

A Note on Smoothed Functional Inverse Regression

L. Forzani and R.D. Cook

University of Minnesota

Abstract

Estimation in the context of functional data analysis is almost always non parametric, since the object to be estimated lives in an infinite dimensional space. That is the case for the functional linear model with a real response and a process as covariables. In a recent paper Ferré and Yao state that the estimation of the Effective Dimension Reduction (EDR) subspace via SIR has parametric order. We will show in this note that a strong condition is needed for their statement to be true.

keywords and phrases: Dimension Reduction, Functional Data Analysis, Inverse regression

1 Introduction

Functional sliced inverse regression is the generalization of slice inverse regression (SIR; Li, 1991) to the infinite dimensional setting. Functional SIR was introduced by Dauxois, Ferré and Yao (2001), and Ferré and Yao (2003). Those papers show that root- n consistent estimators can not be expected. Ferré and Yao (2005) claimed a new method of estimation that is root- n consistent. We argue that their results is not true under the conditions that they stated, but may be so when the covariance operator Γ of the covariable X is restricted. More specifically, root- n consistency may be achievable when Γ has an spectral decomposition with eigenfunctions of the covariance operator Γ_e of $E(X|Y)$ or of the orthogonal complement of Γ_e . The EDR subspace can then be estimated as the span of the eigenfunctions of Γ_e , and therefore root- n consistency follows from the root- n consistency of principal component analysis for functional data (Dauxois, Pousse, and Romain, 1982).

2 The setting in Ferré and Yao (2005)

Let (X, Y) be a random variable that takes values in $L^2[a, b] \times \mathbb{R}$. X is a centered stochastic process with finite fourth moment. Then the covariance operators of X and $E(X|Y)$ exist and are denoted Γ and Γ_e , and Γ is a Hilbert-Smith operator that is assumed to be positive definite.

Ferré and Yao (2005) assume the usual linearity condition for sliced inverse regression extended to functional data in the context of the model

$$Y = g(\langle \theta_1, X \rangle, \dots, \langle \theta_D, X \rangle, \epsilon),$$

where g is a function in $L^2[a, b]$, ϵ is a centered real random variable, $\theta_1, \dots, \theta_D$ are D independent functions in $L^2[a, b]$ and $\langle \cdot, \cdot \rangle$ indicates the usual interior product in $L^2[a, b]$. They called $\text{span}(\theta_1, \dots, \theta_D)$ the Effective Dimension Reduction (EDR) subspace. Then, under their linearity condition the EDR subspace contains the Γ -orthonormal eigenvectors of $\Gamma^{-1}\Gamma_e$ associated with the positive eigenvalues. If an additional coverage condition is assumed then a basis for the EDR subspace will be the Γ -orthonormal eigenvectors of $\Gamma^{-1}\Gamma_e$ associated with the D positive eigenvalues. Therefore the goal is to estimate the subspaces generated by those eigenvectors. Since Γ is one-to-one and because of the coverage condition, the dimensions of $R(\Gamma_e)$ and $R(\Gamma^{-1}\Gamma_e)$ are both D . Here, $R(B)$ denotes the range of an operator B , which is the set of functions $B(f)$ with f belonging to the domain $T(B)$ of the operator B .

To estimate Γ_e it is possible to slice the range of Y (Ferré and Yao, 2003) or to use a kernel approximation (Ferré and Yao, 2005). Under the conditions on the model, L^2 consistency and the central limit theorem follow for the estimators of Γ_e . To approximate Γ , in general, the sample covariance operator is used and consistency and central limit theorem for the approximation of Γ follow (Dauxois, Pousse and Romain, 1982).

In a finite-dimensional context, the estimation of the EDR space does not pose any problem since Γ^{-1} is accurately estimated by the inverse of the empirical covariance matrix of X . This is not true for functional inverse regression when, as assumed by Ferré and Yao (2005), Γ is a Hilbert-Schmidt operator with infinite rank: the inverse is ill-conditioned if the range of Γ is not finite dimensional. Regularization of the $\hat{\Gamma}$ can be used to overcome this difficulty. Estimation of Γ_e is easier, since Γ_e has finite rank. Because of the non continuity of the inverse of a Hilbert-Smith operator, Ferré and Yao (2003) can not get a root- n consistent estimator of the EDR subspace. To overcome that difficulty Ferré and Yao (2005, Section 4) made the following comment:

Under our model, $\Gamma^{-1}\Gamma_e$ has finite rank. Then, it has the same eigen subspace associated with positive eigenvalues as $\Gamma_e^+\Gamma$, where Γ_e^+ is a generalized inverse of Γ_e .

They use this comment to justify estimating the EDR subspace from the spectral decomposition of a root- n consistent sample version of $\Gamma_e^+\Gamma$. However, the conclusion $R(\Gamma^{-1}\Gamma_e) = R(\Gamma_e^+\Gamma)$ – in Ferré and Yao’s comment is not true in the context used by them, but may hold in a more restricted context. More specifically, additional structure seems necessary to equate $R(\Gamma_e^+\Gamma)$, the space that can be estimated, with $R(\Gamma^{-1}\Gamma_e)$ the space that we wish to know. For clarity and to study the implications of Ferré and Yao’s claim we will use

Condition A: $R(\Gamma^{-1}\Gamma_e) = R(\Gamma_e^+\Gamma)$.

Condition A is equivalent to Ferré and Yao's claim stated previously. If Condition A were true then it would seem possible to estimate the eigenvectors of $\Gamma^{-1}\Gamma_e$ more directly by using eigenvectors of the operator Γ_e . In the next section we give justification for these claims, and provide necessary conditions for regressions in which Condition A holds.

3 The results

We first give counter examples to show that Condition A is not true in the context used by Ferré and Yao (2005), even in the finite dimensional case. Consider

$$\Gamma = \begin{pmatrix} 2 & 1 \\ 1 & 4 \end{pmatrix} \text{ and } \Gamma_e = \begin{pmatrix} 2 & 0 \\ 0 & 0 \end{pmatrix},$$

then $R(\Gamma^{-1}\Gamma_e) = \text{span}((4, -1)')$ but $R(\Gamma_e^+\Gamma) = \text{span}((1, 0)')$ and so $R(\Gamma^{-1}\Gamma_e) \neq R(\Gamma_e^+\Gamma)$.

For the infinite dimensional case we consider $L^2[0, 1]$ and any orthonormal basis $\{\phi_i\}_{i=1}^\infty$ of $L^2[0, 1]$. We define $f = \sum_{i=1}^\infty a_i\phi_i$ with $a_i \neq 0$ and $\sum_{i=1}^\infty a_i^2 < \infty$. We define Γ as the operator in $L^2[0, 1]$ with eigenfunctions ϕ_i and corresponding eigenvalue λ_i . We ask that $\lambda_i > 0$ for all i and $\sum_{i=1}^\infty \lambda_i^2 < \infty$. These conditions guarantee that Γ is a Hilbert-Smith operator and strictly positive definite. Let $h = \Gamma(f)$; by definition, $h \in T(\Gamma^{-1})$. Now $h \notin \text{span}(f)$. In fact, suppose $h = cf$. Then

$$h = \Gamma(f) = \sum_{i=1}^\infty \lambda_i \langle f, \phi_i \rangle \phi_i = c \sum_{i=1}^\infty \langle f, \phi_i \rangle \phi_i.$$

Now, since $\langle f, \phi_i \rangle = a_i \neq 0$ for all i we have $\lambda_i = c$ for all i , contradicting the fact that $\sum_{i=1}^\infty \lambda_i^2 < \infty$.

Define the operator Γ_e to be the identity operator in $\text{span}(h)$ and 0 in $\text{span}(h)^\perp$. The generalized inverse of such operator coincides with Γ_e . Now, $R(\Gamma^{-1}\Gamma_e) = \text{span}(f)$ and $R(\Gamma_e^+\Gamma) = \text{span}(h)$ and from the fact that $h \notin \text{span}(f)$ we get $R(\Gamma^{-1}\Gamma_e) \neq R(\Gamma_e^+\Gamma)$.

The next three lemmas give implications of Condition A.

Lemma 1. *If Condition A holds then $R(\Gamma_e) = R(\Gamma^{-1}\Gamma_e)$.*

Proof. Given a set $B \subset L^2[0, 1]$, let us denote by B^\perp its orthogonal complement using the usual interior product in $L^2[a, b]$. The closure of the set B , denoted by \bar{B} , will be the smallest closed set (using the topology defined through the usual interior product) containing B . For an operator B from $L^2[a, b]$ into itself, let B^* denote its adjoint operator, again using the usual interior product.

Let $\{\beta_1, \dots, \beta_D\}$ denote the D eigenfunctions, with eigenvalues nonzero, of $\Gamma_e^+\Gamma$. If Condition A is true then

$$\text{span}(\beta_1, \dots, \beta_D) = R(\Gamma^{-1}\Gamma_e) = R(\Gamma_e^+\Gamma) \subset R(\Gamma_e^+).$$

By definition of generalized inverse (Groetsch, 1977) we have

$$R(\Gamma_e^+) = N(\Gamma_e)^\perp = \overline{R(\Gamma_e^*)} = \overline{R(\Gamma_e)} = R(\Gamma_e)$$

where we use the fact that Γ_e is self-adjoint and the fact that $R(\Gamma_e)$ has dimension D and therefore is closed. Since $R(\Gamma_e)$ has dimension D , the result follows. \square

Lemma 1 shows that we can construct $\text{span}(\beta_1, \dots, \beta_D)$ from the D eigenfunctions of Γ_e associated with nonzero eigenvalues. From Daxouis, Pousse and Romain (1982), the eigenvectors of the approximate Γ_e^n converge to the eigenvectors of Γ_e at the root- n rate (Γ_e^n and Γ_e have finite rank D and therefore they are compact operators). Therefore we can approximate $\text{span}(\beta_1, \dots, \beta_D)$ at the same rate. Let us note that the D eigenfunctions of Γ_e need not be Γ -orthogonormals.

Lemma 2. *Under Condition A we have $R(\Gamma\Gamma_e) \subset R(\Gamma_e)$.*

Proof. Since Γ is one to one, $\overline{R(\Gamma)} = L^2[a, b]$. On the other hand, by hypothesis, $R(\Gamma_e) \subset T(\Gamma^{-1})$. From the definition of the inverse of an operator (Groetsch, 1977) we have that $\Gamma\Gamma^{-1} = \mathcal{I}_d$ in $T(\Gamma^{-1})$, where \mathcal{I}_d indicates the identity operator. Now, let us take $v \in R(\Gamma\Gamma_e)$. Then $v = \Gamma\Gamma_e w$ for some $w \in L^2[a, b]$ and therefore $\Gamma^{-1}v = \Gamma_e w = \Gamma^{-1}\Gamma_e h$ for some $h \in L^2[a, b]$ (this last inequality follows from Lemma 1). Since Γ^{-1} is one to one (in its domain) we get $v = \Gamma_e h \in R(\Gamma_e)$. \square

In mathematical terms, $R(\Gamma\Gamma_e) \subset R(\Gamma_e)$ implies that $R(\Gamma_e)$ is an invariant subspace of the operator Γ (see Conway, 1990, page 39). That, in turn, implies that Γ has a spectral decomposition with eigenfunctions that live in $R(\Gamma_e)$ or its orthogonal complement, as indicated by the following lemma, the finite dimensional form of which was stated by Cook, Li and Chiaromonte (2006).

Lemma 3. *Suppose Condition A is true. Then Γ has a spectral decomposition with eigenfunctions on $R(\Gamma_e)$ or $R(\Gamma_e)^\perp$.*

Proof. Let v be an eigenvector of Γ associated to the eigenvalue $\lambda > 0$. Since $R(\Gamma_e)$ is closed (for being finite dimensional), $v = u + w$ with $u \in R(\Gamma_e)$ and $w \in R(\Gamma_e)^\perp$. Since from Lemma 2, $\Gamma u \in R(\Gamma_e)$ and $\Gamma w \in R(\Gamma_e)^\perp$ we have that u and w are also eigenvectors of Γ if both u and w are different from zero. Otherwise v belongs to $R(\Gamma_e)$ or $R(\Gamma_e)^\perp$.

Now, let $\{v_i\}_{i=1}^\infty$ be a spectral decomposition of Γ . We can assure that there is a enumerable quantity since Γ is compact in $L^2[0, 1]$. From what we said above $v_i = u_i + w_i$ with u_i and w_i eigenvectors in $R(\Gamma_e)$ and $R(\Gamma_e)^\perp$ respectively. Now, we consider $\{u_i : u_i \neq 0\}$ and $\{w_i : w_i \neq 0\}$. Clearly they form a spectral decomposition of Γ with eigenfunctions on $R(\Gamma_e)$ or $R(\Gamma_e)^\perp$.

\square

4 Conclusions

SIR has proven to be a useful method in finite dimensions. One of its advantages is that it yields a root- n consistent estimator of the EDR subspace without pre-specifying a parametric model. In the functional case, on the other hand, one needs to estimate the inverse of a Hilbert-Smith operator with infinite rank. Consequently functional SIR would not normally yield a root- n consistent estimator, and we were surprised to see Ferré and Yao's (2005) claim of root- n consistency. It turns out that their result is not generally true but may hold in a more restricted context.

We proved that a sufficient condition to achieve root- n consistency is that the covariance of the covariables has an spectral decomposition with eigenfunctions living either in the range of the covariance of the expectation of the covariables given the response or in its orthogonal complement. As a consequence a more direct estimation of such subspace is possible.

Since FDA is a relative new area, we do not know if Condition A is generally reasonable in practice. Further study is needed to resolve such issues.

Acknowledgments

This work was supported in part by grant DMS-0405360 from the U.S. National Science Foundation.

References

- Conway, J. B. (1990). *A Course in Functional Analysis*, 2nd ed. Springer, New York.
- Cook, R. D., Li, B. and Chiaromonte, F. (2006). Reductive Multivariate Linear Models. Preprint.
- Dauxois, J., Ferre, L, Yao, A.. (2001). Un modèle semi-paramétrique pour variables aléatoires. *C. R. Acad Paris* **333**, 947-952.
- Dauxois, J., Pousse, A. and Romain, Y. (1982). Asymptotic theory for the principal component analysis of a vector random function: Some applications to statistical inference. *J. Mult. Anal.* **12**, 136–154.
- Ferre, L., Yao, A. F. (2003). Functional sliced inverse regression analysis. *Statistics* **37**, 475–488.
- Ferre, L., Yao, A. F. (2005). Smoothed Functional Inverse Regression. *Statistica Sinica* **15**, 665-683.
- Groetsch, C.W. (1977). *Generalized inverses of Linear Operators*. Marcel Dekker, Inc. New York.

Li, K. C. (1991). Sliced inverse regression for dimension reduction (with discussion). *J. Amer. Statist. Assoc.* **86**, 316-342.