# Statistical Inverse Problems and Instrumental Variables

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# outline

# Keller’s definition of an inverse problem

*“We call two problems* inverses *of one another if the formulation of each involves all or part of the solution of the other. Often, for historical reasons, one of the two problems has been studied extensively for some time, while the other is newer and not so well understood. In such cases, the former problem is called the direct problem, while the latter is called the inverse problem.”*

J.B. Keller. Inverse Problems. *Am. Math. Mon., 83:107-118*, 1976

# Hadamard's definition of well-posedness

**Definition**

*A problem is called well-posed if*

1. *there exists a solution to the problem (existence),*
2. *there is at most one solution to the problem (uniqueness),*
3. *the solution depends continuously on the data (stability).*

Otherwise the problem is called ill-posed.

# ill-posedness in terms of operator equations

Suppose the inverse problem can be formulated as an operator equation

$$F(a) = u$$

where $x$ denotes the unknown solution and $y$ the given data.
Then the inverse problem is well-posed in the sense of Hadamard if

1. $F$ is surjective (existence)
2. $F$ in injective (uniqueness)
3. $F^{-1}$ is continuous (stability)

Typically, the third condition is violated for inverse problems!

# first kind integral equations

Find a function $a$ such that

$$\int k(x,y)a(y)\,dy = u(x) \qquad \text{for all } x.$$

# identification of parameters in differential equations

**Estimate a parameter *a* in a differential equation given noisy measurements of the solution *u*!**

The parameter-to-solution operator $F : a \mapsto u$ is defined only implicitely via the differential equation and typically nonlinear even if the differential equation is linear.

The unknown parameter *a* might be

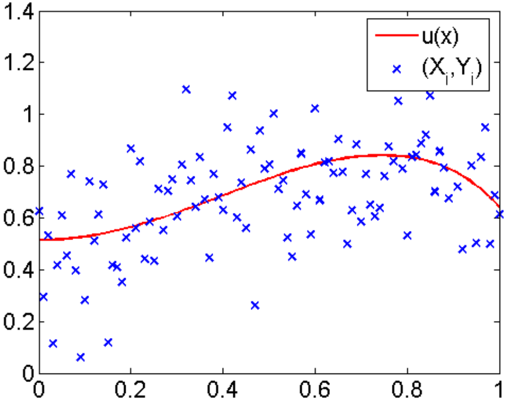
- a coefficient in the differential equation,
- a boundary condition or an initial condition,
- a parametrization of the shape of a domain.

# outline

# nonparametric regression: random design

Estimate a function $u$ in some smoothness class $\mathcal{F}$ given i.i.d. random variables $(X_i, Y_i)$, $i = 1, \ldots, n$ such that

$$\mathbf{E}(Y|X = x) = u(x),$$
$$\mathbf{E}((Y - u(x))^2|X = x) < \infty.$$



# nonparametric regression: deterministic design

Estimate a function $u$ in some smoothness class $\mathcal{F}$ given

$$Y_i = u\left(x_i^{(n)}\right) + \sigma\left(x_i^{(n)}\right)\epsilon_i, \qquad i = 1, \dots, n$$

where $\epsilon_i$ are independent random variables satisfying

$$\mathbf{E}\epsilon_i = 0, \qquad \mathbf{E}\epsilon_i^2 = 1.$$

# estimating functions in white noise

Estimate a function $u$ in some smoothness class $\mathcal{F}$ given a process

$$dY_t^{(n)} = u(t)dt + \frac{\sigma(t)}{\sqrt{n}} dB_t + \delta_n(t)dt$$

where $B_t$ is Brownian motion and $\delta_n$ is a (small) drift term.

**Under mild assumptions every nonparametric regression problem is asymptotically equivalent to a white noise problem.** (Brown & Low, Ann. Stat., 1996)

# Hilbert-space processes

Let $\mathcal{Y}$ be a Hilbert space.

- A Hilbert-space process is a continuous linear operator

$$\xi : \mathcal{Y} \to L^2(\Omega, \mathcal{P}, P).$$

  Every Hilbert-space valued random variable $\Xi$ satisfying $\mathbf{E}\|\Xi\|^2 < \infty$ can be identified with a Hilbert-space process $\varphi \mapsto \langle \Xi, \varphi \rangle$, $\varphi \in \mathcal{Y}$, but not vice versa.
  Notation: $\langle \xi, \varphi \rangle := \xi\varphi$, $\varphi \in \mathcal{Y}$.
- The covariance $\mathbf{Cov}_\xi \in L(\mathcal{Y})$ of $\xi$ is defined implicitly by $\langle \mathbf{Cov}_\xi \varphi_1, \varphi_2 \rangle = \mathbf{Cov}\left(\langle \xi, \varphi_1 \rangle, \langle \xi, \varphi_2 \rangle\right)$ for all $\varphi_1, \varphi_2 \in \mathcal{Y}$.

# statistical inverse problem

estimate $a$ given

$$Y = F(a) + \sigma\xi + \delta\zeta$$

$F : D(F) \subset \mathcal{X} \to \mathcal{Y}$ Fréchet differentiable and one-to-one, $\mathcal{X}, \mathcal{Y}$ separable Hilbert spaces.

$F^{-1}$ is not continuous!

| | |
|---|---|
| $\xi$ | normalized stochastic noise (a Hilbert space process in $\mathcal{Y}$) |
| $\sigma \geq 0$ | stochastic noise level |
| $\zeta \in \mathcal{Y}$ | normalized deterministic noise, $\|\zeta\| = 1$ |
| $\delta \geq 0$ | deterministic noise level |

# outline

# spectral theorem for compact self-adjoint operators

## Theorem (Spectral theorem for compact self-adjoint operators)

*Let $A : \mathcal{X} \to \mathcal{X}$ be a linear, compact, self-adjoint operator. Then:*

- *There exists a complete orthonormal system $\{a_j : j \in \mathbb{N}\}$ of $\mathcal{X}$ consisting of eigenvectors of $A$.*
- *If $\lambda_j$ denote the corresponding eigenvalues, then*

$$Aa = \sum_{j \in \mathbb{N}} \lambda_j \langle a, a_j \rangle a_j$$

  *for all $a \in \mathcal{X}$.*
- *The only possible accumulation point of the sequence eigenvalues $\lambda_j$ is $0$.*

# singular value decomposition

## Theorem and Definition (singular value decomposition)

*Let $T \in L(\mathcal{X}, \mathcal{Y})$ be compact with* $\dim R(T) = \infty$*, and let $P \in L(\mathcal{X})$ denote the orthogonal projection onto $N(T)$. Then there exist singular values $\sigma_0 \geq \sigma_1 \geq \cdots > 0$ and orthonormal systems $\{a_0, a_1, \ldots\} \subset \mathcal{X}$ and $\{u_0, u_1, \ldots\} \subset \mathcal{Y}$ such that*

$$
\begin{aligned}
a &= \sum_{n=0}^{\infty} \langle a, a_n \rangle a_n + Pa \\
Ta &= \sum_{n=0}^{\infty} \sigma_n \langle a, a_n \rangle u_n.
\end{aligned}
$$

*for all $a \in \mathcal{X}$. A system $\{(\sigma_n, a_n, u_n)\}$ with these properties is called a singular system of $T$. The singular values $\sigma_n = \sigma_n(T)$ are uniquely determined by $T$ and satisfy $\sigma_n(T) \to 0$ as $n \to \infty$.*

# spectrum

## Definition

*Let $A : \mathcal{X} \to \mathcal{X}$ be bounded. Then*

$$\rho(A) := \{z \in \mathbb{C} : A - zI \text{ bijective and } (A - zI)^{-1} \text{ bounded}\}$$

*is called the resolvent set of A. $\sigma(A) := \mathbb{C} \setminus \rho(A)$ is called the spectrum of A.*

It follows from Riesz theory that the spectrum of a compact operator is the union of $\{0\}$ and the set of eigenvalues.

# Compact self-adjoint operators are unitarily equivalent to multiplication operators

Let $A \in L(X)$ be compact and self-adjoint and $A\varphi = \sum_{j=1}^{\infty} \lambda_j \langle \varphi, \varphi_j \rangle \varphi_j$ a spectral decomposition.

- We define the operator $W : l^2(\mathbb{N}) \to X$ by $W(f) := \sum_{j \in \mathbb{N}} f(j)\varphi_j$. Here $l^2(\mathbb{N})$ is the Hilbert space of all functions $f : \mathbb{N} \to \mathbb{C}$ with the norm $\|f\|^2 := \sum_{j \in \mathbb{N}} |f(j)|^2$. By Parseval's equality, $W$ is a unitary operator.
- Its inverse is given by $(W^{-1}\varphi)(j) = \langle \varphi, \varphi_j \rangle$ for $j \in \mathbb{N}$.
- With this notation, the spectral decomposition can be written as

$$W^{-1}AW = M_\lambda$$

  where the multiplication operator $M_\lambda \in L(l^2(\mathbb{N}))$ is defined by $(M_\lambda f)(j) = \lambda_j f(j)$, $j \in \mathbb{N}$.

# Convolution operators are unitarily equivalent to multiplication operators

Let $k \in L^1(\mathbb{R}^d)$ satisfy $k(x) = \overline{k(-x)}$ for $x \in \mathbb{R}^d$. Then the convolution operator $(A\varphi)(x) := \int_{\mathbb{R}^d} k(x-y)\varphi(y)\,\mathrm{d}y$ is self-adjoint in $L(X)$.

- Recall that the Fourier transform

$$(\mathcal{F}\varphi)(\omega) := \int_{\mathbb{R}^d} e^{-2\pi i\langle \omega, x\rangle}\varphi(x)\,\mathrm{d}x, \qquad \omega \in \mathbb{R}^d$$

  is unitary on $L^2(\mathbb{R}^d)$.
- Due to the symmetry of $k$, the function $\lambda := \mathcal{F}k$ is real-valued, and it is bounded since $k \in L^1(\mathbb{R}^d)$.
- Introducing the multiplication operator $M_\lambda \in L(L^2(\mathbb{R}^d))$, $(M_\lambda f)(\omega) := \lambda(\omega) f(\omega)$, the Convolution Theorem implies that

$$\mathcal{F}A\mathcal{F}^{-1} = M_\lambda.$$

# Halmos' version of the spectral theorem

**Theorem (spectral theorem for bounded self-adjoint operators)**

*Let $A \in L(X)$ be self-adjoint. Then there exist a locally compact space $\Omega$, a positive Borel measure $\mu$ on $\Omega$, a unitary map*

$$W : L^2(\Omega, d\mu) \longrightarrow X,$$

*and a real-valued function $\lambda \in C(\Omega)$ such that*

$$W^{-1}AW = M_\lambda,$$

*where $M_\lambda \in L(L^2(\Omega, d\mu))$ is the multiplication operator defined by $(M_\lambda f)(\omega) := \lambda(\omega)f(\omega)$ for $f \in L^2(\Omega, d\mu)$ and $\omega \in \Omega$.*

# functional calculus

Let $\mathcal{M}(\sigma(A))$ denote the algebra of bounded measurable functions $f : \sigma(A) \to \mathbb{R}$.

## Theorem and Definition

*For $f \in \mathcal{M}(\sigma(A))$ an operator $f(A) \in L(\mathcal{X})$,*

$$f(A) := W M_{f\circ\lambda} W^{-1}$$

*is well defined and self-adjoint.*
*The mapping $f \mapsto f(A)$ is a norm-decreasing algebra homomorphism from $\mathcal{M}(\sigma(A))$ to $L(\mathcal{X})$, i.e.*

1. $(\alpha f + \beta g)(A) = \alpha f(A) + \beta g(A)$,
2. $(f \cdot g)(A) = f(A)g(A)$,
3. $\|f(A)\| \leq \|f\|_\infty$

*for all $\alpha, \beta \in \mathbb{R}$ and $f, g \in \mathcal{M}(\sigma(A))$.*

# properties of the functional calculus

- For $f_0(\lambda) := 1$ and $f_1(\lambda) := \lambda$ we have $f_0(A) = I$ and $f_1(A) = A$.
- If $p(\lambda) = \sum_{j=0}^{m} c_j \lambda^j$ is a polynomial, then we get the usual definition $p(A) = \sum_{j=0}^{m} c_j \lambda^j$.
- Expressions like $(\mu I + A)^{-1}$ and $\exp(A)$ also agree with the usual definitions.

# outline

# Picard criterion

## Theorem (Picard criterion)

*Let $T \in L(\mathcal{X}, \mathcal{Y})$ be a compact and injective operator with dense range. Let $\{(\sigma_n, a_n, u_k)\}$ be a singular system of $T$. Then the equation*

$$Ta = u$$

*is solvable if and only if the Picard criterion*

$$\sum_{n=0}^{\infty} \frac{1}{\sigma_n^2} \left|\langle u, u_n \rangle\right|^2 < \infty$$

*is satisfied. Then the solution is given by*

$$a = \sum_{n=0}^{\infty} \frac{1}{\sigma_n} \langle u, u_n \rangle \, a_n.$$

# degree of ill-posedness

The solution formula $a = \sum_{n=0}^{\infty} \frac{1}{\sigma_n} \langle u, u_n \rangle \, a_n$ nicely illustrates the ill-posedness of linear operator equations with a compact operator: Since $1/\sigma_n \to \infty$, the Fourier modes corresponding to large $n$ are amplified without bound.

We say that the equation $Ta = u$ is

- mildly ill-posed if the singular values decay to 0 at a polynomial rate, i.e. if there exist constants $C, p > 0$ such that $\sigma_n \geq Cn^{-p}$ for all $n \in \mathbb{N}$.
- Otherwise the problem is called severely ill-posed.
- If there exist constants $C, p > 0$ such that $\sigma_n \leq C \exp(-n^p)$, we call the problem exponentially ill-posed.

# spectral cut-off

One possibility to restore stability in the exact reconstruction formula $a = \sum_{n=0}^{\infty} \frac{1}{\sigma_n} \langle u, u_n \rangle a_n$ is to truncate the series, i.e. to compute

$$R_\alpha u := \sum_{\{n : \sigma_n \geq \alpha\}} \frac{1}{\sigma_n} \langle u, u_n \rangle a_n .$$

for some regularization parameter $\alpha > 0$. This is called spectral cut-off or truncated singular value decomposition.

questions:

- choice of $\alpha$?
- convergence? In which sense?

# disadvantages of spectral cut-off

- a singular value decomposition is known explicitely only for a small number of problem
- the numerical computation of a singular value decomposition is prohibitively expensive for many problems.

# Tikhonov regularization

- Solving $Ta = Y$ is equivalent to finding the minimum of the functional $a \mapsto \|Ta - Y\|^2$ in $\mathcal{X}$. Of course, the solution to this minimization problem again does not depend continuously on the data!
- To restore stability we add a penalty term to the functional and minimize

$$J_\alpha(a) := \frac{1}{2}\|Ta - Y\|^2 + \frac{\alpha}{2}\|a - a_0\|^2.$$

The parameter $\alpha > 0$ is called regularization parameter, and $a_0$ is an initial guess of $a^\dagger$. If no initial guess is known, we take $a_0 = 0$.

# Tikhonov regularization

## Theorem

*The Tikhonov functional $J_\alpha$ has a unique minimum $\widehat{a}_\alpha$ in $\mathcal{X}$ for all $\alpha > 0$, $Y \in \mathcal{Y}$, and $a_0 \in \mathcal{X}$. This minimum is given by*

$$\widehat{a}_\alpha = (T^*T + \alpha I)^{-1}(T^*Y + \alpha a_0).$$

*The operator $T^*T + \alpha I$ is boundedly invertible, so $\widehat{a}_\alpha$ depends continuously on $Y$.*

# iterated Tikhonov regularization

- Once we have computed the Tikhonov solution $\widehat{a}_\alpha$ we may find a better approximation by applying Tikhonov regularization again using $\widehat{a}_\alpha$ as initial guess $a_0$.
- This leads to iterated Tikhonov regularization:

$$\begin{aligned} \widehat{a}_{\alpha,0} &:= 0 \\ \widehat{a}_{\alpha,n+1} &:= (T^*T+\alpha I)^{-1}(T^*Y+\alpha\widehat{a}_{\alpha,n}), \qquad n \geq 0 \end{aligned}$$

- Note that only one operator $T^*T+\alpha I$ has to be inverted to compute $\widehat{a}_{\alpha,n}$ for any $n \in \mathbb{N}$. If we use, e.g., the *LU* factorization to apply $(T^*T+\alpha I)^{-1}$, the computation of $\widehat{a}_{\alpha,n}$ for $n \geq 2$ is not much more expensive than the computation of $\widehat{a}_{\alpha,1}$.

# Landweber iteration

- idea: minimize the functional $J_0(a) = \|Ta - Y\|^2$ by the steepest decent method
- The direction of steepest decent is $-T^*(Ta - Y)$.
- Choosing a fixed step-size parameter $\mu > 0$ leads to the recursion formula

$$\begin{aligned} a_0 &= 0, \\ a_{k+1} &= a_k - \mu T^*(Ta_k - Y), \qquad n \geq 0. \end{aligned}$$

# Landweber iteration

- An analysis shows that $\mu$ should be chosen such that $\mu\|T^*T\| \leq 1$
- It follows by induction that the *n*th Landweber iterate is given by

$$a_k = \sum_{j=0}^{k-1} (I - \mu T^*T)^j \mu T^* Y.$$

# accelerating Landweber iteration: Krylov subspaces

- The $n$th Landweber iterate belongs the Krylov subspace defined by

$$\mathcal{K}_k(T^*T, T^*Y) := \operatorname{span}\{(T^*T)^j T^*Y : j = 1, \dots, n\}$$

- Since the computation of any element of $\mathcal{K}_k(T^*T, T^*Y)$ requires only (at most) $n$ applications of $T^*T$, one may try to look for better approximations in the Krylov subspace $\mathcal{K}_k(T^*T, T^*Y)$.
- The conjugate gradient method applied to the normal equation $T^*Ta = T^*y$ is characterized by the optimality condition

$$\|T\widehat{a}_k - Y\| = \min_{a \in \mathcal{K}_k(T^*T, T^*Y)} \|Ta - Y\|.$$

# conjugate gradient method

$$
\begin{aligned}
&\widehat{a}_0 = 0; \quad d_0 = Y; \quad p_1 = s_0 = T^* d_0 \\
&\text{for } k = 1, 2, \ldots, \text{ unless } s_{k-1} = 0 \\
&\qquad q_k = T p_k \\
&\qquad \alpha_k = \|s_{k-1}\|^2 / \|q_k\|^2 \\
&\qquad \widehat{a}_k = \widehat{a}_{k-1} + \alpha_k p_k \\
&\qquad d_k = d_{k-1} - \alpha_k q_k \\
&\qquad s_k = T^* d_k \\
&\qquad \beta_k = \|s_k\|^2 / \|s_{k-1}\|^2 \\
&\qquad p_{k+1} = s_k + \beta_k p_k
\end{aligned}
$$

Note that $\widehat{a}_k$ depends nonlinearly on $Y$!

# regularization methods: notation

- We consider a family of *continuous* (not necessarily linear) operators $R_\alpha : \mathcal{Y} \to \mathcal{X}$ defined for $\alpha$ in some index set $A$ which approximate the *unbounded* operator $T^{-1}$
- Let $\overline{\alpha} : (0, \infty) \times \mathcal{Y} \to A$ be a parameter choice rule. For a given noisy data $Y = Ta + \delta\zeta$ with noise level $\delta > 0$ and normalized error $\|\zeta\| \le 1$ the exact solution is approximated by

$$a \approx R_{\overline{\alpha}(\delta, Y)} Y.$$

Examples:

- Tikhonov regularization: $R_\alpha = (\alpha I + T^*T)^{-1} T^*$
- spectral cutoff: $R_\alpha u := \sum_{\{n : \sigma_n \ge \alpha\}} \frac{1}{\sigma_n} \langle u, u_n \rangle \, a_n$

# regularization methods: deterministic definition

## Definition

- *The pair $(R, \overline{\alpha})$ is called a convergent regularization method for the problem $Ta = u$ if the worst case error tends to 0 with the noise level, i.e.*

$$\sup\left\{\left\|R_{\overline{\alpha}(\delta,Y)}(Y) - a\right\| : Y = Ta + \delta\zeta, \|\zeta\| \leq 1\right\} \xrightarrow{\delta\to 0} 0$$

*for all $a \in \mathcal{X}$.*

- *$\overline{\alpha}$ is called an a-priori parameter choice rule if $\overline{\alpha}(\delta, Y)$ depends only on $\delta$. Otherwise $\overline{\alpha}$ is called an a-posteriori parameter choice rule.*

# regularization methods: stochastic definition

## Definition

*The pair* $(R, \overline{\alpha})$ *is called a* *consistent regularization method* *for estimating a given data* $Y = Ta + \sigma\xi$ *if the expected error tends to* 0 *with the noise level, i.e.*

$$\mathbf{E}\left\{\left\|R_{\overline{\alpha}(\sigma, Ta+\sigma\xi)}(Ta + \sigma\xi) - a\right\|^2\right\} \xrightarrow{\sigma \to 0} 0$$

*for all* $a \in \mathcal{X}$.

Sometimes convergence in expectation is replaced by convergence in probability:

$$\mathbb{P}\left\{\left\|R_{\overline{\alpha}(\sigma, Ta+\sigma\xi)}(Ta + \sigma\xi) - a\right\| > \epsilon\right\} \xrightarrow{\sigma \to 0} 0$$

for all $a \in \mathcal{X}$ and all $\epsilon > 0$.

# deterministic error decomposition

Let $\alpha \in A = \mathbb{R}$ and assume that $R_\alpha$ are linear operators with $R_\alpha u \to T^{-1}u$ as $\alpha \to 0$ for all $u \in R(T)$. Then the total error can be decomposed by the triangle inequality

$$\|R_\alpha Y - T^{-1}u\| \leq \|R_\alpha Y - R_\alpha u\| + \|R_\alpha u - T^{-1}u\|$$

into

- a propagated data noise error $\|R_\alpha Y - R_\alpha u\| \leq \delta\|R_\alpha\|$, which explodes as $\alpha \to 0$ and
- an approximation error $\|R_\alpha u - T^{-1}u\|$, which tends to 0 as $\alpha \to 0$

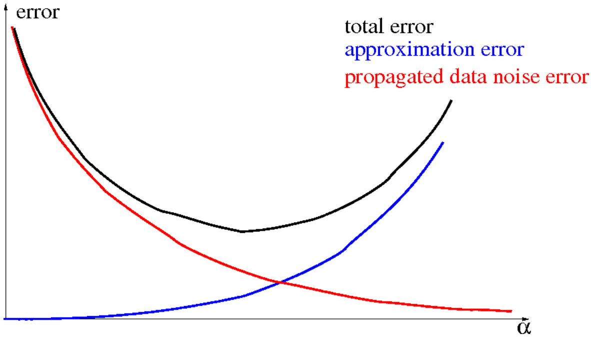
We have a trade-off between accuracy (small $\alpha$) and stability (large $\alpha$).

# bias-variance decomposition

Let $Y = u + \sigma\xi$ with $\mathbf{E}\xi = 0$. Then

$$\begin{aligned}
\mathbf{E}\|R_\alpha Y - T^{-1}u\|^2 &= \mathbf{E}\|R_\alpha Y - R_\alpha u\|^2 + \mathbf{E}\|R_\alpha u - T^{-1}u\|^2 \\
&\quad + \mathbf{E}\sigma\langle\xi, R_\alpha^*(R_\alpha u - T^{-1}u)\rangle \\
&= \sigma^2\mathbf{E}\|R_\alpha\xi\|^2 + \|R_\alpha u - T^{-1}u\|^2
\end{aligned}$$

# balancing the error components



# spectral description of regularization methods

- All regularization methods discussed so far[1] are of the form
$$R_\alpha g^\delta := g_\alpha(T^*T)T^*Y.$$
with some functions $g_\alpha \in C([0, \|T^*T\|])$ depending on some regularization parameter $\alpha > 0$.
- Then the reconstruction error for exact data is given by
$$a - a_\alpha = (I - g_\alpha(T^*T)T^*T)a = r_\alpha(T^*T)a$$
with
$$r_\alpha(\lambda) := 1 - \lambda g_\alpha(\lambda), \qquad \lambda \in [0, \|T^*T\|].$$

[1] For the CGNE method $r_\alpha$ also depends on $Y$!

# spectral description of regularization methods

| | $g_\alpha(\lambda)$ | $r_\alpha(\lambda)$ |
|---|---|---|
| Tikhonov | $\frac{1}{\lambda+\alpha}$ | $\frac{\alpha}{\lambda+\alpha}$ |
| it. Tikhonov | $\frac{(\lambda+\alpha)^n-\alpha^n}{\lambda(\lambda+\alpha)^n}$ | $\left(\frac{\alpha}{\lambda+\alpha}\right)^n$ |
| spectral cut-off | $\begin{cases} \lambda^{-1}, & \lambda \geq \alpha \\ 0, & \lambda < \alpha \end{cases}$ | $\begin{cases} 0, & \lambda \geq \alpha \\ 1, & \lambda < \alpha \end{cases}$ |
| Landweber ($\alpha = \frac{1}{k+1}$) | $\sum_{j=0}^{k-1}(1-\lambda)^j$ | $(1-\lambda)^n$ |
| Showalter | $\lambda^{-1}(1-\exp(\lambda/\alpha))$ | $\exp(\lambda/\alpha)$ |

# outline

# error-free parameter choice rules

**Theorem (Bakushinskii's theorem)**

*Let $T : \mathcal{X} \to \mathcal{Y}$ be one-to-one with dense range. Assume there exists a convergent regularization method $(R_\alpha, \overline{\alpha})$ for $Ta = u$ with a parameter choice rule $\overline{\alpha}(\delta, Y)$, which depends only on $Y$, but not on $\delta$. Then $T^{-1}$ is continuous.*

Remark: The analogous result for a white noise is false since for a white noise process $Y = u + \sigma\xi$ with $u \in \mathcal{Y}$ and $\mathbf{Cov}_\xi = I$ the variance $\sigma^2$ can be estimated reliably.

# negative results

We consider regularization methods $(R_\alpha, \overline{\alpha})$ which satisfy the following assumptions:

- $R_\alpha \in L(\mathcal{Y}, \mathcal{X})$ for all $\alpha \in A \subset (0, \infty)$
- $\lim_{\delta \to 0} \sup \{\overline{\alpha}(\delta, u + \delta\xi) : \|\xi\| \leq 1\} = 0$ for all $u \in R(T)$.
- $R_\alpha$ converges pointwise to $T^{-1}$:

$$\lim_{\alpha \to 0} R_\alpha u = T^{-1} u \qquad \text{for all } u \in R(T).$$

## Theorem

*Assume that $T^{-1}$ is unbounded and the assumptions above hold true. Then*

- *the operators $R_\alpha$ cannot be uniformly bounded with respect to $\alpha$ and*
- *the operators $R_\alpha T$ cannot be norm convergent to $I$ as $\alpha \to 0$.*

# arbitrarily slow convergence

## Theorem

*Assume that there exist a regularization method* $(R_\alpha, \overline{\alpha})$ *for* $Ta = u$ *and a continuous function* $f : [0, \infty) \to [0, \infty)$ *with* $f(0) = 0$ *such that*

$$\sup \left\{ \left\| R_{\overline{\alpha}(\delta, Y)} Y - T^{-1} u \right\| : Y \in \mathcal{Y}, \|Y - u\| \le \delta \right\} \le f(\delta)$$

*for all* $u \in R(T)$ *with* $\|u\| \le 1$ *and all* $\delta > 0$. *Then* $T^{-1}$ *is continuous.*

# general source conditions

## Assumption (SC)

*a satisfies a source condition*

$$a = \Lambda(T^*T)w,$$

*where* $\Lambda : [0,\infty) \to [0,\infty)$ *is continous, monotonely increasing, and* $\Lambda(0) = 0$

Most important examples:

- Hölder-type source conditions: natural for mildly ill-posed problems, i.e. finitely smoothing operators

$$\Lambda(t) = t^\mu, \qquad \mu > 0$$

- logarithmic source conditions: natural for exponentially ill-posed problems, e.g. integral operators with infinitely smooth kernels or inverse problems in pde's with partial measurements of the solution

$$\Lambda(t) = (-\ln t)^{-p}, \qquad p > 0$$

# How to use source conditions

Recall that the approximation error is $a - \widehat{a}_\alpha = r_\alpha(T^*T)a$ with $r_\alpha(t) \to 0$ for all $t$ and $r_\alpha(0) = 1$

- By the spectral theorem $T^*T = W^{-1}M_\lambda W$ we have

$$\|r_\alpha(T^*T)a\| = \|r_\alpha(\lambda) \cdot W^{-1}a\|_{L^2}$$

  which may tend to 0 arbitrarily slowly depending on $a$.

- If $a = \Lambda(T^*T)w$, we get

$$\begin{aligned} \|r_\alpha(T^*T)a\| &= \|r_\alpha(T^*T)\Lambda(T^*T)w\| \\ &\leq \sup_{t\in\sigma(T^*T)} |r_\alpha(t)\Lambda(t)|\,\|w\| \end{aligned}$$

- Since $\Lambda(0) = 0$ we can expect norm convergence, $\|r_\alpha\Lambda\|_{L^\infty(\sigma(T^*T))} \stackrel{\alpha\to 0}{\longrightarrow} 0$, and the problem is reduced to the estimation of the univariate function $r_\alpha \cdot \Lambda$.

# assumptions on regularization methods

## Assumption (R)

- $\sup_{t\in\sigma(T^*T)} |g_\alpha(t)| \leq \frac{C_V}{\alpha}$ *for all* $\alpha > 0$
- *There exists a number* $\nu_0 > 0$ *called* *qualification* *of the method such that*

$$\sup_{t\in\sigma(T^*T)} |t^\nu r_\alpha(t)| \leq \gamma_\nu \alpha^\nu \quad \textit{for all } \alpha \textit{ and } 0 \leq \nu \leq \nu_0.$$

- *The smoothness is covered by the regularization:*

$$\sup_{t\in\sigma(T^*T)} |\Lambda(t) r_\alpha(t)| \leq \gamma_\Lambda \Lambda(\alpha) \quad \textit{for all } \alpha. \tag{2}$$

# discussion of Assumption (R)

## Lemma

*If $t \mapsto t^{\nu_0}/\Lambda(t)$ is increasing in a neighborhood of 0, then (2) is satisfied.*

see Mathé & Pereverzev (2003) and Hohage (2000) for the special case $\Lambda(t) = (-\ln t)^{-p}$.

Assumption (R) holds true for all commonly used linear regularization methods, in particular

- Landweber iteration with any $\nu_0 \in \mathbb{R}$ (but with very large constants for large $\nu$)
- $\nu$-methods with $\nu_0 = \nu$
- Tikhonov regularization with $\nu_0 = 1$
- spectral cut-off with any $\nu_0 \in \mathbb{R}$

# deterministic error estimate

**Theorem**

*If Assumptions (SC) and (R) hold true and*

$$Y = Ta + \delta\zeta$$

*with* $\zeta \in \mathcal{Y}$, $\|\zeta\| = 1$, *then*

$$\|a - \widehat{a}_\alpha\| \leq \gamma_\Lambda \Lambda(\alpha)\|w\| + \sqrt{\frac{C_V(1+\gamma_0)}{\alpha}}\delta.$$

# optimality

Under some mild additional assumptions on $\Lambda$ the following optimality result holds true:

## Theorem

*With an appropriate a-priori parameter choice rule using smoothness information on the solution all methods under consideration are of optimal order up to their qualification in the sense that*

$$\inf_{\alpha>0} \|a - \widehat{a}_\alpha\| \le C \inf_{\Phi:\mathcal{Y}\to\mathcal{X}} \sup_{\tilde{a}\in F_\Lambda, \|\zeta\|\le\delta} \|\Phi(T\tilde{a} + \delta\zeta) - \tilde{a}\|$$

*for all* $\delta > 0$ *with* $F_\Lambda := \{\Lambda(T^*T)\tilde{w} : \|\tilde{w}\| \le 1\}$.

# outline

# Morozov's discrepancy principle

For a fixed parameter $\tau \geq 1$ choose the largest $\alpha > 0$ for which $\|T\widehat{a}_\alpha - g^\delta\| \leq \delta$. Here $\widehat{a}_\alpha := R_\alpha Y$ denotes the reconstruction for the regularization parameter $\alpha$.

$$\alpha(\delta, Y) := \sup\{\alpha > 0 : \|T\widehat{a}_\alpha - Y\| \leq \tau\delta\}$$

Do not try to fit the noise!

For iterative methods such as Landweber iteration, the discrepancy principle consists in stopping the iteration at the first index $K$ for which $\|Ta_K^\delta - Y\| \leq \tau\delta$.

# convergence rate result

If $\tau > \sup_{\alpha,t} |r_\alpha(t)||$, the exact solution satisfies $a = (T^*T)^\nu w$ and the regularization method has qualification $\geq \nu + \frac{1}{2}$, then the regularization method with the discrepancy principle converges of optimal order:

$$\|\hat{a}_\alpha - a\| \leq C\delta^{\frac{2\nu}{2\nu+1}}$$

# discussion of discrepancy principle

- easy to implement, in particular for iterative methods, most often used parameter choice rule
- reduces qualification by $\frac{1}{2}$. E.g. one only gets optimal rates of convergence for Hölder index $\nu \leq \frac{1}{2}$ instead of $\nu \leq 1$.
- Not well defined for white noise since $\|Y\| = \infty$. For discrete stochastic noise, the discrepancy principle typically chooses $\alpha$ too large, but typically it works reasonably well for sample sizes $\approx 100$.

For a further analysis of linear statistical inverse problems, in particular estimates on the variance term $\mathbf{E}\|R_\alpha \xi\|^2$ see

N. Bissantz, T. Hohage, A. Munk, F. Ruymgaart. *Convergence rates of general regularization methods for statistical inverse problems and applications.* SIAM J. Numer. Anal, 45:2610-2636, 2007.