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Speed of Estimation in Positron Emission Tomography

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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 idealisation 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 the exact minimax rates of convergence of estimation, for all possible estimators, over suitable smoothness classes of functions. For indirect data and (in practice unobservable) direct data, these rates are $n^{-p/(p+2)}$ and $(n/\log n)^{-p/(p+1)}$ respectively, for densities in a class corresponding to bounded square-integrable p th derivatives. We obtain numerical values for equivalent sample sizes for a particular class of orthogonal series estimators, based on the eigenfunctions of the Radon transform.

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1 Introduction

Tomography is a non-invasive 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 labeled 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. Some references are given in Sections 2 and 3 below.

In a typical tomography scan, a large number, perhaps ten million, 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? As will be explained below, the observations are not direct observations in the usual statistical sense, because the original positions of the detected emissions in the brain are not known. All that the equipment is able to detect is a tube in space within which each particular emission took place, and thus the observations can be thought of as *indirect observations* of the phenomenon of interest. This incompleteness, or indirectness, of the observed data is of course a standard feature of *linear inverse problems* in general, and PET is just one concrete example of such problems.

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 amount of 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.

This paper has several objectives. We provide a continuous formulation of a simplified model of the PET reconstruction problem. This allows us to 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. This continuous framework is flexible enough to include the estimators proposed in the literature for practical use, and reviewed in Section 3 below. These estimators are mostly based on a discretisation of the problem; although the continuous



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formulation might be used as the basis for practical reconstructions, our orientation in the present paper is mainly theoretical. We do not consider explicitly the iterative non-linear algorithms proposed for practical use, but instead we establish a lower bound (over a suitable smoothness class of functions) to the rate of convergence of *all* estimators. We then show that this rate bound is sharp by computing the rate of convergence of a particularly simple linear density estimate based on orthogonal series. For these estimators, and for a surrogate to the mean integrated square error, we give some numerical values for equivalent sample sizes, and these are discussed in Section 4 below.

Concluding sections of the paper test the sensitivity of our results to perturbations in our mathematical idealisation. We consider the effect of allowing for the three dimensional nature of the problem and for error measures incorporating local variation and find that our qualitative conclusions are not significantly affected.

We have tried to present our results in such a way that readers prepared to take the more technical details on trust need read the first four sections only.

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, Ibragimov and Hasminskii, and Birgé. 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.

A basic tool throughout the paper is the singular value decomposition (SVD) of the Radon transform linking, in a sense that will be discussed below, the unknown density with the observed data. Even when we do not know the SVD, as in one modification of the PET problem discussed in Section 10, the lower and upper bounds differ by only logarithmic terms.

Although we unashamedly concentrate on positron emission tomography, our methods are relevant to other indirect estimation problems as well, especially when the singular value decomposition is available, as is discussed briefly in the concluding Section 11.

2. The positron emission tomography problem

2.1 Introduction

We study the positron emission tomography (or PET) problem in this paper for two reasons. Firstly, it is of important practical interest in its own right, and secondly it is a typical example of a problem involving *indirect observation* of the probability distribution of actual interest. Other such problems arise in tomography of different kinds, as well as in many other fields, and a detailed study of one particular indirect observation problem will yield insight into the more general cases.

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.

The radioactive tagging of the glucose gives rise to emissions of positrons distributed as a Poisson process in 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 lain. However (for equipment of the kind being considered at the moment) it is not possible to detect the position of the emission on the line. In practice the sensors are of finite size and so what is actually observed is the numbers of emissions over a period of time falling in various *detector tubes*, each tube made up of the cylindrical volume between a pair of detectors. There are various simplifying assumptions made in the description we have given. For example, in reality the positrons may well travel a finite distance before annihilation and, furthermore, once the annihilation has taken place the two photons may fly off at an angle of slightly less than 180° to one another. For further discussion of the problem see the papers mentioned above, and also Section 1.3 of Deans (1983).

2.2 An idealised problem and the Radon transform

The problem we shall consider in detail is an idealised 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 Fig. 2.1) 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 B and C of the intersection of l with the detector circle are observed exactly.

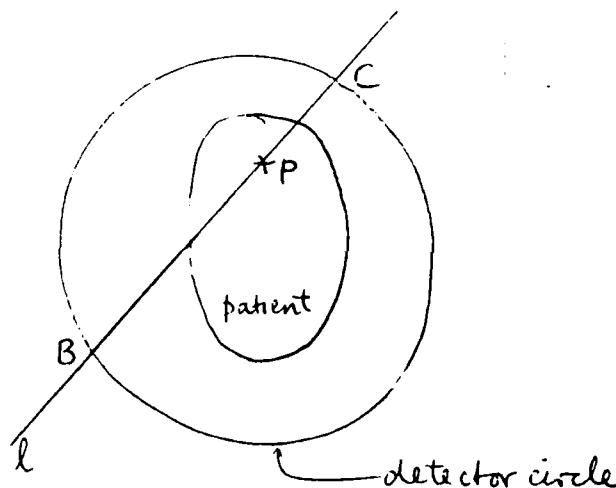


Figure 2.1: *The patient and the detector circle*

Give the name *detector space* to the space of all possible unordered pairs BC of points on the detector circle, and call *brain space* the original disc in the plane enclosed by the detector ring. Brain space is parametrised either by cartesian or standard polar coordinates; elements of detector space are parametrised as (s, φ) as shown in Figure 2.2. The parameter s , $0 \leq s \leq 1$, gives the length of the perpendicular from the origin to the detected line BC , while φ , $0 \leq \varphi \leq 2\pi$, gives the orientation of this perpendicular.

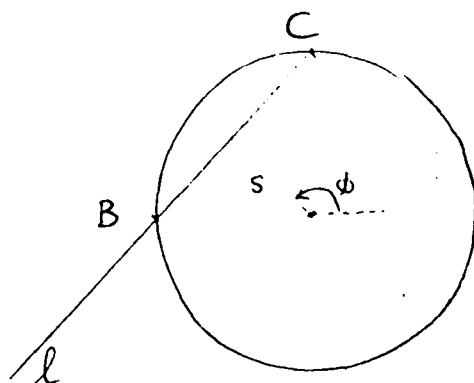


Figure 2.2: Parametrising the line l

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. The factor π^{-1} is included to make μ integrate to 1. On detector space, define a measure λ by $d\lambda(s, \varphi) = 2\pi^{-2}(1-s^2)^{\frac{1}{2}} ds d\varphi$. This measure also integrates to 1; the reason for the form of λ will be explained in a moment.

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

$$Pf(s, \varphi) = \frac{1}{2} (1-s^2)^{-\frac{1}{2}} \int_{-\sqrt{1-s^2}}^{\sqrt{1-s^2}} f(s \cos \varphi - t \sin \varphi, s \sin \varphi + t \cos \varphi) dt \quad (2.1)$$

The integral in (2.1) is the so-called *Radon transform* of the density f , namely the line integral of f along the line l with co-ordinates (s, φ) in detector space. The Radon transform has been the subject of much study; see, for example, Marr (1974) and Deans (1983). Since the length of the segment BC is $2(1-s^2)^{\frac{1}{2}}$, 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 will 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.

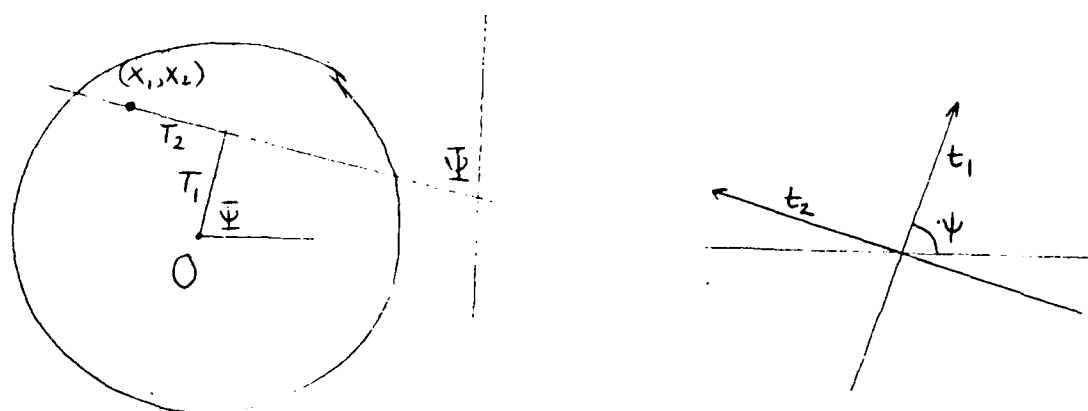


Figure 2.3: Rotating the coordinates

It remains to demonstrate the correctness of (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 2.3; we take $0 \leq \Psi \leq \pi$ for definiteness, and 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 rotating the axes in brain space by an angle ψ , so that

$$x_1 = t_1 \cos \psi - t_2 \sin \psi \quad \text{and} \quad x_2 = t_1 \sin \psi + t_2 \cos \psi.$$

The Jacobian of this transformation is 1, and so with respect to $dt_1 dt_2 d\psi$ we have

$$f_{T_1, T_2, \Psi}(t_1, t_2, \psi) = \pi^{-2} f(t_1 \cos \psi - t_2 \sin \psi, t_1 \sin \psi + t_2 \cos \psi)$$

$$\text{on } \|t\| \leq 1 \text{ and } 0 \leq \psi \leq \pi.$$

Now integrate t_2 out, over the relevant range, to give

$$f_{T_1, \Psi}(t_1, \psi) = \pi^{-2} \int_{-\sqrt{1-t_1^2}}^{\sqrt{1-t_1^2}} f(t_1 \cos \psi - t_2 \sin \psi, t_1 \sin \psi + t_2 \cos \psi) dt_2$$

To give the coordinates in detector space of the detected photon pair set

$$(s, \phi) = \begin{cases} (t_1, \psi) & \text{if } t_1 \geq 0 \\ (-t_1, \psi + \pi) & \text{if } t_1 < 0. \end{cases}$$

This transformation again has unit Jacobian, and has the property that $s \cos \phi = t_1 \cos \psi$ and $s \sin \phi = t_1 \sin \psi$, so that the joint density with respect to $ds d\phi$ is

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

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

3. Outline of our strategy

Statisticians are accustomed to dealing with samples of various sizes and have a certain kind of (sometimes misguided) intuition about what constitutes, say, a "large" data set, and what kind of information can be extracted from such a data set. Tukey and Tukey (1981, p. 194) even attempt to formalise this intuition by suggesting the use of letters of the alphabet A-G as a scale of "numerosity" of the data set. Vardi, Shepp and Kaufman (1985), in their paper describing the PET problem, discuss the use of data sets of 10^7 observed emissions, but because of the indirect nature of the observation process it is not immediately clear how much information such a data set would convey. In this paper we shall attempt to gain some feeling for this question by comparing the accuracy with which an emission density can be estimated from indirect observations with the accuracy that could be obtained if the emissions were observed in their original positions in the brain.

We shall make this comparison in two related ways. The first is the equivalent sample size approach described in the introduction. An alternative, somewhat cruder way of evaluating the efficiency of statistical techniques is to consider the *doubling ratio*, defined to be the relative increase $r = \tilde{n}/n$ in the number of observations needed to halve the root mean square error of estimation. In the case of the estimation of functions, a doubling ratio can of course be calculated with reference to the root mean integrated square error. For standard estimation procedures involving a finite number of parameters the root mean square error is exactly $O(n^{-1/2})$ and so the doubling ratio is equal to 4, at least asymptotically. We shall calculate and compare the doubling ratios, for a particular estimation method, for the direct and indirect cases in the PET problem, and for suitable restrictions on the class of true densities f . Of course, the estimation accuracy achieved, and hence the doubling ratio, depend on the estimation method being used. We shall concentrate most attention on a linear estimation procedure, based on a class of orthogonal series density estimators. The orthogonal series we shall use arises from the singular value decomposition of the Radon transform.

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 Heusman (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) and Jones, Silverman and Wilson (1988). A recent survey of algorithms is given by Tanaka (1987).

As a broad generalisation, one might say that many of the algorithms, especially those based on maximum or penalised likelihood, share some common features. They are typically non-linear and iterative, and respect the fact that the emission density is necessarily non-negative. For these reasons such algorithms are difficult to study analytically with regard to issues such as quality of approximation.

Our strategy is to seek crude qualitative information about the nature of the reconstruction problem, exploiting the continuous formulation given in Section 2.2. The continuous formulation has several virtues:

- 1) it gives a (simplified) model of the actual physics of the problem;
- 2) no grouping or discretisation of the data is involved, so we can use it for lower bounds on *all* estimation procedures, in whatever way the data are actually discretised in practice;
- 3) the singular value decomposition of the Radon transform can be applied to examine what kinds of features are well reconstructed;
- 4) it may provide a framework for construction of alternative algorithms.

We shall study the rates of convergence associated with estimation methods as the sample size increases. We shall show that there is a lower bound to the rate of convergence under a smoothness assumption on the class of unknown emission densities. This lower bound will apply to all estimators, linear or non-linear, iterative or not. To establish that this lower bound is sharp, we evaluate explicitly the rate of convergence of our specific estimator sequence based on orthogonal series. Though this estimator is linear in the (empirical Fourier coefficients of the) data, and non-iterative, it turns out to achieve the same rate of convergence as optimal non-linear estimators. An obvious question, which we intend to investigate in future work, is whether our linear estimator is at all useful as a practical method for finite samples.

The remainder of this paper is set out as follows. For the benefit of readers prepared to take technical details on trust, Section 4 summarises our main conclusions in terms of equivalent sample sizes and doubling ratios. In Section 5 the singular value decomposition of the Radon transform is reviewed, and details are given of the smoothness conditions that we shall place on the unknown density f . Roughly

speaking, a density f will be in smoothness class $B_{p,C}$ if its p th derivatives have square integral bounded by C^2 , the integral being with respect to a particular dominating measure. The higher p is, the more smoothness is imposed on the functions in $B_{p,C}$. Our linear estimation methods are introduced in Section 6, and in Sections 7 and 8 we derive the best possible rate of convergence that can be achieved by these linear estimators over any particular class $B_{p,C}$. Section 9 contains the main part of the argument that shows that essentially nothing is lost, at least in terms of rates, by considering only a special class of linear estimators, since the rates they achieve cannot be bettered by any other estimators, linear or non-linear. It has already been noted in Section 2 that we are considering a highly simplified physical model for positron emission tomography, and in Section 10 we shall consider the ramifications of making slightly more realistic assumptions. Firstly we consider error measures that incorporate derivative information, and secondly we explore the effect of the length-biased sampling introduced by our choice of a two-dimensional idealisation of what is really a three-dimensional problem. Section 11 briefly indicates other classes of indirect estimation problems to which the methods of this paper apply. There is, finally, an appendix containing technical details and proofs of some of the results presented in the main part of the paper.

We close this section with some remarks about discretisation. Most, if not all, current estimation methods in PET depend on various discretisations. For example, there is usually a finite number (say $m=128$) of detector elements in a ring about the patient, and hence a finite number $\frac{1}{2}m(m-1)$ of detector tubes. Only a 'binned' version $P^\dagger f$ of the emission density Pf is observed, and the mapping $f \rightarrow P^\dagger f$ will have a null space about which nothing can be said (even asymptotically in n) without employing further information about f . We do not attempt to discuss discretisation effects in this paper, since our focus is on the continuous idealisation of the PET problem and its attendant simplicity. Thus our results can be construed either as theoretical limits that apply regardless of discretisation, or as being applicable should "position-sensitive detectors" become available for data collection. Our results should be realistic for combinations of sample size and discretisation level for which, over the appropriate smoothness class, the maximum bias due to discretisation is small relative to the total minimax mean square error for that sample size. This maximum bias can be calculated, at least in principle, once a particular detector geometry and division of the image space into pixels have been specified. All this assumes, of course, that the sample size is large enough for the asymptotics to be useful!

4. Main conclusions of the paper

4.1 Equivalent sample sizes

Our main conclusions are in terms of the minimax rates of convergence of the estimation of f based on n observations. The maximum is taken over f in the smoothness class $B_{p,C}$ and the minimum is over all possible estimators based on a data set of size n .

Suppose the observations are taken directly, in other words that the exact position of each emission in brain space is known. Then we shall show that, for fixed p and C , the minimax mean integrated square error in the estimation of f is exactly of order $r_D(n)$, where

$$r_D(n) = c_{D,n}(\log n/n)^{p/(p+1)}. \quad (4.1)$$

and $c_{D,n}$ is a sequence of unspecified positive constants bounded away from zero and infinity. On the other hand, for an indirect sample of size n , where only the emissions as actually recorded in detector space are observed, the minimax mean integrated square error is exactly of order $r_I(n)$, where

$$r_I(n) = c_{I,n}(1/n)^{p/(p+2)}. \quad (4.2)$$

and $c_{I,n}$ is again a sequence of unspecified positive constants bounded away from zero and infinity.

It is now straightforward to draw some *qualitative* conclusions about equivalent sample sizes. Suppose we have an indirect sample of n detected emissions. Let $m(n)$ be the equivalent direct sample size, that is the number of emissions whose original positions in the brain would allow us to estimate f with the same accuracy. Some simple algebra from (4.1) and (4.2) yields the order of magnitude of the equivalent sample size as

$$m(n) \sim \frac{p+1}{p+2} \left[\frac{c_{D,n}}{c_{I,n}} \right]^{\frac{p+1}{p}} n^{(p+1)/(p+2)} \log n. \quad (4.3)$$

Perhaps not surprisingly, the equivalent sample size depends in order of magnitude 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 (4.3) 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 localised areas of high metabolic activity may lead to discontinuities, certainly in high

derivatives of f and possibly in f itself. The value $p = 1$ would correspond to f having square-integrable first weak derivative. These matters are discussed further in Section 5.

Immediate quantitative conclusions cannot be drawn directly from (4.3), both because the constants $c_{D,n}$ and $c_{L,n}$ are not known and because we lack information on the accuracy of (4.3) for a fixed finite value of n . Somewhat more precise statements can be made for the linear orthogonal series estimators studied in Sections 6 to 8 below. Let $r_{LD}(n)$ and $r_{LJ}(n)$ denote the minimax mean integrated square error when considering only *linear* estimators. Since it is still not possible to evaluate the constants in (4.1) and (4.2) for $r_{LD}(n)$ and $r_{LJ}(n)$, we introduce certain surrogate error measures in Section 7 whose ratio to mean integrated square error always lies in the interval $[1-m_C, 1+m_C]$, where $m_C = 2^{(1-p)/2}C$.

Our measures depend on certain constants c_1, c_2, c_3, d_1, d_2 and d_3 , the values of all of which are given in Section 8 below. The constants c_i depend on both smoothness p and radius C , while the d_i depend only on p . For $x > 1$ define a function $\alpha(x)$ as the solution to $\alpha \log \alpha = x$; then $\alpha(x)$ can be found numerically when required and is asymptotic to $x/\log x$ for large x . Define a sequence η_n by

$$\eta_n = d_3 \{ \alpha(c_3 n) \}^{1/(p+1)}.$$

Then the minimax surrogate risks $r_{LD}^*(n)$ and $r_{LJ}^*(n)$ satisfy

$$r_{LD}^*(n) = c_1 n^{-1} \eta_n (\log \eta_n + c_2) + O(n^{-1} \eta_n^{1/2}) \quad (4.4)$$

$$= d_1 C^{2(p+1)} (\log n/n)^{p/(p+1)} + O\{n^{-p/(p+1)} (\log n)^{-1/(p+1)}\} \quad (4.5)$$

and

$$r_{LJ}^*(n) = d_2 C^{4(p+2)} n^{-p/(p+2)} + O(n^{-(p+1)/(p+2)} \log n). \quad (4.6)$$

The form (4.5) for r_{LD}^* is more transparent, but the error term has the same polynomial order as the leading term; the error term in (4.4) is of lower order and so we use (4.4) in numerical computations.

The risks (4.5) and (4.6) naturally increase with the constant C , which specifies a radius of the smoothness class $B_{p,C}$. For definiteness we take $C^2 = 2^{p-1}$; this turns out (see Section 5) to be the largest value for which all f in $B_{p,C}$ are guaranteed to be non-negative probability densities, so long as $p \geq 1$. As C increases, r_{LJ}^* increases faster than r_{LD}^* in relative terms; this is a further consequence of the greater difficulty of the indirect estimation problem.

TABLE 4.1

Equivalent direct sample sizes $m(n)$ to achieve the same surrogate minimax mean integrated square error 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

The explicit equivalent sample size $m(n)$ for given values of n and p follows by ignoring the error terms in (4.4) and (4.6), and then solving $r_{LD}^*(m) = r_{LI}^*(n)$ for m . Some representative cases are given in Table 4.1. 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.

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 10^7 direct observations were available.

4.2 Comparing the doubling ratios

We now return to general non-linear estimators and use the results of Section 4.1 to compare the doubling ratios for the direct and indirect estimation cases. This will yield an alternative interpretation of the rates of convergence (4.1) and (4.2). The doubling ratio for the direct case can be found by solving the equation $r_D(\tilde{n})/r_D(n) = \frac{1}{2}$ numerically, if we neglect finite sample variation in the "constant" of proportionality $c_{D,\tilde{n}}/c_{D,n}$, which we conjecture approaches 1 as $n \rightarrow \infty$, and is in any case bounded away from zero and infinity. For the direct case, because of the logarithmic term, the doubling ratio depends on n and for $p = 2$ and $n = 10^7$ is approximately equal to 9. Thus if the data could be observed directly approximately 9 times as many data points would be required to halve the RMS error. For the indirect case there is no log term, and so as long as n is large and $c_{I,\tilde{n}}/c_{I,n}$ is ignored, the doubling ratio will be approximately equal to 16 for $p = 2$. The ratio $I(p)$ of the doubling ratio for the indirect case to that for the direct case can be taken as a measure of the inefficiency incurred due to the indirect observation of the data. For $p = 2$, the calculations given here yield $I(2) = 16/9$ approximately. As one would expect, the inefficiency $I(p)$ increases as

the amount of smoothness assumed decreases; see the values plotted in Figure 4.1. Of course, any interpretation of the doubling ratio must be guarded because the calculations we have performed take no account of finite-sample phenomena that disappear in asymptotics.

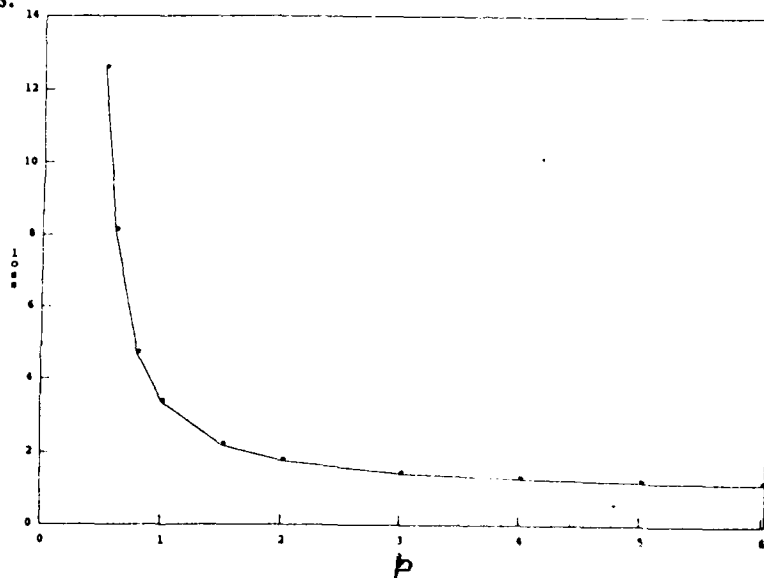


Figure 4.1: Inefficiency $I(p)$ for indirect estimation relative to direct estimation assuming p square-integrable derivatives.

5. The Radon transform and smoothness classes

The normalised Radon transform (2.1) expresses the observed density g as a linear transform Pf of the unknown emission density f . In this section we shall study the singular value decomposition (SVD) of P ; this decomposition is the key to our study in subsequent sections of the loss of information about f due to indirect observation.

To establish notation, we follow Davison (1983) and review briefly the singular value decomposition. Let H and K be Hilbert spaces and $P : H \rightarrow K$ 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

(i)

$$P\varphi_\nu = b_\nu\psi_\nu,$$

so that given f in H ,

$$Pf = \sum_\nu b_\nu \langle f, \varphi_\nu \rangle \psi_\nu;$$

- (ii) the $\{\varphi_\nu\}$ span the orthogonal complement of the kernel of P , $(\ker P)^\perp$;
- (iii) the $\{\psi_\nu\}$ span the range of P ;
- (iv) given g in K , the \tilde{f} of smallest norm which minimises $\|P\tilde{f} - g\|$ is

$$\tilde{f} = \sum_{\nu} b_{\nu}^{-1} \langle g, \psi_{\nu} \rangle \varphi_{\nu}.$$

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 introduced in Section 7 below.

In the PET model described in Section 2, H is the space $L^2(B, \mu)$ of functions on brain space which are square-integrable with respect to the dominating measure μ , where $B = \{x \in \mathbb{R}^2, \|x\| \leq 1\}$. Correspondingly, K is the space $L^2(D, \lambda)$ of detector-space functions square-integrable relative to λ , where $D = \{(s, \varphi) : 0 \leq s \leq 1, 0 \leq \varphi \leq 2\pi\}$.

The operator $P : L^2(B, \mu) \rightarrow L^2(D, \lambda)$ is the normalised Radon transform of (2.1). As mentioned there, it can be thought of as an averaging, or conditional expectation operator. 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 with norm 1 and, by arguments involving characteristic functions, that 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; see references in Marr (1974, Note in Proof) and Deans (1983, Section 7.6).

Since the underlying spaces are two dimensional, we need double indices, specifically $\nu \in N = \{(l, m) : m = 0, 1, 2, \dots; l = m, m-2, \dots, -m\}$. In brain space, an orthonormal basis for $L^2(B, \mu)$ is given by

$$\varphi_{\nu}(r, \theta) = (m+1)^{\frac{1}{2}} Z_m^l(r) e^{i l \theta} \quad \nu = (l, m) \in N, (r, \theta) \in B, \quad (5.1)$$

where Z_m^l denotes the *Zernike polynomial* of degree m and order l , familiar in optics; see, for example, Deans (1983, Section 7.6), or Born and Wolf (1975, Chapter 9.2.1 and Appendix VII). Zernike polynomials arise naturally from a study of the action of rotation on $L^2(B, \mu)$, satisfy the orthogonality relation $\int_0^1 Z_{l+2s}^l(r) Z_{l+2s}^l(r) r dr = \frac{1}{2} (|l| + 2s + 1)^{-1} \delta_{st}$, and can be expressed in terms of the more general family of Jacobi polynomials. These and other properties together with a list of the first few

polynomials are given in the above references.

In detector space the corresponding orthonormal functions in $L^2(D, \lambda)$ are

$$\psi_\nu(s, \varphi) = U_m(s) e^{il\varphi} \quad \nu = (l, m) \in N, \quad (s, \varphi) \in D \quad (5.2)$$

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

$$b_\nu = (m+1)^{-1/2} \quad \nu = (l, m) \in N. \quad (5.3)$$

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 (5.1) and (5.2) 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

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

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.

In Section 7, we carry out a worst-case analysis of various estimators in the PET problem. This worst-case analysis is performed over a suitable class \mathbf{B} of emission densities f in brain space. For reasons of mathematical tractability, this class is taken to be a particular ellipsoid in the Hilbert space $H = L^2(B, \mu)$. In terms of the real version of the orthonormal basis $\{\varphi_\nu\}$, the ellipsoid \mathbf{B} is specified by an array of constants $\{a_\nu\}$ and a threshold C :

$$\mathbf{B} = \{f = \sum f_\nu \varphi_\nu : \sum a_\nu^2 f_\nu^2 < C^2\}.$$

Our immediate goal is to discuss the interpretation of this ellipsoid condition for specific arrays $\{a_\nu\}$. In the simple case where $\{\varphi_\nu\}$ is the sequence of trigonometric polynomials on 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. Thus ellipsoid conditions can amount to the imposition of smoothness and integrability requirements.

To describe specific ellipsoids in the double-index 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 $N' = \{(j, k) : j \geq 0, k \geq 0\}$. Now let

$$\mathbf{B}_{p,C} = \{f: f_{00} = 1, \sum_{(j,k) \in N' \setminus (0,0)} (j+1)^p (k+1)^p |f_{jk}|^2 < C^2\}. \quad (5.4)$$

It is shown in the appendix that $f = f(x_1, x_2) \in L^2(B, \mu)$ lies in $\mathbf{B}_{p,\infty}$ if and only if f has p weak derivatives that are square integrable on B with respect to the *modified* dominating measure $d\mu_{p+1}(x_1, x_2) = (p+1)(1-x_1^2-x_2^2)^p d\mu(x_1, x_2)$. This condition is of course somewhat weaker than requiring square-integrability for μ . It arises because a family of derivatives such as $(\partial/\partial x)\varphi_\nu$ is orthogonal (after a simple linear transformation) with respect to μ_2 and *not* μ_1 . When iterated p times, this yields a condition on μ_{p+1} . This same technical phenomenon also occurs in recent work of Cox (1987). To summarise, in spite of the change in dominating measure, $\mathbf{B}_{p,C}$ can be regarded as imposing a set of smoothness and integrability conditions: the higher p is, the smoother are the functions allowed in $\mathbf{B}_{p,C}$.

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 $\mathbf{B}_{p,C}$ 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 traditionally done using Sobolev embedding theorems, but in the series setting, a direct argument given in the Appendix leads to the following sharp estimate:

$$\text{If } p \geq 1, \sup_{f \in \mathbf{B}_{p,C}} \sup_{x \in B} |f(x) - 1| \leq C 2^{(1-p)/2}. \quad (5.5)$$

This bound is attained only by linear functions, for example $f(x_1, x_2) = 1 + 2^{(1-p)/2} C x_1$. Thus if $p \geq 1$, $f(x) \geq 0$ on $|x| \leq 1$ so long as $C \leq 2^{(p-1)/2}$. Of course, the more smoothness that is assumed, the larger the allowable values of C .

Note also that if $g = Pf$, then

$$\sup_y |g(y) - 1| \leq \sup_x |f(x) - 1| \quad (5.6)$$

since P is an averaging operator.

6. Some density estimators

In this section we shall construct two linear estimators of the density f , one based on direct observations from f and one based on "indirect" observations from the density g in detector space. Of course, in practice observations cannot be taken from f itself and only indirect observations are possible. Both the estimators are based on orthogonal expansions in series derived from the singular value decomposition of the Radon transform discussed in Section 5 above. It is not our intention that the estimators we construct should actually be used in practice, because they would be inefficient computationally and would not necessarily yield non-negative estimates. The non-linear methods that are most useful in practice (see, for example, Vardi, Shepp and Kaufman, 1985, and Jones, Silverman and Wilson, 1988) are difficult to analyse mathematically; in any case we shall show that the weighted orthogonal series estimators introduced in this section are, in a certain sense, asymptotically optimal even among non-linear methods. Orthogonal series estimators of probability density functions have been the subject of considerable attention in the literature, particularly in the univariate case. See, for example, Silverman (1985, Section 2.7), Wertz (1978, Chapter 5), Kronmal and Tarter (1968) and Prakasa Rao (1983, Sections 2.2 and 3.3).

Suppose, first, that we have independent observations X_1, \dots, X_n drawn from the density f in brain space. The basic idea of the orthogonal series method is to expand f as the series

$$f = \sum_{\nu} f_{\nu} \varphi_{\nu} \quad (6.1)$$

and then to obtain suitable estimates of the coefficients f_{ν} , which are substituted into (6.1) to give an estimate of f . The indices ν in (6.1) are each double subscripts (l, m) as explained in Section 5 above.

Define empirical coefficients ξ_{ν} by

$$\xi_{\nu} = n^{-1} \sum_{i=1}^n \varphi_{\nu}(X_i). \quad (6.2)$$

The ξ_{ν} depend on n , but this dependence will not be expressed explicitly. Since, for each ν , $E\xi_{\nu} = \int \varphi_{\nu} f d\mu = f_{\nu}$, each ξ_{ν} will be an unbiased estimator of the corresponding coefficient f_{ν} . For reasons explained in Silverman (1985, Section 2.7), in order to obtain a good estimate of the density f it is necessary to 'taper' the ξ_{ν} by a suitable collection of tapering weights w_{ν} . The direct estimate \hat{f} of f that we shall consider is defined by setting

$$\hat{f}_{\nu} = w_{\nu} \xi_{\nu}, \quad \text{so that} \quad \hat{f} = \sum w_{\nu} \xi_{\nu} \varphi_{\nu}. \quad (6.3)$$

We shall see in Section 7 below that the appropriate choice of weights will depend on the smoothness conditions assumed for the density f .

Turn now to the indirect estimation of f from a sample Y_1, \dots, Y_n from the density $g = Pf$ in detector space. It was shown in Section 5 above that the expansion $g = \sum g_\nu \psi_\nu$ of g in terms of the eigenfunctions ψ_ν in detector space is obtained by setting $g_\nu = b_\nu f_\nu$, where the array (b_ν) is as defined in equation (5.3). Define empirical coefficients η_ν by

$$\eta_\nu = n^{-1} \sum_{i=1}^n \psi_\nu(Y_i). \quad (6.4)$$

For each ν , η_ν will be an unbiased estimator of g_ν and so $b_\nu^{-1} \eta_\nu$ will be an unbiased estimator of f_ν . As before, we introduce an array of tapering weights u_ν , and define an estimator f^* of f by

$$f^* = \sum u_\nu b_\nu^{-1} \eta_\nu \phi_\nu, \quad \text{so that } f^* = \sum u_\nu b_\nu^{-1} \eta_\nu \phi_\nu. \quad (6.5)$$

It will again be the case that the ideal choice of weights will depend on the smoothness conditions assumed for f , and this will be discussed in the next section.

7. Choosing the weights

7.1 Results for a fixed true density

In this section we shall investigate how the weights w_ν and u_ν should be chosen to yield good estimates of the density f . We shall also consider various consequences of the ideal choice of weights. Our work on the choice of weights depends on some simple sampling properties of the estimates \hat{f} and f^* , and it is these that we study first of all.

For any fixed density f define constants σ_ν^2 by

$$\begin{aligned} \sigma_\nu^2 &= \text{var } \varphi_\nu(X_1) = \int \varphi_\nu^2 f d\mu - \left(\int \varphi_\nu f d\mu \right)^2 \\ &= \int \varphi_\nu^2 f d\mu - f_\nu^2 \end{aligned} \quad (7.1)$$

It was shown in Section 6 that

$$E\xi_\nu = f_\nu \quad (7.2)$$

and it follows from (7.1) and the independence of the X_i that

$$\text{var } \xi_v = n^{-1} \text{var } \varphi_v(X_1) = n^{-1} \sigma_v^2 \quad (7.3)$$

We shall judge closeness of the estimator \hat{f} to the true density f by the mean integrated square error $E \int (\hat{f} - f)^2 d\mu$. Though some authors (see for example Devroye and Györfi, 1985) prefer other criteria of accuracy of density estimation, mean integrated square error is both intuitively attractive and, particularly in the present context, mathematically tractable. Because of the orthonormality of the φ_v with respect to μ ,

$$\int (\hat{f} - f)^2 d\mu = \sum_v (\hat{f}_v - f_v)^2 = \sum_v (w_v \xi_v - f_v)^2. \quad (7.4)$$

Thus, using (7.2) and (7.3), we have

$$\begin{aligned} E \int (\hat{f} - f)^2 d\mu &= \sum_v \{w_v^2 \text{var } \xi_v + (E w_v \xi_v - f_v)^2\} \\ &= \sum_v \{n^{-1} w_v^2 \sigma_v^2 + (1 - w_v)^2 f_v^2\} \end{aligned} \quad (7.5)$$

Some simple algebra from (7.5) gives the optimal choice of the weights w_v in the sense of minimum mean square error. To minimise (7.5), we set

$$w_v = f_v^2 / (f_v^2 + n^{-1} \sigma_v^2) \quad (7.6)$$

and then the mean integrated square error is $M_{\text{direct}}(f)$, where

$$M_{\text{direct}}(f) = \sum_v n^{-1} \sigma_v^2 f_v^2 / (f_v^2 + n^{-1} \sigma_v^2). \quad (7.7)$$

It is important to note that the optimal weights w_v themselves depend on the unknown density f , and so, even if the observations X_1, \dots, X_n were known, it would not be possible in general to attain this optimal mean integrated square error. The quantity $M_{\text{direct}}(f)$ is the minimum possible mean integrated square error for any weight array, and should be thought of as a benchmark against which any actual weight sequence can be compared.

For the indirect estimator f^* , some very similar calculations can be performed. Define constants τ_v^2 by

$$\tau_v^2 = \text{var } \psi_v(Y_i) = \int \psi_v^2 g d\lambda - g_v^2, \quad (7.8)$$

so that, as before,

$$\text{var } \eta_v = n^{-1} \tau_v^2.$$

Making use of (6.5) we have

$$E \int (f^* - f)^2 d\mu = E \sum_v (f_v^* - f_v)^2 = E \sum_v (b_v^{-1} u_v \eta_v - f_v)^2$$

$$\begin{aligned}
&= \sum_{\nu} (b_{\nu}^{-2} u_{\nu}^2 \text{var } \eta_{\nu} + (E b_{\nu}^{-1} u_{\nu} \eta_{\nu} - f_{\nu})^2) \\
&= \sum_{\nu} \{n^{-1} b_{\nu}^{-2} u_{\nu}^2 \tau_{\nu}^2 + (1 - u_{\nu})^2 f_{\nu}^2\} \quad (7.9)
\end{aligned}$$

A comparison of (7.5) and (7.9) shows that the squared bias term has the same form in both cases, but the variance terms are inflated by a factor of b_{ν}^{-2} in the indirect case. To counteract this inflation, the optimally chosen u_{ν} decay faster than the w_{ν} given in equation (7.6). By very similar manipulations to those leading to (7.6), the optimal choice of weights u_{ν} will be given by

$$u_{\nu} = f_{\nu}^2 / (f_{\nu}^2 + n^{-1} b_{\nu}^{-2} \tau_{\nu}^2) \quad (7.10)$$

and the minimum possible mean integrated square error $M_{\text{indirect}}(f)$ for the density f will be

$$M_{\text{indirect}}(f) = \sum_{\nu} n^{-1} b_{\nu}^{-2} \tau_{\nu}^2 f_{\nu}^2 / (f_{\nu}^2 + n^{-1} b_{\nu}^{-2} \tau_{\nu}^2) \quad (7.11)$$

7.2 Results for densities constrained to lie in a given class

The work of Section 7.1 gave expressions for the best possible mean integrated square error for a particular density f . By contrast, we shall now find densities that are least favourable to estimate within a particular class, in terms of order of magnitude of mean integrated square error. This will be a preliminary to the discussion of the comparisons between direct and indirect estimation. We shall also find the weights that should be used to minimize, in order of magnitude, the maximum mean square error for densities in a particular class.

Consider a smoothness class of densities $\mathbf{B} = \mathbf{B}_{p,C}$ as defined in Section 5 above. Let $m_C = 2^{(1-p)/2} C$, and assume that C is chosen sufficiently small that $m_C < 1$. From (5.5) it will follow that $\inf_{\mathbf{B}} f \geq 1 - m_C$ and $\sup_{\mathbf{B}} f \leq 1 + m_C$, and these bounds on f will imply bounds on σ_{ν}^2 . For any $\nu \neq (0,0)$, we will have

$$\sigma_{\nu}^2 \leq \int \varphi_{\nu}^2 f \, d\mu \leq (1 + m_C) \int \varphi_{\nu}^2 \, d\mu = 1 + m_C \quad (7.12)$$

and

$$\begin{aligned}
\sigma_{\nu}^2 &= E\{\varphi_{\nu}(X_1) - f_{\nu}\}^2 = \int (\varphi_{\nu} - f_{\nu})^2 f \, d\mu \\
&\geq (1 - m_C) \int (\varphi_{\nu} - f_{\nu})^2 \, d\mu \geq (1 - m_C) \int \varphi_{\nu}^2 \, d\mu \\
&= 1 - m_C \quad (7.13)
\end{aligned}$$

since $\int \varphi_{\nu} \, d\mu = 0$ and $\int \varphi_{\nu}^2 \, d\mu = 1$.

Since φ_{00} is constant, we have $\sigma_{00}^2 = 0$ for all f and so the weight w_{00} will always be set equal to 1. The sums in (7.5) and (7.7) can be taken over all v except $(0,0)$ without changing their value. Let

$$m_0(f, w) = \sum_v \{n^{-1}w_v^2 + (1-w_v)^2 f_v^2\} \quad (7.14)$$

and define

$$M_0(f) = \min_w m_0(f, w) = \sum_v n^{-1} f_v^2 / (f_v^2 + n^{-1}). \quad (7.15)$$

The bounds (7.12) and (7.13) ensure that the ratio between $M_{\text{direct}}(f)$ and $M_0(f)$ lies in the interval $[1-m_C, 1+m_C]$, and so is uniformly bounded above and below for all n and all f in \mathbf{B} . Hence using $m_0(f, w)$ as a surrogate for mean integrated square error will have no effect in order of magnitude.

Consider, now, the maximization of $M_0(f)$ over \mathbf{B} . We recall a lemma of Pinsker (1980, Lemma 1). Subtracting a Lagrange multiplier term $\gamma_0 \sum a_v^2 f_v^2$ from $M_0(f)$ it can be seen by standard calculus that the maximizer satisfies

$$f_v^2 = n^{-1}(\gamma_0^{-1/2} a_v^{-1} - 1)_+ \quad (7.16)$$

and that the maximum value

$$\max_{\mathbf{B}} M_0(f) = n^{-1} \sum_v (1 - \gamma_0^{1/2} a_v)_+ \quad (7.17)$$

where γ_0 is chosen to ensure that

$$n^{-1} \sum a_v^2 (\gamma_0^{-1/2} a_v^{-1} - 1)_+ = C^2. \quad (7.18)$$

The weight array corresponding to the (f_v^2) of (7.16) will be given by

$$w_v = (1 - \gamma_0^{1/2} a_v)_+. \quad (7.19)$$

Regarded as a function of the vectors (f_v^2) and (w_v) , $m_0(f, w)$ is convex over (w_v) for fixed (f_v^2) and linear, and hence concave, over (f_v^2) for fixed (w_v) . The domain of both (w_v) and (f_v^2) is the convex set of all non-negative sequences. It follows by the usual arguments of optimisation theory (see, for example, Whittle, 1971) that the 'maximin' solution of (7.17) is also a solution to the problem

$$\min_w \max_{f \in \mathbf{B}} m_0(f, w)$$

and that the minimizing weights are those given by (7.19). Any density f satisfying (7.16) will be least favourable in the class \mathbf{B} . The quantity in (7.17) will be, in order of magnitude, the minimax mean integrated square error for the direct estimation of f

over the class \mathbf{B} .

Now turn to the case of indirect estimation. The nature (2.1) of $Pf(s, \varphi)$ as an average of f over a certain line segment in the unit disc implies that, taking inf and sup over \mathbf{B} ,

$$\inf f \leq \inf Pf \leq \sup Pf \leq \sup f$$

and hence that the bounds (7.12) and (7.13) also apply to the τ_v^2 . As a surrogate for the mean integrated square error $\int (f^* - f)^2 d\lambda$ we use

$$m_1(f, u) = \sum_v \{n^{-1} b_v^{-2} u_v^2 + (1 - u_v)^2 f_v^2\}, \quad (7.20)$$

and again the relative error of the surrogate is at most m_C . Analogous arguments to those for the direct case show that

$$\begin{aligned} \min_u \max_{f \in \mathbf{B}} m_1(f, u) &= \max_{f \in \mathbf{B}} \min_u m_1(f, u) \\ &= n^{-1} \sum b_v^{-2} (1 - \gamma_1^{\frac{1}{2}} a_v)_+ \end{aligned} \quad (7.21)$$

with γ_1 chosen to ensure that

$$n^{-1} \sum a_v^2 b_v^{-2} (\gamma_1^{-\frac{1}{2}} a_v^{-1} - 1)_+ = C^2. \quad (7.22)$$

The minimum and maximum in (7.21) are attained by choosing as optimum weights

$$u_v = (1 - \gamma_1^{\frac{1}{2}} a_v)_+ \quad (7.23)$$

and as least favourable density any f for which

$$f_v^2 = n^{-1} b_v^{-2} (\gamma_1^{-\frac{1}{2}} a_v^{-1} - 1)_+. \quad (7.24)$$

To summarize this section, we have found, within a bounded factor, the minimax mean integrated square error over the class \mathbf{B} for the estimation of f both from direct and indirect observations. In both cases the weights are chosen as best possible for the class \mathbf{B} . Although the expressions may appear to be inelegant and intractable, we use them in the next section to obtain orders of magnitude for the minimax mean integrated square errors. Comparing these orders of magnitude will give an indication of how much information is lost by using indirect rather than direct observations. Although we have restricted attention in this section to a very special class of linear estimators, we shall show later on that the minimax rates are not altered by extending attention to all estimators of f , whether linear or non-linear.

8. Rates of convergence for orthogonal series estimators

In this section we shall make use of the results of Section 5 above to find the orders of magnitude of the minimax mean integrated square errors for direct and indirect observations. The calculations involve little more than the approximation of sums by integrals and some simple calculus.

We shall use the (j, k) parametrisation of Section 5, so that all the expansions of Section 7 became sums over (j, k) with $j = 0, 1, \dots$ and $k = 0, 1, \dots$. The smoothness class **B** will be taken to be, for a fixed $p > 0$,

$$\mathbf{B} = \{f: f_{00} = 1 \text{ and } \sum (j+1)^p (k+1)^p f_{jk}^2 \leq C^2\} \quad (8.1)$$

so that, following (5.4),

$$a_{jk}^2 = (j+1)^p (k+1)^p. \quad (8.2)$$

As discussed in Section 5, the singular values are given by

$$b_{jk} = (1+j+k)^{-1} \text{ for all } j \text{ and } k. \quad (8.3)$$

The following integral approximation lemma will be used repeatedly. It is obtained heuristically by approximating sums by integrals and its proof is given in the appendix. As in Section 5, the notation \approx is used to connect two quantities whose ratio is uniformly bounded above and below away from zero. The quantity γ in (8.4) is Euler's constant, 0.57722... .

Lemma 8.1

For any η , let $\sum_{(\eta)}$ denote a sum over $\{(j, k): 1 \leq (j+1)(k+1) \leq \eta\}$.

For fixed $r \geq 0$, as η tends to infinity,

$$\sum_{(\eta)} (j+1)^r (k+1)^r = (r+1)^{-1} \eta^{r+1} \{\log \eta + 2\gamma - (r+1)^{-1}\} + O(\eta^{r+1/2}) \quad (8.4)$$

and

$$\sum_{(\eta)} (j+k+1)(j+1)^r (k+1)^r = \frac{1}{3} \pi^2 (r+2)^{-1} \eta^{r+2} + O(\eta^{r+1} \log \eta). \quad (8.5)$$

Consider first the direct estimation of f . We will have $\gamma_0 a_v^2 \leq 1$ if and only if $(j+1)(k+1) \leq \gamma_0^{-1/p}$ and so the $(\cdot)_+$ in (7.17) and (7.18) may be replaced by (\cdot) if the sums over all v are replaced by $\sum_{(\eta)}$ with $\eta = \gamma_0^{-1/p}$. Performing this replacement, and applying (8.4), equation (7.18) becomes

$$\begin{aligned} C^2 &= n^{-1} \sum_{(\eta)} (\gamma_0^{-1/2} a_v - a_v^2) \\ &= n^{-1} \sum_{(\eta)} \{ \gamma_0^{-1/2} (j+1)^{p/2} (k+1)^{p/2} - (j+1)^p (k+1)^p \} \end{aligned}$$

$$= n^{-1} \eta^{p+1} (a_1 \log \eta + b_1) + n^{-1} O(\eta^{p+\frac{1}{2}}), \quad (8.6)$$

where $a_1 = p(p+1)^{-1}(p+2)^{-1}$ and $b_1 = 2\gamma a_1 - \{4(p+2)^{-2} - (p+1)^{-2}\}$. Let $\eta_n = \eta_n(C, p)$ be the solution for η of equation (8.6); this will be studied below. Apply similar manipulations to the minimax surrogate mean integrated square error (7.17) to obtain

$$\begin{aligned} r_{LD}^*(n) &= \max_{\mathbf{B}} M_0(f) = n^{-1} \sum_{(\eta)} (1 - \gamma_0^{\frac{1}{2}} a_v) \\ &= p(p+2)^{-1} n^{-1} \eta_n \{ \log \eta_n + 2\gamma - (p+4)(p+2)^{-1} \} + n^{-1} O(\eta_n^{\frac{1}{2}}). \end{aligned} \quad (8.7)$$

This yields equation (4.4) with the values for the constants $c_1 = p(p+2)^{-1}$ and $c_2 = 2\gamma - (p+4)/(p+2)$. It is easily seen that $\eta_n \sim (n/\log n)^{1/(p+1)}$ and that $\max_{\mathbf{B}} M_0(f) \sim (n/\log n)^{-p/(p+1)}$.

We can obtain more precise results by a more careful analysis of equation (8.6). As in Section 4, denote by $\alpha(x)$ the solution of the equation $\alpha \log \alpha = x$. The substitution $\eta = \exp(-b_1/a_1) y^{1/(p+1)}$ reduces equation (8.6) to the form

$$y \log y = a_1^{-1} C^2 n (p+1) \exp\{(p+1)b_1/a_1\}. \quad (8.8)$$

It follows that

$$\eta_n = d_3 \{ \alpha(c_3 n) \}^{1/(p+1)} \quad (8.9)$$

with $c_3 = a_1^{-1} C^2 (p+1) \exp\{(p+1)b_1/a_1\}$ and $d_3 = \exp(-b_1/a_1)$. Substituting back into (8.7) gives, after some algebra using the fact that $\alpha(x) = (x/\log x) \{1 + o(1)\}$ for large x ,

$$r_{LD}^*(n) \sim d_1 C^{2/(p+1)} (\log n/n)^{p/(p+1)} \quad (8.10)$$

where $d_1 = (p+1)^{1/(p+1)} \{ p(p+2)^{-1} (p+1)^{-1} \}^{p/(p+1)}$.

It was shown in Section 7 that the true minimax mean integrated square error will have asymptotic behaviour of the same rate as its surrogate, and hence it follows in particular that, as $n \rightarrow \infty$, for the estimator \hat{f} as defined in Section 6,

$$\min_w \max_{f \in \mathbf{B}} E \int (\hat{f} - f)^2 d\mu = \max_{f \in \mathbf{B}} \min_w E \int (\hat{f} - f)^2 d\mu \sim (n/\log n)^{-p/(p+1)}. \quad (8.11)$$

Exactly the same steps can be carried out for indirect estimation. This time set $\tilde{\eta} = \gamma_1^{-1/p}$ and write equation (7.22) in the form

$$\begin{aligned} C^2 &= n^{-1} \sum_{(\eta)} (j+k+1) \{ \gamma_1^{-\frac{1}{2}} (j+1)^{p/2} (k+1)^{p/2} - (j+1)^p (k+1)^p \} \\ &= a_2 n^{-1} \tilde{\eta}^{p+2} + n^{-1} O(\tilde{\eta}^{p+1} \log \tilde{\eta}). \end{aligned} \quad (8.12)$$

where $a_2 = (\pi^2/3) p(p+2)^{-1} (p+4)^{-1}$. Ignore the error term and solve for $\tilde{\eta}$ to obtain $\tilde{\eta}_n = (nC^2/a_2)^{1/(p+2)}$. Substituting back into (7.21) and performing some algebra gives the required equation (4.6) for the minimax surrogate mean integrated square error $r_{LD}^*(n)$, with the constant $d_2 = \frac{1}{2} \{ \pi^2 p/3(p+4) \}^{p/(p+2)} (p+2)^{2/(p+2)}$. Hence it follows,

using the equivalence of the surrogate mean integrated square error and the true mean integrated square error, that

$$\min_u \max_{f \in B} E \int (f^* - f)^2 d\mu = \max_{f \in B} \min_u E \int (f^* - f)^2 d\mu = n^{-p/(p+2)}. \quad (8.13)$$

Let us now turn to the question of equivalent sample sizes discussed in Section 4, namely the (approximate) solution of the equation $r_{LD}^*(m) = r_{LD}^*(n)$ for given n . A simple, and very asymptotic, calculation uses relations (4.5) and (4.6), with the error terms ignored, to conclude that

$$m(n) \approx C^{-2/(p+2)} a_3 n^{(p+1)/(p+2)} \log n,$$

where

$$\begin{aligned} a_3 &= (p+1)(p+2)^{-1} (d_1/d_2)^{(p+1)/p} \\ &= C^{-2/(p+2)} 2^{(p+1)/2} p^{1/(p+2)} (p+1)^{1/p} (p+2)^{-2-2(p+1)/p(p+2)} \{3\pi^{-2}(p+4)\}^{(p+1)/(p+2)}. \end{aligned}$$

This apparently fearsome constant decreases innocuously from 0.27 to 0.055 as p increases from 1 to 10 and is well fit by the function $0.006 + 0.533p^{-1} - 0.276p^{-2}$ over this range!

A more accurate procedure is to solve $r_{LD}^*(m) = r_{LD}^*(n)$ using the approximation (8.7) for $r_{LD}^*(m)$ instead of (8.10). For values of n such as 10^7 and 10^8 considered in Table 4.1, it is best to solve for $m(n)$ numerically using (8.7) and (4.6), ignoring the error terms. Each evaluation of $r_{LD}^*(m)$ in turn requires that η_n is found from (8.9), performing a numerical evaluation of the function α . Table 4.1 contains the results of this procedure for selected values of p .

To summarise this section, we have shown that, for the linear weighted orthogonal series estimators, the optimum rate of consistency in mean integrated square error is reduced 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 non-linear estimators.

9. Lower bounds

In this section we establish lower bounds on the rates of convergence to the density f of estimators based on direct and indirect observations. These lower bounds apply to arbitrary (even non-linear) estimators, and show that the minimax rates obtained by the simple series estimators of Section 7 cannot be improved. The 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.

We write $\tilde{f}(x) = \tilde{f}(x, X^n)$ for an arbitrary estimator of the unknown density $f(x)$ based on n direct observations $X^n = (X_1, \dots, X_n)$ drawn i.i.d. from $f(x)$. Correspondingly, we write $\tilde{f}^*(x) = \tilde{f}^*(x, Y^n)$ for an arbitrary estimator of f based on n indirect observations $Y^n = (Y_1, \dots, Y_n)$ drawn i.i.d. from $g(x) = (Pf)(x)$. The notation $B_{p,C}$ will denote the ellipsoid (5.4), with C chosen so as to ensure that all members are probability densities.

Theorem 9.1: Let $p \geq 1$. There exist constants $c = c(p, C)$ and $c' = c'(p, C)$ such that in the direct estimation problem

$$\inf_{\tilde{f}} \sup_{f \in B_{p,C}} E \|\tilde{f} - f\|^2 \geq c(n/\log n)^{-p/(p+1)}, \quad (9.1)$$

and in the indirect problem

$$\inf_{\tilde{f}^*} \sup_{f \in B_{p,C}} E \|\tilde{f}^* - f\|^2 \geq c' n^{-p/(p+2)}. \quad (9.2)$$

Remark: It will be apparent from the proof that explicit expressions for c and c' could be obtained. However, the values obtained by the present method may well be very conservative, and our present goal is to obtain crude qualitative insights. The problem of obtaining exact constants in (9.1) and (9.2) is open and perhaps of some technical interest.

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" $\tau(\epsilon)$ 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 optimisation problem for the particular operator in question. This viewpoint was taken recently by Donoho and Liu (1987) in their study of estimation of linear functionals.

We begin with step (ii), which is formulated in slightly greater generality than needed for Theorem 9.1. We then return to step (i) to compute the particular moduli occurring in (9.1) and (9.2).

Suppose there are available n i.i.d. observations $Y^{(n)} = (Y_1, \dots, Y_n)$ from a density $g(y)d\lambda(y)$, $y \in D$, and that we wish to estimate $f = Qg$, where $Q : (K, \|\cdot\|_K) \rightarrow (H, \|\cdot\|_H)$ is a linear operator between the inner product spaces K and H .

(For the PET application, in the indirect case we take $H = L^2(B, \mu)$ and K as the linear subspace of $L^2(D, \lambda)$ which is the range of the normalised Radon transform P of Section 2. Each space has the inner product norm and Q is taken to be P^{-1} . In the direct case, $H = K = L^2(B, \mu)$ and $Q = I$.)

Denote by $\tilde{f}(Y^{(n)})$ an arbitrary estimator of f based on the data $Y^{(n)}$ from g . Lower bounds to the estimation error $\|\tilde{f}(Y^{(n)}) - f\|_H$ depend on a generalised modulus of continuity of the operator Q mapping g to f .

We suppose that $g \in G \subset K$. In our applications the parameter space G will be a translate $V + g^\circ$ of a set V that is balanced about the origin ($v \in V \Rightarrow -v \in V$). Typically g° would be the uniform density.

Suppose that M is a finite dimensional subspace of K . A set $U = M \cap \{v \in K : \|v\|_K \leq r\}$ will be called a finite-dimensional ball of radius r ; we denote the radius of such a ball by $r(U)$. The dimension, $d(U)$, of the ball is the dimension of M . We shall need a dimension-normalised measure of radius $\rho(U) = d(U)^{-1/2}r(U)$.

The generalised modulus of continuity of Q over the parameter space V (and G) may now be defined as

$$\tau(\varepsilon) = \sup_{\substack{U \subset V \\ \rho(U) = \varepsilon}} \inf_{v \in U : \|v\|_K = r(U)} \|Qv\|_H, \quad (9.3)$$

where the supremum is taken over finite dimensional balls of the type described above. Loosely speaking, $\tau(\varepsilon)$ measures the increase of the singular values of Q relative to the parameter space V at resolution range ε .

Notice that if Q is a linear functional (so that $(H, \|\cdot\|_H) = (\mathbb{R}, |\cdot|)$), the above definition reduces to

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

which is the modulus of continuity studied by Donoho and Liu (1987).

The significance of the modulus functional is that an (often sharp) lower bound for the rate of convergence of $\|\tilde{f}(Y^{(n)}) - Qg\|$ over G 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 G :

$$\text{For some } B < \infty, K(g_\alpha, g_\beta) \leq B \|g_\alpha - g_\beta\|_K^2 \text{ for all } g_\alpha, g_\beta \in G. \quad (9.4)$$

Proposition 9.2 If condition (9.4) holds, there exist constants c_1, c_2 such that

$$\inf_{\tilde{f}_n} \sup_{g \in G} E_g \|\tilde{f}_n(Y^{(n)}) - Qg\|_H^2 \geq c_1 \tau^2(c_2 n^{-1/2})$$

Proof

1. The estimation problem is at least as hard as a discrimination problem. Choose a subset $F^\circ = \{f_1, \dots, f_M\} \subset F = Q(G)$ that is 2δ -distinguishable: namely $\|f_\alpha - f_\beta\| > 2\delta$ if $\alpha \neq \beta$. Pick a corresponding subset $G^\circ = \{g_1, \dots, g_M\} \subset G$ with $g_\alpha \in Q^{-1}f_\alpha$ (for the moment, we don't assume that Q is one-to-one). Given an estimator \tilde{f} , define a discrimination rule $\varphi(Y^{(n)}) = \varphi(Y^{(n)}, \tilde{f}) \rightarrow F^\circ$ that picks the closest element in F° to $\tilde{f}(\cdot, Y^{(n)})$. Hence, if $\varphi(Y^{(n)}) \neq f \in F^\circ$, then necessarily $\|\tilde{f} - f\| > \delta$. Thus the maximum risk of \tilde{f} is minorised by the average discrimination error rate

$$\begin{aligned} \sup_{g \in G} E_g \|\tilde{f} - Qg\|^2 &\geq \delta^2 \sup_{f \in F^\circ} P_f(\|\tilde{f} - f\| > \delta) \\ &\geq \frac{\delta^2}{M} \sum_{\alpha=1}^M P_{g_\alpha}(\varphi(Y^n) \neq f_\alpha). \end{aligned}$$

2. The average error rate in discriminating amongst M hypotheses P_α^n (where here $P_\alpha^n(dy^n) = \prod_{i=1}^n g_\alpha(y_i) \lambda(dy_i)$ is the density of n i.i.d. observations from g_α) can be minorised in terms of the Kullback-Leibler discrepancies

$$\begin{aligned} K(P_\alpha^n, P_\beta^n) &= \int \log \frac{dP_\alpha^n}{dP_\beta^n} dP_\alpha^n \\ &= n \int \log \frac{g_\alpha(y)}{g_\beta(y)} g_\alpha(y) d\lambda(y). \end{aligned}$$

This is done by convexity methods (Fano's lemma of information theory, see Ibragimov and Hasminskii (1981, p.323), and Birgé's version (1983, p.196)) and yields

$$\frac{1}{M} \sum_{\alpha=1}^M P_\alpha^n(\varphi(Y^n) \neq f_\alpha) \geq 1 - \frac{\sup_{1 \leq \alpha, \beta \leq M} K(P_\alpha^n, P_\beta^n) + \log 2}{\log(M-1)}.$$

3. Since the observations are i.i.d., $K(P_\alpha^n, P_\beta^n) = nK(g_\alpha, g_\beta)$. Using the assumption (9.4), the conclusion of 1. and 2. becomes

$$\sup_{g \in G} E_g \|\tilde{f}_n - Qg\|^2 \geq \delta^2 \left\{ 1 - \frac{nB \sup_{1 \leq \alpha, \beta \leq M} \|g_\alpha - g_\beta\|_K^2 + \log 2}{\log(M-1)} \right\}, \quad (9.5)$$

where, by construction, $\|Qg_\alpha - Qg_\beta\| = \|f_\alpha - f_\beta\| \geq 2\delta$.

4. To evaluate the lower bound (9.4), we relate M and δ , the cardinality and separation of members of F° , to the metric dimension properties of G . The idea is to choose sufficiently many hypotheses g_α (M large) that are sufficiently close ($\|g_\alpha - g_\beta\|$ small) that the average discrimination error, and hence the maximum estimation risk, is at least $\delta^2/2$.

From the definition of the modulus $\tau(\varepsilon)$, choose a finite dimensional ball $U \subset V$ so that $\rho(U) = \varepsilon$ and $\inf\{\|Qv\|_H : v \in U, \|v\|_K = r(U)\} \geq \tau(\varepsilon)/2$. Choose $v_1, \dots, v_M \in U$ such that $\|v_\alpha - v_\beta\|_K \geq r(U)/2$, and define g_α as $g^\circ + v_\alpha$ (this ensures that $g_\alpha \in G$). Thus, at the same time $\|g_\alpha - g_\beta\|_K \leq 2r(U)$ while, from the choice of U ,

$$\|Qg_\alpha - Qg_\beta\| \geq \frac{\tau(\varepsilon)}{2} \frac{\|g_\alpha - g_\beta\|}{r(U)} \geq \frac{\tau(\varepsilon)}{4}.$$

so that we may choose $2\delta = \tau(\varepsilon)/4$.

A useful lemma of approximation theory asserts that a k dimensional ball of radius r contains an $r/2$ distinguishable subset of cardinality at least 2^k (e.g. Lorentz, 1966, p.905). Thus $M \geq 2^{d(U)}$, and collecting all the bounds, the right side of (9.5) is bounded below by

$$\begin{aligned} & \left[\frac{\tau(\varepsilon)}{8} \right]^2 \left\{ 1 - \frac{nB4r^2(U) + \log 2}{\log(2^{d(U)} - 1)} \right\} \\ & \geq \frac{\tau^2(\varepsilon)}{64} \left\{ 1 - \frac{c_3 nr^2(U)}{d(U)} \right\} = \frac{\tau^2(\varepsilon)}{64} (1 - c_3 n \varepsilon^2) \end{aligned}$$

where c_3 is an appropriate constant and $\varepsilon = \rho(U) = d(U)^{-1/2} r(U)$. Now set ε so that $c_3 n \varepsilon^2 = \frac{1}{2}$ and the proof of Proposition 9.2 is complete.

Note: Assumption (9.4) will be satisfied if the densities g_α and g_β are bounded above and below:

$$0 < B_1 \leq g_\alpha(y), g_\beta(y) \leq B_2 < \infty. \quad (9.6)$$

Indeed, their Kullback-Leibler discrepancy is bounded above by their L^2 distance:

$$\begin{aligned} K(g_\alpha, g_\beta) &= \int \log \frac{g_\alpha}{g_\beta} g_\alpha d\lambda \\ &\leq c_1(B_1, B_2) \int \frac{(g_\beta - g_\alpha)^2}{g_\alpha} d\lambda \leq c_2(B_1, B_2) \|g_\alpha - g_\beta\|^2. \end{aligned}$$

(since $-\log y \leq 1 - y + c(y-1)^2$ for $y > y_0(c)$ where $y_0(c) \rightarrow 0$ as $c \rightarrow \infty$).

The condition (9.6) will hold for the smoothness classes $\mathbf{B}_{p,C}$ of Section 5 so long as $p \geq 1$ and $C < 2^{(p-1)/2}$; see (5.5) and (5.6).

We now return to the PET setting to compute the moduli $\tau(\varepsilon)$ for Theorem 9.1. In fact, we don't have to solve the optimisation problem exactly — a reasonable lower bound to $\tau(\varepsilon)$ will suffice.

Begin with the direct estimation problem, in which $H = K = L^2(B, \mu)$ and $Q = I$. Thus $\mathbf{G} = \mathbf{B}_{p,C}$, $g = f$, and so we revert to the notation of previous sections. It is convenient to restrict to balls of the form

$$U_J(r) = \{f : \sum_{v \in J} f_v^2 \leq r^2, f_v = 0 \text{ on } J^c\}.$$

(Since we always deal with probability densities, from now on we make the convention that $f_{00} = 1$ and that $J \cup J^c = N \setminus (0,0)$.) Hence, $\tau^2(\varepsilon) \geq \tau_1^2(\varepsilon) = \sup\{r^2 : U_J(r) \subset \mathbf{G} \text{ and } r^2 = \varepsilon^2 |J|\} = \varepsilon^2 \sup\{|J| : U_J(\varepsilon |J|^{1/2}) \subset \mathbf{G}\}$. To pack as many dimensions as possible into \mathbf{G} , consider J of the form $J_\eta = \{v : a_v^2 \leq \eta\} = \{j \geq 0, k \geq 0 : (j+1)(k+1) \leq \eta^{1/p}\}$. From Lemma 8.1,

$$|J_\eta| = \eta^{1/p} \log \eta^{1/p} \{1 + o(1)\}. \quad (9.7)$$

Now, if $r^2 \leq C^2 \eta^{-1}$, then $U_{J_\eta}(r) \subset \mathbf{G}$ and hence $C_{J_\eta}(C \eta^{-1/2}) \subset \mathbf{G}$. This says that the radius of the ball that can be squeezed into \mathbf{G} decreases as the number of dimensions ("frequencies") is increased. Thus $\tau_1^2(\varepsilon) \geq C^2 \eta^{-1}(\varepsilon)$ where $\eta(\varepsilon)$ is the solution to $\varepsilon^2 |J_\eta| = C^2 \eta^{-1}$. Using (9.7) we find that

$$\tau^2(\varepsilon) \geq M(\varepsilon^2 \log \varepsilon^{-2})^{p/(p+1)},$$

so that $\tau^2(c n^{-1/2}) \geq M(\log n/n)^{p/(p+1)}$,

which establishes (9.1), the first part of Theorem 9.1.

For the indirect estimation problem, we take $H = L^2(B, \mu)$, $K =$ the Hilbert subspace of $L^2(D, \lambda)$ generated by the orthonormal set of singular functions $\{\psi_v\}$. We take $Q = P^{-1}$, so that $Q\psi_v = b_v^{-1} \phi_v$. Functions $g \in K$ have expansions $\sum g_v \psi_v$, and

we now consider balls $U_J(r) = \{g : \sum_{v \in J} g_v^2 \leq r^2, g_v = 0 \text{ on } J^c\}$. On such balls it is easy to compute a lower bound to $\tau_Q(\varepsilon)$ using the singular values of Q :

$$\begin{aligned} \tau^2(\varepsilon) &\geq \tau_1^2(\varepsilon) = \sup\{r^2 \inf_{v \in J} b_v^{-2} : U_J(r) \subset G \text{ and } r^2 = \varepsilon^2 |J|\} \\ &= \varepsilon^2 \{|J| \inf_J b_v^{-2} : U_J(\varepsilon |J|^{1/2}) \subset G\} \end{aligned}$$

The parameter space $G = P(\mathbf{B}_p, C) = \{g : \sum_v a_v^2 b_v^{-2} g_v^2 \leq C^2\}$. Now we seek not only to pack many dimensions into G , but also to use subspaces where $b_v^{-2} = j+k+1$ is large. Consider therefore J of the form

$$J_\eta = \{j \geq 0, k \geq 0 : (j+1)(k+1) \leq \eta^{1/p}, j+k+1 \geq \alpha \eta^{1/p}\}.$$

In the appendix it is shown that

$$|J_\eta| = c_\alpha \eta^{1/p} + O(1) \quad \text{as } \eta \rightarrow \infty. \quad (9.8)$$

Now $\sum_{J_\eta} a_v^2 b_v^{-2} g_v^2 \leq \eta \cdot \eta^{1/p} \sum_{J_\eta} g_v^2 \leq C^2$ if $\sum_{J_\eta} g_v^2 \leq C^2 \eta^{-(p+1)/p}$.

Hence $U_{J_\eta}(C \eta^{-(p+1)/2p}) \subset G$ and thus

$$\tau_1^2(\varepsilon) \geq C^2 \eta(\varepsilon)^{-(p+1)/p} \alpha \eta^{1/p} = C^2 \eta^{-1}(\varepsilon),$$

where this time $\eta(\varepsilon)$ is the solution to $\varepsilon^2 |J_\eta| = C^2 \eta^{-(p+1)/p}$, which yields $\tau_1^2(\varepsilon) \geq M \varepsilon^{2p/(p+2)}$. Consequently, $\tau^2(c n^{-1/2}) \geq M n^{-p/(p+2)}$, which establishes (9.2) and completes the proof of Theorem 9.2.

Remark

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 s^{th} 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 p^{th} weak derivative.

10. Some remarks on sensitivity to assumptions

In Sections 2 to 5 we formulated a particular idealised model for the PET problem, together with one formal structure for comparing the minimax error of estimators and the costs of indirect observation. Obviously it is important to ask how the results change with modifications to the assumptions or error criteria. We discuss two rather different such perturbations in this section. While this is certainly not a complete sensitivity analysis, the results obtained below are broadly consistent with those of the previous sections.

10.1 Alternative error measures taking account of derivatives

Our use of integrated squared error to measure discrepancy between estimator and unknown function has shortcomings. For example, being a pointwise measure L^2 pays no attention to local spatial variations. Our results extend easily to a class of losses that also measure the closeness of derivatives of the estimate to the true unknown function; these losses take more account of the "shape" of the function than does L^2 .

It is noted in the Appendix that the norm

$$\int |f|^2 d\mu_1 + \int \sum_{\substack{r,s \geq 0 \\ r+s=q}} |D_x^r D_y^s f|^2 d\mu_{p+1} \quad (10.1)$$

is equivalent to the norm

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

Thus errors measured in norms equivalent to (10.1) will be equivalent to loss functions of the form $L(\hat{f}, f) = \sum_{\nu} c_{\nu}^2 (\hat{f}_{\nu} - f_{\nu})^2$, where $c_{\nu}^2 = c_{jk}^2 = (j+1)^q (k+1)^q$.

To extend the upper bound results of Section 8 to this setting, note that the minimax risk for linear estimates over the ellipsoid $B_{p,C}$ is given by

$$n^{-1} \sum_{(\eta)} (c_{\nu}^2 v_{\nu}^2 - c_{\nu} v_{\nu}^2 a_{\nu} \lambda^{\frac{1}{2}}),$$

where $v_{\nu}^2 = \sigma_{\nu}^2$ in the direct case and $\tau_{\nu}^2 b_{\nu}^{-2}$ in the indirect case, and λ is chosen to satisfy $n^{-1} \lambda^{-\frac{1}{2}} \sum_{(\eta)} (a_{\nu} c_{\nu} v_{\nu}^2 - a_{\nu}^2 v_{\nu}^2) = C^2$. So long as $q < p$, we obtain 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.

It follows by an extension of the method of Section 9 that these are in fact the exact rates of convergence. The 2δ -distinguishable set F° and the ball $U_J(r) = \{f : \sum_{\nu \in J} c_{\nu}^2 f_{\nu}^2 \leq r^2, f_{\nu} = 0 \text{ on } J^c\}$ are now constructed in the $|||\cdot|||$ norm. By defining

$$J_\eta = \{v: a_v^2 c_v^{-2} \leq \eta, c_v^2 > \alpha^q \eta^{q/(p-q)}, b_v^2 < \alpha \eta^{-1/(p-q)}\},$$

one ensures that, for some fixed $\alpha \in (0, 1)$,

$$\sup_{U_j(r)} \frac{|||Pf|||^2}{|||f|||^2} \leq \alpha \eta^{-1/(p-q)} \alpha^{-q} \eta^{-q/(p-q)}.$$

With these changes, the lower bounds can be derived from (9.5) just as in Section 9.

10.2 Results for the length-biased sampling model

Here we explore the effects of incorporating tube-length sampling bias into the idealised model of Section 2. We are not able to obtain equal upper and lower rates of convergence, but the ratio of our bounds grows more slowly than $\log n$. Since the upper rate is the same as for the basic model of Section 2, we conclude that ignoring the tube-length bias does not have a great effect on our overall qualitative conclusions.

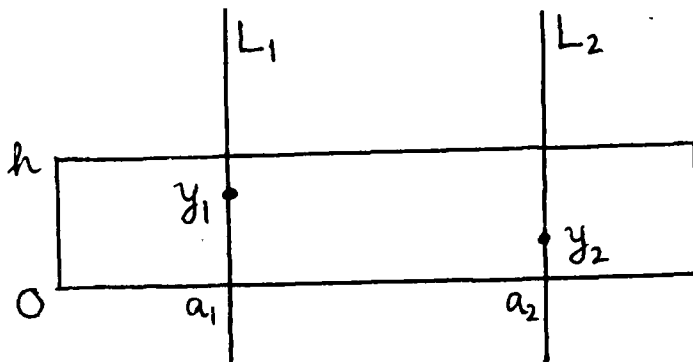


Figure 10.1: Vertical cross-section of a detector ring

The tube length bias arises because the direction of emissions is uniform in \mathbb{R}^3 , not just in the plane of detectors. Consider a detector tube of length l and height h (see Figure 10.1), and vertical lines L_i with abscissae a_i ($i=1,2$). An emission is detected if the two photons hit the opposite ends of the tube. We assume that $h \ll l$ and hence that the emission density is constant in the vertical direction. If an emission occurs with abscissa a_1 , denote its probability of detection by $P(D|a_1)$. A simple symmetry argument shows that $P(D|a_1)$ does not depend on the value of $a_1 \in [0, l]$. Indeed, let $p_{a_2|a_1}(y_2|y_1)$ denote the conditional density of the intercept on L_2 of an emission at y_1 on L_1 . This density is symmetric in its arguments: $p_{a_2|a_1}(y_2|y_1) = p_{a_1|a_2}(y_1|y_2)$. Writing \mathcal{L}_{a_1, a_2} for the collection of intercepts (y_1, y_2) determining a line hitting both ends of the tube, we see that

$$P(D|a_1) = \int_{\mathcal{L}_{a_1, a_2}} p_{a_2|a_1}(y_2|y_1) \frac{dy_1}{h} dy_2$$

$$\begin{aligned}
 &= \int_{L_{a_1, a_2}} p_{a_1|a_2}(y_1|y_2) \frac{dy_2}{h} dy_1 \\
 &= P(D|a_2).
 \end{aligned}$$

Since $P(D|a_1)$ is independent of a_1 and $h \ll l$, it follows that

$$P(D|a_1) = P(D|0) = \frac{1}{\pi} \int_0^h \tan^{-1} \left[\frac{y}{l} \right] + \tan^{-1} \left[\frac{h-y}{l} \right] \frac{dy}{h} = \frac{h}{\pi l}$$

Thus the probability of detection is inversely proportional to the length of the tube, namely $2(1-s^2)^{\frac{1}{2}}$ for a tube with co-ordinates (s, φ) . The dominating measure $\lambda(ds, d\varphi) = 2\pi^{-2}(1-s^2)^{\frac{1}{2}} ds d\varphi$ in detector space should therefore be adjusted by a factor proportional to $(1-s^2)^{-\frac{1}{2}}$ yielding a new dominating measure $\lambda_2(ds, d\varphi) = ds d\varphi/2\pi$, which is just Lebesgue measure on detector space.

Alternatively, one can explicitly build the three dimensional structure into the derivation by assuming that there is a detection *cylinder* of height h , not necessarily small. The observed density of detected lines (which now has four arguments) is a weighted Radon line transform of the unknown emission density. In the limit as $h \rightarrow 0$, one recovers the planar version, incorporating the tube length correction, which has the form, up to a proportionality constant,

$$\tilde{g}(s, \varphi) ds d\varphi = 4h^2 g_0(s, \varphi) + O(h^4(1-s^2)^{-3/2}) ds d\varphi$$

where

$$g_0(s, \varphi) = \frac{1}{2}(1-s^2)^{-\frac{1}{2}} \int f(s \cos \varphi - t \sin \varphi, s \sin \varphi + t \cos \varphi) dt$$

as before.

A new difficulty arises because $g_0(s, \varphi)$ does *not* in general integrate to 1 against $ds d\varphi/2\pi$. Indeed it may be checked that

$$\begin{aligned}
 \beta(f) &= \int_0^1 \int_0^{2\pi} g_0(s, \varphi) \frac{ds d\varphi}{2\pi} = \frac{1}{2} \int_B K(|x|^2) f(x) d\mu(x) \\
 &= \frac{1}{2} \sum_{\substack{m \geq 0 \\ \text{even}}} (m+1)^{-3/2} f_{0m}
 \end{aligned} \tag{10.2}$$

where $K(m) = \int_0^{\pi/2} (1-m \sin^2 \theta)^{-\frac{1}{2}} d\theta$ is the complete elliptic integral of the first kind, and f_{0m} is the Fourier coefficient of f for the (radial) singular function $\varphi_\nu(x)$ with $\nu = (0, m)$. To obtain a probability density in detector space (relative to $ds d\varphi/2\pi$) we set

$$\begin{aligned}
g(s, \varphi) &= (P_2 f)(s, \varphi) = (Pf)(s, \varphi) / \beta(f) \\
&= \frac{1}{2(1-s^2)^{\frac{1}{2}} \beta(f)} \int f(s \cos \varphi - t \sin \varphi, s \sin \varphi + t \cos \varphi) dt \quad (10.3)
\end{aligned}$$

We are unable to duplicate the analysis of previous sections for lack of the explicit singular value decomposition of $P : L^2(B, \mu) \rightarrow L^2(D, dsd\varphi)$ (in fact, we don't even know if P is L^2 -bounded here!). Instead we adopt some *ad hoc* devices.

To compute an upper bound via orthogonal series, we modify the basis functions in detector space into a non-orthogonal set $\tilde{\psi}_\nu = 4\pi^{-1}(1-s^2)^{\frac{1}{2}}\psi_\nu$, which nevertheless have the property that $E\tilde{\psi}_\nu = \beta^{-1}(f) \int \psi_\nu Pf d\lambda = \beta^{-1}b_\nu f_\nu$. From the empirical Fourier coefficients $\eta_\nu = n^{-1} \sum \tilde{\psi}_\nu(Y_i)$, and assuming for the moment that $\beta = \beta(f)$ is known, we form the natural estimate

$$\tilde{f}(x) = \sum_\nu u_\nu \beta b_\nu^{-1} \eta_\nu \phi_\nu(x). \quad (10.4)$$

where u_ν are, as always, tapering weights.

In practice, the bounded linear functional $\beta(f)$ must be estimated, which we can expect to do at rate $n^{-\frac{1}{2}}$. Indeed, since $b_{00} = f_{00} = 1$, an $n^{\frac{1}{2}}$ -consistent estimator of $\beta^{-1}(f)$ is given by $\eta_{00} = n^{-1} \sum \tilde{\psi}_{00}(Y_i) = 4\pi^{-1} n^{-1} \sum_i (1-S_i^2)^{\frac{1}{2}}$. This indicates, but of course does not fully prove, that the rate of convergence of the estimate of f , which will be slower than $n^{-\frac{1}{2}}$, does not depend on whether $\beta(f)$ is known or not.

We thus compute the best choice of weights (u_ν) and find the worst MSE over $B_{p,C}$ for the resulting estimator of the form (10.4). First we note some inequalities:

$$\pi/4 \leq \beta(f), \quad \sup_{B_{p,C}} \beta(f) = 1 + C3^{-3/2}2^{-p} \quad (10.5)$$

and

$$\tau_\nu^2 = \text{var } \tilde{\psi}_\nu(Y) \leq E|\tilde{\psi}_\nu|^2(Y) \leq 16\pi^{-2}. \quad (10.6)$$

(The first inequality in (10.5) follows from the bound $K(m) \geq \pi/2$ in (10.2), and the second by maximising the second expression in (10.2)). These inequalities allow us to use the surrogate mean square error (7.20) in the same fashion as in Sections 7 and 8. Hence we obtain the *same* rate $n^{-p/(p+2)}$ as an *upper bound* to the minimax rate of convergence in this modified setting.

Even though we don't have the SVD of P here, the lower bound approach of Section 9 yields some information. The new feature emerges in bounding the term

$$\sup_{1 \leq \alpha, \beta \leq M} \|Pf_\alpha - Pf_\beta\|_0^2 \text{ in (9.4), where } \|\cdot\|_0 \text{ is now the norm of } L^2(D, dsd\varphi/2\pi).$$

The difficulty is that $\psi_\nu = b_\nu^{-1}P\phi_\nu$ are no longer orthogonal or of norm 1. We

employ the following lemmas

Lemma 10.1

Let $\{\varphi_1, \dots, \varphi_m\}$ be an orthonormal basis for a linear space M and $P : M \rightarrow N$ a linear operator. Then there exists a subspace $M' \subset M$ of dimension at least $[m/2]$ such that

$$\sup_{M'} \|Pf\|^2 / \|f\|^2 \leq 2 \operatorname{ave}(\|P\varphi_i\|^2) \leq 2 \max(\|P\varphi_i\|^2)$$

Lemma 10.2

$$\|\psi_{lm}\|_0^2 \leq \int_0^{\pi/2} \frac{\sin^2(m+1)\theta}{\sin \theta} d\theta \approx \log m \quad \text{as } m \rightarrow \infty.$$

Lemma 10.1 is used to isolate a subset of $I_{\eta, \zeta}$ (in Section 9) and a corresponding subspace of dimension $|I_{\eta, \zeta}|/2$ on which $\|P\|^2 \leq 2 \max_i \{b_v^2 \|\psi_v\|_0^2\}$. Now, Lemma 10.2 bounds this by $2\zeta \log \eta$. Except for this extra factor of $\log \eta$, the proof continues as before to yield the modified *lower* rate bound of $(n/\log n)^{-p/(p+2)}$.

Of course, at least one of these bounds is not sharp, but their ratio is $(\log n)^{p/(p+2)}$, which is negligible relative to any positive power of n .

11. 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 (1987), Nychka and Cox (1984), Jones, Silverman and Wilson (1988) and Wilson (1988).

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 $K(Pf_1^{(n)}, Pf_2^{(n)}) = \frac{1}{2}n \int \{Pf_1(t) - Pf_2(t)\}^2 \lambda(dt)$, so that the lower bound methods of Section 9 immediately apply. Upper bound results are given, for

example, by Nychka and Cox (1984).

For a generic one-dimensional problem with singular value decomposition $P\varphi_v = b_v\varphi_v$, $b_v \sim v^{-\beta}$, and with ellipsoid determined by $a_v^2 = v^{2\alpha}$, 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).

Appendix: Proofs

A.1 Smoothness and ellipsoids

In this section we indicate the proof of the statement immediately following (5.4). We employ Gegenbauer (ultraspherical) polynomials as normalised in Magnus, Oberhettinger and Sony (1966, p.218 ff) or Gradshteyn and Ryzhik (1980, p.827). Define probability measures μ_α on B by $d\mu_\alpha = \alpha(1-|x|)^{2\alpha-1}d\mu(x)$. An orthogonal basis for $L^2(B, \mu_\alpha)$ is given by the polynomials

$$\tilde{\varphi}_{jk}^\alpha = (2\pi)^{-1} \int_0^{2\pi} e^{i(j-k)\theta} C_{j+k}^\alpha(x \cdot u_\theta) d\theta \quad j, k \geq 0, u_\theta = (\cos \theta, \sin \theta)^T. \quad (\text{A.1})$$

Consider the conditional expectation operator $(Pf)(s, \theta) = E\{f(X) | u_\theta^T X = s\}$ where $X \sim \mu_\alpha$. We view the polynomials $\tilde{\varphi}_{lm}^\alpha$ as the pullback by the adjoint P^* of the singular functions $e^{i\theta} C_m^\alpha(s)$ of PP^* . This construction of the SVD of P is explained in Johnstone (1988), following Davison (1981, 1983) but with different notation and normalisations.

In terms of the basis (A.1), the differentiation operators $D_z = \frac{1}{2}(\partial/\partial x_1 - i\partial/\partial x_2)$ and $D_{\bar{z}} = \frac{1}{2}(\partial/\partial x_1 + i\partial/\partial x_2)$ have a very simple action. Since $(d/dt)C_m^\alpha = 2\alpha C_{m-1}^{\alpha-1}$, we have, setting $\tilde{\varphi}_{jk} = 0$ if $j \wedge k = 0$,

$$D_z \tilde{\varphi}_{jk}^\alpha = \alpha \tilde{\varphi}_{j-1, k}^{\alpha+1} \quad \text{and} \quad D_{\bar{z}} \tilde{\varphi}_{jk}^\alpha = \alpha \tilde{\varphi}_{j, k-1}^{\alpha+1}.$$

The raising of the index from α to $\alpha+1$ leads us from the original measure μ of Section 2 to the family μ_α .

It is shown in Johnstone (1988) that if $f = \sum_{j, k \geq 0} c_{jk} \tilde{\varphi}_{jk}^1$ and $r+s=p$, then

$$\begin{aligned} \|D_z^r D_{\bar{z}}^s f\|_{\mu_{p+1}}^2 &= p! \sum_{\substack{j \geq r \\ k \geq s}} c_{jk}^2 \|\tilde{\varphi}_{j-r, k-s}^{p+1}\|_{\mu_{p+1}}^2 \\ &= \sum_{\substack{j \geq r \\ k \geq s}} c_{jk}^2 a_{jk}^2 \|\tilde{\varphi}_{jk}^1\|_{\mu_1}^2 \end{aligned}$$

where, for $j \geq r$ and $k \geq s$,

$$(j+1)^{\mathcal{P}}(k+1)^{\mathcal{P}}(p+1)^{-2\mathcal{P}+1} \leq a_{jk}^2 \leq (j+1)^{\mathcal{P}}(k+1)^{\mathcal{P}}(p+1)^{2\mathcal{P}}.$$

It can also be shown that $\tilde{\varphi}_{lm}^1 = (1+m)^{-\frac{1}{2}} \varphi_{lm}$, where $\{\varphi_{lm}\}$ is the orthonormal basis as defined in (5.1). It follows, by standard arguments of analysis (see, for example, Gilbarg and Trudinger, 1977) that $f = \sum f_{jk} \varphi_{jk}$ has weak derivatives of order p in $L^2(B, \mu_{p+1})$ if and only if

$$\sum_{j, k \geq p} (j+1)^{\mathcal{P}}(k+1)^{\mathcal{P}} |f_{jk}|^2 < \infty. \quad (\text{A.2})$$

If, in addition, f is required to be in $L^2(B, \mu)$, then the sum in (A.2) should be extended to the range $\{(j, k) : j \geq 0, k \geq 0\}$.

A.2 Proof of (5.5)

It is easily seen that the ellipsoid B has exactly the same description in terms of either the real or the complex form of the basis (5.1), as long as $a_{-l, m}^2 = a_{l, m}^2$. In the latter form, we find

$$f(r, \theta) = \sum_{(l, m) \in N} f_{lm} (m+1)^{\frac{1}{2}} e^{il\theta} Z_m^l(r).$$

Zernike polynomials have the properties

$$Z_m^{-l} = Z_m^l ; \sup_{0 \leq r \leq 1} |Z_m^l(r)| = Z_m^l(1) = 1.$$

These may be derived from 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 Szegő (1939, Section 7.2, p.163), applied to the polynomials $Q_s^l(t) = P_s^{0, l}(2t - 1)$ as s varies. Hence

$$|f-1| \leq \sum_{N \setminus (0,0)} (m+1)^{\frac{1}{2}} |f_{lm}|$$

Changing the index set from (l, m) to (j, k) as in Section 5, and setting $x_{jk} = (j+1)^{p/2} (k+1)^{p/2} |f_{jk}| / C$, we obtain

$$\sup_{B_{p,C}} |f-1| \leq C \sup_{N' \setminus (0,0)} \sum (j+k+1)^{\frac{1}{2}} (j+1)^{-p/2} (k+1)^{-p/2} x_{jk}$$

where $N' = \{(j, k) : j \geq 0, k \geq 0\}$, and the supremum is taken over arrays $\{x_{jk}\}$ with $\sum_{N' \setminus (0,0)} x_{jk}^2 \leq 1$. Thus, so long as $p \geq 1$,

$$\begin{aligned} \sup_{B_{p,C}} |f-1| &\leq C \sup_{N' \setminus (0,0)} (j+k+1)^{\frac{1}{2}} (j+1)^{-p/2} (k+1)^{-p/2} \\ &= C \sup_{m \geq 1} (m+1)^{\frac{1}{2}} (m+1)^{-p/2} \\ &= C 2^{(1-p)/2}. \end{aligned}$$

The supremum is clearly attained when $m=1$, which implies that the corresponding density f is linear.

A.3 Proof of Lemma 8.1

We transform the sums in (8.4) and (8.5) by replacing $j+1$ by j and $k+1$ by k ; denote by $\sum_{[\eta]}$ the sum over the transformed range $\{(j, k) : j \geq 1, k \geq 1 \text{ and } jk \leq \eta\}$. Then the sums (8.4) and (8.5) become

$$\sum_{[\eta]} j^r k^r \quad \text{and} \quad \sum_{[\eta]} (j^{r+1} k^r + j^r k^{r+1} - j^r k^r) \quad (\text{A.3})$$

respectively. Using symmetry in (j, k) , we decompose the first sum in (A.3) as

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

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

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

which yields the result of (8.4).

For the second sum in (A.3), we use an integral approximation, valid for $s \geq 0$ and $x \geq 1$,

$$\sum_{j=1}^{[x]} j^s = (s+1)^{-1} x^{s+1} + c_{sx} x^s, \quad 0 \leq |c_{sx}| \leq c_s, \quad (\text{A.4})$$

which follows from the bounds

$$(s+1)^{-1} [x]^{s+1} \leq \int_0^{[x]} t^s ds \leq \sum_{j=1}^{[x]} j^s \leq \int_1^{[x+1]} t^s ds \leq (s+1)^{-1} [x+1]^{s+1}.$$

To evaluate the sums $\sum_{[\eta]} j^{r+1} k^r = \sum_{[\eta]} j^r k^{r+1}$ in (A.3), we now employ (A.4) as follows, assuming throughout that η is an integer:

$$\begin{aligned} \sum_{[\eta]} j^{r+1} k^r &= \sum_{k=1}^{\eta} k^r \sum_{j=1}^{[\eta k^{-1}]} j^{r+1} \\ &= \sum_{k=1}^{\eta} k^r (r+2)^{-1} (\eta k^{-1})^{r+2} + \sum_{k=1}^{\eta} k^r c_{r+1, \eta, k} (\eta k^{-1})^{r+1} \\ &= (r+2)^{-1} \eta^{r+2} \sum_1^{\eta} k^{-2} + O(\eta^{r+1} \sum_1^{\eta} k^{-1}) \\ &= \frac{1}{6} \pi^2 (r+2)^{-1} \eta^{r+2} + O(\eta^{r+1} \log \eta). \end{aligned} \quad (\text{A.5})$$

Since the sum $\sum_{[\eta]} j^r k^r$ has already been shown to be $O(\eta^{r+1} \log \eta)$, substituting (A.5) back into (A.3) completes the proof of (8.5).

A.4 Proof of (9.8)

Throughout this proof, let $\xi = \eta^{1/p}$, and use χ to denote the indicator function of a set. In terms of indicator functions, the required equation (9.8) can be rewritten as

$$|J_\eta| = \sum_{j,k \geq 1} \chi\{jk \leq \xi, j+k \geq \alpha\xi+1\} = c_\alpha \eta^{1/p} + O(1). \quad (\text{A.6})$$

To establish (A.6), define $x(\xi) = \frac{1}{2}(\alpha\xi+1) - \frac{1}{2}\{(\alpha\xi+1)^2 - 4\xi\}^{\frac{1}{2}}$, so that x is the smaller solution of the equations $xy = \xi$, $x+y = \alpha\xi+1$. Assume that ξ is sufficiently large that x is real. It is easily seen that $x(\xi) = \alpha^{-1} + O(\xi^{-1})$.

Provided x is real, the sum in (A.6) can be re-expressed as

$$\begin{aligned} & 2 \sum_{j=1}^{[x]} \sum_k \chi\{\alpha\xi+1-j \leq k \leq j^{-1}\xi\} \\ &= 2 \sum_{j=1}^{[x]} \{(j^{-1}-\alpha)\xi + (j-1)\} + O(x) = c_\alpha \xi + O(1), \end{aligned}$$

as required.

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