Regularization of statistical inverse problems

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framework and notations

unknown quantity: $a \in H$, $H$ real, separable Hilbert space
observable quantity: $u \in L^2(\Omega, \mu)$, $\Omega$ metric space, $\mu$ Borel measure

operator equation: $F(a) = u + \text{“noise”}$

$F : D(F) \subset H \rightarrow L^2(\Omega, \mu)$ (possibly nonlinear) one-to-one operator

Unlike in a Bayesian view on inverse problems (cf. e.g. Kaipio, Päivärinta, Somersalo et al.), $a$ is considered as an unknown parameter, not as a random variable!

exact solution: $a^\dagger \in D(F) \subset H$

exact data: $u^\dagger := F(a^\dagger)$. 
statistical model

measured data are random variables

\[ Y_i = u^\dagger(X_i) + v(X_i)\epsilon_i, \quad i = 1, \ldots, n. \]

\( v : \Omega \to [0, \infty) \) variance function.
\( \epsilon_i \) are independent, identically distributed random variables satisfying

\[ \mathbb{E} \epsilon_i = 0, \quad \text{Var} \epsilon_i = 1. \]

Both \( v \) and the distribution of the \( \epsilon_i \)'s are unknown!

measurement points: \( X_i \in \Omega \). Either random variables, independent of \( \epsilon_i \) (random design) or deterministic quantities (deterministic design).
Our aim is to construct estimators

\[(Y_i, X_i)_{i=1,\ldots,n} \mapsto \hat{a}_n \quad (\mathbb{R} \times \Omega)^n \rightarrow D(F)\]

such that the expected error \(\mathbf{E} \|\hat{a}_n - a^\dagger\|^2\) is as small as possible uniformly for all possible solutions \(a^\dagger \in D(F)\).

In particular, we want the family of estimators to be consistent in the sense that

\[\lim_{n \to \infty} \mathbf{E} \|\hat{a}_n - a^\dagger\|^2 = 0\]

for all \(a^\dagger \in D(F)\). Moreover, we would like to estimate the speed of convergence if \(a^\dagger\) belongs to certain smoothness classes.
method of Ruymgaart el al. for linear problems

van Rooij & Ruymgaart 1992, 1996; Mair & Ruymgaart 1996

Let $F = T$ be a linear integral operator

$$(Ta)(x) = \int k(x, t)f(t) \, dt.$$ 

We multiply the eq. $Ta = u^\dagger$ from the left by an operator $Q : L^2(\mu) \to H$ such that $QT$ is self-adjoint and positive definite (usually $Q = T^*$):

$$QTa = Qu$$

Obviously, for $Q = T^*$ this introduces additional ill-posedness. However, it is possible under reasonable assumptions on the kernel $k$ to construct an estimator $\hat{q}_n$ of $q^\dagger := Qu^\dagger$ which is unbiased, $\sqrt{n}$-consistent ($E \hat{q}_n = q^\dagger$ and $\text{Var} \hat{q}_n \leq \frac{C}{n}$). In the simplest case, this estimator is given by

$$\hat{q}_n := \frac{1}{n} \sum_{i=1}^{n} k(X_i, \cdot)Y_i.$$
An estimator of $a$ can be obtained by applying a regularized inverse $R_\alpha \approx (QT)^{-1}$ to $\hat{q}_n$:

$$\hat{a}_{\alpha,n} := R_\alpha \hat{q}_n$$

Such regularized inverses can be constructed by any linear regularization method, e.g.

- **Tikhonov regularization**: $R_\alpha = (\alpha I + QT)^{-1}$
- **Landweber iteration**: $R_k = \sum_{j=0}^{k-1} k - 1(I - QT)^j$
- **spectral cut-off**
- ...
decomposition of the MISE

Let $f_\alpha = R_\alpha q^\dagger = \mathbf{E} \hat{a}_{\alpha,n}$. Then the mean integrated square error (MISE) satisfies:

$$\mathbf{E} \| \hat{a}_{\alpha,n} - a^\dagger \|^2 = \mathbf{E} \| \hat{a}_{\alpha,n} - a_{\alpha} \|^2 + \| a_{\alpha} - a^\dagger \|^2$$

The bias is exactly the approximation error in deterministic theory. The variance term corresponds to the data noise error, but should be treated differently.
Halmos version of spectral theorem

**Theorem:** Let $A : H \rightarrow H$ be a, bounded, self-adjoint linear operator. Then there exists a measure space $(S, \Sigma)$, a function $\rho \in L^\infty(S, \Sigma)$, and a unitary operator $U : H \rightarrow L^2(S, \Sigma)$ such that

$$A = U^* M_\rho U$$

where $M_\rho : L^2(S, \Sigma) \rightarrow L^2(S, \Sigma)$ is the multiplication operator

$$(M_\rho \varphi)(\sigma) := \rho(\sigma) \varphi(\sigma).$$
convergence rate results

It has been shown in a number of situations that for spectral cut-off with a suitable choice of regularization parameters the MISE converges to 0 at an order-optimal rate as $n \to \infty$. (Garza, Hall, Mair, Rooij, Ruymgaart, . . .)

These cases include compact operators with singular-values behaving like $\sigma_n(T) \sim \frac{1}{n^\gamma}$, $\gamma > 0$ (mildly-ill-posed problems) or $\sigma_n(T) \sim (\ln n)^{-p}$, $p > 0$ (exponentially ill-posed problems).

For Tikhonov regularization a convergence rate analysis for mildly ill-posed problems has been provided by Nychka and Cox, 1988,89 in a special setting involving reproducing kernel Hilbert spaces.
assumptions on spectral data of operator

Assume that \( \rho \in L^1(S, \Sigma) \) and that \( R(\alpha) := \tilde{\Sigma}(\{\rho > \alpha\}) \), \( \alpha \geq 0 \) satisfies

1. \( S'(\alpha) \leq R(\alpha) \leq S(\alpha) + c \) for some \( c > 0 \)
2. \( S'' \leq 0 \)
3. \( \alpha S'(\alpha) \) is integrable
4. \( \lim_{\alpha \to 0} \alpha S(\alpha) = 0 \)
5. There exists \( C \in (0, 2) \) s.t. \( S'''(\alpha) \leq C \frac{S'(\alpha)}{\alpha} \) for all \( \alpha \in (0, \bar{\alpha}] \).

Motivation:
2: \( R \) is decreasing
3: \( -\int_0^{\infty} \alpha dR(\alpha) = \int_S \rho d\Sigma < \infty \) as \( \rho \in L^1(\Sigma) \).
4. \( \lim_{\alpha \to 0} \alpha R(\alpha) = \lim_{\alpha \to 0} \int_S \alpha 1_{\rho \geq \alpha} d\Sigma = 0 \) by dominated convergence

5. holds true if \( QT \) is compact with \( \sigma_n(QT) \sim n^{-\gamma}, \gamma > 1 \) or \( \sigma_n(QT) \sim (\ln n)^{-p}, p > 0 \).
convergence of spectral regularization methods

**Theorem:** (Bissantz, H., Munk & Ruymgaart) Under the assumptions above, the variance term of all commonly used spectral regularization methods (in particular Tikhonov regularization, Landweber iteration and $\nu$-methods) is uniformly bounded by a constant times the variance term of spectral cut-off.

**Corollary:** The methods above converge at the same (optimal) rate as $n \to \infty$ if no saturation effects occur.
There has been a lot of work on consistency and convergence rates for linear statistical inverse problems (see Evans & Stark, 2002 for a recent review), but very little on nonlinear problems.

**nonlinear method of regularization (MOR):**

\[ \hat{a}_n = \arg\min_{a \in D(F)} \sum_{j=1}^{n} |(Fa)(X_j) - Y_j|^2 + \alpha_n \|a - a_0\|^2_H \]

\( \alpha_n > 0 \) regularization parameter, \( a_0 \) a-priori guess.

**O’Sullivan, 1990:** consistency and convergence rate result for a special class of nonlinear problems, which are well-posed if \( L^2(\Omega) \) is replaced by a Sobolev space \( W^s(\Omega) \) (nonlinear extension of the approach of Nychka & Cox).
another approach

For many inverse problems in partial differential equations, the exact data function \( u^\dagger \in L^2(\Omega) \) enjoys certain a-priori known smoothness properties. Therefore, we can reliably estimate \( u^\dagger \) itself from the given data. However, we will have to sacrifice unbiasedness of the estimator \( \hat{u}_n \in L^2(\Omega) \).

In the second step we determine an estimate \( \hat{a}_n \) of \( a^\dagger \in D(F) \) by computing a minimizer of the functional

\[
a \mapsto \sum_{j=1}^{n} \| F(a) - \hat{u}_n \|^2 + \alpha_n \| a - a_0 \|_H^2, \quad a \in D(F).
\]

Again, \( \alpha_n > 0 \) is a regularization parameter and \( a_0 \) an a-priori guess.
example: inverse obstacle scattering problem

$K \subset \mathbb{R}^m$ star-shaped, $m = 2, 3$

$u_i(x) = e^{ikx \cdot d}$ incident wave,

$d \in \mathbb{R}^m, |d| = 1$ direction,

$k^{-1} \approx \text{diam } K$ wave number

direct problem: Given $K$ and $u_i$ determine a scattered field $u_s$ such that

- $\Delta u_s + k^2 u_s = 0$ in $\mathbb{R}^m \setminus K$
- $r^{\frac{m-1}{2}} \left( \frac{\partial u_s}{\partial r} - ik u_s \right) \xrightarrow{r \to \infty} 0$
- $u = 0$ on $\partial K$, $u := u_i + u_s$

inverse problem: Given the far field pattern $u_\infty$ of $u_s$ and $u_i$, find the obstacle $K$!
Illustration of the reconstruction algorithm

Data

Step 1: Estimation of far field pattern

Step 2: Estimation of shape

Variance $\sqrt{\nu}$ estimated by 0.3005 (0.3000)

$\frac{\|\hat{u}_{100} - u_{\infty}\|}{\|\hat{u}_{100}\|}$ estimated by 0.1321 (0.1349)
The MOR has the apparent advantage that only one regularization parameter has to be chosen whereas in our method both steps involve the choice of a regularization parameter. However, if we aim at a completely data-driven method, it is actually advantageous both for practical and theoretical reasons to tackle the simpler problem of estimating $u$ without information on the variance of the data errors in a first step.

The choice of the regularization parameter in the second step can be done by well-known methods from deterministic regularization theory since we have obtained reliable information on the data error in the first step.
local polynomial estimators

data: \( Y_i = u(X_i) + \epsilon_i, i = 1, \ldots, n \)

aim: Estimate \( u \in L^2(\Omega), \Omega \subset \mathbb{R}^d \) smooth, bounded

Let \( K : \mathbb{R}^d \rightarrow \mathbb{R} \) be a smooth symmetric weight function (kernel) such that \( \int_{\mathbb{R}^d} x x^T K(x) \, dx = \mu_2(K) I_d \) with \( \mu_2(K) > 0 \) (e.g. the Gauss bell function).

The polynomial estimator of \( u \) at \( x \in \Omega \) of degree \( p = 0, 1, \ldots \) and bandwidth \( h > 0 \) is defined as \( \hat{u}_n(x; h, p) := \varphi(x) \) where \( \varphi \) is the \( d \)-variate polynomial of degree \( \leq p \) which solves the minimization problem

\[
\sum_{i=1}^n |\varphi(x - X_i) - Y_i|^2 h^{-d} K \left( \frac{x - X_i}{h} \right) = \min!
\]
convergence of local polynomial estimators

**Theorem:** Assume that

- $\Omega \subset \mathbb{R}^d$ is a smooth, bounded domain and $u^\dagger \in C^2(\overline{\Omega})$.

- $K$ is continuous, has compact support, $\int x x^T K(x) \, dx = \mu_2(K) I$ for some constant $\mu_2(K) > 0$, and all odd-order moments of $K$ vanish, i.e. $\int x_1^{\kappa_1} \cdots x_d^{\kappa_d} K(x) \, dx = 0$ for all combinations of integers $\kappa_1, \ldots, \kappa_d \geq 0$ with $\sum_{i=1}^d \kappa_i$ odd.

- The bandwidth $h = h(n)$ tends to 0 as $n \to \infty$ such that $nh^d \to \infty$.

Define $R(K) := \int_{\mathbb{R}^d} K(x)^2 \, dx$ and denote by $H_{u^\dagger}(x)$ the Hessian of $u^\dagger$ at $x \in \Omega$. Then the linear polynomial estimator is well defined with probability tending to 1 and satisfies

$$
\mathbb{E} \left( \| \hat{u}_n (\cdot; h) - u^\dagger \|_{L^2(\Omega)}^2 | X_1, \ldots, X_n \right) = \frac{h^4}{4} \mu_2(K)^2 \int_{\Omega} (\text{Tr} \, H_{u^\dagger}(x))^2 \, dx \\
+ \frac{1}{nh^d} R(K) \int_{\Omega} v(x) \, dx + o_P \left( \frac{1}{nh^d} + h^4 \right).
$$
estimation of the variance

Let the $n \times n$-matrix $W = (w_{ij})$ be defined through the linear mapping

$$\hat{u}_n(X_i) = \sum_{i=1}^{n} w_{ij} Y_j, \; i = 1, \ldots, n.$$ 

The variance $v := \text{Var} \epsilon_i$ of the measurement errors can be estimated by

$$\hat{v}_n := \frac{1}{\nu} \sum_{i=1}^{n} |Y_i - \hat{u}_n(X_i)|^2.$$ 

The constant $\nu = n - 2 \sum_{i=1}^{n} w_{ij} + \sum_{i=1}^{n} \sum_{j=1}^{n} w_{ij}^2$ is chosen such that $\mathbb{E} \hat{v}_n = v$ if $u$ is a polynomial of degree $\leq p$.

It can be shown that the estimator $\hat{v}$ is asymptotically optimal and $\sqrt{n}$-consistent. (Wagner, 1999)
assumptions

- uniqueness: \( F(a_1) = F(a_2) \Rightarrow a_1 = a_2 \)

- \( F \) is weakly sequentially closed, i.e. if a sequence \((a_n)_{n \in \mathbb{N}} \subset D(F)\) converges weakly to some \( a \in D(F) \), \( a_n \rightharpoonup a \) and if \( F(a_n) \rightharpoonup u \) for some \( u \in G \), then \( a \in D(F) \) and \( F(a) = u \).

- \( \mathbf{E} \| \hat{u}_n - u^\dagger \|^2 = O(\beta_n^2) \) for some sequence \( \beta_n \to 0 \).
Theorem: (Bissantz, H. & Munk)
Under the assumptions listed above, let \( \hat{a}_n \) denote a (not necessarily unique) solution to the minimization problem

\[
\| F(a) - \hat{u}_n \|^2 + \alpha_n \| a - a_0 \|^2 = \min_{a \in D(F)} a \in D(F)
\]

and assume that the regularization parameters \( \alpha_n > 0 \) are chosen such that

\[
\alpha_n \to 0, \quad \frac{\beta_n^2}{\alpha_n} \to 0 \quad \text{as } n \to \infty.
\]

Then

\[
\mathbf{E} \| \hat{a}_n - a^\dagger \|^2 \to 0 \quad \text{as } n \to \infty.
\]
convergence plots for the scattering problem

Left: \( \| \hat{u}_{n,\infty} - u_{\infty}^\dagger \|_{L^2} \) over \( n \). Right: \( \| \hat{a}_n - a^\dagger \|_{H^s} \) over \( n \).

The solid lines connect the mean values for each sample size.
convergence rate result

Theorem: (Bissantz, H. & Munk) Assume that:

- $F$ is Fréchet differentiable.
- $D(F)$ is convex, and that there exists a Lipschitz constant $L > 0$ such that
  $$\|F'[a_1] - F'[a_2]\| \leq L\|a_1 - a_2\| \quad \text{for all } a_1, a_2 \in D(F).$$

- source condition: There exists $w \in \tilde{H}$ such that
  $$a^\dagger - a_0 = F'[a^\dagger]^* w, \quad L\|w\| < 1$$

- $E \|\hat{u}_n - u^\dagger\|^2 = O(\beta_n^2)$ for some sequence $\beta_n \to 0$.

Then, for a choice of regularization parameters satisfying $\alpha_n \sim \beta_n$, any sequence $\hat{a}_n$ of minimizers to the Tikhonov functional obeys

$$E \|\hat{a}_n - a^\dagger\|^2 = O(\beta_n), \quad \text{and} \quad E \|F(\hat{a}_n) - u^\dagger\|^2 = O(\beta_n^2).$$

(cf. result of Engl, Kunisch & Neubauer, 1989 in deterministic theory)
potential optimality of the convergence rate

Consider the linear integral operator $F : L^2([0, 1]) \to L^2([0, 1])$,

$$(Fa)(x) := \int_0^1 k(x, y)a(y) \, dy$$

with kernel

$$k(x, y) := \begin{cases} x(1 - y), & x \leq y, \\ y(1 - x), & y > x. \end{cases}$$

The source condition $a^\dagger \in R(F)$ is equivalent to

$$(u^\dagger)^{(4)} \in L^2([0, 1])$$

$$u^\dagger(0) = u^\dagger(1) = (u^\dagger)''(0) = (u^\dagger)''(1) = 0.$$ 

For this smoothness class, cubic polynomial estimators with bandwidth $h \sim n^{-1/9}$ convergence with the rate

$$\mathbb{E} \|\hat{u}_n - u^\dagger\|^2 = O(n^{-8/9})$$

i.e. $\beta_n = n^{-4/9}$. Hence, by the previous theorem,

$$\mathbb{E} \|\hat{a}_n - a^\dagger\|^2 = O\left(n^{-4/9}\right).$$
potential optimality, cont’d

On the other hand, Mair & Ruymgaart (1996) have shown the lower bound (or *mini-max rate*)

\[
\inf_{\hat{a}_n \in \mathcal{A}_n} \sup_{a^\dagger \in \{Fw: \|w\| \leq 1\}} \mathbb{E} \|\hat{a}_n - a^\dagger\|^2 \geq cn^{-4/9}.
\]

Here \(c > 0\) is a constant, and \(\mathcal{A}_n\) denotes the class of all mappings \(\hat{a}_n : ([0, 1] \times \mathbb{R})^n \to L^2([0, 1])\).

Since the upper bound is of the same order as the lower bound, the convergence of our method is optimal up to a constant for this example.
a groundwater filtration problem

\[ a \quad \text{diffusivity of the sediment} \]
\[ u \quad \text{piezometric head} \]
\[ g \quad \text{sinks and sources of water} \]
\[ \Omega \subset \mathbb{R}^d \quad \text{smooth domain} \]

differential equation:

\[ \nabla a \nabla u = g \quad \text{in } \Omega \]
\[ u = 0 \quad \text{on } \partial \Omega. \]

We introduce the parameter-to-solution operator

\[ F : D(F) \subset H^s_0(\Omega) \to L^2(\Omega) \quad \text{with} \quad D(F) := \{ a \in H^s_0(\Omega) : a \geq \underline{a} \} \]

where \( s > d/2 \) and \( \underline{a} \in (0, \infty) \) by

\[ F'(a) := u. \]
verification of the assumptions

- uniqueness: Richter, 1981 under the assumption that the right hand side $g$ be positive and Hölder continuous.

- weak closedness ... an argument involving compactness of embedding operators $H^s \hookrightarrow H^{s'}$ with $s > s' > d/2$

- $F$ is Fréchet differentiable, and the differential equation can be formally differentiated w.r.t. $a$:

\[
\nabla a \nabla (u'[a]h) = -\nabla h \nabla u, \quad u|_{\partial \Omega} = 0
\]

- $F'$ is Lipschitz continuous since $F$ is twice continuously differentiable.

- source condition: For $d = 1$ the source condition can be interpreted as a smoothness condition (see Engl, Hanke, Neubauer, 96). For $d \geq 2$ a precise characterization is not known.
groundwater filtration problem: results