

METHODOLOGY AND CONVERGENCE RATES FOR FUNCTIONAL LINEAR REGRESSION

Peter Hall¹ and Joel L. Horowitz²

ABSTRACT. In functional linear regression the slope “parameter” is a function. Therefore, in a nonparametric context, it is determined by an infinite number of unknowns. Its estimation involves solving an ill-posed problem, and has points of contact with a range of methodologies, including statistical smoothing and deconvolution. The standard approach to estimating the slope function is based explicitly on functional principal components analysis, and consequently on spectral decomposition in terms of eigenvalues and eigenfunctions. We discuss this approach in detail, and show that in certain circumstances, optimal convergence rates are achieved by the PCA technique. An alternative approach, based on quadratic regularisation, is suggested, and shown to have advantages from some points of view.

KEYWORDS. Deconvolution, dimension reduction, eigenfunction, eigenvalue, linear operator, minimax optimality, nonparametric, principal components analysis, smoothing, quadratic regularisation.

SHORT TITLE. Functional linear regression.

AMS (2000) SUBJECT CLASSIFICATION: Primary, 62J05; Secondary, 62G20.

¹ Centre for Mathematics and its Applications, Australian National University, Canberra, ACT 0200, Australia. The research of Peter Hall was supported in part by an ARC grant.

² Department of Economics, Anderson Hall, Northwestern University, 2001 Sheridan Road, Evanston, IL 60208-2600, USA. The research of Joel L. Horowitz was supported in part by NSF Grants SES 9910925 and SES 0352675.

1. INTRODUCTION

In functional linear regression, data pairs (X_i, Y_i) are generated by the model

$$Y_i = a + \int_{\mathcal{I}} b X_i + \epsilon_i, \quad 1 \leq i \leq n. \quad (1.1)$$

The X_i 's are random functions, \mathcal{I} denotes the interval on which each such function is defined, the intercept a and the errors ϵ_i are scalars, and the slope b , the main target of our interest in this paper, is a function. The model (1.1) is applicable in a wide range of settings, including many where data are becoming available only through new developments in technology.

For example, in near-infrared spectroscopy applied to data on different cereal-grain types (for example, different varieties of wheat), $X_i(t)$ denotes the intensity of reflected radiation recorded at the spectrometer when the wavelength equals t , and Y_i denotes the level of a particular protein, for the i th cereal type. By constructing the linear regression at (1.1) we can predict, from data on a new function X , the level of protein for that cereal type. This is especially useful in practice, since the explanatory variables X_i are very easy and inexpensive to observe in the field, using hand-held equipment, whereas direct calculation of Y_i requires expensive, and time-consuming, analysis in a laboratory. There is an extensive literature on this problem; see, for example, Shenk and Westerhaus (1991) and Wesley *et al.* (1999).

Once an estimator, \hat{b} , of the slope, b , is available, it is straightforward to estimate the intercept, a , for example as the average of the values of $Y_i - \int_{\mathcal{I}} \hat{b} X_i$. Therefore, much interest in the literature focuses on estimating b . The conventional approach, discussed for example by Ramsay and Silverman (1997, Chapter 10; 2002), is based on principal components analysis or PCA. Although this method has been discussed widely (e.g. Ferraty and Vieu (2000), Cuevas *et al.* (2002) and Cardot and Sarda (2003)), relatively little is known about convergence rates of estimators, apart from upper bounds. In this paper we shall give optimal convergence rates in this problem, and discuss PCA-based estimators which attain those rates. The known upper bounds for convergence rates are an order of magnitude greater than the minimax-optimal rates derived in this paper.

An alternative approach, based on Tikhonov, or quadratic, regularisation (Tik-

honov, 1963), will also be addressed. To our knowledge this approach has not been considered before in functional data analysis, although it has wide application to the solution of other ill-posed problems. In particular, quadratic regularisation methods are increasingly studied in the statistics literature; see, for example, work of Efromovich and Koltchinskii (2001) and Cavalier *et al.* (2002) on optimality properties.

We shall show that the Tikhonov regularisation approach is also able to achieve optimal convergence rates, and that it is robust against potential problems caused by tied, or closely spaced, eigenvalues in the spectral decomposition on which PCA is based. The difficulties that close eigenvalues can cause for PCA will be discussed using an example.

The estimation of slope and intercept parameters in functional linear regression has points in common with a range of smoothing and deconvolution problems, where dimension reduction is involved. See, for example, Stefanski and Carroll (1990), Fan (1991, 1993) and Delaigle and Gijbels (2002). Work on statistical smoothing is particularly extensive, and is relatively well-known to readers, so we shall not attempt to survey it here. The problem of estimating slope in functional linear regression is also related to that of estimating the point-spread function in image analysis, when the true image, or test pattern, is known. Here, too, significant work has been done; see e.g. Yang *et al.* (1994) and Kundur and Hatzinakos (1998).

Of course, the literature on linear inverse problems is very much larger than this. In the statistics setting it includes work of Donoho (1995) and Johnstone (1999), using wavelet and vaguelette methods, and of van Rooij and Ruymgaart (1996) on optimal convergence rates. There is also closely related work in economics on the subjects of panel data (Horowitz and Markatou, 1996), covariate measurement error (Li and Hsiao, 2004), and estimation with instrumental variables (e.g., Newey *et al.*, 1999; Blundell and Powell, 2003; Darolles *et al.*, 2002; Newey and Powell, 2002; Hall and Horowitz, 2005). In statistics, there is related work on errors-in-variables problems (e.g., Carroll *et al.*, 1995). There is a small but increasing literature on applications of functional regression to longitudinal data analysis. See, for example, Staniswalis and Lee (1998) and Chiou *et al.* (2003).

2. METHODOLOGY

We shall assume we observe independent and identically distributed data $(X_1, Y_1), \dots, (X_n, Y_n)$, where each explanatory variable X_i is a square-integrable random function on the compact interval \mathcal{I} . The response variables Y_i are generated by the model (1.1). It will be supposed that the errors ϵ_i are independent and identically distributed, with finite variance and zero mean, and that the errors are also independent of the explanatory variables. Our goal is to discuss estimators of b , and to describe the rate at which they converge to the true function.

We begin by describing standard functional linear regression methodology, as discussed by, for example, Ramsay and Silverman (1997, Chapter 10). It is founded on spectral expansions of both the covariance of X and its estimator, and is constructed as follows.

Let (X, Y, ϵ) denote a generic (X_i, Y_i, ϵ_i) , and put $K(u, v) = \text{cov}\{X(u), X(v)\}$, $\bar{X} = n^{-1} \sum_i X_i$ and

$$\hat{K}(u, v) = \frac{1}{n} \sum_{i=1}^n \{X_i(u) - \bar{X}(u)\} \{X_i(v) - \bar{X}(v)\}.$$

Write the spectral expansions of K and \hat{K} as

$$K(u, v) = \sum_{j=1}^{\infty} \kappa_j \phi_j(u) \phi_j(v), \quad \hat{K}(u, v) = \sum_{j=1}^{\infty} \hat{\kappa}_j \hat{\phi}_j(u) \hat{\phi}_j(v), \quad (2.1)$$

where

$$\kappa_1 > \kappa_2 > \dots > 0, \quad \hat{\kappa}_1 \geq \hat{\kappa}_2 \geq \dots \geq 0 \quad (2.2)$$

are the eigenvalue sequences of linear operators with kernels K and \hat{K} , respectively, and ϕ_1, ϕ_2, \dots and $\hat{\phi}_1, \hat{\phi}_2, \dots$ are the respective orthonormal eigenvector (in fact, eigenfunction) sequences. We interpret $(\hat{\kappa}_j, \hat{\phi}_j)$ as an estimator of (κ_j, ϕ_j) .

During the review process, it has been suggested that the case where $\sum_j \kappa_j$ diverges might be explored. For example, the context $\kappa_j \sim j^{-\alpha}$, with α close to either 0 or $\frac{1}{2}$, might provide particular challenges. We agree that this setting is of mathematical interest. However, it should be noted that if $\text{var } X(t)$ is bounded in

t then $\sum_j \kappa_j < \infty$. The case of unbounded covariance does not arise commonly in applied work.

Both the sequences $\{\phi_j\}$ and $\{\hat{\phi}_j\}$ are complete in the class of square-integrable functions on \mathcal{I} . The fact that each κ_j is strictly positive implies that the linear operator corresponding to K , taking a function ϕ to $K\phi$ defined by $(K\phi)(u) = \int K(u, v) \phi(v) dv$, is strictly positive definite. (To economise on notation we use the symbol K for both the kernel and the operator.) We determine the signs of ϕ_j and $\hat{\phi}_j$, in cases where sign is important, by insisting that $\int_{\mathcal{I}} \hat{\phi}_j \phi_j \geq 0$. This can be done without loss of generality, for example by changing the sign of $\hat{\phi}_j$ to match that of ϕ_j , since switching the signs of ϕ_j and $\hat{\phi}_j$ results in commensurate changes of sign for generalised Fourier coefficients, such as the quantities \hat{b}_j and \hat{g}_j which we shall introduce below. Therefore, $\int_{\mathcal{I}} \hat{\phi}_j \phi_j > 0$ can be assumed without altering the values taken by estimators.

A model equivalent to (1.1) is

$$Y_i - \mu = \int_{\mathcal{I}} b(X_i - x) + \epsilon_i, \quad 1 \leq i \leq n,$$

where $x = E(X_i)$ and $\mu = E(Y_i) = a + \int bx$, with x denoting a deterministic function on \mathcal{I} . It follows that, if we define $g(u) = E[(Y - \mu) \{X(u) - x(u)\}]$, where (X, Y) represents a generic pair (X_i, Y_i) , then

$$Kb = g.$$

Moreover, if we write $b = \sum_j b_j \phi_j$ and $g = \sum_j g_j \phi_j$, then $b_j = \kappa_j^{-1} g_j$. This suggests the estimator

$$\hat{b}(u) = \sum_{j=1}^m \hat{b}_j \hat{\phi}_j(u), \quad (2.3)$$

where the truncation point m is a smoothing parameter, $\hat{b}_j = \hat{\kappa}_j^{-1} \hat{g}_j$, $\hat{g}_j = \int \hat{g} \hat{\phi}_j$,

$$\hat{g}(u) = \frac{1}{n} \sum_{i=1}^n (Y_i - \bar{Y}) \{X_i(u) - \bar{X}(u)\} \quad (2.4)$$

and $\bar{Y} = n^{-1} \sum_i Y_i$.

Next we suggest an alternative method, which uses a ridge parameter, ρ , rather than the cut-off, m , as the smoothing parameter. Let $\widehat{K}^+ = (\widehat{K} + \rho I)^{-1}$ denote the inverse of the operator $\widehat{K} + \rho I$, where $\rho > 0$ and I is the identity operator. Define

$$\tilde{b} = \widehat{K}^+ \hat{g} = \frac{1}{n} \sum_{i=1}^n (Y_i - \bar{Y}) \widehat{K}^+ \{X_i(u) - \bar{X}(u)\}, \quad (2.5)$$

where \hat{g} is as at (2.4). Then \tilde{b} is an estimator alternative to \hat{b} .

3. THEORETICAL PROPERTIES

First we treat the standard functional linear regression estimator \hat{b} , defined at (2.3). The Karhunen-Loève expansion of the random function X is given by

$$X - E(X) = \sum_{j=1}^{\infty} \xi_j \phi_j,$$

where the random variables $\xi_j = \int_{\mathcal{I}} (X - EX) \phi_j$ have zero means and variances $E(\xi_j^2) = \kappa_j$, and are uncorrelated. Let $C > 1$ denote a constant. Concerning the distributions of the random function X and the errors ϵ in the model at (1.1), we shall assume that

$$X \text{ has finite fourth moment, in that } \int_{\mathcal{I}} E(X^4) < \infty; E(\xi_j^4) \leq C \kappa_j^2 \text{ for all } j; \text{ and the errors } \epsilon_i \text{ are identically distributed with zero mean and variance not exceeding } C. \quad (3.1)$$

Of the eigenvalues κ_j we ask that

$$\kappa_j - \kappa_{j+1} \geq C^{-1} j^{-\alpha-1} \quad \text{for } j \geq 1. \quad (3.2)$$

This condition prevents the spacings between adjacent order statistics from being too small. It also implies a lower bound on the rate at which κ_j decreases: κ_j must not be less than a constant multiple of $j^{-\alpha}$. The importance of (3.2) to ensuring Theorem 1, below, will be discussed following Theorem 2.

Of the Fourier coefficients b_j and exponents α and β we suppose that

$$\begin{aligned} |b_j| &\leq C j^{-\beta}, \\ \alpha &> 1, \quad \frac{1}{2} \alpha + 1 < \beta. \end{aligned} \quad (3.3)$$

The first part of (3.3) can be viewed in at least two ways: as a definition of β , in terms of a given sequence b_j , or as a condition that the generalised Fourier coefficients b_j not decrease too quickly. The basis with respect to which these coefficients are defined is determined by the context of the problem, and more particularly by the covariance function K , rather than outside the problem. This is not unnatural, for at least two related reasons. Firstly, the basis ϕ_1, ϕ_2, \dots is canonical in the functional-data problem, since it is the unique basis with respect to which the function X can be expressed as a generalised Fourier series (its Karhunen-Loève expansion) with uncorrelated coefficients. It gives the most rapidly convergent representation of X , when speed of convergence is defined in an L_2 sense. Second, as discussed in section 1, the representation with respect to this basis is fundamental to the most popular method for estimating b , and so is particularly deserving of study.

Note that the assumption that K is bounded, or even the milder condition $\int_{\mathcal{I}} \text{var} \{X(u)\} du < \infty$, entails $\sum_j \kappa_j < \infty$; and that (3.2) implies $\kappa_j \geq C j^{-\alpha}$, for a constant $C > 0$. Therefore, boundedness of K , and (3.2), imply that $\alpha > 1$, which is the second part of (3.3). The assumption $\frac{1}{2}\alpha + 1 < \beta$ in (3.3) asks that the function b be sufficiently smooth relative to K , where smoothness of K is expressed relative to the spectral decomposition of this function. (More concisely, b should be sufficiently smooth relative to the lower bound on the smoothness of K that is implied by the condition $\kappa_j \geq C j^{-\alpha}$.) Since $\alpha > 1$ then a sufficient condition for $\frac{1}{2}\alpha + 1 < \beta$ is $\alpha \leq \beta$, which can be interpreted as asking that the function b be no less smooth than the lower bound on the smoothness of K implied by (3.2).

Of the tuning parameter m we assume that

$$m \asymp n^{1/(\alpha+2\beta)}. \quad (3.4)$$

In (3.4), the relation $r_n \asymp s_n$, for positive r_n and s_n , means that the ratio r_n/s_n is bounded away from zero and infinity.

Let $\mathcal{F}(C, \alpha, \beta)$ denote the set of distributions F of (X, Y) that satisfy (3.1)–(3.3) for given values of C , α and β . Let \mathcal{B} denote the class of measurable functions \bar{b} of the data $(X_1, Y_1), \dots, (X_n, Y_n)$, generated by (1.1). We shall frame our next result

in terms of minimax bounds. Below, the upper bound (3.5) shows performance of \hat{b} , and the lower bound (3.6) reflects performance of any estimator of b . The fact that the convergence rate is the same in each instance implies that the rate for \hat{b} is optimal, in a minimax sense.

Theorem 1. *If (3.1)–(3.4) hold then*

$$\lim_{D \rightarrow \infty} \limsup_{n \rightarrow \infty} \sup_{F \in \mathcal{F}} P_F \left\{ \int_{\mathcal{I}} (\hat{b} - b)^2 > D n^{-(2\beta-1)/(\alpha+2\beta)} \right\} = 0 \quad (3.5)$$

as $n \rightarrow \infty$. Furthermore,

$$\liminf_{n \rightarrow \infty} n^{(2\beta-1)/(\alpha+2\beta)} \inf_{\bar{b} \in \mathcal{B}} \sup_{F \in \mathcal{F}} \int_{\mathcal{I}} E_F (\bar{b} - b)^2 > 0. \quad (3.6)$$

It follows from (3.5) that for each $F \in \mathcal{F}$,

$$\int_{\mathcal{I}} (\hat{b} - b)^2 = O_p(n^{-(2\beta-1)/(\alpha+2\beta)})$$

The theorem is proved in section 5. The fact that (3.5) is expressed in terms of a probability, rather than an expected value, is not significant. By modifying the estimator \hat{b} using a truncation point, to prevent \hat{b} taking values that are too large, we may state and prove (3.5) in the more traditional form; compare (3.10) below. We do not do this since the present form of \hat{b} is the one actually used by statisticians.

Convergence rates of the form $n^{-(2\beta-1)/(\alpha+2\beta)}$ are generic to a large class of noisy inverse problems, where the difficulty of inverting the operator is an increasing function of α , and the smoothness of the target function is an increasing function of β . For example, this rate arises in the context of problems discussed by Cavalier *et al.* (2002). See equation (7) there, and note that the appropriate values of the components of that formula are $\lambda_i = 1$ for $1 \leq i \leq m$ and $\lambda_i = 0$ otherwise, $\theta_i = b_i$, $\sigma_i^2 = \text{var}(\xi_i)$ and $\epsilon^2 = n^{-1}$. Of course, Theorem 1 cannot be derived from the results of Cavalier *et al.* (2002), but since the problem is of the same broad type then the rates enjoy the same form, and have exactly the same formula if we make the substitutions above. Connections of this nature are frequently highlighted in the literature, for nonlinear inverse problems (see e.g. Natterer, 1984; Neubauer,

1989) as well as linear ones. In particular, similar remarks can be made about the rates given by Hall and Horowitz (2005).

Next we address the alternative estimator \tilde{b} , at (2.5), where the smoothing parameter is the ridge, ρ , rather than the cut-off, m . Assumptions (3.2)–(3.4) are respectively replaced by:

$$j^{-\alpha} \leq C \kappa_j, \quad (3.7)$$

$$|b_j| \leq C j^{-\beta}, \quad \alpha > 1, \quad \alpha - \frac{1}{2} < \beta, \quad (3.8)$$

$$\rho \asymp n^{-\alpha/(\alpha+2\beta)}. \quad (3.9)$$

Let $\mathcal{G}(C, \alpha, \beta)$ denote the set of distributions F of (X, Y) that satisfy (3.1), (3.7) and (3.8) for given values of C , α and β .

The result below is a direct analogue of Theorem 1 in the case of \tilde{b} , rather than \hat{b} , except that we replace the probability bound (3.5) by one on expected value.

Theorem 2. *If (3.1) and (3.7)–(3.9) hold then*

$$\sup_{F \in \mathcal{G}} \int_{\mathcal{I}} E_F(\tilde{b} - b)^2 = O(n^{-(2\beta-1)/(\alpha+2\beta)}) \quad (3.10)$$

as $n \rightarrow \infty$. Furthermore,

$$\liminf_{n \rightarrow \infty} n^{(2\beta-1)/(\alpha+2\beta)} \inf_{\tilde{b} \in \mathcal{B}} \sup_{F \in \mathcal{G}} \int_{\mathcal{I}} E_F(\tilde{b} - b)^2 > 0. \quad (3.11)$$

A proof of (3.10) can be developed along the lines of that of Theorem 4.1 of Hall and Horowitz (2005), and so will not be given here; and a proof of (3.11) is identical to that of (3.6). There is no close connection between the convergence rates in (3.10) and in Hall and Horowitz (2005). In fact, the only significant linkage is that both rates are obtained by using Tikhonov regularisation to solve a linear inverse problem. From a conventional statistical viewpoint our work is much closer to that of linear regression in a large number of dimensions than it is to instrumental variables problems.

Condition (3.7) is weaker than (3.2). For example, the latter excludes cases where two or more of the eigenvalues κ_j are close together, in particular where they

are tied. (When employing the approach at (2.5) it is not necessary to assume strict inequality among the κ_j 's.) Indeed, (3.5) in Theorem 1 can fail, and (3.10) in Theorem 2 hold, if closely-spaced eigenvalues are permitted. This is perhaps best illustrated by an example, which we give below in a setting where there are long strings of tied eigenvalues. The assumption of perfect ties can be relaxed, by permitting the κ_j 's to be very close to one another but not identical. The argument there is more complex, however.

Let γ, τ denote constants satisfying $1 < \gamma \leq \alpha\tau$, and let j_k equal the least integer not less than $k^{k\tau}$. Put $\mathcal{J}_k = \{j_k, j_k + 1, \dots, j_{k+1} - 1\}$, and define $\kappa_j = k^{-k\gamma}$ for all $j \in \mathcal{J}_k$. Then, for j in this range,

$$\kappa_j = k^{-k\gamma} \geq k^{-k\alpha\tau} \geq j_k^{-\alpha} \geq j^{-\alpha}, \quad (3.12)$$

and also, $j_{k+1}/j_k \sim e^\tau k^\tau$ as k increases. Property (3.12) implies (3.7), but (3.2) fails because of the ties.

Those ties mean that the functions ϕ_j , for j in the block \mathcal{J}_k , are not even identifiable. Indeed, any permutation of the function sequence ϕ_j , $j \in \mathcal{J}_k$, is equally appropriate, since within-blocks permutations of the ϕ_j 's do not lead to violation of the condition that the κ_j 's are non-decreasing. For the same reason, while the (unordered) set of function estimators, $\widehat{\Phi}_k = \{\hat{\phi}_j : j \in \mathcal{J}_k\}$, converges to the set $\Phi_k = \{\phi_j : j \in \mathcal{J}_k\}$ as $n \rightarrow \infty$, for each k , the individual estimators $\hat{\phi}_j$ are not consistent for the respective functions ϕ_j .

If the sum at (2.3) is taken over a whole number of blocks \mathcal{J}_k , this inconsistency does not cause any difficulties estimating the slope function b . There are problems, however, if the integer m at (2.3) falls mid-way through one of the blocks \mathcal{J}_k . For definiteness, take m to equal the integer part of $n^{1/(\alpha+2\beta)}$, thereby satisfying (3.4). Define $k_0 = k_0(n)$ to be the unique value of k such that $m \in \mathcal{J}_k$. Then, along an infinite sequence, \mathcal{N} say, of values of n , it is true that

$$\frac{1}{2} (j_{k_0} + j_{k_0+1}) \leq m \leq j_{k_0+1} - 1. \quad (3.13)$$

Condition (3.13) ensures that the set of integers $j \in \mathcal{J}_{k_0}$ that lie between j_{k_0} and m comprises at least half of \mathcal{J}_{k_0} . Moreover, since $j_{k+1}/j_k \sim e^\tau k^\tau$, then for all

sufficiently large $n \in \mathcal{N}$, the value of

$$\frac{1}{m} \#\{j : j \in \mathcal{J}_{k_0} \text{ such that } 1 \leq j \leq m\}$$

converges to 1 as $n \rightarrow \infty$. Call these properties (P).

An argument based on symmetry shows that, if $p = \hat{p}$ is the random permutation of \mathcal{J}_{k_0} defined to minimise any given symmetric measure of performance of $\hat{\Phi}$ as an estimator of Φ_j , for example to minimise

$$\sum_{j \in \mathcal{J}_{k_0}} \int_{\mathcal{I}} (\hat{\phi}_j - \phi_{p(j)})^2,$$

then \hat{p} is uniformly distributed on the set of all permutations of \mathcal{J}_{k_0} . From this it may be shown, using properties (P) and letting $n \rightarrow \infty$ through values in \mathcal{N} , that (3.5) fails.

4. NUMERICAL PROPERTIES

This section summarises the results of a Monte Carlo investigation of the finite-sample performance of the estimators \hat{b} and \tilde{b} discussed in section 2. Samples of sizes $n = 100$ and 500 were generated from the model (2.1), with $\mathcal{I} = [0, 1]$, $a = 0$, and the errors ϵ_i distributed as normal $N(0, \sigma_\epsilon^2)$, where $\sigma_\epsilon = 0.5$ or 1 . We took $b = \sum_{1 \leq j \leq 50} b_j \phi_j$ and $X = \sum_{1 \leq j \leq 50} \gamma_j Z_j \phi_j$, where (a) $b_1 = 0.3$ and $b_j = 4(-1)^{j+1}j^{-2}$ for $j > 1$, (b) the γ_j 's were deterministic coefficients, (c) $\phi_1 \equiv 1$ and $\phi_{j+1} = 2^{1/2} \cos(j\pi t)$ for $j \geq 1$, and (d) the Z_j 's were uniformly distributed on $[-3^{1/2}, 3^{1/2}]$. In particular, each Z_j had zero mean and unit variance.

Two sets of the γ_j 's were used. In the first, $\gamma_j = (-1)^{j+1}j^{-\alpha/2}$, with $\alpha = 1.1, 1.5, 2$ or 4 . For these coefficients the eigenvalues of the operator K were $\kappa_j = j^{-\alpha}$ and were distinct. In the remainder of this section we label these eigenvalues ‘‘well spaced.’’ In the second set, $\gamma_1 = 1$, $\gamma_j = 0.2(-1)^{j+1}(1 - 0.0001j)$ if $2 \leq j \leq 4$, and $\gamma_{5j+k} = 0.2(-1)^{5j+k+1}\{(5j)^{-\alpha/2} - 0.0001k\}$ for $j \geq 1$ and $0 \leq k \leq 4$. This set of γ_j 's generated blocks of κ_j 's that were nearly equal when j was not too large, and we refer to it as the ‘‘closely spaced’’ case. The theoretical arguments presented in section 3 suggest that the performance of \hat{b} can be poor in this setting.

All our results represent averages over 1000 Monte Carlo replications for each parameter setting. The quantities denoted by Bias², Var and MISE in Tables 1 and 2 are Monte Carlo approximations to integrated squared bias, integrated variance and mean integrated squared error, respectively, computed on a grid of 50 equally spaced points on \mathcal{I} . The values of m and ρ , for given n , σ_ϵ , α and a given set of γ_j 's, were chosen to minimise MISE.

Table 1 shows that in the case of well-spaced eigenvalues the MISE of \hat{b} is smaller than that of \tilde{b} for almost all values of the other design parameters. However, it follows from Table 2 that in the closely-spaced case the MISE of \tilde{b} is nearly always smaller than that of \hat{b} . Thus, in terms of MISE, neither estimator dominates the other.

Both tables reveal that there is a general tendency for MISE to decrease as α increases. This does not contradict (3.5) or (3.10), since those results describe the behaviour of MISE as a function of n for fixed α and β , not the behaviour of MISE as a function of α or β for fixed n .

5. DERIVATION OF THEOREM 1

5.1. Proof of (3.5). We begin by defining notation used in the proof. Given a sequence c_n of positive constants, we shall use $O_p(c_n)$ and $o(c_n)$ to denote random variables R_n and r_n , respectively, which satisfy:

$$\lim_{D \rightarrow \infty} \limsup_{n \rightarrow \infty} \sup_{F \in \mathcal{F}} P_F(|R_n| > D c_n) = 0,$$

$$\lim_{n \rightarrow \infty} \sup_{F \in \mathcal{F}} P_F(|r_n| > D c_n) = 0 \quad \text{for each } D > 0.$$

Similarly, a deterministic quantity $A_n = A_n(F)$ which is written as $A_n = O(c_n)$, will be understood to satisfy

$$\sup_{n \geq 1} c_n^{-1} \sup_{F \in \mathcal{F}} |A_n(F)| < \infty.$$

Next we state subsidiary results concerning distances between the spectra of two operators. Let L denote a general positive-semidefinite linear operator, and

write L also for the kernel of that operator. Let the spectral decomposition of L be

$$L(u, v) = \sum_{j=1}^{\infty} \lambda_j \psi_j(u) \psi_j(v). \quad (5.1)$$

We assume the terms are ordered in such a way that $\lambda_1 \geq \lambda_2 \geq \dots \geq 0$. Given univariate functions p and q , and a symmetric bivariate function M , put $\|M\| = (\iint_{\mathcal{I}^2} M^2)^{1/2}$. Write $\int pq$ and $\int Mpq$ for

$$\int_{\mathcal{I}} p(u) q(u) du, \quad \iint_{\mathcal{I}^2} M(u, v) p(u) p(v) du dv,$$

respectively. Further, denote by $\int Mp$ the function of which the value at u is $\int_{\mathcal{I}} M(u, v) p(v) dv$, and define $\delta_j = \min_{1 \leq k \leq j} (\kappa_k - \kappa_{k+1})$.

The following pair of results may be derived from theory developed by Bhatia, Davis and McIntosh (1983):

$$\sup_{j \geq 1} |\kappa_j - \lambda_j| \leq \|K - L\|, \quad \sup_{j \geq 1} \delta_j \|\phi_j - \psi_j\| \leq 8^{1/2} \|K - L\|. \quad (5.2)$$

In framing the second bound here we use the convention that $\int \psi_j \phi_j \geq 0$, which determines the sign of ψ_j in those cases where choice of sign has an impact on the validity of (5.2).

The following lemma will be proved in section 5.2.

Lemma 5.1. *If we may write $\psi_j - \phi_j = \chi_j + \Delta_j$, for functions χ_j and Δ_j , then*

$$\begin{aligned} & \left| (\kappa_j - \lambda_j) \left(1 + \int \chi_j \phi_j \right) - \int (K - L) (\phi_j + \chi_j) \phi_j \right| \\ & \leq \|\Delta_j\| \left\{ |\kappa_j - \lambda_j| + \left\| \int (K - L) \phi_j \right\| \right\}. \end{aligned} \quad (5.3)$$

Furthermore, if $\inf_{k: k \neq j} |\lambda_j - \kappa_k| > 0$ then

$$\psi_j - \phi_j = \sum_{k: k \neq j} (\lambda_j - \kappa_k)^{-1} \phi_k \int (L - K) \psi_j \phi_k + \phi_j \int (\psi_j - \phi_j) \phi_j. \quad (5.4)$$

Put $\widehat{\Delta} = \|\widehat{K} - K\|$, and define the event \mathcal{E}_m by

$$\mathcal{E}_m = \mathcal{E}_m(n) = \left\{ \frac{1}{2} \kappa_m \geq \widehat{\Delta} \right\}.$$

That is, \mathcal{E}_m denotes the set of all realisations such that, for sample size n , $\frac{1}{2} \kappa_m \geq \widehat{\Delta}$. Below, when we say that a bound is valid when \mathcal{E}_m holds, this should be interpreted as stating that the bound is valid for all realisations for which $\frac{1}{2} \kappa_m \geq \widehat{\Delta}$. It is not a statement that relates to a conditioning argument, in the sense that conditioning is usually interpreted in probability theory.

Write $\hat{b}_j = \check{b}_j + \hat{\kappa}_j^{-1}(S_{j1} + S_{j2} + S_{j3})$, where $\hat{\kappa}_j \check{b}_j = \int g \phi_j$, $S_{j1} = \int (\hat{g} - g) \phi_j$, $S_{j2} = \int g (\hat{\phi}_j - \phi_j)$ and $S_{j3} = \int (\hat{g} - g) (\hat{\phi}_j - \phi_j)$. In this notation,

$$\begin{aligned} \sum_{j=1}^m (\hat{b}_j - \check{b}_j)^2 &\leq 3 \sum_{j=1}^m \hat{\kappa}_j^{-2} (S_{j1}^2 + S_{j2}^2 + S_{j3}^2) \leq 12 \sum_{j=1}^m \kappa_j^{-2} (S_{j1}^2 + S_{j2}^2 + S_{j3}^2) \\ &\leq 12 \sum_{j=1}^m \kappa_j^{-2} (S_{j1}^2 + S_{j2}^2) + 12 \|\hat{g} - g\|^2 \sum_{j=1}^m \kappa_j^{-2} \|\hat{\phi}_j - \phi_j\|^2, \end{aligned} \quad (5.5)$$

where the first inequality holds universally; the second inequality, which is obtained using the first part of (5.2), is valid provided the event \mathcal{E}_m holds; and the third inequality employs the bound $|S_{j3}| \leq \|\hat{g} - g\| \|\hat{\phi}_j - \phi_j\|$.

Note that, provided \mathcal{E}_m holds,

$$\begin{aligned} \sum_{j=1}^m (\check{b}_j - b_j)^2 &= \sum_{j=1}^m \left(\frac{\hat{\kappa}_j - \kappa_j}{\hat{\kappa}_j \kappa_j} \right)^2 \left(\int g \phi_j \right)^2 \leq 4 \sum_{j=1}^m \left(\frac{\hat{\kappa}_j - \kappa_j}{\kappa_j^2} \right)^2 \left(\int g \phi_j \right)^2 \\ &= 4 \sum_{j=1}^m \kappa_j^{-2} b_j^2 (\hat{\kappa}_j - \kappa_j)^2. \end{aligned} \quad (5.6)$$

Define $\widehat{\Delta}_j = \|\int (\widehat{K} - K) \phi_j\|$. Using (5.3) with $\chi_j \equiv 0$, and then applying both parts of (5.2), we obtain:

$$\left| \hat{\kappa}_j - \kappa_j - \int (\widehat{K} - K) \phi_j \phi_j \right| \leq \|\hat{\phi}_j - \phi_j\| (|\hat{\kappa}_j - \kappa_j| + \widehat{\Delta}_j) \leq \delta_j^{-1} \widehat{\Delta} (\widehat{\Delta} + \widehat{\Delta}_j). \quad (5.7)$$

Combining (5.6) and (5.7), and defining $\widehat{\Delta}_{jj} = |\int (\widehat{K} - K) \phi_j \phi_j|$, we deduce that, if \mathcal{E}_m holds,

$$\sum_{j=1}^m (\check{b}_j - b_j)^2 \leq 8 \sum_{j=1}^m \kappa_j^{-2} b_j^2 \widehat{\Delta}_{jj}^2 + 16 \widehat{\Delta}^2 \sum_{j=1}^m (\delta_j \kappa_j)^{-2} b_j^2 (\widehat{\Delta}^2 + \widehat{\Delta}_j^2). \quad (5.8)$$

We shall prove in section 5.3 that, under the conditions of the theorem,

$$E(\widehat{\Delta}^2) + E(\widehat{\Delta}_j^2) = O(n^{-1}), \quad E(\widehat{\Delta}_{jj}^2) = O(n^{-1} \kappa_j^2), \quad (5.9)$$

uniformly in j . In particular, (5.9) entails $\widehat{\Delta} = O_p(n^{-1/2})$. Now, (3.2) and (3.4) imply that $n^{1/2}\kappa_m \rightarrow \infty$ as $n \rightarrow \infty$, and so the first part of (5.9) implies that $P(\mathcal{E}_m) \rightarrow 1$. Therefore, since the result (3.5) that we wish to prove relates only to probabilities of differences, not to moments of differences, then it suffices to work with bounds that are established under the assumption that \mathcal{E}_m holds, since the contrary case contributes only $o(1)$ to the probability on the left-hand side of (3.5).

In our arguments below we shall use the property $\widehat{\Delta} = O_p(n^{-1/2})$ without further reference. Now, the conditions in Theorem 1 imply that $\delta_j^{-1} \leq C_1 j^{\alpha+1}$, whence it follows that

$$\begin{aligned} n^{-1} \sum_{j=1}^m \kappa_j^{-2} b_j^2 \kappa_j^2 &\leq C_2 n^{-1} \sum_{j=1}^m j^{-2\beta} \leq C_3 n^{-1}, \\ n^{-2} \sum_{j=1}^m (\delta_j \kappa_j)^{-2} b_j^2 &\leq C_4 n^{-2} \sum_{j=1}^m j^{4\alpha-2\beta+2} \leq C_5 n^{-2} s(n), \end{aligned} \quad (5.10)$$

where C_1, \dots, C_5 are positive constants and $s(n)$ equals $n^{(4\alpha-2\beta+3)/(\alpha+2\beta)}$ if the exponent is strictly positive, equals $1 + \log n$ if the exponent vanishes, and equals 1 otherwise. Combining (5.8)–(5.10) we deduce that

$$\sum_{j=1}^m (\check{b}_j - b_j)^2 = O_p\{n^{-1} + n^{-2} s(n)\} = o_p(n^{-(2\beta-1)/(\alpha+2\beta)}). \quad (5.11)$$

Observe too that

$$\begin{aligned} \int_{\mathcal{I}} \left\{ \sum_{j=1}^m b_j \hat{\phi}_j(u) - b(u) \right\}^2 du &\leq 2 \int_{\mathcal{I}} \left[\sum_{j=1}^m b_j \{\hat{\phi}_j(u) - \phi_j(u)\} \right]^2 du + 2 \sum_{j=m+1}^{\infty} b_j^2 \\ &\leq 2m \sum_{j=1}^m b_j^2 \|\hat{\phi}_j - \phi_j\|^2 + 2 \sum_{j=m+1}^{\infty} b_j^2. \end{aligned} \quad (5.12)$$

Combining (5.5), (5.11) and (5.12) we find that

$$\begin{aligned} \int (\hat{b} - b)^2 &\leq 3 \sum_{j=1}^m (\hat{b}_j - \check{b}_j)^2 + 3 \sum_{j=1}^m (\check{b}_j - b_j)^2 + 3 \sum_{j=1}^m \int \left(\sum_{j=1}^m b_j \hat{\phi}_j - b \right)^2 \\ &\leq 36 \sum_{j=1}^m \kappa_j^{-2} (S_{j_1}^2 + S_{j_2}^2) + 36 \sum_{j=1}^m (m b_j^2 + \|\hat{g} - g\|^2 \kappa_j^{-2}) \|\hat{\phi}_j - \phi_j\|^2 \\ &\quad + 6 \sum_{j=m+1}^{\infty} b_j^2 + o_p(n^{-(2\beta-1)/(\alpha+2\beta)}). \end{aligned} \quad (5.13)$$

Simple moment calculations show that $E\|\hat{g} - g\|^2 = O(n^{-1})$, and clearly, $\sum_{j \geq m+1} b_j^2 = O(n^{-(2\beta-1)/(\alpha+2\beta)})$. It will be proved in section 5.3 that

$$E(S_{j1}^2) = O(n^{-1}\kappa_j), \quad (5.14)$$

whence it follows that $\sum_{j \leq m} \kappa_j^{-2} S_{j1}^2 = O_p(n^{-(2\beta-1)/(\alpha+2\beta)})$. Combining these results and (5.13) we see that (3.5) will follow if we prove that

$$\begin{aligned} & \sum_{j=1}^m j^{2\alpha} \left\{ \int g(\hat{\phi}_j - \phi_j) \right\}^2 \\ & + \sum_{j=1}^m (m j^{-2\beta} + n^{-1} j^{2\alpha}) \|\hat{\phi}_j - \phi_j\|^2 = O_p(n^{-(2\beta-1)/(\alpha+2\beta)}). \end{aligned} \quad (5.15)$$

Derivation of this property requires bounds on $\hat{\phi}_j - \phi_j$, which we now discuss.

Take $L = \widehat{K}$, $\lambda_j = \hat{\kappa}_j$ and $\psi_j = \hat{\phi}_j$ in Lemma 5.1. Formula (5.4) yields $\|\hat{\phi}_j - \phi_j\|^2 = \hat{u}_j^2 + \hat{v}_j^2$, where

$$\hat{u}_j^2 = \sum_{k: k \neq j} (\hat{\kappa}_j - \kappa_k)^{-2} \left\{ \int (\widehat{K} - K) \hat{\phi}_j \phi_k \right\}^2$$

and $\hat{v}_j^2 = \left\{ \int (\hat{\phi}_j - \phi_j) \phi_j \right\}^2$. Now, \hat{u}_j equals the length of the projection of $\hat{\phi}_j - \phi_j$ into the plane perpendicular to ϕ_j ; hence it also equals the projection of $\hat{\phi}_j$ into that plane. Also, $\int \hat{\phi}_j \phi_j$ equals the length of the projection of $\hat{\phi}_j$ onto ϕ_j . Therefore, by Pythagoras' Theorem, $(\int \hat{\phi}_j \phi_j)^2 + \hat{u}_j^2 = \|\hat{\phi}_j\|^2 = 1$, whence it follows that $\int \hat{\phi}_j \phi_j = (1 - \hat{u}_j^2)^{1/2}$. Hence,

$$\hat{v}_j^2 = \left(1 - \int \hat{\phi}_j \phi_j \right)^2 = \left\{ 1 - (1 - \hat{u}_j^2)^{1/2} \right\}^2 = 2 \left\{ 1 - (1 - \hat{u}_j^2)^{1/2} \right\} - \hat{u}_j^2,$$

which implies that

$$\|\hat{\phi}_j - \phi_j\|^2 = 2 \left\{ 1 - (1 - \hat{u}_j^2)^{1/2} \right\} \leq 2 \hat{u}_j^2. \quad (5.16)$$

Let $C > 0$, and define

$$\mathcal{F}_m = \mathcal{F}_m(n) = \left\{ (\hat{\kappa}_j - \kappa_k)^{-2} \leq 2(\kappa_j - \kappa_k)^{-2} \leq C n^{2(\alpha+1)/(\alpha+2\beta)} \right\},$$

i.e. the set of realisations such that, for sample size n , $(\hat{\kappa}_j - \kappa_k)^{-2} \leq 2(\kappa_j - \kappa_k)^{-2} \leq C n^{2(\alpha+1)/(\alpha+2\beta)}$. Observe that

$$\left\{ \int (\hat{K} - K) \hat{\phi}_j \phi_k \right\}^2 \leq 2 \left\{ \int (\hat{K} - K) \phi_j \phi_k \right\}^2 + 2 \hat{w}_{jk}^2, \quad (5.17)$$

where $\hat{w}_{jk}^2 = \left\{ \int (\hat{K} - K) (\hat{\phi}_j - \phi_j) \phi_k \right\}^2$. Note too that, uniformly in $1 \leq j \leq m$,

$$\max(\kappa_j - \kappa_{j+1}, \kappa_{j-1} - \kappa_j) \geq C_1 j^{-(\alpha+1)} \geq C_2 n^{-(\alpha+1)/(\alpha+2\beta)},$$

where C_1, C_2 denote positive constants; and that, since $\beta > \frac{1}{2}\alpha + 1$, $n^{-1/2} = o(n^{-(\alpha+1)/(\alpha+2\beta)})$. These properties, and the fact that $|\hat{\kappa}_j - \kappa_j| \leq \hat{\Delta} = O_p(n^{-1/2})$, imply that, if the constant C in the definition of \mathcal{F}_m is chosen sufficiently large, then $P(\mathcal{F}_m) \rightarrow 1$ as $n \rightarrow \infty$. Therefore, as in the case of \mathcal{E}_n , since (3.5) relates only to probabilities of differences, it suffices to work with bounds that are established under the assumption that \mathcal{F}_m holds. In this case,

$$\sum_{k: k \neq j} (\hat{\kappa}_j - \kappa_k)^{-2} \hat{w}_{jk}^2 \leq C n^{2(\alpha+1)/(\alpha+2\beta)} \sum_{k=1}^{\infty} \hat{w}_{jk}^2. \quad (5.18)$$

Using Parseval's identity and the Cauchy-Schwarz inequality we may prove that

$$\sum_{k=1}^{\infty} \hat{w}_{jk}^2 = \int_{\mathcal{I}} \left[\int_{\mathcal{I}} (\hat{K} - K)(u, v) (\hat{\phi}_j - \phi_j)(v) dv \right]^2 du \leq \hat{\Delta}^2 \|\hat{\phi}_j - \phi_j\|^2. \quad (5.19)$$

Combining (5.17)–(5.19) we deduce that, provided \mathcal{F}_m holds,

$$\hat{u}_j^2 \leq 2 \sum_{k: k \neq j} (\hat{\kappa}_j - \kappa_k)^{-2} \left\{ \int (\hat{K} - K) \phi_j \phi_k \right\}^2 + 2 C n^{2(\alpha+1)/(\alpha+2\beta)} \hat{\Delta}^2 \|\hat{\phi}_j - \phi_j\|^2.$$

Substituting into (5.16) we find that

$$(1 - 4 C n^{2(\alpha+1)/(\alpha+2\beta)} \hat{\Delta}^2) \|\hat{\phi}_j - \phi_j\|^2 \leq 4 \sum_{k: k \neq j} (\hat{\kappa}_j - \kappa_k)^{-2} \left\{ \int (\hat{K} - K) \phi_j \phi_k \right\}^2. \quad (5.20)$$

Recall that $\hat{\Delta} = O_p(n^{-1/2})$, and observe that, since $\beta > \frac{1}{2}\alpha + 1$, we have $n^{2(\alpha+1)/(\alpha+2\beta)} \cdot n^{-1} \rightarrow 0$. Therefore, noting that $P(\mathcal{F}_m) \rightarrow 1$, we deduce that

(5.20) implies:

$$\begin{aligned} \|\hat{\phi}_j - \phi_j\|^2 &\leq 4 \{1 + o_p(1)\} \sum_{k:k \neq j} (\hat{\kappa}_j - \kappa_k)^{-2} \left\{ \int (\hat{K} - K) \phi_j \phi_k \right\}^2 \\ &\leq 8 \{1 + o_p(1)\} \sum_{k:k \neq j} (\kappa_j - \kappa_k)^{-2} \left\{ \int (\hat{K} - K) \phi_j \phi_k \right\}^2, \end{aligned} \quad (5.21)$$

where the “ $o_p(1)$ ” terms are of that order uniformly in $1 \leq j \leq m$. We shall show in section 5.3 that

$$n \sum_{k:k \neq j} (\kappa_j - \kappa_k)^{-2} E \left\{ \int (\hat{K} - K) \phi_j \phi_k \right\}^2 = O(j^2), \quad (5.22)$$

uniformly in $1 \leq j \leq m$. Results (5.21) and (5.22) together imply that

$$\begin{aligned} \sum_{j=1}^m (m j^{-2\beta} + n^{-1} j^{2\alpha}) \|\hat{\phi}_j - \phi_j\|^2 &= O_p(mn^{-1} + m^{2\alpha+3}n^{-2}) \\ &= o_p(n^{-(2\beta-1)/(\alpha+2\beta)}). \end{aligned} \quad (5.23)$$

Observe next that

$$\begin{aligned} \int g(\hat{\phi}_j - \phi_j) &= \sum_{k:k \neq j} g_k (\hat{\kappa}_j - \kappa_k)^{-1} \int (\hat{K} - K) \hat{\phi}_j \phi_k + g_j \int (\hat{\phi}_j - \phi_j) \phi_j \\ &= T_{j1} + T_{j2} + T_{j3} + T_{j4}, \end{aligned} \quad (5.24)$$

where

$$\begin{aligned} T_{j1} &= \sum_{k:k \neq j} g_k (\kappa_j - \kappa_k)^{-1} \int (\hat{K} - K) \phi_j \phi_k, \\ T_{j2} &= \sum_{k:k \neq j} g_k \{ (\hat{\kappa}_j - \kappa_k)^{-1} - (\kappa_j - \kappa_k)^{-1} \} \int (\hat{K} - K) \phi_j \phi_k, \\ T_{j3} &= \sum_{k:k \neq j} g_k (\hat{\kappa}_j - \kappa_k)^{-1} \int (\hat{K} - K) (\hat{\phi}_j - \phi_j) \phi_k \end{aligned}$$

and $T_{j4} = g_j \int (\hat{\phi}_j - \phi_j) \phi_j$. Let C_1, C_2, \dots denote positive constants. Since $|g_k| \leq C_1 k^{-(\alpha+\beta)}$, then, if \mathcal{F}_m holds,

$$\begin{aligned} T_{j2}^2 &\leq C_2 \left\{ \sum_{k:k \neq j} k^{-(\alpha+\beta)} \frac{|\hat{\kappa}_j - \kappa_j|}{(\kappa_j - \kappa_k)^2} \left| \int (\hat{K} - K) \phi_j \phi_k \right| \right\}^2 \\ &\leq C_3 \left\{ \sum_{k:k \neq j} k^{-2(\alpha+\beta)} \frac{(\hat{\kappa}_j - \kappa_j)^2}{(\kappa_j - \kappa_k)^4} \right\} \left[\sum_{k=1}^{\infty} \left\{ \int (\hat{K} - K) \phi_j \phi_k \right\}^2 \right] \\ &= C_4 (\hat{\kappa}_j - \kappa_j)^2 \hat{\Delta}_j^2 \sum_{k:k \neq j} k^{-2(\alpha+\beta)} (\kappa_j - \kappa_k)^{-4}. \end{aligned}$$

Now,

$$\begin{aligned}
\sum_{k=2j}^{\infty} k^{-2(\alpha+\beta)} (\kappa_j - \kappa_k)^{-4} &\leq C_5 \kappa_j^{-4} \sum_{k=2j}^{\infty} k^{-2(\alpha+\beta)} \leq C_6 j^{2\alpha-2\beta+1}, \\
\sum_{k=1}^{j/2} k^{-2(\alpha+\beta)} (\kappa_j - \kappa_k)^{-4} &\leq C_7 \sum_{k=1}^{j/2} k^{-2(\alpha+\beta)} \kappa_k^{-4} \leq C_8 \sum_{k=1}^{j/2} k^{2\alpha-2\beta} \\
&\leq C_9 \begin{cases} 1 & \text{if } \alpha + \frac{1}{2} < \beta \\ 1 + \log j & \text{if } \alpha + \frac{1}{2} = \beta \\ j^{2\alpha-2\beta+1} & \text{if } \alpha + \frac{1}{2} > \beta, \end{cases} \\
\sum_{k=j/2}^{2j} k^{-2(\alpha+\beta)} (\kappa_j - \kappa_k)^{-4} &\leq \sum_{k=j/2}^{2j} k^{-2(\alpha+\beta)} (j/\kappa_j)^4 (1 + |j - k|)^{-4} \\
&\leq C_{10} j^{2\alpha-2\beta+4}.
\end{aligned}$$

Therefore,

$$\sum_{k:k \neq j} k^{-2(\alpha+\beta)} (\kappa_j - \kappa_k)^{-4} \leq C_{11} (1 + j^{2\alpha-2\beta+4} + \log j), \quad (5.25)$$

whence, using (5.2) and (5.9),

$$\begin{aligned}
\sum_{j=1}^m j^{2\alpha} T_{j2}^2 &\leq C_{12} \sum_{j=1}^m (\hat{\kappa}_j - \kappa_j)^2 \hat{\Delta}_j^2 (j^{2\alpha} \log n + j^{4\alpha-2\beta+4}) \\
&= O_p \left\{ n^{-1} \sum_{j=1}^m E(\hat{\Delta}_j^2) (j^{2\alpha} \log n + j^{4\alpha-2\beta+4}) \right\} \\
&= O_p \left\{ n^{-2} \sum_{j=1}^m (j^{2\alpha} \log n + j^{4\alpha-2\beta+4}) \right\} \\
&= O_p \{ n^{-2} (m^{2\alpha+1} \log n + m^{4\alpha-2\beta+5}) \} = o_p(n^{-(2\beta-1)/(\alpha+2\beta)}). \quad (5.26)
\end{aligned}$$

If \mathcal{F}_m holds then

$$\begin{aligned}
|T_{j3}| &\leq C_{13} \sum_{k:k \neq j} k^{-(\alpha+\beta)} |\kappa_j - \kappa_k|^{-1} \left| \int (\hat{K} - K) (\hat{\phi}_j - \phi_j) \phi_k \right| \\
&\leq C_{14} \sum_{k:k \neq j} k^{-(\alpha+\beta)} |\kappa_j - \kappa_k|^{-1} \|\hat{\phi}_j - \phi_j\| \\
&\quad \times \int |\phi_k(u)| \left[\int \{\hat{K}(u, v) - K(u, v)\}^2 dv \right]^{1/2} du \\
&\leq C_{15} \hat{\Delta} \|\hat{\phi}_j - \phi_j\| \sum_{k:k \neq j} k^{-(\alpha+\beta)} |\kappa_j - \kappa_k|^{-1} \\
&\leq C_{16} \hat{\Delta} \|\hat{\phi}_j - \phi_j\|, \quad (5.27)
\end{aligned}$$

where the last inequality follows using the argument leading to (5.25). From (5.27), using (5.21) and (5.22), it may be shown that

$$\sum_{j=1}^m j^{2\alpha} T_{j3}^2 = O_p\left(n^{-2} \sum_{j=1}^m j^{2\alpha+2}\right) = o_p(n^{-(2\beta-1)/(\alpha+2\beta)}). \quad (5.28)$$

More simply,

$$\sum_{j=1}^m j^{2\alpha} T_{j4}^2 \leq C_{17} \sum_{j=1}^m j^{-2\beta} \|\hat{\phi}_j - \phi_j\|^2 = O_p(n^{-1}). \quad (5.29)$$

Combining (5.24), (5.26), (5.28) and (5.29) we deduce that

$$\sum_{j=1}^m j^{2\alpha} \left\{ \int g(\hat{\phi}_j - \phi_j) \right\}^2 \leq 4 \sum_{j=1}^m j^{2\alpha} T_{j1}^2 + o_p(n^{-(2\beta-1)/(\alpha+2\beta)}). \quad (5.30)$$

We shall prove in section 5.3 that

$$\sum_{j=1}^m j^{2\alpha} E(T_{j1}^2) = O(n^{-(2\beta-1)/(\alpha+2\beta)}). \quad (5.31)$$

The desired result (5.15) follows from (5.23), (5.30) and (5.31); this completes the proof of (3.5).

5.2. Proof of Lemma 5.1. To derive (5.3) observe that, on subtracting the expansions of K and L at (2.1) and (5.1), respectively, we obtain an expansion of $K - L$. Multiplying both sides of this by $\psi_j(u) \phi_j(v)$, and integrating over u and v , we deduce that

$$(\kappa_j - \lambda_j) \int \psi_j \phi_j - \int (K - L) \psi_j \phi_j = 0. \quad (5.32)$$

Since $\psi_j = \phi_j + \chi_j + \Delta_j$ then

$$\left| \int \psi_j \phi_j - 1 - \int \chi_j \phi_j \right| = \left| \int \Delta_j \phi_j \right| \leq \|\Delta_j\|, \quad (5.33)$$

$$\begin{aligned} \left| \int (K - L) (\psi_j - \phi_j - \chi_j) \phi_j \right|^2 &= \left| \int (K - L) \Delta_j \phi_j \right|^2 \\ &\leq \left(\int \Delta_j^2 \right) \int_{\mathcal{I}} \left[\int_{\mathcal{I}} \{K(u, v) - L(u, v)\} \phi_j(u) du \right]^2 dv. \end{aligned} \quad (5.34)$$

Result (5.3) follows from (5.32)–(5.34).

The expansions of K and L , at (2.1) and (5.1), may be used to prove that

$$\lambda_j (\psi_j - \phi_j) = \int K (\psi_j - \phi_j) + \int (L - K) \psi_j - (\lambda_j - \kappa_j) \phi_j .$$

Multiplying both sides by ϕ_k , and integrating, we deduce that

$$\lambda_j \int (\psi_j - \phi_j) \phi_k = \kappa_k \int (\psi_j - \phi_j) \phi_k + \int (L - K) \psi_j \phi_k - (\lambda_j - \kappa_j) \delta_{jk} ,$$

where δ_{jk} denotes the Kronecker delta. Equivalently, provided $\lambda_j \neq \kappa_k$,

$$\int (\psi_j - \phi_j) \phi_k = (\lambda_j - \kappa_k)^{-1} \int (L - K) \psi_j \phi_k - \delta_{jk} .$$

Result (5.4) follows from this formula and the fact that

$$\psi_j - \phi_j = \sum_{k=1}^{\infty} \phi_k \int (\psi_j - \phi_j) \phi_k .$$

5.3. *Proofs of (5.9), (5.14), (5.22) and (5.31).* Direct calculation shows that $E(\widehat{K} - K)^2 = O(n^{-1})$, uniformly on $\mathcal{I} \times \mathcal{I}$. It follows that $E(\widehat{\Delta}^2) = O(n^{-1})$. Note too that, by Parseval's identity, $\widehat{\Delta}^2 = \sum_j \widehat{\Delta}_j^2$, and so $\sup_j E(\widehat{\Delta}_j^2) = O(n^{-1})$.

This gives the first part of (5.9). To derive the second part, assume without loss of generality that $E(X) = 0$, and observe that

$$\int (\widehat{K} - K) \phi_j \phi_k = n^{-1} \sum_{i=1}^n (\xi_{ij} \xi_{ik} - E\xi_j \xi_k) - \bar{\xi}_j \bar{\xi}_k , \quad (5.35)$$

where $\xi_{ij} = \int X_i \phi_j$, $\bar{\xi}_j = n^{-1} \sum_i \xi_{ij}$ and ξ_j denotes a generic ξ_{ij} . Therefore, using the fact that $E(\xi_j^4) \leq C_1 (E\xi_j^2)^2$, where $C_1 > 0$ does not depend on j , we deduce that

$$E(\widehat{\Delta}_{jj}^2) = E \left\{ n^{-1} \sum_{i=1}^n (\xi_{ij}^2 - E\xi_j^2) - \bar{\xi}_j^2 \right\}^2 \leq n^{-1} C_2 (E\xi_j^2)^2 = n^{-1} C_2 \kappa_j^2 ,$$

where C_2 does not depend on j . This implies the second part of (5.9).

To prove (5.14), observe that

$$\begin{aligned} \int (\hat{g} - g) \phi_j &= n^{-1} \sum_{i=1}^n \left\{ \xi_{ij} \int b X_i - \bar{\xi}_j \int b \bar{X} - E \left(\xi_{ij} \int b X_i \right) \right\} \\ &\quad + n^{-1} \sum_{i=1}^n (\xi_{ij} \epsilon_i - \bar{\xi}_j \bar{\epsilon}), \end{aligned}$$

where $\bar{\epsilon} = n^{-1} \sum_i \epsilon_i$. It may thus be proved that

$$n E \left\{ \int (\hat{g} - g) \phi_j \right\}^2 \leq C_3 \left\{ \text{var} \left(\xi_j \int b X \right) + \text{var} (\xi_j) \right\} \leq C_4 (E \xi_j^4)^{1/2} \leq C_5 \kappa_j,$$

which implies (5.14).

To obtain (5.22), note that by (5.35) and the fact that $E(\xi_j^4) \leq C_1 (E \xi_j^2)^2$,

$$n E \left\{ \int (\hat{K} - K) \phi_j \phi_k \right\}^2 \leq C_6 E(\xi_j^2 \xi_k^2) \leq C_7 (E \xi_j^4 \cdot E \xi_k^4)^{1/2} \leq C_8 \kappa_j \kappa_k,$$

uniformly in k and k . Result (5.22) follows directly, on substitution and employing the argument leading to (5.25).

Again using (5.35),

$$T_{j1} = n^{-1} \sum_{i=1}^n \sum_{k: k \neq j} g_k (\kappa_j - \kappa_k)^{-1} \{ \xi_{ij} \xi_{ik} - E(\xi_{ij} \xi_{ik}) - \bar{\xi}_j \bar{\xi}_k \},$$

from which it may be proved that, since $E(|\xi_{k_1} \dots \xi_{k_4}|) \leq \prod_{\ell} (E \xi_{k_\ell}^4)^{1/4}$,

$$\begin{aligned} n E(T_{j1}^2) &\leq C_9 E \left\{ \xi_j \sum_{k: k \neq j} g_k (\kappa_j - \kappa_k)^{-1} \xi_k \right\}^2 \\ &\leq C_{10} (E \xi_j^4)^{1/2} \left\{ \sum_{k_1: k_1 \neq j} \dots \sum_{k_4: k_4 \neq j} E(|\xi_{k_1} \dots \xi_{k_4}|) \right. \\ &\quad \left. \times \prod_{\ell=1}^4 |g_{k_\ell} (\kappa_j - \kappa_{k_\ell})^{-1}| \right\}^{1/2} \\ &\leq C_{11} \kappa_j \left(\sum_{k: k \neq j} \left| \frac{g_k \kappa_k}{\kappa_j - \kappa_k} \right| \right)^4 \leq C_{12} \kappa_j, \end{aligned}$$

uniformly in j . Therefore, $\sum_{j \leq m} j^{2\alpha} E(T_{j1}^2) \leq C_{10} n^{-1} m^{\alpha+1}$, which implies (5.31).

5.4. *Proof of (3.6).* Let $\mathcal{I} \equiv [0, 1]$, $\phi_1 \equiv 1$ and $\phi_{j+1}(t) = 2^{-1/2} \cos(j\pi t)$ for $j \geq 1$. Put $b_j = \theta_j j^{-\beta}$ for $L_{n+1} \leq j \leq 2L_n$, and $b_j = 0$ otherwise, where L_n denotes the integer part of $n^{1/(2\beta+1)}$ and each θ_j is either 0 or 1. Let $\kappa_j = j^{-\alpha}$ and write Z_1, Z_2, \dots for independent random variables all with the uniform distribution on $[-3^{1/2}, 3^{1/2}]$. Note that $E(Z_j) = 0$ and $E(Z_j^2) = 1$, and that the Z_j 's are observable if X is observable, since $Z_j = j^{\alpha/2} \int_{\mathcal{I}} X \phi_j$.

Set $X = \sum_j j^{-\alpha/2} Z_j \phi_j$ and

$$Y = \int_{\mathcal{I}} b X + \epsilon = \sum_{j=L_{n+1}}^{2L_n} \theta_j j^{-(\alpha+2\beta)/2} Z_j + \epsilon,$$

where the error ϵ is taken to be Gaussian with zero mean. Then we may write $b = \sum_{L_{n+1} \leq j \leq 2L_n} \theta_j j^{-\beta} \phi_j$, and if \bar{b} is an estimator of b ,

$$\bar{\theta}_j = j^\beta \int_{\mathcal{I}} \bar{b} \phi_j \tag{5.36}$$

is an estimator of θ_j . An argument based on the Neyman-Pearson lemma shows that

$$\lim_{n \rightarrow \infty} \inf_{L_{n+1} \leq j \leq 2L_n} \inf_{\bar{\theta}_j} \sup^* E(\bar{\theta}_j - \theta_j)^2 > 0,$$

where \sup^* denotes the supremum over all 2^{L_n} different distributions of (X, Y) obtained by taking different choices of $\theta_{L_{n+1}}, \dots, \theta_{2L_n}$, and $\inf_{\bar{\theta}_j}$ represents the infimum over all measurable functions $\bar{\theta}_j$ of the data. Therefore, if an estimator \check{b} is given, and $\check{\theta}_{L_{n+1}}, \dots, \check{\theta}_{2L_n}$ are the respective estimators of $\theta_{L_{n+1}}, \dots, \theta_{2L_n}$ obtained by substituting \check{b} for \bar{b} in (5.36), then for constants $D_1, D_2 > 0$ which do not depend on choice of the measurable function \check{b} ,

$$\begin{aligned} \sup^* \int_{\mathcal{I}} E_F(\check{b} - b)^2 &= \sup^* \sum_{j=L_{n+1}}^{2L_n} j^{-2\beta} E_F(\check{\theta}_j - \theta_j)^2 \\ &\geq D_1 \sum_{j=L_{n+1}}^{2L_n} j^{-2\beta} \geq D_2 n^{-(2\beta-1)/(\alpha+2\beta)}. \end{aligned}$$

This proves (3.6).

REFERENCES

- BHATIA, R., DAVIS, C. AND MCINTOSH, A. (1983). Perturbation of spectral subspaces and solution of linear operator equations. *Linear Algebra Appl.* **52/53**, 45–67.
- BLUNDELL, R. AND POWELL, J.L. (2003). Endogeneity in nonparametric and semiparametric regression models. In: *Advances in Economics and Econometrics: Theory and Applications*, Dewatripont, M., Hansen, L.-P. and Turnovsky, S.J., eds, vol. 2, pp. 312–357. Cambridge, UK: Cambridge University Press.
- CARDOT AND SARDA, P. (2003). Linear regression models for functional data. <http://www.quantlet.org/hizirjsp/sarda-cardot/sarda-cardot.pdf>
- CARROLL, R.J., RUPPERT, D. AND STEFANSKI, L.A. (1995). *Measurement Error in Nonlinear Models*. Chapman & Hall, London.
- CAVALIER, L., GOLUBEV, G.K., PICARD, D. AND TSYBAKOV, A.B. (2002). Oracle inequalities for inverse problems. *Ann. Statist.* **30**, 843–874.
- CHIOU, J.M., MÜLLER, H.-G. AND WANG, J.-L. (2003). Functional quasi-likelihood regression models with smooth random effects. *J. Roy. Statist. Soc. Ser. B* **65**, 405–423.
- CUEVAS, A., FEBRERO, M. AND FRAIMAN, R. (2002). Linear functional regression: the case of fixed design and functional response. *Canad. J. Statist.* **30**, 285–300.
- DAROLLES, S., FLORENS, J.-P. AND RENAULT, E. (2002). Nonparametric instrumental regression. Working paper, GREMAQ, University of Social Science, Toulouse.
- DELAIGLE, A. AND GIJBELS, I. (2002). Estimation of integrated squared density derivatives from a contaminated sample. *J. R. Stat. Soc. Ser. B* **64**, 869–886.
- DONOHU, D.L. (1995). Nonlinear solution of linear inverse problems by wavelet-vaguelette decomposition. *Appl. Comput. Harmon. Anal.* **2**, 101–126.
- EFROMOVICH, S. AND KOLTCHINSKII, V. (2001). On inverse problems with unknown operators. *IEEE Trans. Inform. Theory* **47**, 2876–2894.
- FAN, J. (1991). On the optimal rates of convergence for nonparametric deconvolution problems. *Ann. Statist.* **19**, 1257–1272.
- FAN, J. (1993). Adaptively local one-dimensional subproblems with application to a deconvolution problem. *Ann. Statist.* **21**, 600–610.
- FARAWAY, J.J. (1997). Regression analysis for a functional response. *Technometrics* **39**, 254–261.
- FERRATY, F. AND VIEU, P. (2000). Fractal dimensionality and regression estimation in semi-normed vectorial spaces. *C.R. Acad. Sci. Paris Sér. I* **330**,

139–142.

- HALL, P. AND HOROWITZ, J.L. (2005). Nonparametric methods for inference in the presence of instrumental variables. *Ann. Statist.*, forthcoming.
- HOROWITZ, J.L. AND MARKATOU, M. (1996). Semiparametric estimation of regression models for panel data. *Rev. Econom. Stud.* **63**, 145–168.
- JOHNSTONE, I.M. (1999). Wavelet shrinkage for correlated data and inverse problems: adaptivity results. *Statist. Sinica* **9**, 51–83.
- KUNDUR, D. AND HATZINAKOS, D. (1998). A novel blind deconvolution scheme for image restoration using recursive filtering. *IEEE Trans. Sig. Process.* **46**, 375–390.
- LI, T. AND HSIAO, C. (2004). Robust estimation of generalised linear models with measurement errors. *J. Econometrics* **118**, 51–65.
- NATTERER, F. (1984). Error bounds for Tikhonov regularization in Hilbert scales. *Applicable Anal.* **18**, 29–37.
- NEUBAUER, A. (1989). Tikhonov regularisation for nonlinear ill-posed problems: optimal convergence rates and finite-dimensional approximation. *Inverse Problems* **5**, 541–557.
- NEWHEY, W.K. AND POWELL, J.L. (2002). Instrumental variable estimation of nonparametric models. *Econometrica*, to appear.
- NEWHEY, W.K., POWELL, J.L. AND VELLA, F. (1999). Nonparametric estimation of triangular simultaneous equations models. *Econometrica* **67**, 565–603.
- RAMSAY, J.O. AND SILVERMAN, B.W. (1997). *Functional Data Analysis*. Springer, New York.
- RAMSAY, J.O. AND SILVERMAN, B.W. (2002). *Applied Functional Data Analysis: Methods and Case Studies*. Springer, New York.
- SHENK, J.S. AND WESTERHAUS, M.O. (1991). Population definition, sample selection, and calibration procedures for near infrared reflectance spectroscopy. *Crop Science* **31**, 469–474.
- STANISWALIS, J.G. AND LEE, J.J. (1998). Nonparametric regression analysis of longitudinal data. *J. Amer. Statist. Assoc.* **93**, 1403–1418.
- STEFANSKI, L. AND CARROLL, R.J. (1990). Deconvoluting kernel density estimators. *Statistics* **21**, 169–184.
- TIKHONOV, A.N. (1963). On the solution of incorrectly put problems and the regularisation method. In: *Outlines Joint Sympos. Partial Differential Equations* (Novosibirsk, 1963), pp. 261–265. Acad. Sci. USSR Siberian Branch, Moscow.
- VAN ROOIJ, A.C.M. AND RUYMGAART, F.H. (1996). Asymptotic minimax rates for abstract linear estimators. *J. Statist. Plann. Inference* **53**, 389–402.

- WESLEY, I.J., UTHAYAKUMARAN, S., ANDERSSSEN, R.S., CORNISH, G.B., BEKES, F., OSBORNE, B.G. AND SKERRITT, J.H. (1999). A curve-fitting approach to the near infrared reflectance measurement of wheat flour proteins which influence dough quality. *J. Near Infrared Spectrosc.* **7**, 229–240.
- YANG, Y., GALATSANOS, N.P. AND STARK, H. (1994). Projection-based blind deconvolution. *J. Optical Soc. Amer. Ser. A* **11**, 2401–2409.

TABLE 1: Results of Monte Carlo Experiments for Well-Spaced Eigenvalues

σ_ε	n	α	ρ	a_n	$\text{Bias}^2(\hat{b})$	$\text{Bias}^2(\tilde{b})$	$\text{Var}(\hat{b})$	$\text{Var}(\tilde{b})$	$\text{MISE}(\hat{b})$	$\text{MISE}(\tilde{b})$	
0.5	100	1.1	2	0.4	0.158	1.150	0.843	1.340	1.001	2.490	
		1.5	2	0.38	0.148	1.289	0.718	0.759	0.866	2.048	
		2.0	2	0.28	0.140	1.202	0.676	0.622	0.816	1.824	
		4.0	2	0.10	0.134	1.344	2.225	0.611	2.359	1.955	
	500	1.1	3	0.28	0.016	0.717	0.236	0.480	0.251	1.197	
		1.5	3	0.22	0.015	0.663	0.254	0.364	0.269	1.027	
		2.0	2	0.12	0.139	0.416	0.146	0.441	0.285	0.857	
		4.0	2	0.032	0.139	0.460	0.409	0.493	0.548	0.953	
	1.0	100	1.1	2	1.0	0.161	2.709	2.034	1.203	2.195	3.913
			1.5	2	0.75	0.149	2.401	2.221	1.019	2.370	3.420
			2.0	2	0.50	0.139	2.047	2.395	1.034	2.534	3.081
			4.0	1	0.25	3.257	2.302	0.501	0.788	3.758	3.090
500		1.1	2	0.50	0.142	1.438	0.408	0.758	0.549	2.197	
		1.5	2	0.35	0.138	1.164	0.425	0.702	0.563	1.866	
		2.0	2	0.10	0.139	0.314	0.514	2.279	0.654	2.593	
		4.0	2	0.10	0.139	1.386	1.647	0.472	1.786	1.858	

TABLE 2: Results of Monte Carlo Experiments for Closely Spaced Eigenvalues

σ_ε	n	α	m	ρ	$\text{Bias}^2(\hat{b})$	$\text{Bias}^2(\tilde{b})$	$\text{Var}(\hat{b})$	$\text{Var}(\tilde{b})$	$\text{MISE}(\hat{b})$	$\text{MISE}(\tilde{b})$
0.5	100	1.1	1	0.22	3.526	2.502	0.141	0.585	3.398	3.087
		1.5	1	0.22	3.257	2.487	0.131	0.455	3.389	2.942
		2.0	1	0.20	3.259	2.403	0.126	0.454	3.385	2.857
		4.0	1	0.20	3.260	2.402	0.130	0.433	3.390	2.835
	500	1.1	5	0.08	0.002	1.463	2.510	0.574	2.512	2.037
		1.5	5	0.06	0.002	1.212	2.604	0.623	2.606	1.835
		2.0	5	0.04	0.006	0.846	2.528	0.783	2.535	1.629
		4.0	5	0.04	0.006	0.780	2.500	0.640	2.506	1.420
1.0	100	1.1	1	0.42	3.260	3.127	0.533	0.856	3.793	3.983
		1.5	1	0.42	3.271	3.031	0.512	0.706	3.783	3.736
		2.0	1	0.32	3.260	2.822	0.540	0.937	3.799	3.759
		4.0	1	0.36	3.262	2.954	0.496	0.760	3.758	3.713
	500	1.1	1	0.20	3.258	2.379	0.109	0.532	3.367	2.911
		1.5	1	0.14	3.262	2.078	0.109	0.729	3.372	2.807
		2.0	1	0.12	3.262	1.922	0.103	0.762	3.366	2.684
		4.0	1	0.12	3.256	1.818	0.107	0.695	3.363	2.514