.g. L^2, Besov norm, modulation space norm]:

$$|||f_a^+||| \sim |||f_a^-|||$$

$\rightsquigarrow$ do not resolve occuring instability!

Less classical approach:
atoll functions (see A., Daubechies, Grohs, Yin):
change notion of solution (give up on global phase factor) $\rightsquigarrow$ stability restored
(relies heavily on holomorphy property of $V_\varphi f$
$\rightsquigarrow$ Bargmann trafo)

Image classification

$\rightsquigarrow$ slides