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SPEED OF ESTIMATION IN POSITRON EMISSION TOMOGRAPHY AND RELATED INVERSE PROBLEMS

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Several algorithms for image reconstruction in positron emission tomography (PET) have been described in the medical and statistical literature. We study a continuous idealization of the PET reconstruction problem, considered as an example of bivariate density estimation based on indirect observations. Given a large sample of indirect observations, we consider the size of the equivalent sample of observations, whose original exact positions would allow equally accurate estimation of the image of interest. Both for indirect and for direct observations, we establish exact minimax rates of convergence of estimation, for all possible estimators, over suitable smoothness classes of functions. A key technical device is a modulus of continuity appropriate to global function estimation. For indirect data and (in practice unobservable) direct data, the rates for mean integrated square error are $n^{-p/(p+2)}$ and $(n/\log n)^{-p/(p+1)}$, respectively, for densities in a class corresponding to bounded square-integrable pth derivatives. We obtain numerical values for equivalent sample sizes for minimax linear estimators using a slightly modified error criterion. Modifications of the model to incorporate attenuation and the third dimension effect do not affect the minimax rates. The approach of the paper is applicable to a wide class of linear inverse problems.

1. Introduction. Tomography is a noninvasive technique for reconstructing the internal structure of an object of interest, often in a medical context. Positron emission tomography (PET) deals with the estimation of the amount and location of a radioactively labelled metabolite on the basis of particle decays indirectly observed outside the body. Emission tomography in general, and PET in particular, has been the subject of considerable recent research in nuclear medicine, and has attracted the interest of statisticians as an example of a reconstruction problem involving incomplete and noisy data.

The formulation of the PET problem we shall consider is basically that given by Shepp and Vardi (1982) and Vardi, Shepp and Kaufman (1985). Following their convention we shall consider a particular PET experiment, where the brain is scanned by counting radioactive emissions from tagged glucose. The distribution of glucose within the brain corresponds to the glucose uptake mechanism, and so a map of the glucose distribution within the brain gives an indication of the pattern of the brain's metabolic activity. In the idealization we shall consider, following Vardi, Shepp and Kaufman (1985), the radioactive tagging of the glucose gives rise to emissions of positrons distributed as a Poisson process in

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space and time; the spatial intensity of emissions is the same as the distribution of glucose. Each positron that is emitted annihilates with a nearby electron and yields two photons that fly off in opposite directions along a line with uniformly distributed orientation. One or more rings of sensors placed around the patient's head make it possible to detect the photon pairs and hence, for each emission that is detected, to give a line on which the point of emission must have occurred. However, for equipment of the kind discussed here, it is not possible to detect the position of the emission on the line.

The PET problem is just one of a large number of statistical problems involving *indirect observations* of the phenomenon of interest; in our case the observations are indirect in that the emissions themselves are not observed directly. Such problems arise, for example, in geophysics, in stereology and wherever linear deconvolution with known filter is required. Our aim in the present paper is not just to study the PET problem but also to develop theory that can be applied in many other contexts.

In a typical PET scan, a large number, perhaps one to ten million, of radioactive emissions are recorded, and the image of interest, a slice through the patient's brain or body, is reconstructed in some way from this apparently vast data set. But is ten million observations really a large sample in this kind of context? One way of gaining some insight into the problem is to think in terms of *equivalent sample sizes*. We make some smoothness assumptions about the image of interest and then ask how accurately it could possibly be reconstructed given a particular indirect sample. The equivalent sample size would be the number of emissions whose *original* positions could yield an equally accurate estimate. The equivalent sample size gives, in terms more attuned to usual statistical intuition, a quantification of the information actually available from our sample of ten million indirectly observed emissions, and hence gives an idea of how much is lost by the indirect nature of the observation process.

In Section 2 we formulate the reconstruction problem as an example of nonparametric bivariate density estimation based on indirect data; in fact, an example of a linear inverse problem in a function space. The function we estimate is the intensity function of emissions in the slice through the brain. A key feature of our treatment is the explicit singular value decomposition of the transform linking the unknown density with that of the observed data. The main conclusions of the paper are summarized in Section 3. In particular, we give in Section 3 a table of explicit equivalent sample sizes, admittedly for our mathematical idealization of the PET problem. In Section 4 we confine attention to linear estimators and to intensities falling in a suitable smoothness class of functions. We find the exact minimax rates of consistency, that is, the rate for the least favourable density and the best linear estimator. We then show, in Section 5, that these rates cannot be improved by extending consideration to all possible estimators, linear or nonlinear. Thus, we do not consider particular iterative nonlinear algorithms proposed elsewhere for practical use, but instead we establish the best possible performance achievable by any estimator.

Section 6 of the paper considers modifications of our mathematical idealization in order to take account of attenuation of the emitted photons and of the

three dimensional nature of the problem. Our broad conclusions carry over when these effects are incorporated. In Section 7, we extend our results to some error measures based on the derivatives as well as the values of the images and their reconstructions. Finally, in Section 8, we make some concluding remarks, and mention some possible issues for future research.

A subsidiary objective of the paper is to illustrate, in a relatively simple and concrete setting, the general approach to deriving lower bounds to estimation risk developed by Le Cam [(1985), for example], Ibragimov and Hasminskii (1981) and Birgé (1983). This method relates the best possible speed of estimation (in a given "global" metric) to the metric entropy structure of the parameter space. We need a minor modification to handle the present indirect estimation setting, introducing a form of "modulus of continuity" of the inverse transform. This material is presented mainly in Section 5.

There is a substantial literature on practical algorithms for reconstruction in the PET setting. An extensive survey covering the period up to 1979 is given by Budinger, Gullberg and Huesman (1979); this includes adaptation of methods from X-ray transmission tomography and the orthogonal series method of Marr (1974). Maximum likelihood methods were proposed by Rockmore and Macovski (1977); they were implemented via the EM algorithm by Shepp and Vardi (1982) [see also Vardi, Shepp and Kaufman, (1985)] and modified in various ways, to incorporate smoothing, by Geman and McClure (1985), Snyder and Miller (1985), Silverman, Jones, Wilson and Nychka (1990) and Green (1990). Some practical illustration of the orthogonal series method introduced in the present paper is given by Jones and Silverman (1989). A recent survey of algorithms is given by Tanaka (1987). Papers considering noise limitations in X-ray and transmission tomography include Chesler, Rieder and Pelc (1977) and Tretiak (1978, 1979). The focus of these papers differs from ours in that they consider estimation of a fixed finite number of real-valued functions of a particular unknown intensity, using discrepancies based on variance rather than mean square error.

2. Mathematical model and technical preliminaries.

2.1. *An idealized problem and the Radon transform.* In our idealized version of the PET problem, the ring of detectors defines a slice of the patient's head, and the reconstruction aims to display a picture of the glucose density within that slice. Emissions that give rise to photon pairs, one or both of which miss the detector ring, will go unrecorded. Bearing this in mind, we shall regard the slice as a plane and consider an essentially two-dimensional problem where (see Figure 1) emissions take place in the plane according to some density within a detector circle taken to be the unit circle in the plane. An emission at P gives rise to a photon pair whose directions of flight lie in the plane along a line l through P with random, uniformly distributed, orientation. The finite size of the detectors is ignored and it is assumed that the points Q and R of the intersection of l with the detector circle are observed exactly.

Give the name *detector space* to the space D of all possible unordered pairs QR of points on the detector circle, and call *brain space* the original disc B in

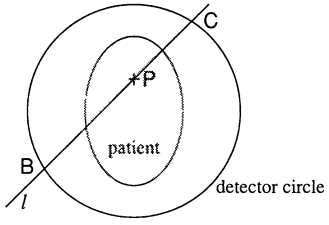

FIG. 1. *The patient and the detector circle.*

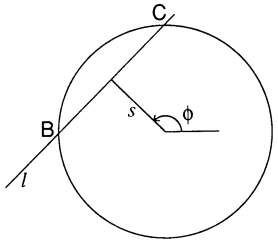

FIG. 2. *Parametrizing the line l.*

the plane enclosed by the detector ring. Assume that coordinates are chosen so that B is the unit disc. Brain space is parametrized by either Cartesian or standard polar coordinates. To parametrize detector space, let s be the length of the perpendicular from the origin to the detected line QR as in Figure 2, and φ the orientation of this perpendicular. Thus D is $\{(s, \varphi): 0 \leq s \leq 1, 0 \leq \varphi \leq 2\pi\}$.

We now define dominating measures on brain space and on detector space. Define a measure μ on brain space to be $\pi^{-1} \times$ Lebesgue measure, so that $d\mu(r, \theta) = \pi^{-1} r\, dr\, d\theta$ for $0 \leq r \leq 1$ and $0 \leq \theta < 2\pi$ if polar coordinates are used, and $d\mu(x_1, x_2) = \pi^{-1}\, dx_1\, dx_2$ for $\|x\| \leq 1$ in Cartesian coordinates. On detector space, define a measure λ by $d\lambda(s, \varphi) = 2\pi^{-2}(1 - s^2)^{1/2}\, ds\, d\varphi$. Both μ and λ integrate to 1.

Suppose an emission takes place at a point distributed with probability density $f(x_1, x_2)$ with respect to μ in brain space. Let $g = Pf$ be the probability density in detector space, with respect to λ, of the corresponding detection of a pair of photons, so that the mapping P maps the actual density of emissions to the corresponding observable density in detector space. We shall show below that Pf is given by

(2.1)

$$Pf(s, \varphi) = \tfrac{1}{2}(1 - s^2)^{-1/2} \int_{-\sqrt{(1-s^2)}}^{\sqrt{(1-s^2)}} f(s \cos \varphi - t \sin \varphi, s \sin \varphi + t \cos \varphi)\, dt.$$

The integral in (2.1) is the so-called *Radon transform* [see Marr (1974) and

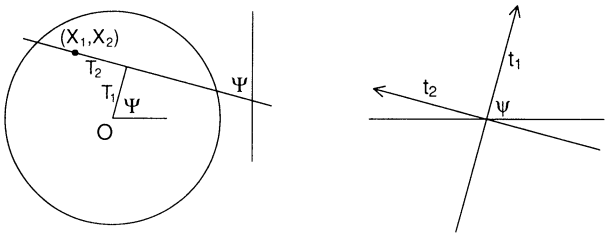

FIG. 3. *Transforming the coordinates.*

Deans (1983)] of the density f, namely the line integral of f along the line l with coordinates (s, φ) in detector space. Since the length of the segment QR is $2(1 - s^2)^{1/2}$, it can be seen at once that $Pf(s, \varphi)$ is the average of f over the part of l that intersects the detector disc $\|x\| \leq 1$. If f is the uniform density in brain space, so that $f(x_1, x_2) = 1$ for all $\|x\| \leq 1$, then we shall have $Pf(s, \varphi) = 1$ for all s and φ. Thus the probability measure λ in detector space is the detector space distribution corresponding to the uniform measure μ in brain space.

It remains to verify (2.1). Suppose an emission takes place at (X_1, X_2) and that the corresponding photon pair has trajectory at angle Ψ as shown in Figure 3; taking $0 \leq \Psi \leq \pi$ for definiteness, the joint probability density with respect to $dx_1\, dx_2\, d\psi$ on $\|x\| \leq 1$ and $0 \leq \psi \leq \pi$ is given by

$$f_{X_1, X_2, \Psi}(x_1, x_2, \psi) = \pi^{-2} f(x_1, x_2)$$

using the definition of μ and the fact that Ψ is independent of X_1 and X_2. Now change variables by setting

$$S = |X_1 \cos\Psi + X_2 \sin\Psi|,$$

$$\Phi = \begin{cases} \Psi & \text{if } X_1 \cos\Psi + X_2 \sin\Psi \geq 0, \\ \Psi + \pi & \text{otherwise,} \end{cases}$$

$$T = -X_1 \sin\Psi + X_2 \cos\Psi;$$

the variables (S, Φ) are the coordinates of the detected photon pair. After making the transformation, which has unit Jacobian, and integrating out the unobserved variable T, we obtain the joint density with respect to $ds\, d\varphi$,

$$f_{S,\Phi}(s, \varphi) = \pi^{-2} \int_{-\sqrt{(1-s^2)}}^{\sqrt{(1-s^2)}} f(s\cos\varphi - t\sin\varphi,\ s\sin\varphi + t\cos\varphi)\, dt.$$

The density (2.1) with respect to λ follows at once from the definition of λ.

2.2. *Estimators and loss functions.* In this section, we define various classes of estimator of f that we shall be considering, as well as two measures of the accuracy of estimation of f. The proofs of the three propositions stated in this section are given in the Appendix.

Two particular classes of estimator are of obvious interest. Let $\mathcal{T}_D(n)$ be the class of all possible estimators based on a sample of n independent *direct*

observations in brain space from the density f. Let $\mathscr{T}_I(n)$ be the class of all estimators of f based on a sample of n *indirect* observations, i.e., observations in detector space drawn from the density Pf. It will also be important in some of our work to concentrate attention on those estimators that are *linear estimators*. An estimator $\hat{f}$ based on observations $Z_1, \ldots, Z_n$ is called linear if there exists a weight function $w(x, z)$ such that $\int w(x, z)\, d\mu(x) = 1$ for all z in the space of the observations, and

$$\hat{f}(x) = n^{-1} \sum_{i=1}^{n} w(x, Z_i) \quad \text{for all } x \text{ in } B. \tag{2.2}$$

Let $\mathscr{T}_{LD}(n)$ be the set of all linear estimators based on a direct sample of size n subject to the additional condition $\int\int w(x, x')^2\, d\mu(x)\, d\mu(x') < \infty$, and let $\mathscr{T}_{LI}(n)$ be the set of all linear estimators of f based on an indirect sample of size n for which $\int\int w(x, y)^2\, d\mu(x)\, d\lambda(y) < \infty$. The additional square integrability conditions are mild; they ensure that $\hat{f}$ has finite mean integrated square error if f is bounded.

One natural measure of the accuracy of an estimator $\hat{f}$ is the mean integrated square error $M(\hat{f}; f) = E_f \int_B (\hat{f} - f)^2\, d\mu$. By standard calculations,

$$M(\hat{f}; f) = \int \left[\operatorname{var}_f \hat{f}(x) + \left\{ E_f \hat{f}(x) - f(x) \right\}^2 \right] d\mu(x), \tag{2.3}$$

where the suffix f indicates that the mean and variance are calculated for data drawn from f in the direct case and Pf in the indirect case. We define the *surrogate mean integrated square error* $M^*(\hat{f}; f)$ by replacing the variance term in (2.3) by the corresponding term calculated for the uniform density on brain space

$$M^*(\hat{f}; f) = \int \left[\operatorname{var}_1 \hat{f}(x) + \left\{ E_f \hat{f}(x) - f(x) \right\}^2 \right] d\mu(x), \tag{2.4}$$

where var_1 denotes a variance calculated with respect to data drawn from the probability measure μ in the direct case and λ in the indirect case. An important relation between the surrogate and the true mean integrated square error for *linear* estimators is given by the following lemma.

PROPOSITION 2.1. *Suppose that f is bounded above and below away from zero. Then, for all $\hat{f}$ in $\mathscr{T}_{LD}(n)$ or in $\mathscr{T}_{LI}(n)$*

$$\inf_B f(x) \le M(\hat{f}; f)/M^*(\hat{f}; f) \le \sup_B f(x).$$

2.3. *The singular value decomposition of the Radon transform.* The singular value decomposition (SVD) of the normalized Radon transform P defined in (2.1) is the key to our study of the loss of information about f due to indirect observation. To establish notation, let H and K be Hilbert spaces and P: $H \to K$ a bounded linear operator. Under suitable conditions, there exist orthonormal sets of functions ($\{\varphi_\nu\}$ in H and $\{\psi_\nu\}$ in K) and positive real numbers $\{b_\nu\}$, the singular values of P, such that the $\{\varphi_\nu\}$ span the orthogonal complement of the kernel of P, the $\{\psi_\nu\}$ span the range of P, and $P\varphi_\nu = b_\nu \psi_\nu$ for all ν.

Thus P is diagonal in the bases $\{\varphi_\nu\}$ and $\{\psi_\nu\}$. If a singular value b_ν is small, then noise encountered in estimation of the component of f along φ_ν will be amplified by a factor of b_ν^{-1}. Some form of regularization method [Tikhonov and Arsenin (1977)] is needed to deal with this instability, and one such method, based on tapered orthogonal series, will be exploited in Section 4.

In our PET model, H is the space $L^2(B, \mu)$ of functions on brain space that are square-integrable with respect to the dominating measure μ. Correspondingly, K is the space $L^2(D, \lambda)$ of detector-space functions square-integrable relative to λ. Suppose that $X = (X_1, X_2)$ is drawn at random (according to μ) from brain space B. If a direction φ is specified by $u_\varphi = (\cos\varphi, \sin\varphi)$, then

$$Pf(s, \varphi) = E\{ f(X) | u_\varphi \cdot X = s \}$$

From this representation it follows at once that P is a bounded operator from $L^2(B, \mu)$ to $L^2(D, \lambda)$ with norm 1 and, by arguments involving characteristic functions, it is one-to-one.

The SVD of the Radon transform in this specific setting appears to have been first derived by workers in optics and tomography; we now review its properties, drawing material from Born and Wolf [(1975), Chapter 9.2.1 and Appendix VII], Marr (1974) and Deans [(1983), Section 7.6]. Since the underlying spaces are two dimensional, we need double indices, specifically $\nu \in N = \{(l, m)\colon m = 0, 1, 2, \ldots; l = m, m-2, \ldots, -m\}$. In brain space, an orthonormal basis for $L^2(B, \mu)$ is given by

$$\varphi_\nu(r, \theta) = (m+1)^{1/2} Z_m^{|l|}(r) e^{il\theta}, \qquad \nu = (l, m) \in N, (r, \theta) \in B, \tag{2.5}$$

where Z_m^k denotes the *Zernike polynomial* of degree m and order k. Zernike polynomials satisfy the orthogonality relation $\int_0^1 Z_{k+2s}^k(r) Z_{k+2t}^k(r) r\, dr = \frac{1}{2}(k + 2s + 1)^{-1}\delta_{st}$ and can be expressed in terms of the more general family of Jacobi polynomials. They arise naturally from a study of the action of rotation on $L^2(B, \mu)$.

The corresponding orthonormal functions in $L^2(D, \lambda)$ are

$$\psi_\nu(s, \varphi) = U_m(s) e^{il\varphi}, \qquad \nu = (l, m) \in N, (s, \varphi) \in D \tag{2.6}$$

where $U_m(\cos\theta) = \sin(m+1)\theta / \sin\theta$ are the Chebyshev polynomials of the second kind. We have $P\varphi_\nu = b_\nu \psi_\nu$, with the singular values $b_\nu = b_{lm}$ specified by

$$b_\nu = (m+1)^{-1/2}, \qquad \nu = (l, m) \in N. \tag{2.7}$$

The relatively slow decay of the singular values with degree m (independently of l) suggests that the costs of indirect observation in the PET problem are not inordinately large.

Since we work with *real* densities f, we may identify the complex bases (2.5) and (2.6) with equivalent real orthonormal bases in a standard fashion. For example $f = \sum f_\nu \varphi_\nu = \sum \tilde{f}_\nu \tilde{\varphi}_\nu$, where

$$\tilde{\varphi}_{l,m} = \begin{cases} \sqrt{2}\ \mathrm{Re}(\varphi_{l,m}) & \text{if } l > 0, \\ \varphi_{0,m} & \text{if } l = 0, \\ \sqrt{2}\ \mathrm{Im}(\varphi_{l,m}) & \text{if } l < 0 \end{cases}$$

and similarly for the real coefficients $\tilde{f}_{l,m}$. From now on, we suppress the tildes in the notation and use whichever basis is convenient.

2.4. *Smoothness classes.* In our subsequent analysis, we place constraints on the unknown density f over brain space by assuming it lies in a particular class $\mathscr{F}$. For reasons of mathematical tractability, this class is taken to be a particular ellipsoid $\mathscr{F}$ in the Hilbert space $H = L^2(B, \mu)$, specified by an array of constants $\{a_\nu\}$ and a threshold c:

$$\mathscr{F} = \left\{ f = \sum f_\nu \varphi_\nu : \sum a_\nu^2 f_\nu^2 \leq c \right\}. \tag{2.8}$$

Ellipsoid conditions can amount to the imposition of smoothness and integrability requirements. For example in the simple case where $\{\varphi_\nu\}$ is the sequence of trigonometric polynomials in a bounded interval $[0, 2\pi]$ in one dimension and $a_\nu \sim \nu^{-p}$, $\sum a_\nu^2 f_\nu^2 < \infty$ if and only if the periodic function f has p square-integrable derivatives on the interval.

To describe specific ellipsoids in the PET problem, it is useful to transform the index set N by the change of variables $j = (m + l)/2$, $k = (m - l)/2$ into the lattice orthant $N' = \{(j, k);\ j \geq 0, k \geq 0\}$. Using the real version of the basis $\{\varphi_\nu\}$, let

$$\mathscr{F}_{p,C} = \left\{ f \in H : f_{00} = 1, \sum (j+1)^p (k+1)^p f_{jk}^2 \leq 1 + C^2 \right\}. \tag{2.9}$$

This set is characterized by the following proposition.

PROPOSITION 2.2. *The function f in H lies in some $\mathscr{F}_{p,C}$ if and only if f has p weak derivatives that are square integrable on B with respect to the modified dominating measure $d\mu_{p+1}(x) = (p+1)(1 - \|x\|^2)^p \, d\mu(x)$.*

The condition derived in Proposition 2.2 is of course somewhat weaker than requiring square-integrability with respect to μ and the reason for the modification of the dominating measure is discussed in the proof; a similar technical phenomenon occurs in Cox (1988). Nevertheless, $\mathscr{F}_{p,C}$ can be regarded as imposing a set of smoothness and integrability conditions: The higher p is, the smoother are the functions allowed in $\mathscr{F}_{p,C}$.

How smooth are the functions that we are trying to reconstruct? In X-ray transmission tomography, there may be discontinuities, or at least sharp jumps, in tissue density across the boundaries of various regions. As noted by Natterer (1980, 1986), functions that are piecewise smooth with jumps only along smooth curves lie in Sobolev spaces corresponding to $p < \frac{1}{2}$ square integrable (fractional) derivatives. In emission tomography, with its inherently lower resolution, it may perhaps be reasonable to postulate somewhat smoother emission densities of the labelled metabolite. In any case, our theory is presented for arbitrary values of the smoothness $p > 0$ wherever possible.

To ensure that elements of $\mathscr{F}_{p,C}$ are bona fide probability densities, some further restrictions are needed. To have total mass 1, we require $f_{00} = 1$. By restricting the constant C that governs the ellipsoid size, we can ensure that

$f(x) \geq 0$. This is a consequence of the following proposition.

PROPOSITION 2.3. *Suppose* $p \geq 1$ *and* $f \in \mathcal{F}_{p,C}$. *Then*

$$\sup_{x \in B} |f(x) - 1| \leq C2^{(1-p)/2}. \tag{2.10}$$

Equality is attained in (2.10) *if* f *is a linear function of* x.

It follows from the proposition that $\mathcal{F}_{p,C}$ will be a class of nonnegative functions on B if and only if $C \leq 2^{(p-1)/2}$. Note also that if $g = Pf$, then

$$\sup_{y} |g(y) - 1| \leq \sup_{x} |f(x) - 1| \tag{2.11}$$

since P is an averaging operator.

3. Main conclusions of the paper.

3.1. *Arbitrary estimators.* We use minimax mean integrated square error as our basic approach to the quantification of the information available in a given sample. The maximum is taken over a smoothness class $\mathcal{F}_{p,C}$ of unknown functions f, and the minimum is then taken over a class of estimators $\mathcal{T}$, whose specification takes account of whether the sample is direct or indirect. We define the various classes of estimators as in Section 2.2 above, and the smoothness classes $\mathcal{F}_{p,C}$ as in Section 2.4.

Suppose we have a sample from a density f and an estimator $\hat{f}$ of f based on that sample. As assessment of the accuracy of $\hat{f}$ that does not depend on a *particular* unknown f can be obtained by merely restricting f to lie in a fixed class, for example $\mathcal{F}_{p,C}$ for some fixed p and C, and finding the maximum mean integrated square error

$$R(\hat{f}) = \sup_{f \in \mathcal{F}_{p,C}} M(\hat{f}; f). \tag{3.1}$$

The maximum risk gives an indication of how well any given estimator will perform, but a large value of $R(\hat{f})$ might indicate either that there is not much information in the sample or that an inefficient estimator is being used. Because we are interested in the experiment itself rather than any particular estimator, we consider the minimum value of $R(\hat{f})$ over suitable classes of estimators $\hat{f}$.

Define

$$r_D(n) = \inf_{\hat{f} \in \mathcal{T}_D(n)} R(\hat{f}) \tag{3.2}$$

and

$$r_I(n) = \inf_{\hat{f} \in \mathcal{T}_I(n)} R(\hat{f}). \tag{3.3}$$

These minimax risks quantify the information about the unknown density inherent in direct and indirect data sets of size n, in a manner that is independent of the method of estimation. Comparing their relative values gives an

indication of how much information is lost because data can only be observed indirectly in practice.

We can now state our first main result, which gives exact orders of magnitude for $r_D(n)$ and $r_I(n)$ for fixed p and C. The condition placed on C is precisely that needed to ensure that all elements of $\mathscr{F}_{p,C}$ are positive probability densities. Here and subsequently we use the notation $a_n \approx b_n$ to mean that the sequences $\{a_n\}$ and $\{b_n\}$ satisfy $\inf_n(a_n/b_n) > 0$ and $\sup_n(a_n/b_n) < \infty$.

THEOREM 3.1. *For fixed $p \geq 1$ and $0 < C < 2^{(p-1)/2}$, with the definitions* (3.1)–(3.3),

$$r_D(n) \approx (\log n/n)^{p/(p+1)} \tag{3.4}$$

and

$$r_I(n) \approx (1/n)^{p/(p+2)}. \tag{3.5}$$

The proof of Theorem 3.1 is given in Sections 4 and 5 below. It can be seen from (3.4) and (3.5) that the effect of the indirect nature of the observations taken in practice is to reduce somewhat the rate at which the minimax risk converges to zero. Suppose, for example, $p = 1$, corresponding to f having square-integrable first weak derivatives. Then (neglecting the logarithmic term) the rate is reduced from $n^{-1/2}$ to $n^{-1/3}$ by taking indirect rather than direct observations. Note that both these rates are slower than the n^{-1} rate usually obtained for mean square error in parametric statistics; this is because, even with the restriction that f lies in $\mathscr{F}_{p,C}$, the space of possible parameters is infinite dimensional.

Theorem 3.1 also leads to some qualitative conclusions about equivalent sample sizes. Define the *equivalent sample size* $m(n)$ to a given indirect sample size n to be the number of emissions knowledge of whose original positions in the brain would allow us to estimate f with the same minimax accuracy, so that

$$r_D(m(n)) = r_I(n). \tag{3.6}$$

Some simple algebra from (3.4) and (3.5) yields the order of magnitude of the equivalent sample size as

$$m(n) \approx n^{(p+1)/(p+2)} \log n. \tag{3.7}$$

Perhaps not surprisingly, the order of magnitude of the equivalent sample size depends on the smoothness assumptions made on the density f. The smoother f is assumed to be, the larger will be the index p. Hence for very smooth densities the power in (3.7) will be close to 1 and little will be lost as a result of the indirect nature of the observation process. However, in reality, we ought not to assume that the true emission density necessarily varies very smoothly, since tissue boundaries and/or localized areas of high metabolic activity may lead to discontinuities, certainly in high derivatives of f and possibly in f itself.

3.2. *Linear estimators.* More precise numerical quantitative conclusions cannot be drawn directly from (3.7), because Theorem 3.1 only gives orders of

TABLE 1
Constants needed for Theorem 3.2. Euler's constant $\gamma_E = 0.57722\ldots$.

$c_1 = \exp(-c_8/c_7)$	$c_5 = (p+1)^{1/(p+1)}c_7^{p/(p+1)}$
$c_2 = c_7^{-1}(p+1)\exp\{(p+1)c_8/c_7\}$	$c_6 = \frac{1}{2}\{\pi^2 p/3(p+4)\}^{p/(p+2)}(p+2)^{2/(p+2)}$
$c_3 = p(p+2)^{-1}$	$c_7 = p(p+1)^{-1}(p+2)^{-1}$
$c_4 = 2\gamma_E - (p+4)/(p+2)$	$c_8 = 2\gamma_E c_7 - \{4(p+2)^{-2} - (p+1)^{-2}\}$

magnitude for the relevant risks. We are able, however, to give explicit approximate numerical equivalent sample sizes for minimax risks calculated restricting attention to linear estimators and using as a measure of error the surrogate mean integrated square error M^* defined in (2.4). By analogy to (3.2) and (3.3) define *surrogate linear minimax risks* $r^*_{LD}(n)$ and $r^*_{LI}(n)$ by

$$r^*_{LD}(n) = \inf_{\hat{f}\in\mathscr{T}_{LD}(n)} \sup_{f\in\mathscr{F}_{p,C}} M^*(\hat{f}; f) \tag{3.8}$$

and

$$r^*_{LI}(n) = \inf_{\hat{f}\in\mathscr{T}_{LI}(n)} \sup_{f\in\mathscr{F}_{p,C}} M^*(\hat{f}; f). \tag{3.9}$$

The second main result gives leading terms of asymptotic expansions for r^*_{LD} and r^*_{LI}. The leading orders of magnitude are exactly the same as those given for the corresponding quantities in Theorem 3.1, and so the restriction to linear estimators does not affect the rates of convergence available. All the constants c_j depend only on the smoothness p and are collected in Table 1. One of our reasons for introducing surrogate mean integrated square error is that we have been able to derive these more precise expressions and, hence, obtain numerical results. The other reason is that the result of Theorem 3.2 is a key step in the proof of Theorem 3.1.

THEOREM 3.2. *For* $x > 1$, *let* $\alpha(x)$ *denote the solution to* $\alpha\log\alpha = x$, *and set*

$$\eta_n^{p+1} = c_1^{p+1}\alpha(c_2 nC^2). \tag{3.10}$$

Then, provided $0 < C \le 2^{(p-1)/2}$,

$$r^*_{LD}(n) = c_3 n^{-1}\eta_n(\log\eta_n + c_4) + O(n^{-1}\eta_n^{1/2}) \tag{3.11}$$

$$= c_5 C^{2/(p+1)}(\log n/n)^{p/(p+1)}\{1 + o(1)\} \tag{3.12}$$

and

$$r^*_{LI}(n) = c_6 C^{4/(p+2)}n^{-p/(p+2)} + O(n^{-(p+1)/(p+2)}\log n). \tag{3.13}$$

The form (3.12) for r^*_{LD} is more transparent, but the error term can be shown to have the same polynomial order as the leading term; the error term in (3.11) is of lower order and so we use (3.11) in numerical computations. Of course, $\alpha(x)$ can be found numerically when required and is asymptotic to $x/\log x$ for large x.

For any particular indirect sample size n, the approximate equivalent sample size $m^*(n)$ can be found: Equate the expressions (3.11) for $r^*_{LD}(m^*)$ and (3.13) for

TABLE 2
Equivalent direct sample sizes $m^*(n)$ to achieve the same surrogate linear minimax risk over smoothness class p as for an indirect sample of size n.

	$n = 10^7$	$n = 10^8$	ratio $m(10^8) / m(10^7)$
$p = 1$	1.93×10^5	1.03×10^6	5.34
$p = 2$	4.85×10^5	3.12×10^6	6.44
$p = 5$	1.29×10^6	1.05×10^7	8.09

$r_{LI}^*(n)$, neglect the lower order terms and solve numerically for m^*. For definiteness we take $C^2 = 2^{p-1}$, the largest value for which all f in $\mathcal{F}_{p,C}$ are nonnegative probability densities, so long as $p \geq 1$ (Proposition 2.3). Some representative cases are given in Table 2. As expected, the equivalent sample size increases as the assumed amount of smoothness rises. If technology allows an order of magnitude increase in the amount of data collected, then the equivalent direct sample sizes increase by a factor of between 5 and 8, this factor itself increasing with assumed smoothness.

For the quantity $m^*(n)$ the asymptotic constant of proportionality in the expression corresponding to (3.7) can be found. A simple calculation uses relations (3.12) and (3.13), with the error terms ignored, to conclude that

$$m^*(n) = (p+1)(p+2)^{-1}(c_5/c_6)^{(p+1)/p}C^{-2/(p+2)} \times n^{(p+1)/(p+2)} \log n\{1 + o(1)\}.$$

In summary, our results confirm intuition that for the PET problem, the amount of information available is still substantial, but it is by no means as great as if a sample of the same number of direct observations were available.

4. Convergence rates for linear estimators. The main aim of this section is to prove Theorem 3.2, which gives the asymptotic behaviour of the surrogate risks (2.4) for linear estimators. It is a consequence of Propositions 2.1 and 2.3 that, provided $C < 2^{(p-1)/2}$, the ratio of exact to surrogate mean integrated square error for linear estimates will be bounded above and below away from 0 uniformly over $\mathcal{F}_{p,C}$. Since $\mathcal{T}_{LD}(n)$ and $\mathcal{T}_{LI}(n)$ are subclasses of $\mathcal{T}_D(n)$ and $\mathcal{T}_I(n)$, respectively, it then follows that the orders of magnitude of $r_D(n)$ and $r_I(n)$ are bounded above by those obtained in Theorem 3.2 for surrogate linear minimax risks. Once Theorem 3.2 has been proved, the proof of Theorem 3.1 will be completed in Section 5 by showing that these are also lower bounds.

4.1. *Structure of the linear minimax estimator.* We consider the indirect case first; the argument we shall use will apply to the direct case also. We start by defining some notation. Suppose that $\hat{f}$ is in $\mathcal{T}_{LI}(n)$. For ν and π in N define $w_{\nu\pi} = \int w(x, y)\varphi_\nu(x)\psi_\pi(y)\, d\mu(x)\, d\lambda(y)$; because of the condition

$\int\int w^2\,d\mu\,d\lambda < \infty$, standard functional analysis gives that, in the L^2 sense,

$$w(x, y) = \sum_{\nu}\sum_{\pi} w_{\nu\pi}\varphi_{\nu}(x)\psi_{\pi}(y). \tag{4.1}$$

As in Sections 2.3 and 2.4, we expand f as $\Sigma f_{\nu}\varphi_{\nu}$. We write W for the infinite matrix $(w_{\nu\pi})$ and $\mathbf{f}$ for the vector (f_{ν}). The index set of all vectors and matrices will be the set N; the subscript $(0,0)$ will be written as 0 for simplicity. Since $\int f\,d\mu = 1$, the coefficient $f_0 = 1$. Write $B = \operatorname{diag}(b_{\nu})$, the singular values of the operator P. Let $\mathbf{e}_{\nu}$ be the vector $(\delta_{\nu\pi}\colon\ \pi \in N)$. The first lemma gives a matrix form for the surrogate mean integrated square error of the linear estimator $\hat{f}$.

LEMMA 4.1. *With the above definitions,*

$$M^*(\hat{f}; f) = n^{-1}\operatorname{tr} W\big(I - \mathbf{e}_0\mathbf{e}_0^T\big)W + \mathbf{f}^T(I - WB)^T(I - WB)\mathbf{f}. \tag{4.2}$$

PROOF. Write $\hat{f} = \Sigma\hat{f}_{\nu}\varphi_{\nu}$. From (4.1) it follows that $\hat{\mathbf{f}} = W\boldsymbol{\eta}$, where $\eta_{\nu} = n^{-1}\Sigma_i\psi_{\nu}(Y_i)$. Each Y_i has density $g = \Sigma g_{\nu}\psi_{\nu}$, where $\mathbf{g} = B\mathbf{f}$, and for each ν, $E_f\eta_{\nu} = \int\psi_{\nu}g\,d\lambda = g_{\nu}$, so that $E_f\boldsymbol{\eta} = B\mathbf{f}$. Hence $E_f\hat{\mathbf{f}} = WB\mathbf{f}$, and the integrated square bias

$$\int\big(E_f\hat{f} - f\big)^2\,d\mu = \|E\hat{\mathbf{f}} = \mathbf{f}\|^2 = \|WB\mathbf{f} - \mathbf{f}\|^2 = \|(I - WB)\mathbf{f}\|^2. \tag{4.3}$$

If f is the uniform density, then $\mathbf{f} = \mathbf{e}_0$ and so, writing E_1 for an expectation relative to the uniform density f, $E_1\boldsymbol{\eta} = B\mathbf{e}_0 = \mathbf{e}_0$, since $b_0 = 1$.

By the orthonormality of the ψ_{ν}, the matrix $E_1\boldsymbol{\eta}\boldsymbol{\eta}^T = n^{-1}I$ and so $\boldsymbol{\eta}$ has covariance matrix $n^{-1}(I - \mathbf{e}_0\mathbf{e}_0^T)$ under the uniform distribution. Thus, the surrogate variance term

$$\begin{aligned}\int \operatorname{var}_1\hat{f}\,d\mu &= E_1\|\hat{\mathbf{f}} - E_1\hat{\mathbf{f}}\|^2 = E_1\|W(\boldsymbol{\eta} - E_1\boldsymbol{\eta})\|^2 \\ &= n^{-1}\operatorname{tr} W\big(I - \mathbf{e}_0\mathbf{e}_0^T\big)W^T\end{aligned} \tag{4.4}$$

by a standard multivariate calculation. To complete the proof, substitute (4.3) and (4.4) into the definition (2.4) of surrogate mean integrated square error. □

Our second lemma provides an expression for the surrogate linear minimax risk and gives the general form of the minimax estimator. The smoothness class $\mathscr{F}$ is defined as in (2.8) and (2.9) to be $\mathscr{F} = \{f\colon\ f_0 = 1, \mathbf{f}^TA\mathbf{f} \le 1 + C^2\}$, where we write $A = \operatorname{diag}(a_{\nu}^2)$ and assume that $a_0 = 1$, $\sup a_{\nu}^2 = \infty$ and that every f in $\mathscr{F}$ is nonnegative.

LEMMA 4.2.

$$\inf_{\hat{f}\in\mathscr{T}_{LI}(n)}\sup_{f\in\mathscr{F}} M^*(\hat{f}; f) = n^{-1}\sum b_{\nu}^{-2}\big(1 - a_{\nu}\gamma^{1/2}\big)_+, \tag{4.5}$$

where γ *is chosen to ensure that*

$$n^{-1}\sum_{\nu\neq 0} b_\nu^{-2}a_\nu^2\left(\gamma^{-1/2}a_\nu^{-1}-1\right)_+ = C^2. \tag{4.6}$$

The minimax estimator is given by setting, in (4.1),

$$w_{\nu\pi} = \delta_{\nu\pi} \text{ for } \nu = 0 \quad \text{and} \quad w_{\nu\pi} = \delta_{\nu\pi}b_\nu^{-1}\left(1-\gamma^{1/2}a_\nu\right)_+ \text{ otherwise.} \tag{4.7}$$

The form of the minimax estimator is worth noting, since it corresponds to a *diagonal* matrix of weights and, hence, is an estimator of the form $\hat{f}(x) = n^{-1}\Sigma b_\nu^{-1}u_\nu\psi_\nu(Y_i)\varphi_\nu(x)$. Although the derivation of the estimator has been performed for theoretical reasons, some examples of the use of estimators of this kind are given by Jones and Silverman (1989). Similar results to Lemma 4.2 exist for standard regression [for example, Pinsker (1980) and Speckman (1985)] and for other nonparametric problems [for example, Buckley, Eagleson and Silverman (1988)]. Our proof is an extension of that of Speckman [(1985), pages 981–982].

PROOF OF LEMMA 4.2. The condition $\int w(x, y)\,d\mu(x) = 1$ for all y implies that $w_{00} = 1$ and $w_{0\nu} = 0$ for $\nu \neq 0$. Let $\mathcal{W}$ be the set of matrices W satisfying this condition and for which $\Sigma\Sigma w_{\nu\pi}^2 < \infty$; the matrices W in $\mathcal{W}$ correspond precisely to the estimators $\hat{f}$ in $\mathcal{T}_{LI}(n)$. We use Lemma 4.1 and find the minimax value of the expression (4.2) over W in $\mathcal{W}$ and f in $\mathcal{F}$. Let

$$J(W) = \sup_{f\in\mathcal{F}}\left\{\|(I-WB)\mathbf{f}\|^2 + n^{-1}\operatorname{tr} W\left(I-\mathbf{e}_0\mathbf{e}_0^T\right)W^T\right\}. \tag{4.8}$$

Let W^0 be the matrix $\operatorname{diag}(w_{\nu\nu})$; we show that $J(W) \geq J(W^0)$ and, hence, that we may restrict attention to diagonal matrices in $\mathcal{W}$.

For fixed κ in N, $\kappa \neq 0$, let $\mathcal{F}_\kappa$ be the set $\{f = 1 + f_\kappa\varphi_\kappa,\ a_\kappa^2 f_\kappa^2 \leq C^2\}$. Then

$$\begin{aligned}
\sup_{\mathcal{F}_\kappa}\|(I-WB)\mathbf{f}\|^2 &= \sup_{\mathcal{F}_\kappa}\sum_\nu\left(w_{\nu 0} + w_{\nu\kappa}b_\kappa f_\kappa - f_\nu\right)^2 \\
&\geq \sup_{\mathcal{F}_\kappa}\left\{w_{\kappa 0} + \left(w_{\kappa\kappa}b_\kappa - 1\right)f_\kappa\right\}^2 \qquad (4.9)\\
&\geq \left(1 - w_{\kappa\kappa}b_\kappa\right)^2 C^2/a_\kappa^2,
\end{aligned}$$

by picking out the κ term from the summation and performing some elementary algebra. Again by restricting the sum, we have

$$\operatorname{tr} W\left(I-\mathbf{e}_0\mathbf{e}_0^T\right)W^T = \sum_{\nu\neq 0}\sum_{\pi\neq 0} w_{\nu\pi}^2 \geq \sum_{\nu\neq 0} w_{\nu\nu}^2. \tag{4.10}$$

Restricting the supremum to f in $\cup\mathcal{F}_\kappa$ and substituting (4.9) and (4.10), we obtain

$$J(W) \geq \sup_{\kappa\neq 0}\left(1 - w_{\kappa\kappa}b_\kappa\right)^2 C^2/a_\kappa^2 + n^{-1}\sum_{\nu\neq 0} w_{\nu\nu}^2 = J(W^0) \tag{4.11}$$

by checking that every inequality in our argument is an exact equality when W is diagonal.

Let $\gamma = \sup_{\kappa \neq 0}(1 - w_{\kappa\kappa}b_\kappa)^2 a_\kappa^{-2}$. Now reason from (4.11) as in Speckman (1985) to obtain (4.7); then substitute into the expression for $J(W^0)$ in (4.11) and minimize over γ to complete the proof. □

To obtain corresponding results for the direct case, set the operator P to the identity in the whole of the preceding argument. The minimax surrogate risk $r_{LD}^*(n)$ is given by (4.5) and (4.6) with all b_ν set to 1. The minimax estimator $n^{-1}\sum_{i,\nu} w_{\nu\nu}\varphi_\nu(X_i)\varphi_\nu(x)$ is a probability density estimate of tapered orthogonal series form as introduced and studied by Watson (1969).

4.2. *Integral approximation of the minimax risks.* In this subsection we explicitly approximate the expression (4.5), and the corresponding expression for the direct case, to complete the proof of Theorem 3.2. We set $\mathscr{F} = \mathscr{F}_{p,C}$ as in (2.4) so that $a_{jk}^2 = (j+1)^p(k+1)^p$. The key to our treatment is the following approximation lemma, obtained by approximating sums by integrals.

LEMMA 4.3. *For any η, let $\sum_{(\eta)}$ denote a sum over*

$$\{(j,k): 1 < (j+1)(k+1) \leq \eta\}.$$

For fixed $r \geq 0$, as $\eta \to \infty$,

$$\sum_{(\eta)} (j+1)^r(k+1)^r = (r+1)^{-1}\eta^{r+1}\left\{\log \eta + 2\gamma_E - (r+1)^{-1}\right\} + O\left(\eta^{r+1/2}\right), \tag{4.12}$$

where γ_E is Euler's constant, and

$$\sum_{(\eta)} (j+k+1)(j+1)^r(k+1)^r = \tfrac{1}{3}\pi^2(r+2)^{-1}\eta^{r+2} + O\left(\eta^{r+1}\log \eta\right). \tag{4.13}$$

PROOF. For the proof, we transform the sums by replacing $j+1$ by j and $k+1$ by k; denote by $\sum_{[\eta]}$ the sum over the transformed range $\{(j,k): j \geq 1, k \geq 1 \text{ and } 1 < jk \leq \eta\}$. By symmetry in (j,k), the sum in (4.12) satisfies

$$1 + S = \sum_{[\eta]} j^r k^r = 2\sum_{k=1}^{[\eta^{1/2}]} k^r \sum_{j=1}^{[\eta k^{-1}]} j^r - \sum_{j=1}^{[\eta^{1/2}]}\sum_{k=1}^{[\eta^{1/2}]} j^r k^r.$$

From the relation $\Sigma_{j=1}^{t} j^r = (r+1)^{-1}t^{r+1} + O(t^r)$, we obtain

$$\begin{aligned} S &= 2(r+1)^{-1}\sum_{k=1}^{[\eta^{1/2}]} k^r\left\{\left[\eta k^{-1}\right]^{r+1} + O(\eta^r k^{-r})\right\} \\ &\quad - \left\{(r+1)^{-1}\left[\eta^{1/2}\right]^{r+1} + O(\eta^{r/2})\right\}^2 - 1 \\ &= 2(r+1)^{-1}\eta^{r+1}\sum_{k=1}^{[\eta^{1/2}]} k^{-1} - \sum_{k=1}^{[\eta^{1/2}]} k^r\left\{\left(\eta k^{-1}\right)^{r+1} - \left[\eta k^{-1}\right]^{r+1}\right\} \\ &\quad - (r+1)^{-2}\eta^{r+1} + O(\eta^{r+1/2}) \\ &= 2(r+1)^{-1}\eta^{r+1}\left\{\tfrac{1}{2}\log\eta + \gamma + O(\eta^{-1/2})\right\} - (r+1)^{-2}\eta^{r+1} \\ &\quad + O(\eta^{r+1/2}), \end{aligned} \tag{4.14}$$

which yields the result of (4.12).

To deal with (4.13), we need an integral approximation, valid for $s \geq 0$ and $x \geq 1$,

$$\sum_{j=1}^{[x]} j^s = (s+1)^{-1}x^{s+1} + c_{sx}x^s, \qquad 0 \leq |c_{sx}| \leq c_s, \tag{4.15}$$

which follows from the bounds $(s+1)^{-1}[x]^{s+1} \leq \int_0^{[x]} t^s\,ds \leq \Sigma_{j=1}^{[x]} j^s \leq \int_1^{[x+1]} t^s\,ds \leq (s+1)^{-1}[x+1]^{s+1}$. Assuming that η is an integer, it then follows that

$$\begin{aligned} 1 + \sum_{[\eta]} j^{r+1}k^r &= \sum_{k=1}^{\eta} k^r \sum_{j=1}^{[\eta k^{-1}]} j^{r+1} \\ &= \sum_{k=1}^{\eta} k^r(r+2)^{-1}\left(\eta k^{-1}\right)^{r+2} + \sum_{k=1}^{\eta} k^r c_{r+1,\eta,k}\left(\eta k^{-1}\right)^{r+1} \\ &= (r+2)^{-1}\eta^{r+2}\sum_{1}^{\eta} k^{-2} + O\left(\eta^{r+1}\sum_{1}^{\eta} k^{-1}\right) \\ &= \tfrac{1}{6}\pi^2(r+2)^{-1}\eta^{r+2} + O(\eta^{r+1}\log\eta). \end{aligned} \tag{4.16}$$

To complete the proof of (4.13), transform the sum to $\Sigma_{[\eta]}(j^{r+1}k^r + j^r k^{r+1} - j^r k^r)$. Then substitute (4.16) for each of the first two terms and use (4.15) to absorb the third term into the error. □

COMPLETION OF PROOF OF THEOREM 3.2. We will have $\gamma a_\nu^2 \leq 1$ if and only if $(j+1)(k+1) \leq \gamma^{-1/p}$ and so the $(\ )_+$ in (4.6) and (4.7) may be replaced with $(\ )$ if the sums over all ν are replaced by $\Sigma_{(\eta)}$ with $\eta = \gamma^{-1/p}$. The constants c_r will be defined as in Table 1.

In the direct case, we replace $\mathscr{T}_{LI}$ in (4.5) by $\mathscr{T}_{LD}$ and set all b_ν to 1. Applying (4.12), (4.6) becomes

$$\begin{aligned} C^2 &= n^{-1}\sum_{(\eta)}\left(\gamma^{-1/2}a_\nu - a_\nu^2\right) \\ &= n^{-1}\sum_{(\eta)}\left\{\gamma^{-1/2}(j+1)^{p/2}(k+1)^{p/2} - (j+1)^p(k+1)^p\right\} \\ &= n^{-1}\eta^{p+1}(c_7\log\eta + c_8) + n^{-1}O\left(\eta^{p+1/2}\right). \end{aligned} \tag{4.17}$$

The substitution $\eta = c_1 y^{1/(p+1)}$ reduces equation (4.17) with the error term omitted to the form $y\log y = c_2 nC^2$; it follows that η_n as defined in (3.10) is the solution for η of this equation. Apply similar manipulations to (4.5) to obtain

$$r_{LD}^*(n) = n^{-1}\sum_{(\eta)}\left(1 - \gamma^{1/2}a_\nu\right) = c_3 n^{-1}\eta_n\{\log\eta_n + c_4\} + n^{-1}O\left(\eta_n^{1/2}\right),$$

completing the proof of (3.11). To prove (3.12), substitute the definition of η_n into (3.11) and use the fact that that $\alpha(x) = (x/\log x)\{1 + o(1)\}$ for large x.

For the indirect case, we use the values (2.7) for the b_ν. Equation (4.6) then becomes

$$\begin{aligned} C^2 &= n^{-1}\sum_{(\eta)}(j+k+1)\left\{\gamma^{-1/2}(j+1)^{p/2}(k+1)^{p/2} - (j+1)^p(k+1)^p\right\} \\ &= c_9 n^{-1}\eta^{p+2} + n^{-1}O\left(\eta^{p+1}\log\eta\right). \end{aligned} \tag{4.18}$$

where $c_9 = (\pi^2/3)p(p+2)^{-1}(p+4)^{-1}$. Set $\tilde{\eta}_n = (nC^2/c_9)^{1/(p+2)}$, the solution to (4.18) with the error omitted. Then the solution to (4.18) with the error included satisfies $\eta = \tilde{\eta}_n + O(\log\tilde{\eta}_n)$. Substitute back into (4.5), apply Lemma 4.3 and perform some elementary algebra to obtain (3.13) and, hence, to complete the proof of Theorem 3.2. □

To summarize this section, we have shown that, for linear estimators, the indirect nature of the PET observations reduces the minimax rate of consistency in mean integrated square error from $O\{(n/\log n)^{-p/(p+1)}\}$ to $O(n^{-p/(p+2)})$. It will be shown in the next section that these rates of consistency are both best possible even if we allow the class of estimators to be extended to cover all linear and nonlinear estimators.

5. Lower bounds. In this section we establish lower bounds on the rates of consistency of arbitrary estimators based on direct and indirect observations. These lower bounds show that the minimax rates obtained for linear estimators in Section 4 cannot be improved by extending the class of estimators considered. As noted at the beginning of Section 4, this will complete the proof of Theorem 3.1.

5.1. *Moduli of continuity and a general lower bound for global norms.* Our approach is based on Fano's lemma of information theory, as developed by

Ibragimov and Hasminskii [e.g., (1981)] and Birgé (1983), although a slight extension of Birgé's formulation is needed for the indirect observation case. Although we continue to focus on the PET example, it will be seen that the methodology applies quite generally to estimation with global norms in linear inverse problems of both density and regression estimation type.

The convergence rate in the indirect problem clearly depends on the operator P^{-1} mapping the observable density g to the target density f. One convenient approach to computing convergence rates has two parts: (i) compute a "modulus of continuity" $\tau(\varepsilon)$ for P^{-1}, and (ii) argue that a lower bound to the minimax convergence rate is given by (essentially) $\tau(n^{-1/2})$. This approach separates stochastics and analysis: Step (ii) uses the information theory lemma to bound the estimation error by $\tau(n^{-1/2})$, while step (i) is a concrete optimization problem for the particular operator in question. This viewpoint was taken recently by Donoho and Liu (1989) in their study of estimation of linear functionals. We begin with step (ii), which computes a modulus $\sigma(\delta)$ that is more convenient for the problems at hand. We return to step (i) in Section 5.2.

Suppose, in general, there are available n i.i.d. observations $Y^{(n)} = (Y_1, \ldots, Y_n)$ from a density $g(y)\,d\lambda(y)$, $y \in D$ and that we wish to estimate $f = P^{-1}g$. We assume that $f \in \mathscr{F} \subset H$, and that $\mathscr{F}$ is a translate $f^0 + H_0$ of a set H_0 that is balanced about the origin ($h \in H_0 \Rightarrow -h \in H_0$). Let M be a finite-dimensional subspace of H. We write $|M|$ for the dimension of M and $B_M(\delta)$ for the open ball of radius δ about 0 in M. The norm of the restriction of P to M is defined by $\|P\|_M = \sup\{\|Ph\|/\|h\|\colon\ h \in M\}$. Finally, let $\mathscr{M}_\delta = \{M\colon\ B_M(\delta) \subset H_0\}$. The modulus $\sigma(\delta)$ may now be defined as

$$\sigma(\delta) = \delta \inf\{\|P\|_M/|M|^{1/2}\colon\ M \in \mathscr{M}_\delta\}. \tag{5.1}$$

Loosely speaking, $\sigma(\delta)$ measures the decay of the singular values of P relative to the parameter space H_0 at resolution δ. Since σ is strictly increasing, a left-continuous inverse $\tau(\varepsilon) = \sigma^{-1}(\varepsilon)$ can be defined.

Let $\hat{f} \in \mathscr{T}_I(n)$ be an arbitrary estimator based on $Y^{(n)}$. The significance of the modulus functional is that an (often sharp) lower bound for the rate of convergence of $\|\hat{f} - f\|$ over $\mathscr{F}$ is given by $\tau(n^{-1/2})$. For the proof we need an additional assumption bounding the Kullback–Leibler information divergence $K(g_\alpha, g_\beta) = \int \log(g_\alpha/g_\beta) g_\alpha\,d\lambda$ over $\mathscr{G} = P\mathscr{F}$:

(5.2) For some $A < \infty$, $K(g_\alpha, g_\beta) \le A\|g_\alpha - g_\beta\|_K^2$ for all $g_\alpha, g_\beta \in \mathscr{G}$.

This condition will be satisfied provided the densities g in $\mathscr{G}$ are uniformly bounded above and below away from zero. In the context of Theorem 3.1, this is a consequence of (2.11) and (2.10).

PROPOSITION 5.1. *If condition* (5.2) *holds, there exist constants* d_1, d_2 *such that*

$$\inf_{\hat{f} \in \mathscr{T}_I(n)} \sup_{f \in \mathscr{F}} E_f \|\hat{f} - f\|_H^2 \ge d_1 \tau^2\big(d_2 n^{-1/2}\big). \tag{5.3}$$

PROOF. Choose a subset $\mathscr{F}^0 = \{f_1, \ldots, f_r\} \subset \mathscr{F}$ that is 2δ-*distinguishable*: namely, $\|f_\alpha - f_\beta\| > 2\delta$ if $\alpha \ne \beta$. Set $g_\alpha = Pf_\alpha$ and write $K^n(g_\alpha, g_\beta) =$

$n\int \log(g_\alpha/g_\beta)g_\alpha\, d\lambda$, the Kullback–Leibler discrepancy based on a sample of size n.

Consider the discrimination problem of choosing among the r hypotheses $\mathscr{F}^0$. Given an estimator $\hat{f} \in \mathscr{T}_I(n)$, define a discrimination rule $\varphi(Y^{(n)})$ taking values in $\mathscr{F}^0$ that picks the closest element in $\mathscr{F}^0$ to $\hat{f}$. Then, by elementary probability and analysis,

$$\begin{aligned}\sup_{f\in\mathscr{F}} E_f\|\hat{f}-f\|^2 &\geq \sup_{f\in\mathscr{F}^0} E_f\|\hat{f}-f\|^2 \geq \delta^2 \sup_{f\in\mathscr{F}^0} P_f\big(\|\hat{f}-f\|>\delta\big)\\ &\geq \delta^2 r^{-1}\sum_{\alpha=1}^{r} P_{f_\alpha}\big(\|\hat{f}-f_\alpha\|>\delta\big) \geq \delta^2 r^{-1}\sum_{\alpha=1}^{r} P_{f_\alpha}\big\{\varphi(Y^{(n)})\neq f_\alpha\big\},\end{aligned} \tag{5.4}$$

since $\varphi(Y^{(n)}) \neq f_\alpha$ implies that $\|\hat{f}-f_\alpha\| > \delta$, because of the 2δ-distinguishability.

By Birgé's version [(1983), page 196] of Fano's lemma, the average error rate in the discrimination problem can be bounded below as follows:

$$\begin{aligned}&r^{-1}\sum_{\alpha=1}^{r} P_{f_\alpha}\big(\varphi(Y^{(n)})\neq f_\alpha\big)\\ &\quad\geq 1-\Big\{\sup_{1\leq\alpha,\beta\leq r} K^n(g_\alpha,g_\beta)+\log 2\Big\}/\log(r-1).\end{aligned} \tag{5.5}$$

Combining (5.4) and (5.5), and substituting (5.2), we obtain the lower bound

$$\delta^{-2}\sup_{f\in\mathscr{F}} E_f\|\hat{f}-f\|^2 \geq 1-\Big\{nA\sup_{1\leq\alpha,\beta\leq r}\|Pf_\alpha-Pf_\beta\|_K^2+\log 2\Big\}/\log(r-1). \tag{5.6}$$

To make use of this lower bound, we use the metric dimension properties of $\mathscr{F}$ and the operator P to construct a suitable set $\mathscr{F}^0$ for which r is large and $\sup\|Pf_\alpha - Pf_\beta\|_K^2$ is small. From the definition (5.1) of the modulus σ, choose a subspace M of H for which $B_M(4\delta) \subset H_0$ and $4\delta\|P\|_M/|M|^{1/2} \leq 2\sigma(4\delta)$. A useful lemma of approximation theory [e.g., Lorentz (1966), page 905] asserts that a k-dimensional ball of radius R contains an $(R/2)$-distinguishable subset of cardinality at least 2^k. Setting $r = 2^{|M|}$, use this lemma to choose $h_1,\ldots,h_r \in B_M(4\delta)$ such that $\|h_\alpha - h_\beta\| \geq 2\delta$ and define the 2δ-distinguishable set $\mathscr{F}^0$ by $f_\alpha = f^0 + h_\alpha$ for $\alpha = 1,\ldots,r$. By construction, for any α and β,

$$\begin{aligned}&\|Pf_\alpha - Pf_\beta\|_K^2\\ &\quad\leq \|P\|_M^2\|f_\alpha - f_\beta\|^2 \leq \tfrac{1}{4}\delta^{-2}|M|\sigma(4\delta)^2\cdot 64\delta^2 = 16|M|\sigma(4\delta)^2.\end{aligned} \tag{5.7}$$

Substituting back into (5.6), and performing some elementary algebra, we have $\sup_{\mathscr{F}} E_f\|\hat{f}-f\|^2 \geq \delta^2[1 - d_3 n\sigma^2(4\delta)]$ where d_3 is an appropriate constant. Now choose δ so that $d_3 n\sigma^2(4\delta) = \frac{1}{2}$ and the proof of Proposition 5.1 is complete. □

The estimation problem we study can be thought of as estimation of Qg, where $g \in \mathscr{G}$ and Q $(= P^{-1})$ is an unbounded operator. The term "modulus of continuity" might be more appropriately applied to a measure of the rate of

growth of the singular values of Q relative to $\mathscr{G}$. Indeed it is in this form that the similarity to the modulus of Donoho and Liu (1989) is clearer. Now suppose that $\mathscr{G}$ is a translate $g^0 + K_0$ of a set balanced about the origin in K. We denote finite-dimensional balls about 0 in K by U. Define the normalized radius $\rho(U)$ to be the radius of U divided by the square root of the dimension of U.

Define a generalized modulus of continuity of Q over the parameter space K_0 by

$$\tilde{\tau}(\varepsilon) = \sup_{U} \inf_{v \in \partial U} \|Qv\|_H, \tag{5.8}$$

where the supremum is taken over the class of finite dimensional balls $U \subset K_0$ for which $\rho(U) = \varepsilon$. Notice that if Q is a linear *functional* [so that $(H, \|\cdot\|_H) = (\mathbf{R}, |\cdot|)$], the above definition reduces to

$$\tau(\varepsilon) = \sup\{|Qv|: \|v\|_K = \varepsilon \text{ and } tv \in K_0 \text{ for } |t| \le 1\},$$

which is the modulus of continuity studied by Donoho and Liu (1989).

It can be shown that $\tilde{\tau}$ is approximately inversely related to the modulus σ defined at (5.1) in the sense that $\tilde{\tau}(\sigma(\delta)) \le \delta$. Thus $\sigma^{-1}(\varepsilon) \ge \tilde{\tau}(\varepsilon)$, and so the lower rate bounds derived from use of σ are at least as good as those that would follow from $\tilde{\tau}$. It turns out that these rate bounds are in fact equivalent for all the applications discussed in this paper. These results and extensions will be discussed more fully elsewhere.

5.2. *Completion of Proof of Theorem* 3.2. We now return to the PET setting to prove two propositions that complete the proof of Theorem 3.1. Both these are proved by finding reasonable lower bounds to $\tau(\varepsilon)$.

PROPOSITION 5.2. *Subject to the conditions of Theorem* 3.1, *there exists a constant* $d_D(p, C) > 0$ *such that*

$$r_D(n) \ge d_D(\log n/n)^{p/(p+1)}.$$

PROOF. Set $H = K = L^2(B, \mu)$ and $P = I$. Let f^0 be the uniform density and $H_0 = \mathscr{F}_{p,C} - f^0$. A good upper bound for $\sigma(\delta)$ as defined in (5.1) can be obtained by considering high dimensional subspaces M subject to the constraint that $B_M(\delta) \subset H_0$. For large η, let $M_\eta = \text{span}\{\varphi_\nu: a_\nu^2 \le \eta^p\}$. Then $B_{M_\eta}(\delta) \subset H_0$ when $\eta^p \le C^2/\delta^2$. From the definition of $\sigma(\delta)$, it follows that

$$\sigma^2(\delta) \le \delta^2/\sup\{|M_\eta|: \eta^p \le C^2/\delta^2\}.$$

Using χ to denote the characteristic function of a set, $|M_\eta| = \Sigma\chi\{1 < (j+1)(k+1) \le \eta\} = \eta \log \eta\{1 + o(1)\}$ by Lemma 4.3. Hence $\sigma^2(\delta) \le d_4\delta^{2(p+1)/p}/\log \delta^{-2}$, from which it follows that $\tau^2(\varepsilon) \ge d_5(\varepsilon^2 \log \varepsilon^{-2})^{p/(p+1)}$, so that $\tau^2(cn^{-1/2}) \ge d_6(\log n/n)^{p/(p+1)}$. Substitute back into Theorem 5.1 to complete the proof. □

PROPOSITION 5.3. *Subject to the conditions of Theorem* 3.1, *there exists a constant* $d_I(p, C) > 0$ *such that*

$$r_I(n) \ge d_I(1/n)^{p/(p+2)}.$$

PROOF. Now take H and H_0 as above, and let K be the Hilbert subspace of $L^2(D, \lambda)$ generated by the orthonormal set of singular functions $\{\psi_\nu\}$. This time a good bound for $\sigma(\delta)$ must use high-dimensional subspaces [with $B_M(\delta) \subset H_0$] for which in addition $\|P\|_M$ is small. For given η, set $M_\eta = \operatorname{span}\{\varphi_{j0}: \frac{1}{2}\eta \le j + 1 \le \eta\}$. Then $\|P\|^2_{M_\eta} = \max\{b_\nu^2: \varphi_\nu \in M_\eta\} \le 2\eta^{-1}$ and $|M_\eta| \ge [\frac{1}{2}\eta]$. As in the proof of Proposition 5.2, $B_{M_\eta}(\delta) \subset H_0$ if $\eta^p \le C^2/\delta^2$. Substituting into (5.1), we have, for sufficiently small δ,

$$\sigma^2(\delta) \le \delta^2 \inf\{2\eta^{-1}/[\tfrac{1}{2}\eta]: \eta^p \le C^2/\delta^2\} = d_7\delta^{2(p+2)/p}.$$

Consequently $\tau^2(\varepsilon) \ge d_8\varepsilon^{2p/(p+2)}$ and $\tau^2(cn^{-1/2}) \ge d_9 n^{-p/(p+2)}$, which, as above, can be substituted into Proposition 5.1 to complete the proof. □

We close this section by remarking that Ibragimov and Hasminskii (1981) and Stone (1982) have shown that the minimax rate of convergence of global mean integrated square error for *direct* nonparametric density and regression problems is $n^{-2p/(2p+d)}$, where p is the assumed amount of smoothness and d is the dimension, $d = 2$ in our case. They consider classes of functions constrained by a Hölder continuity condition of order $\alpha \in (0, 1]$ on the sth derivative, so that $p = s + \alpha$. The extra $\log n$ term in the rate of convergence $(\log n/n)^{2p/(2p+d)}$ obtained in the present paper reflects the slightly reduced smoothness imposed by requiring only square-integrability of the pth weak derivative.

6. Biased sampling and attenuation. In any practical PET scan, not all pairs of emitted photons are detected. We shall show in this section that two of the main reasons for this incompleteness of sampling can be placed within the same mathematical framework, and that our results can, in part, be extended to account for them. Under mild assumptions, the incompleteness of sampling has no effect on the minimax rate of consistency found in Theorem 3.1.

6.1. *The effect of the third dimension.* Up to now, we have considered the detectors as forming a circle in the plane, and we have assumed that all the paths of emitted photons fall in this plane. Of course, in reality the detectors form a ring of finite thickness $d > 0$, and the orientation of the line of flight of the photons is uniformly distributed in $\mathbf{R}^3$. We shall assume that the emission density is constant over the thickness of the cylindrical slab enclosed by the detector ring. Only emissions taking place in this slab will be considered, since only they have any chance of being detected at all.

Given any emission, the photon line-of-flight is now parametrized by three coordinates (s, φ, φ'), where (s, φ) are the coordinates in detector space of the projection of the line onto the detector plane, and the *vertical angle* φ' $(-\pi/2 < \varphi' \le \pi/2)$ is the angle between the line and its projection. The assumption that the line has uniformly distributed direction implies that, independently of (s, φ), the vertical angle has probability density $\frac{1}{2}\cos\varphi'\, d\varphi'$. An emission line will only be detected if its vertical angle is such that both photons hit the detector ring. If the emission is detected, only the coordinates s and φ are observed.

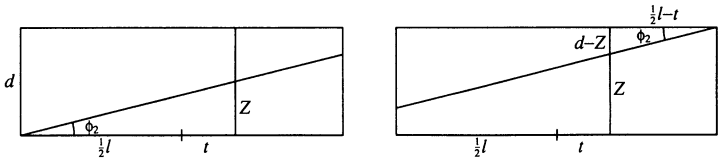

FIG. 4. *The two cases for* φ_2.

Condition on a particular s and φ, and let $l = 2(1 - s^2)^{1/2}$, the length of the corresponding detector tube. Assume that an emission takes place at distance t from the centre of the tube and at vertical position Z as shown in Figure 4. Assume that the projection of the line of flight of the emitted photons has coordinates (s, φ). Let $(-\varphi_1, \varphi_2)$ be the range of vertical angles over which both photons will hit the detectors. For given φ_1 and φ_2 the probability of detection will be

$$\int_{-\varphi_1}^{\varphi_2} \tfrac{1}{2} \cos \varphi' \, d\varphi' = \tfrac{1}{2}(\sin \varphi_1 + \sin \varphi_2).$$

We have (see Figure 4)

$$\tan \varphi_2 = \begin{cases} Z/\left(t + \tfrac{1}{2}l\right) & \text{if } Z < \left(t + \tfrac{1}{2}l\right)d/l, \\ (d - Z)/\left(\tfrac{1}{2}l - t\right) & \text{otherwise.} \end{cases}$$

By assumption, Z is uniformly distributed over $(0, d)$. By elementary calculus, the expected value of $\sin \varphi_2$ over this distribution of Z is equal to

$$\begin{aligned} & d^{-1} \int_0^{(l/2+t)d/l} \sin\left[\tan^{-1}\left\{z/\left(\tfrac{1}{2}l + t\right)\right\}\right] dz \\ & \quad + d^{-1} \int_{(l/2+t)d/l}^{1} \sin\left[\tan^{-1}\left\{(d - z)/\left(\tfrac{1}{2}l - t\right)\right\}\right] dz \\ & = d^{-1}\left(\tfrac{1}{2}l + t\right) \int_0^{d/l} \sin(\tan^{-1} u) \, du + d^{-1}\left(\tfrac{1}{2}l - t\right) \int_0^{d/l} \sin(\tan^{-1} u) \, du \\ & = d^{-1} l \left\{\left(1 + d^2/l^2\right)^{1/2} - 1\right\}. \end{aligned} \tag{6.1}$$

By symmetry, the expected value of $\sin \varphi_1$ and, hence, the expected probability of detection conditional on s, t and φ, will also be equal to the expression in (6.1). Note that this probability is independent of t and only depends on the tube length l. Letting $a_{3D}(s, \varphi)$ be the probability that an emission in tube (s, φ) is actually detected, if follows from (6.1) that

$$a_{3D}(s, \varphi) = \left\{4(1 - s^2)d^{-2} + 1\right\}^{1/2} - 2(1 - s^2)^{1/2} d^{-1}.$$

This quantity increases as s increases, reflecting the fact that emissions in

shorter tubes (large s) are more likely to be detected. We have, finally,

$$0 < (1 + 4d^{-2})^{1/2} - 2d^{-1} \leq a(s, \varphi) \leq 1 \quad \text{for all } s \in [0,1].$$

6.2. *Attenuation.* The other effect we shall consider is *attenuation*, defined as being the loss of a detection caused by the absorption or scattering of one of the photons in flight. Let us model the probability of such loss of a photon as it travels between $\mathbf{x}$ and $\mathbf{x} + d\mathbf{x}$ as $\mu(\mathbf{x})|d\mathbf{x}|$ and assume that $\mu(\mathbf{x})$ is bounded. Suppose an emission occurs at a point $\mathbf{x}_0$ and that y is the line of flight of the emitted photons. Let $y_+(\mathbf{x}_0)$ and $y_-(\mathbf{x}_0)$ be the half-lines of y emanating from $\mathbf{x}_0$, and assume y intersects the detector ring. By standard Poisson process theory, the probability that neither photon will be lost is given by

$$\exp\left\{-\int_{y_+(\mathbf{x}_0)} \mu(\mathbf{x})\, d\mathbf{x}\right\} \exp\left\{-\int_{y_-(\mathbf{x}_0)} \mu(\mathbf{x})\, d\mathbf{x}\right\} = \exp\left\{-\int_y \mu(\mathbf{x})\, d\mathbf{x}\right\}$$

$$= a_A(s, \varphi) \quad \text{say.}$$

Just as in Section 6.1, the probability that the emission will be detected depends only on the detector tube (s, φ) and is independent of the emission's position within that tube. In general, if both effects are considered, the probability that any particular detection will not be lost will be $a_{3D}(s, \varphi)a_A(s, \varphi)$. Both effects are important in PET; intensities reconstructed ignoring them can, in practice, be too low by a factor of three in the centre of the image (F. Natterer, personal communication). A common technique for correcting for attenuation is to estimate it separately, for example by a transmission scan.

6.3. *A general framework and the extension of our results.* The two effects we have discussed can be combined by assuming the existence of a function $a(s, \varphi)$, $0 < a(s, \varphi) \leq 1$ such that a positron emission at (x_1, x_2) gives rise to a detection at (S, Φ) as defined in Section 2.1 with probability $a(S, \Phi)$ conditional on (S, Φ); with probability $1 - a(S, \Phi)$ the detection is lost. It follows from this formulation that the *observed* detections will form a *biased sample* with density in detector space with respect to $d\lambda(s, \varphi)$

$$g_a(s, \varphi) = P_a f(s, \varphi) = a(s, \varphi)Pf(s, \varphi) \Big/ \int_D Pf(s, \varphi')a(s, \varphi')\, d\lambda(s, \varphi').$$

Let $\mathscr{T}_B(n)$ be the class of all estimators of f based on a sample of size n from $P_a f$, and let $r_B(n)$ be the minimax mean integrated square error over $\hat{f}$ in $\mathscr{T}_B(n)$ and f in $\mathscr{F}_{p,C}$.

THEOREM 6.1. *Suppose that* $\inf_D a(s, \varphi) = a_0 > 0$, *and make the assumptions of Theorem* 3.1. *Then*

$$r_B(n) \approx n^{-p/(p+2)}. \tag{6.2}$$

PROOF. The order of magnitude in (6.2) is of course the same as that obtained for unbiased indirect estimation in (3.5).

Suppose, first, that f is the least favourable density in $\mathscr{F}_{p,C}$ for estimation by estimators in $\mathscr{T}_I(n)$. Let $n' = [\frac{1}{2}a_0 n]$. Suppose $Y_1, Y_2, \ldots$ is an i.i.d. sequence drawn from Pf. Construct an i.i.d. sequence $Z_1, \ldots$ from $P_a f$ by including each Y_i in the sequence with probability $a(Y_i) \geq a_0$. Let $\hat{f}$ be the estimator of f based on $Z_1, \ldots, Z_{n'}$ using the minimax estimator in $\mathscr{T}_B(n')$, so that $M(\hat{f}; f) \leq r_B(n')$. Now let N be the number of $Y_1, \ldots, Y_n$ that are included in the Z_j sequence, and let $\hat{f}_1$ be equal to $\hat{f}$ if $N \geq n'$ and 1 otherwise. Since $\hat{f}_1$ is based on $Y_1, \ldots, Y_n$, and since f is least favourable for $\mathscr{T}_I(n)$, we have $M(\hat{f}_1; f) \geq r_I(n)$. By an elementary argument, $M(\hat{f}_1; f) \leq M(\hat{f}; f) + P(N < n') \int (f - 1)^2 \, d\mu$, so that $r_B(n') \geq r_I(n) - P(N < n')$, making use of Proposition 2.3 and the assumption $C < 2^{(p-1)/2}$ to bound $\int (f - 1)^2$ by 1. A crude bound now suffices for $P(N < n')$; since N is stochastically larger than a $Bi(n, a_0)$ random variable, $P(N < n') \leq P\{Bi(n, a_0) \leq \frac{1}{2}na_0\} = O(n^{-1})$ by Chebyshev's inequality. We conclude that $r_B([\frac{1}{2}na_0]) \geq r_I(n) - O(n^{-1})$.

Now reverse the role of biased and unbiased samples throughout the argument. If $Z_1, \ldots$ is an i.i.d. sample from $P_a f$, then a sample $Y_1, \ldots$ from Pf can be constructed by including each Z_i with probability $a_0/a(Z_i)$; this quantity necessarily lies between a_0 and 1. The analogous argument to that used above yields that $r_I([\frac{1}{2}na_0]) \geq r_B(n) - O(n^{-1})$. Applying Theorem 3.1 it now follows that $r_B(n)$ has the same order of magnitude $n^{-p/(p+2)}$ as $r_I(n)$. □

There is, of course, a distinction between a biased sample of n observations drawn from $P_a f$ and a censored sample consisting of all the observations that are detected arising from n emissions in brain space. The censored sample will consist, in the notation of the proof of Theorem 6.1, of N observations from $P_a f$. Implicit in the proof of Theorem 6.1 is a demonstration that the minimax mean integrated square error for estimation based on this censored sample will have the same order of magnitude as $r_I(n)$ under the assumption $a_0 > 0$.

For the third dimension effect, as the detector ring thickness $d \to 0$, we have $a_{3D}(s, \varphi) \sim \frac{1}{4}d(1 - s^2)^{-1/2}$ and $a_0 \to 0$. In the limiting case, the biased sample density will be proportional to $(1 - s^2)^{-1/2} Pf(s, \varphi)$, whose ratio to $Pf(s, \varphi)$ is unbounded as $s \to 1$. Theorem 6.1 no longer applies, but it can be shown that the biased sampling has at most a logarithmic order effect, in that the order of magnitude of $r_B(n)$ lies between $(n \log n)^{-p/(p+2)}$ and $n^{-p/(p+2)}$. This is a consequence of the following more general result on singular biased sampling, whose proof is omitted.

THEOREM 6.2. *Suppose* $p \geq 1$ *and* $0 < C < 2^{(p-1)/2}$.

(a) *If* $\int_D a(s, \varphi)^{-1}(1 - s^2)^{-1} \, d\lambda(s, \varphi) < \infty$, *then there exists* c_1 *such that* $r_B(n) \leq c_1 n^{-p/(p+2)}$.

(b1) *If* $\int_D a(s, \phi)(1 - s^2)^{-1} \, d\lambda(s, \varphi) < \infty$, *then there exists* c_2 *such that* $r_B(n) \geq c_2 n^{-p/(p+2)}$.

(b2) *If* $\int_D a(s, \varphi) \, d\lambda(s, \varphi) < \infty$, *and* $\sup_s (1 - s^2)^{1/2} \int_0^{2\pi} a(s, \varphi) \, d\varphi < \infty$, *then there exists* c_3 *such that* $r_B(n) \geq c_3 (n \log n)^{-p/(p+2)}$.

For $a(s, \varphi) = (1 - s^2)^{-1/2}$, the conditions of (a) and (b2) hold but the integral in (b1) is infinite.

7. Alternative error measures. Our results can be extended to some more general measures of the discrepancy between the estimator and the unknown function than mean integrated square error. We can treat a class of losses that takes into account the closeness of derivatives, as well as values, of the estimate to those of the true unknown function; these losses take more account of the "shape" of the function than does ordinary mean integrated square error.

Define measures μ_p as in Proposition 2.2. It is noted in the Appendix that, for integers $q \geq 0$, the squared norm

$$\int |f|^2 \, d\mu_1 + \sum_{r_1 + r_2 = q} \int |\partial^{r_1 + r_2} f / \partial x_1^{r_1} \, \partial x_2^{r_2}|^2 \, d\mu_{q+1} \tag{7.1}$$

is equivalent to

$$\| f \|_q^2 = \sum_{j,\, k \geq 0} (j + 1)^q (k + 1)^q f_{jk}^2. \tag{7.2}$$

For noninteger values of q, the norm $\| \cdot \|_q$ will be a more general Sobolev norm [Adams (1975)], although some care will be necessary because of the nonstandard dominating measures μ_q; this is a topic for future investigation.

We can now state and prove a theorem that gives the exact minimax rates in the $\| \cdot \|_q$ norm for both direct and indirect estimation. Theorem 3.1 is the special case $q = 0$ and it can be seen that the rates available are both reduced, in a natural way, when higher order norms are used.

THEOREM 7.1. *For fixed* $p \geq 1$, $0 < C < 2^{(p-1)/2}$ *and* $0 \leq q < p$,

$$\inf_{\hat{f} \in \mathcal{T}_D(n)} \sup_{f \in \mathcal{F}_{p,C}} E \| \hat{f} - f \|_q^2 \approx (\log n / n)^{(p-q)/(p+1)}$$

and

$$\inf_{\hat{f} \in \mathcal{T}_I(n)} \sup_{f \in \mathcal{F}_{p,C}} E \| \hat{f} - f \|_q^2 \approx (1/n)^{(p-q)/(p+2)}.$$

PROOF. The proof is analogous to that of Theorem 3.1 and we shall confine ourselves to a brief outline of the necessary changes. Define $c_\nu^2 = c_{jk}^2 = (j + 1)^q (k + 1)^q$ and $\Gamma = \operatorname{diag}(c_\nu)$. To obtain upper bounds, define the surrogate risk $M_q^*(\hat{f}; f) = \Sigma_\nu c_\nu^2 \{\operatorname{var}_1 \hat{f}_\nu + (E_f \hat{f}_\nu - f_\nu)^2\}$. The result corresponding to Proposition 2.1 is immediate. As in Lemma 4.1,

$$M_q^*(\hat{f}; f) = n^{-1} \operatorname{tr} \Gamma W (I - \mathbf{e}_0 \mathbf{e}_0^T) W^T \Gamma + \| \Gamma (I - WB) \mathbf{f} \|^2.$$

As in Lemma 4.2, the minimax surrogate risk for linear estimates over the

ellipsoid $\mathscr{F}_{p,C}$ is given by $n^{-1}\Sigma_{(\eta)}(c_\nu^2 b_\nu^{-2} - c_\nu b_\nu^{-2} a_\nu \gamma^{1/2})$, where γ is chosen to satisfy $n^{-1}\Sigma_{(\eta)}(a_\nu c_\nu b_\nu^{-2}\gamma^{-1/2} - a_\nu^2 b_\nu^{-2}) = C^2$. So long as $q < p$, we obtain surrogate linear minimax rates of convergence equal to $(n/\log n)^{-(p-q)/(p+1)}$ and $n^{-(p-q)/(p+2)}$ in the direct and indirect cases respectively. Clearly it would be possible to obtain more precise results corresponding to Theorem 3.2, but we shall refrain from doing so.

The methods of Section 5 show that these are in fact the exact minimax rates of convergence for the $\|\cdot\|_q$ norm for general estimators. From Proposition 5.1, it is only necessary to compute the modulus $\sigma(\delta)$ of (5.1), now with respect to the $\|\cdot\|_q$ norm on H. This calculation goes as in Propositions 5.2 and 5.3, even using the same definitions of the subspaces M_η. Since the $\|\cdot\|_q$ norm is now used on H, $\|P\|^2_{M_\eta} = \sup\{b_\nu^2 c_\nu^{-2}\colon \varphi_\nu \in M_\eta\}$ and $B_{M_\eta}(\delta) \subset H_0$ if $\eta^{p-q} \le C^2/\delta^2$. With these changes, the proof is completed. □

8. Some concluding remarks. This paper has focused on lower and upper bounds for one particular bivariate density estimation problem for indirect data. The same formalism applies to many other density and regression estimation problems. The celebrated "unfolding" problem for sphere size distributions is an example involving univariate density estimation from indirect data and the singular value decomposition of the Abel transform. For recent results and further references on this problem, see, for example, Hall and Smith (1988), Nychka and Cox (1989), Silverman, Jones, Wilson and Nychka (1990) and Wilson (1989).

Noisy integral equations of the form $y_i = (Pf)(t_i) + \varepsilon_i$ can be treated using our methods, at least under appropriate assumptions on the distributions of (t_i, ε_i). For example, if the observation points t_i follow a known distribution $\lambda(dt)$ and the errors ε_i are independently Gaussian $(0, \sigma^2)$, then the information divergence between the hypotheses f_1 and f_2 is $K(P_{f_1}^{(n)}, P_{f_2}^{(n)}) = \frac{1}{2}n\int\{Pf_1(t) - Pf_2(t)\}^2\lambda(dt)$, so that the lower bound methods of Section 5 immediately apply. Upper bound results are given, for example, by Nychka and Cox (1989).

For a generic one-dimensional problem with singular value decomposition $P\varphi_\nu = b_\nu\varphi_\nu$, $b_\nu \sim \nu^{-\beta}$, and with ellipsoid determined by $a_\nu^2 = \nu^{2\alpha}$, corresponding to "α derivatives," the exact minimax rate of convergence of the mean square error in $n^{-2\alpha/(2\alpha+2\beta+1)}$. This should be compared with the exact rate of $n^{-2\alpha/(2\alpha+1)}$ for the corresponding direct case. Related calculations for a large class of one-dimensional convolution equation models appear in Wahba and Wang (1987).

One important topic for future attention is the effect of the discretization of detector space due to the finite size of the detectors. It is clear intuitively that if the number of detectors is sufficiently large relative to the size of the sample collected, then the minimax rates will not be affected, and of course it would be interesting to quantify this notion more precisely. Some PET machines [see, for example, Snyder and Politte, (1983)] are able to use time-of-flight information to provide an approximate indication of the place in the detector tube where an emission occurs. This is usually accompanied by a loss in detector efficiency and, hence, a smaller sample size n. It would be desirable to extend our framework to

make a quantitative evaluation of this trade-off. Kaufman, Morgenthaler and Vardi (1983) report some earlier work on this issue.

Another issue that could be explored is the further extension of our results to deal with more general metrics on images. Finally there is very little known about the theoretical performance of algorithms commonly used in practice; our results at least provide a framework and a benchmark against which particular algorithms can be judged.

APPENDIX

PROOF OF PROPOSITION 2.1. The proof is elementary. Consider the direct case first. Suppose Ξ is a random variable drawn from the uniform density and that X is a random variable with density f. Then $\operatorname{var}_f \hat{f}(x)/\operatorname{var}_1 \hat{f}(x) = n^{-1} \operatorname{var} w(x, X)/n^{-1} \operatorname{var} w(x, \Xi)$. Now

$$\begin{aligned}\operatorname{var} w(x, X) &\le E\{w(x, X) - Ew(x, \Xi)\}^2 \\ &= \int \{w(x, \xi) - Ew(x, \Xi)\}^2 f(\xi)\, d\mu(\xi) \\ &\le \sup_B f \int \{w(x, \xi) - Ew(x, \Xi)\}^2\, d\xi = \sup_B f \operatorname{var} w(x, \Xi),\end{aligned}$$

and similarly $\operatorname{var} w(x, \Xi) \le \sup_B(1/f)\operatorname{var} w(x, X) = \operatorname{var} w(x, X)/\inf_B f$. Thus $\operatorname{var}_f \hat{f}/\operatorname{var}_1 \hat{f}$, and hence M/M^*, is bounded between $\inf f$ and $\sup f$. In the indirect case an exactly analogous argument bounds M/M^* between $\inf_D Pf$ and $\sup_D Pf$. It follows from (2.1) that $\inf_D Pf \ge \inf_B f$ and that $\sup_D Pf \le \sup_B f$, completing the proof. □

PROOF OF PROPOSITION 2.2. We employ Gegenbauer (ultraspherical) polynomials as normalized in Gradshteyn and Ryzhik [(1980), page 827]. An orthogonal basis for $L^2(B, \mu_\alpha)$ is given by the polynomials

$$\tilde{\varphi}^\alpha_{jk}(\mathbf{x}) = (2\pi)^{-1} \int_0^{2\pi} e^{i(j-k)\theta} C^\alpha_{j+k}(\mathbf{u}_\theta^T \mathbf{x})\, d\theta \qquad j, k \ge 0, \mathbf{u}_\theta = (\cos\theta, \sin\theta)^T.$$

Defining the operator $(P_\alpha f)(s, \theta) = E\{f(\mathbf{X}) | u_\theta^T \mathbf{X} = s\}$, where $\mathbf{X} \sim \mu_\alpha$, the polynomials $\tilde{\varphi}^\alpha_{jk}$ are the pullback by the adjoint P^*_α of the singular functions $e^{i(j-k)\theta} C^\alpha_{j+k}(s)$ of $P_\alpha P^*_\alpha$. This construction of the SVD of P_α is explained in Johnstone (1989), following Davison (1981, 1983) but with different notation and normalizations. It can be shown that $\tilde{\varphi}^1_{jk} = (j + k + 1)^{-1/2} \varphi_{jk}$, so that $f = \Sigma(j + k + 1)^{1/2} f_{jk} \tilde{\varphi}^1_{jk}$.

Let $D_z = \frac{1}{2}(\partial/\partial x_1 - i\,\partial/\partial x_2)$ and $D_{\bar{z}} = \frac{1}{2}(\partial/\partial x_1 + i\,\partial/\partial x_2)$. Since $(d/dt)C^\alpha_m = 2\alpha C^{\alpha-1}_{m-1}$, we have, setting $\tilde{\varphi}_{jk} = 0$ if j or $k < 0$, $D_z \tilde{\varphi}^\alpha_{jk} = \alpha \tilde{\varphi}^{\alpha+1}_{j-1,k}$ and $D_{\bar{z}} \tilde{\varphi}^\alpha_{jk} = \alpha \tilde{\varphi}^{\alpha+1}_{j,k-1}$. The raising of the index from α to $\alpha + 1$ leads us from the original measure μ of Section 2 to the family μ_{p+1}, so that, for example, the family of derivates $D_z \varphi_\nu$ and $D_{\bar{z}} \varphi_\nu$ is orthogonal with respect to μ_2, not μ_1. □

It is shown in Johnstone (1989) that if $r + s = p$, then, for certain constants c_{jkrs} all falling in $[(p+1)^{-2p+1}, (p+1)p^{2p}]$,

$$\int (D_z^r D_{\bar{z}}^s f)^2 \, d\mu_{p+1} = p! \sum_{\substack{j \geq r \\ k \geq s}} (j+k+1) f_{jk}^2 \int \left(\tilde{\varphi}_{j-r,k-s}^{p+1}\right)^2 d\mu_{p+1}$$
$$= \sum_{\substack{j \geq r \\ k \geq s}} c_{jkrs}^2 (j+1)^p (k+1)^p (p+1) f_{jk}^2.$$

Standard arguments of analysis complete the proof. □

PROOF OF PROPOSITION 2.3. In the complex form of the basis, we have

$$f(r,\theta) = \sum_{(j,k) \in N'} f_{jk} (j+k+1)^{1/2} e^{i(j-k)\theta} Z_{j+k}^{|j-k|}(r).$$

Zernike polynomials satisfy $\sup_{0 \leq r \leq 1} |Z_m^l(r)| = Z_m^l(1) = 1$, as a consequence of the representation in terms of Jacobi polynomials: $Z_{l+2s}^l(r) = r^l P_s^{(0,l)}(2r^2 - 1)$, together with the results of Szegö [(1938), page 163], applied to the polynomials $Q_s^l(t) = P_s^{0,l}(2t-1)$ as s varies. Hence

$$\sup |f - 1| \leq \sum_{N' \setminus (0,0)} (j+k+1)^{1/2} |f_{jk}|.$$

The ellipsoid $\mathcal{F}_{p,C}$ has exactly the same description in terms of either the real or the complex form of the basis. Setting $x_{jk} = (j+1)^{p/2}(k+1)^{p/2}|f_{jk}|/C$, we obtain

$$\sup_{\mathcal{F}_{p,C}} \sup |f - 1| \leq C \sup \Bigg\{ \sum_{N' \setminus (0,0)} (j+k+1)^{1/2} (j+1)^{-p/2} (k+1)^{-p/2} x_{jk} : \sum_{N' \setminus (0,0)} x_{jk}^2 \leq 1 \Bigg\}$$
$$\leq C \sup_{N' \setminus (0,0)} (j+k+1)^{1/2} (j+1)^{-p/2} (k+1)^{-p/2} = C 2^{(1-p)/2},$$

provided $p \geq 1$. To complete the proof, note that the linear function $1 + 2^{(1-p)/2} Cr \cos\theta$ falls in $\mathcal{F}_{p,C}$ and satisfies $\sup |f - 1| = C 2^{(1-p)/2}$. □

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