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Saturation spaces for regularization methods in inverse problems

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Abstract

The aim of this article is to characterize the saturation spaces that appear in inverse problems. Such spaces are defined for a regularization method and the rate of convergence of the estimation part of the inverse problem depends on their definition. Here we prove that it is possible to define these spaces as regularity spaces, independent of the choice of the approximation method. Moreover, this intrinsec definition enables us to provide minimax rate of convergence under such assumptions.

Keywords:Linear inverse problems, Regularization methods, structural econometrics

1 Introduction

An inverse problem deals with the estimation of an unknown function φ which is not observed directly but through an implicit relation to solve. Generally speaking, let φ be our functional interest parameter which belongs to a Hilbert space Φ. We denote S a random variable and the associated cumulative distribution function $F \in \mathcal{F}$. Our objective is to study the solution of the relation:

$$A(\varphi, F) = 0 \tag{1.1}$$

where A is an operator defined on $\Phi \times \mathcal{F}$.

Let $S_1, ..., S_n$ be realizations of the random variable S. Since F is unknown, we have to replace it by an estimator F^δ and the associated estimated solution φ^δ is defined through:

$$A(\varphi^\delta, F^\delta) = 0 \tag{1.2}$$

In order to study the convergence of the solution φ^δ of (1.2) to the true solution φ of (1.1), we need to check if the inverse problem is well-posed or not. If the problem is well-posed, then we can define a unique solution stable under small perturbation (like replacing F by F^δ). In that case, under classical regularity assumptions on the true solution φ, we are able to prove the consistency and derive the optimal rate of convergence. Let illustrate that by some examples.

A classical example is the GMM estimation in finite dimension.Let assume $S \in \mathbb{R}^m$ a random vector and F the associated cumulative distribution function; let h be an operator defined on $\mathbb{R}^m \times \Phi$ and valued in $\mathbb{R}^r$. We assume that h is integrable for any φ and consider the following problem:

$$\mathbb{E}_F \left[h(S, \varphi) \right] = 0$$

When φ is finite dimensional, we obtain the usual moment conditions of the GMM method. It has been extensively studied (Hansen 1982, Hall 1993).

Another example in econometrics of well-posed inverse problem is the following.

Consider $S = (X, Y, Z) \in \mathbb{R}^3$ and assume that φ is the solution of:

$$\begin{cases} y'(x) & = m_F(x, y(x)) \\ y(x_0) & = y_0 \end{cases}$$

where $m_F(x, y) = \mathbb{E}\left[Z \,| X = x, Y = y \right]$. A classical economic application has been developed by Hausman and Hausman and Newey on the analysis of the variation of consumer surplus, associated to a variation of price. We can rewrite the problem the following way:

$$\varphi(x) = \int_{x_0}^{x} m_F(t, \varphi(t)) dt$$

The existence and uniqueness of a solution is the result of the application of Cauchy-Lipchitz theorem and under the assumption that $\varphi \in C^2(I)$ where I is a neighborhood of the initial condition (x_0, y_0), we are able to prove the consistency and the optimality of the rate of convergence (see Vanhems and Loubes and Vanhems for an extension).

However, the regularity assumptions imposed of φ in order to achieve the optimal rate of convergence may be more complicated when the inverse problem is not well-posed. In this paper, we will focus on linear ill-posed inverse problem and we want to characterize solutions of:

$$r = T\varphi \tag{1.3}$$

for a specific situation where the exact data r are not known, but only an approximation r^δ such that $\|r - r^\delta\| \leq \delta$. T is a linear compact operator that is supposed to be known. For example, we may think of an observation model $r_i = r_i^\delta + \varepsilon_i$ where ε_i are observation errors. In our setting we will always assume T is known but the result coud easily be extended when T is unknown and is estimated by T^δ. In that case,the observable data are given by the relation:

$$r^\delta = T^\delta \varphi = r + (T^\delta - T)\varphi$$

We will suppose here that our inverse problem is ill-posed. Then, if we consider the equation:

$$r^\delta = T\varphi^\delta \tag{1.4}$$

the solution φ^δ of (1.4) is not a good approximation of φ due to the unboundedness of the inverse operator T^{-1}.

Such kind of ill-posed linear inverse problems occurs frequently in econometrics. For general references, we refer to Cavalier and Tsybakov 2000, Ermakov 189, O'Sullivan 1996. Let us detail for example the case developed by Darolles, Florens Renault 2002.

Note $S = (Y, Z, W)$ a random vector; the probability distribution on S is characterized by its joint cumulative distribution function F. For a given F, we consider the Hilbert space L^2_F of square integrable functions of S and we denote $L^2_F(Y)$, $L^2_F(Z)$, $L^2_F(W)$ the subspaces of L^2_F of functions depending on Y, Z or W only. Then, the objective is to study the function $\varphi \in L^2_F(Z)$ solution of the functional equation:

$$\mathbb{E}\left[Y - \varphi(Z) \,|W\right] = 0 \tag{1.5}$$

This relation can be rewritten in the following way:

$$T\varphi = r$$

where $r = \mathbb{E}\left[Y \,|W\right]$ and $T\varphi = \mathbb{E}\left[\varphi(Z) \,|W\right]$.

Another classical is the deconvolution problem, studied in particular by Carrasco and Florens (2002). Let X a random variable with density f unobserved. The problem to solve is:

$$X = Y + Z$$

We assume that Y and Z are independent variables, with respective densities φ and g; g is known and φ is our interest parameter. The equation to study is then the following:

$$f(x) = \int \varphi(y) g(x-y) dy$$

which an ill-posed integral equation to solve.

More generally speaking, the usual way to solve ill-posed inverse problems is to try to regularize them. The equation we will consider up to the end is the following:

$$T\varphi = r$$

and we will assume that:

$[A1]$: T is a compact operator defined on an hilbert space of L^2-functions Φ.

Then, T^*T is a compact self-adjoint positive operator from Φ to Φ. Therefore, we can define an orthonormal basis of eigenfunctions $(\varphi_i)_{i\geq 0}$ (for the L^2-norm) and positive eigenvalues $\left(\lambda_i^2\right)_{i\geq 0}$ such that:

$$\begin{cases} \lambda_0^2 = \|T\|^2 \\ \forall i \in I\!N, \lambda_{i+1}^2 \leq \lambda_i^2 \\ \lambda_n^2 \underset{n->\infty}{->} 0 \end{cases}$$

In order to have identification of our interest parameter, we need to assume that:

$[A2]$: $\forall i \in I\!N, \lambda_i^2 > 0$

To ensure the overidentification of φ, we need a last assumption:

$[A3]$: $r \in R(T) + N(T^*)$

Then, we consider the unique solution φ of:

$$T^*T\varphi = T^*r$$

Since T^*T is not compact, its inverse is not bounded and the approximated solution obtained when replacing r by r^δ may not converge to the true solution φ. Therefore, we cannot directly inverse the operator T^*T but we try to approximate it by a regularization operator which inverse is continuous and which converges to the true operator T^*T. In what follows, we define a regularization operator R_α which converges to $(T^*T)^{-1}$ as α decreases to zero (but not too fast in order to ensure the stability of the solution). Then we can construct $\varphi_\alpha^\delta = R_\alpha T^* r^\delta$, the regularized estimator of the solution of the ill-posed inverse problem. Write also $\varphi_\alpha = R_\alpha T^* r$ the regularized of the real data r. The estimator should verify $\varphi_\alpha^\delta -> \varphi$ when α and δ go to zero.

There exists various examples of regularization operators. A well-known method is called spectral cut-off. The idea is the following: instead of using the all sequence of eigenvalues, let cut it up to one fixed value and define:

$$\varphi_\alpha = \sum_{i:\lambda_i^2 > \lambda_\alpha^2} \frac{1}{\lambda_i^2} \langle T^* r, \varphi_i \rangle \varphi_i$$

Another possibility, called Tikhonov regularization, is to increase the value of the $\left(\lambda_i^2\right)_{i \geq 0}$ by adding a positive number like:

$$\varphi_\alpha = \sum_{i \geq 0} \frac{1}{\alpha + \lambda_i^2} \langle T^* r, \varphi_i \rangle \varphi_i$$

Generally speaking, this regularization operator depends on a smoothing parameter α which converges to 0. Moreover, in order to prove the convergence of φ_α^δ to φ, we usually have to impose another constraint: $\|\varphi_\alpha - \varphi\|^2 = O(\alpha^\beta)$ where the parameter β controls the convergence of the regularised solution to the true one. We define the space Φ_β such that: $\Phi_\beta = \left\{\varphi; \|\varphi_\alpha - \varphi\|^2 = O(\alpha^\beta)\right\}$.

In what follows, the sub-space defined by this condition is called saturation space. As a matter of fact, such spaces determine the longest sets where a regularization scheme provide estimators converging at an optimal rate of convergence. The objective of our work is then to characterize this condition in terms of regularity assumptions of both the function φ and the operator T. Moreover, under classical smoothness assumptions for the operator T, the space will only depend on φ.

The condition $\varphi \in \Phi_\beta$ is crucial to obtain the rate of convergence and also appears in many ill-posed inverse problems (see for example Loubes Vanhems 2002) but up to now, the link between the space Φ_β, the regularity of the function φ and the operator T was not clearly established.

Therefore, the main goal of this paper is to try to characterize this space Φ_β and we show that its definition is independant of the type of regularization; moreover we can characterize this space only through regularity assumptions on φ, which enables us to check the minimax properties of Darolles Florens Renault estimator.

Even if in this work we only consider linear inverse problems, it is possible to study in a similar way the nonlinear case, when replacing the assumptions over T by assumptions over $DT(\varphi)$ (the differential of T with respect to φ). For a close study of nonlinear inverse problem, we refer to Ludena Loubes 2003.

The plan of this article is the following: we first derive the main characterisation of the space Φ_β; then, we show that using this characterization, we are able to fing the minimax rate of convergence and at last we stress the link with Sobolev spaces.

2 Characterization of saturation spaces for regularization method

Consider the general ill-posed integral linear inverse problem:

$$r = T\varphi$$

where φ is the true functional interest parameter which belongs to an Hilbert space $\Phi \subset L^2(X)$; $L^2(X)$ is the Hilbert space of square integrable real valued functions depending on X, a random real-valued variable. Moreover T is a linear operator defined on $L^2(X)$ to $L^2(Y)$ (with Y a real-valued random variable). At last we define the function r which belongs to an Hilbert space $\Psi \subset L^2(Y)$. Then, $T^* : L^2(Y) -> L^2(X)$ will be the adjoint of T.

We assume that T^*T satisfy the three assumptions $[A1]$, $[A2]$ and $[A3]$ and write (λ_n^2, φ_n) the associated spectral value decomposition and E_λ the spectrum of T^*T. Therefore, we introduce the following integral notation:

$$T^*T\varphi = \sum_n \lambda_n^2 < \varphi, \varphi_n > \varphi_n = \int \lambda dE_\lambda \varphi.$$

We have for every continuous function g:

$$g(L^*L)\varphi = \int g(\lambda) dE_\lambda \varphi = \sum_n g(\lambda_n^2) < \varphi, \varphi_n > \varphi_n. \tag{2.1}$$

As a result, for every regularization scheme R_α, there exists a function g_α such that

$$\begin{aligned} \varphi_\alpha &= \sum_{i \geq 0} g_\alpha(\lambda_i^2) \langle T^*r, \varphi_i \rangle \varphi_i \\ &= \sum_{i \geq 0} \lambda_i^2 g_\alpha(\lambda_i^2) \langle \varphi, \varphi_i \rangle \varphi_i \end{aligned}$$

which is equivalent to

$$\varphi_\alpha = \int \lambda g_\alpha(\lambda) dE_\lambda \varphi$$

For example, the Tikhonov's regularized estimator is defined by a function

$$g_\alpha = \frac{1}{\lambda + \alpha}.$$

Then we have

$$\begin{aligned} \varphi_\alpha - \varphi = g_\alpha(T^*T)T^*r - \varphi &= (g_\alpha(T^*T)T^*T - I)\varphi \\ = \int (\lambda g_\alpha(\lambda) - 1) dE_\lambda \varphi &= f_\alpha(T^*T)\varphi. \end{aligned}$$

where $f_\alpha(\lambda) = \lambda g_\alpha(\lambda) - 1$.

We have also the following useful equality:

$$\|\varphi_\alpha - \varphi\|^2 = \int_0^{\|T\|^2} f_\alpha^2(\lambda) d\|E_\lambda \varphi\|^2. \tag{2.2}$$

At last, define, for $\beta \geq 0$ the set $X_\beta = \left\{ \varphi \in \Phi : \sum_{i\geq 0} \frac{\langle \varphi, \varphi_i \rangle^2}{\lambda_i^{2\beta}} < +\infty \right\}$

Theorem 2.1 *If $\lambda^\beta |f_\alpha(\lambda)|^2 \leq \alpha^\beta$, then*

$$\varphi \in X_\beta \quad \Rightarrow \|\varphi_\alpha - \varphi\|^2 = O(\alpha^\beta) \tag{2.3}$$

If there exists a constant γ such that $\forall \lambda \in [c\alpha, \|T\|^2]$, $\lambda^\beta |f_\alpha(\lambda)|^2 \geq \gamma \alpha^\beta$, then we get the following implication

$$\|\varphi_\alpha - \varphi\|^2 = O(\alpha^\beta) \quad \Rightarrow \varphi \in X_\beta. \tag{2.4}$$

Proof. For the first part, we assume that $\varphi \in X_\beta$. Then,

$$\|\varphi_\alpha - \varphi\|^2 = \sum_{i=0}^{+\infty} f_\alpha^2(\lambda_i^2) \langle \varphi, \varphi_i \rangle^2$$

and

$$f_\alpha^2(\lambda_i^2) \leq \frac{\alpha^\beta}{\lambda_i^{2\beta}}$$

Since $\varphi \in L^2$, we find that $\|\varphi_\alpha - \varphi\|^2 = O(\alpha^\beta)$.

For the second part, using (2.2) we get:

$$\begin{aligned}
\|\varphi_\alpha - \varphi\|^2 &= \int_0^{\|T\|^2} f_\alpha^2(\lambda) d\|E_\lambda \varphi\|^2 \\
&\geq \int_{c\alpha}^{\|T\|^2} f_\alpha^2(\lambda) d\|E_\lambda \varphi\|^2 \geq \gamma^2 \alpha^\beta \int_{c\alpha}^{\|T\|^2} \lambda^{-\beta} d\|E_\lambda \varphi\|^2 \\
&= O(\alpha^\beta).
\end{aligned}$$

As a result, $\int_{c\alpha}^{\|T\|^2} \lambda^{-\beta} d\|E_\lambda \varphi\|^2 = O(1)$, which proves that $\varphi \in X_\beta$. ■

Therefore, we have obtained a first characterization of the saturation space Φ_β that involves the eigenvalues of the operator T^*T and the coefficients $\langle \varphi, \varphi_i \rangle$ of φ in the decomposition on the basis of eigenfunctions $(\varphi_i)_{i\geq 0}$.

The result we present now show more precisely the link between the operator T and the set Φ_β. Indeed, we would like to characterize the saturation space using the smoothing properties of the integral operator T and the following proposition will help us to do so.

Proposition 1 $X_\beta = R\left[(T^*T)^{\beta/2}\right]$

Proof. - Let assume first that $\varphi \in R\left[(T^*T)^{\beta/2}\right]$. Then, we know that: $\exists\psi \in L^2 : \varphi = (T^*T)^{\beta/2}\,\psi$ which is equivalent to

$$\varphi = \sum_{i=0}^{+\infty} \lambda_i^{\beta/2} \langle \psi, \varphi_i \rangle \varphi_i$$

Therefore, we have:

$$\sum_{i=0}^{N} \frac{\langle \varphi, \varphi_i \rangle}{\lambda_i^{\beta/2}} = \sum_{i=0}^{N} \langle \psi, \varphi_i \rangle$$

which converges since $\psi \in L^2$. So, $R\left[(T^*T)^{\beta/2}\right] \subset X_\beta$.

- Assume now that $\varphi \in X_\beta$ and denote $\psi = \sum_{i=0}^{+\infty} \frac{\langle \varphi, \varphi_i \rangle}{\lambda_i^{\beta}} \varphi_i$. We know that ψ exists and belongs to L^2 since $\varphi \in X_\beta$. Moreover, we have: $\varphi = \sum_{i=0}^{+\infty} \lambda_i^{\beta} \langle \psi, \varphi_i \rangle \varphi_i$ and $X_\beta \subset R\left[(T^*T)^{\beta/2}\right]$. ■

As a consequence, under the assumptions of Theorem (2.1), we have the equality of the two sets

$$\Phi_\beta = \{\varphi, : \|\varphi - \varphi_\alpha\|^2 = O(\alpha^\beta)\} = X_\beta = \{\varphi, : \exists \omega \in L^2, \varphi = (T^*T)^{\beta/2}\omega\}.$$

It provides a characterization of the saturation spaces Φ_β in terms of functionnal spaces, independent of the chosen regularization method. As a consequence, the sets Φ_β can be characterized as functional sets, where the regularity of the operator T is linked with the regularity of the function φ.

3 Link with Sobolev spaces

In order to characterize the saturation space Φ_β, we need to assume some regularity conditions on the operator T. We then introduce the notion of fractional Sobolev spaces H^s where $s \in \mathbb{R}_+^*$ and we make the following assumption:

[$A4$]: T is a smoothing operator of order t.with respect to the space H^s

This is equivalent to say that:

$$T : H^s - > H^{s+t}$$

or, using the ellipticity property , that:

$$\forall \varphi \in L^2(X), \|T\varphi\|^2 \sim \|\varphi\|^2_{H^{-t}}$$

Remark 2 *Such a property can be expressed using the kernel function of the integral operator T. Indeed, assume that:*

$$T\varphi(x) = \int k(x, y)\,\varphi(y)dy$$

Then, imposing some regularity on T is equivalent to imposing some derivative properties on the kernel k. For example, in the case developed by Darolles, Florens and Renault, k represents a conditional density.

Therefore, under the assumption $[A4]$, $(T^*T)^{\beta/2}$ is a smoothing operator of order $t\beta$ and we have in particular:

$$(T^*T)^{\beta/2} : L^2(X) -> H^{t\beta}$$

This result is useful to characterize the saturation space Φ_β since under the assumptions of theorem (2.1), we know that $\Phi_\beta = R\left[(T^*T)^{\beta/2}\right]$.

Hence, the condition $\varphi \in \Phi_\beta$ implies that $\varphi \in H^{t\beta}$, the Sobolev space of order $t\beta$. As a consequence, the operator T is such that:

$$T : \Phi_\beta \subset H^{t\beta} \longrightarrow H^{t(1+\beta)}.$$

4 Minimax rate of convergence for inverse problems

The objective of this sectin is to use the result of theorem (2.1) in order to obtain the minimax rate of convergence achieved on Φ_β.

Let introduce first some notations.

$\forall \delta > 0$, and for all subspace $\mathcal{M}$ of $L^2(X)$, define

$$\Omega(\delta, \mathcal{M}) = \sup\{\|\varphi\|, : \varphi \in \mathcal{M}, : \|T\varphi\| \leq \delta\}. \tag{4.1}$$

Set also, for a regularization operator R,

$$\Delta(\delta, \mathcal{M}, R) = \sup\{\|R\varphi^\delta - \varphi\|, : \varphi \in \mathcal{M}, : r^\delta \in \nabla, : \|r - r^\delta\| \leq \delta\}. \tag{4.2}$$

This quantity measures the quality of approximation of the regularization method R for functions in the set $\mathcal{M}$.

Lemma 4.1

$$\Delta(\delta, \mathcal{M}, R) \geq \Omega(\delta, \mathcal{M}).$$

Proof. Let $\varphi \in \mathcal{M}$, such that $\|T\varphi\| \leq \delta$. As a result, for a choice of $r^\delta = 0$, we get $r = T\varphi$ is such that $\|r\| \leq \delta$. Hence, taking the supremum over all $x \in \mathcal{M}$, we get

$$\Delta(\delta, \mathcal{M}, R) \geq \Omega(\delta, \mathcal{M}).$$

■

Thanks to the previous section, we know that:

for $\beta \geq 0$, $X_\beta = \mathcal{R}(T^*T)^{\beta/2} = \{\varphi \in \Phi, : \exists \omega \in L^2(X), : \varphi = (T^*T)^{\beta/2}\omega\}$.

The set X_β can be written using the following decomposition

$$X_\beta = \cup_{\rho>0} X_{\beta,\rho}, \text{with}$$

$$X_{\beta,\rho} = \{\varphi \in \Phi, : \exists \omega \in L^2(X), : \|\omega\| \leq \rho, : \varphi = (T^*T)^{\beta/2}\omega\}.$$

Using Lemma (4.1), a lower bound for $\Omega(\delta, \mathcal{M})$ will give the lower rate of convergence for the approximation method R. This rate determines the difficulty of the issue. The following proposition gives this rate of convergence.

Proposition 4.2

$$\Omega(\delta, X_{\beta,\rho}) = \delta^{\frac{\beta}{\beta+1}} \rho^{\frac{1}{2\rho+1}}.$$

Proof. The proof of the previous result falls into 2 parts and is closely linked with the work of Ludena Loubes.
First, using the definition of X_β we get

$$\begin{aligned} \|\varphi\| &= \|(T^*T)^{\beta/2}\omega\| \\ &\leq \|(T^*T)^{\beta/2+\frac{1}{2}}\omega\|^{\frac{\beta}{\beta+1}} \|\omega\|^{\frac{1}{\beta+1}} \\ &\leq \|(T^*T)^{\frac{1}{2}}\varphi\|^{\frac{\beta}{\beta+1}} \|\omega\|^{\frac{1}{\beta+1}} \\ &\leq \|T\varphi\|^{\frac{\beta}{\beta+1}} \|\omega\|^{\frac{1}{\beta+1}} \\ &\leq \delta^{\frac{\beta}{\beta+1}} \rho^{\frac{1}{\rho+1}}. \end{aligned}$$

Then, recall that the eigenvalues λ_n are decreasing towards 0, as n increases. Hence, set $\delta_n = \rho\lambda_n^{\beta+1}$. As a result

$$\left(\frac{\delta_n}{\rho}\right)^{\frac{1}{\beta+1}} = \lambda_n$$

is an eigenvalues of the operator T^*T. The associated eigenvector φ_n satisfies $\|\varphi_n\| = 1$. Set now

$$\psi_n = \rho(T^*T)^{\beta/2}\varphi_n \in X_{\beta,\rho}.$$

We have

$$\begin{aligned} \psi_n &= \rho(T^*T)^{\beta/2}\varphi_n = \rho\lambda_n^{\beta}\varphi_n \\ &= \delta_n^{\frac{\beta}{\beta+1}} \rho^{\frac{1}{\beta+1}}\varphi_n = \delta_n^{\frac{\beta+2}{\beta+1}} \rho^{-\frac{1}{\beta+1}}\varphi_n. \end{aligned}$$

So, we get

$$\|T\psi_n\|^2 =< T^*T\psi_n, \psi_n >= \delta_n^2.$$

As a consequence

$$\Omega(\delta_n, X_{\beta,\rho}) \geq \|\psi_n\| = \delta_n^{\frac{\beta}{\beta+1}} \rho^{\frac{1}{2\beta+1}},$$

which gives the desired upper bound. ■

For every $\varphi \in \Phi_\beta$, we get the following rate of convergence:

$$\begin{aligned} \|\varphi_\alpha^\delta - \varphi\|^2 &\leq \|\varphi_\alpha^\delta - \varphi_\alpha\|^2 + \|\varphi_\alpha - \varphi\|^2 \\ &\leq O(\alpha^\beta) + \|R_\alpha(r^\delta - r)\|^2 \\ &\leq O(\alpha^\beta) + \frac{\delta}{\alpha}. \end{aligned}$$

An optimal choice for the regularization parameter is $\alpha \sim \delta^{\frac{1}{\beta+1}}$. So, for estimating a function $\varphi \in \Phi_\beta$, an upper bound for the rate of convergence is given by $\delta^{\frac{\beta}{\beta+1}}$. This result, together with Proposition (4.2), prove that the rate of convergence in $\delta^{\frac{\beta}{\beta+1}}$ is a minimax rate of convergence for the inverse problem (1.3).
When T is not observed, we consider an estimate $T_n \to T$. The observable data are then given by the relation

$$r^\delta = T_n\varphi = r + (\hat{L_n} - T)\varphi.$$

As a result we get the following correspondance

$$\delta_n = \|(\hat{T_n} - T)\varphi\|^2.$$

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