Discretization Effects in Statistical Inverse Problems*.$

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The statistical inverse problems considered are those where binned observations are available from a density $g$ related to the density $f$ of real interest by a linear operator equation $g = \mathcal{D}f$. Both the fineness of the discretization and the number of observations taken are important parameters of the problem, and both may be under the control of the experimenter, at least at the design stage of the equipment. A minimax approach over suitable function classes is used, involving the singular value decompositions of $\mathcal{D}$ and the discretization operator. The asymptotic results derived indicate that, for a given number of observations, discretization beyond a certain critical rate essentially will not yield extra information, while at the critical rate of discretization the accuracy of estimation is degraded by a constant factor. Examples of relevant statistical inverse problems—all discussed in detail—include the estimation of a probability density from binned observations, deconvolution, the Wicksell unfolding problem of determining the density of radii of a population of spheres given a random section through the spheres, and the reconstruction of images observed by positron emission tomography.


1. INTRODUCTION

There is a large class of problems, in a variety of fields, that may be considered as being statistical inverse problems. We consider a problem as being a statistical inverse problem under the following circumstances.

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Suppose $\mathcal{D}$ is a space on which we can make observations of data points $Y_1, Y_2, \ldots$. Assume that $\mathcal{D}$ is equipped with a dominating probability measure $\lambda$ and let $\mathcal{G}$ be the space of functions $g$ on $\mathcal{D}$ that are square integrable with respect to $\lambda$. Assume that the observed data have distribution that depends on some $g$ in $\mathcal{G}$, for example by arising from a Poisson process with intensity $ng$ with respect to $\lambda$; here $n$ is an integer giving an index of the amount of data collected.

Although the observations are taken on the space $\mathcal{D}$, the space of real interest is another space $\mathcal{B}$, and the function $g$ is related to a function $f$ on $\mathcal{B}$ by $g = \mathcal{P}f$, where $\mathcal{P}$ is a linear operator. Typically, $f$ is the probability density function of random variables $X_j$ on $\mathcal{B}$ that we cannot observe directly but which give rise to the accessible observations $Y_i$. (It need not be the case that every data point $X$ in $\mathcal{B}$ gives rise to a $Y$ in $\mathcal{D}$; it may be that some $X$ are "lost" and do not give rise to observable $Y$'s.) Our aim is to use the observations $Y_i$ on $\mathcal{D}$ to estimate the function $f$ on $\mathcal{B}$. We assume that $\mathcal{B}$ is equipped with a dominating measure $\mu$ and that $\mathcal{P}$ is a bounded linear operator from $\mathcal{F}$ to $\mathcal{G}$, where $\mathcal{F}$ is the space of functions $f$ on $\mathcal{B}$ that are square integrable with respect to $\mu$. We assume without loss of generality, if necessary replacing $\mathcal{G}$ by the subspace $\mathcal{P}\mathcal{F}$, that the operator $\mathcal{P}$ is surjective.

Suppose further that even the observations $Y_i$ cannot be observed exactly but that they can only be observed in binned or discretized form. To be precise, assume that the space $\mathcal{D}$ is partitioned into bins $D_1, \ldots, D_r$. Let $\mathcal{Q}$ be the discretization operator that maps a function $g$ on $\mathcal{D}$ to a vector defined by

$$
(\mathcal{Q}g)_j = \frac{1}{\lambda(D_j)} \int_{D_j} g d\lambda \quad \text{for } j = 1, \ldots, r.
$$

This vector gives the averages of $g$ over the each of the bins $D_j$. For each $j$ let $n_j$ be the total number of $Y_i$ falling into the bin $D_j$; assume that only the $n_j$ can be actually observed. Under the Poisson process assumption described above, the $n_j$ are independent Poisson random variables with means $n\lambda(D_j)(\mathcal{Q}g)_j$, $j = 1, \ldots, r$. Before discussing the aspects of these problems that we discuss in this paper, it may be helpful to outline some examples.

**Example 1. Density estimation from binned data.** A very simple example, not normally considered as a statistical inverse problem, is that of estimating a continuous probability density function from binned data. Suppose that $\mathcal{B}$ is the interval $[0, 10)$ and that $\mathcal{B}$ is divided into 10 bins $[0, 1), \ldots, [9, 10)$. Suppose that the points $Y_i$ are continuous observations from a density $f$ on the interval $[0, 10)$ but we only observe which bin each $Y_i$ falls in. In this case the operator $\mathcal{P}$ is the identity, and the operator $\mathcal{Q}$ maps $f$ to the 10-vector of averages of $f$ over each of the bins.
EXAMPLE 2. **Deconvolution.** Suppose now that the observations $Y_i$ are the sum of two independent and identically distributed components $X_i$ and $e_i$. However, only a binned version of the $Y_i$ are actually seen, as in Example 1. It is desired to estimate the density $f(x)$ of the $X_i$ using the binned data. The distribution of the additive contaminating noise $e_i$ is assumed known. In addition the $\{X_i\}$ and $\{e_i\}$ are independent. The problem occurs in a wide variety of contexts (e.g., Jansson, 1984). For simplicity, we assume that the $X_i$ and $e_i$ take values in the unit circle. This case arises, for example, in the study of directional data (e.g., Mardia, 1972).

EXAMPLE 3. **The Wicksell “unfolding” problem of stereology.** A classical problem in stereology (Wicksell, 1925) is the following. Suppose a population of spheres is embedded in a medium. The spheres have radii that may be assumed to be drawn independently from a density $f$. A random plane slice is taken through the medium and those spheres that are intersected by the plane furnish the data points $Y_1, Y_2, \ldots$. The basic unfolding problem is to infer the density $f$ of sphere radii from the observed circle radii $Y_i$. For example (Nychka et al., 1984) the spheres might be tumors in an animal’s liver and the random slice could be taken as part of a post mortem examination. There are many other examples in both biological and engineering contexts; see Cruz-Orive (1983) and numerous other papers in the Journal of Microscopy.

In the unfolding problem the space $\mathcal{B}$ is the set of possible sphere radii and the space $\mathcal{D}$ the space of circle radii, so that both $\mathcal{B}$ and $\mathcal{D}$ are the positive half-line or intervals of the form $[0, b]$. It is unusual for the circle radii to be recorded exactly. More often the space $\mathcal{D}$ is divided into bins and the number of circles falling into each bin is recorded.

EXAMPLE 4. **Positron emission tomography.** This problem is the main motivating example for our work. In positron emission tomography (PET) a radioactively labeled metabolite is introduced into the body and gives rise to emissions that are observed by external detectors. For definiteness, let us suppose that it is the patient’s brain that is the organ of interest. Radioactive emissions take place within the brain at positions $X_i$ that cannot be observed directly. Instead, each emission gives rise to a pair of photons that fly off in opposite directions along a line with uniformly distributed orientation. Detectors placed around the patient’s head make it possible to observe (to some degree of accuracy) the photon pairs, and hence to give a line on which the point of emission must have occurred. Usually there is a ring of detectors and so the space $\mathcal{B}$ may be considered as the disk enclosed by the detectors—by suitable choice of units the unit disk. When a photon pair is detected, the observation that is actually made is the pair of detectors that are actuated by photons. In this example the space $\mathcal{D}$ consists of all possible detectable lines of flight of photon pairs. Each (unordered) pair of detectors will give rise to a data
bin in \( \mathcal{D} \), the collection of all photon lines that will be detected by that particular pair of detectors.

1.1 Discretization

The examples we have discussed have in common that they involve the discretization of the observation space. In all cases, it is natural to introduce an index \( N \) of the fineness of the discretization. In the histogram, deconvolution, and stereology examples, \( N \) is simply the number of histogram bins, while in the PET example, the obvious discretization index is the number of detectors. With the general case in mind, we write \( \mathcal{D}_N \) for the discretized observation space with index \( N \) and let \( r(N) \) be the number of bins in \( \mathcal{D}_N \); we let \( \mathcal{G}_N \) be the space of vectors of length \( r(N) \) and define \( \mathcal{G}_N \) to be the discretization map from \( \mathcal{G} \) to \( \mathcal{G}_N \). We write \( \mathcal{P}_N \) for the map \( \mathcal{D}_N \mathcal{P} \) from \( \mathcal{F} \) to \( \mathcal{G}_N \). The space \( \mathcal{G}_N \) will be equipped with an inner product and corresponding norm; for the work of the present paper the inner product is

\[
\langle \mathbf{x}, \mathbf{y} \rangle = \sum x_j y_j \lambda(D_j)
\]

(or some asymptotically equivalent approximation to be described in certain specific examples).

If the observations have the Poisson dependence on \( \mathcal{P}_N g \) as described above, then we refer to the problem as being a density estimation model. It has already been noted that some of the \( X \)'s may be lost and do not give rise to observable \( Y \)'s. For example in the PET case in practice, some of the photons will fly out on lines that do not intersect the detector ring at all, and in the stereology example only those spheres actually intersected by the plane will be recorded at all. As long as the probability of loss depends only on the value of \( X \), and the various \( X \)'s behave independently, the observed counts will of course still have independent Poisson distributions; both these assumptions hold in our formulations of the PET and stereology problems.

Another form of dependence is a regression model. In this case the available data consist of noisy observations of the values of the discretized version of \( g \), so that we observe random variables \( Z_i \) satisfying

\[
Z_i = \langle \mathcal{D}_N g \rangle_i + \varepsilon_i, \quad i = 1, \ldots, r(N),
\]

where the \( \varepsilon_i \) are independent \( N(0, \sigma^2) \) random variables. Problems of this kind occur in very many fields of application. We do not consider the regression model in any detail in the present paper, but our approach can be modified to address it.
1.2 Key Issues

The key issue that we investigate in this paper is the way that the fineness of the discretization interacts with the amount and accuracy of data collected. In the PET example, a natural and important design question concerns the number of detectors. It is intuitively clear that for any given number of detectors there is a point beyond which the accuracy of estimation cannot be improved, no matter how large the sample of emissions observed. Conversely, if we know that only a relatively small sample is to be collected, there may not be much loss in using a machine with a small number of detectors. In terms of the models we have set up, the question we consider is how some measure of estimation accuracy depends on the two parameters \( n \), essentially the sample size, and \( N \), the discretization index.

In the regression case, the parameter \( n \) is replaced by the error variance \( \sigma^2 \), but the basic issue remains the same: Beyond what point should one strive to increase the fineness of the discretization as indexed by \( N \) rather than worrying about the accuracy of individual observations?

There is a substantial statistical literature that is concerned with questions such as how many bins to use with a histogram estimator and a given sample size \( n \). The approach taken in this paper is somewhat different in emphasis, since it is seen that our estimators will almost always further smooth the binned data. We treat discretization as a property of the data rather than as a method for estimation or a proxy for smoothing.

1.3 Singular Value Decompositions and a Simplifying Assumption

Our calculations are based on the singular value decomposition (SVD) of the operator \( \mathcal{P} \). Define norms \( \| \cdot \|_\mathcal{F} \) on \( \mathcal{F} \) and \( \| \cdot \|_\mathcal{G} \) on \( \mathcal{G} \) to be the \( L^2 \) norms with respect to the measures \( \mu \) and \( \lambda \), respectively, and assume that, with respect to these norms, \( \mathcal{P} \) is a bounded linear operator from \( \mathcal{F} \) to \( \mathcal{G} \). Let \( \{ \phi_v \} \) be an orthonormal basis for \( \mathcal{F} \) and let \( \{ \psi_v \} \) be an orthonormal set of functions in \( \mathcal{G} \) such that, for some (possibly complex) singular values \( \{ b_v \} \),

\[
\mathcal{P} \phi_v = b_v \psi_v. \tag{2}
\]

Since we assume that \( \mathcal{P} \) maps \( \mathcal{F} \) onto the whole of \( \mathcal{G} \), it follows that the \( \{ \psi_v \} \) necessarily form an orthonormal basis for \( \mathcal{G} \). A singular value decomposition (2) will always exist since \( \mathcal{P} \) is a bounded linear operator. We can now state the crucial condition for our treatment of the discretization problem.

**Matching SVD assumption.** Given any \( v_1 \) and \( v_2 \), the vectors \( \mathcal{G}_N \psi_{v_1} \) and \( \mathcal{G}_N \psi_{v_2} \) are either parallel or orthogonal on the space \( \mathcal{G}_N \).
Although this is a restrictive assumption, it holds exactly or approximately in a number of important specific problems. Its effect is that the functions $\psi_\nu$ are also singular functions, in a suitable sense, of the discretization operator $\mathcal{D}_N$: it is easy to construct an orthonormal basis $\{x_\nu\}$ of $\mathcal{H}_N$ such that for each $\nu$ there exists $[\nu]$ for which

$$\mathcal{D}_N\psi_\nu = \gamma_\nu x_{[\nu]}$$

for certain constants $\gamma_\nu$.

2. Risk Functions and Classes of Estimators

In this section, we set out in general terms the classes of estimators with which we are concerned and the risk functions that we consider.

2.1 Classes of Functions and Estimators

Crucial to our methodology is the idea of considering minimax estimation over certain classes of functions in $\mathcal{F}$. The classes we consider are translates of ellipsoids $\mathcal{F}_0$ in the space $\mathcal{F}$, specified in terms of a collection of constants $\{a_\nu\}$ and a threshold $C$ by

$$\mathcal{F}_0 = \{f = \sum f_\nu \phi_\nu : f_0 = 1, \sum_{\nu \neq 0} a_\nu^2 f_\nu^2 \leq C^2\}. \tag{4}$$

The condition $f_0 = 1$ is a normalization condition: when $\phi_0 = 1$, it ensures that a nonnegative $f$ is a probability density, and in other cases (such as the Wicksell unfolding problem discussed in detail in Section 5 below) it can correspond to a physically meaningful identifiability constraint. We assume that the $\{a_\nu\}$ and $C$ are chosen to ensure that all members of $\mathcal{F}_0$ are nonnegative. Ellipsoid conditions of the kind (4) can amount to the imposition of smoothness and integrability conditions. For example in the simple case where $f$ is a periodic function on $[0,2\pi]$ and the $\{\phi_\nu\}$ are Fourier functions, an ellipsoid condition with $a_\nu \sim \nu^{-a}$ corresponds to placing a bound on the integral of the squared $\nu$th derivative of $f$; the members of $\mathcal{F}_0$ will all be positive provided $a > \frac{1}{2}$ and $2C^2 \sum_{k=1}^{\infty} k^{-2a} < 1$.

Under the matching SVD assumption, for any fixed $\tilde{N}$ we define an equivalence relation on the set of subscripts $\{\nu\}$ by

$$\nu_1 \sim \nu_2 \text{ if and only if } [\nu_1] = [\nu_2]$$

here $[\nu]$ is as defined in (3) above, so that the equivalence classes correspond to sets of $\psi_\nu$ that are all mapped by $\mathcal{D}_N$ to multiples of the same basis
vector in $\mathcal{G}_N$. The $[\nu]$ can thus be considered as being equivalence classes under $\sim$. We construct a set of representatives $\mathcal{L}_N$ of these equivalence classes by selecting from each $[\nu]$ a $\nu$ that maximises $b_\nu \gamma_\nu$ over the equivalence class: this $\nu$ essentially corresponds to the direction in which least energy is lost under the mapping $\mathcal{D}_N \mathcal{P}$. We assume that $0 \in \mathcal{L}_N$; however, it plays a special role in view of the restriction $f_0 \equiv 1$, so we introduce $\mathcal{L}_N^0 = \mathcal{L}_N \setminus \{0\}$.

Let $\mathcal{F}^L = \text{span}\{ \phi_\nu : \nu \in \mathcal{L}_N^0 \}$ and $\mathcal{F}^H = \{ f = \sum f_\nu \phi_\nu : f_\nu = 0 \text{ for } \nu \in \mathcal{L}_N \}$, so that $\mathcal{F} = \text{span}\{ \phi_0 \} \oplus \mathcal{F}^L \oplus \mathcal{F}^H$. The letters $L$ and $H$ stand for "low frequency" and "high frequency," corresponding to the notion that the composition of the transformation operator $\mathcal{P}$ and the discretization operator $\mathcal{D}_N$ will smooth out more strongly the high-frequency components of the functions. Finally, we define the ellipsoid $\mathcal{F}_D^0 = (\phi_0 + \mathcal{F}^L) \cap \mathcal{F}_0$. The sets $\mathcal{F}^L$, $\mathcal{F}^H$, and $\mathcal{F}_D^0$ all depend on $N$, but this dependence is not expressed in the notation.

We now turn to classes of estimators. We assume that the available data consists of a vector $Z$ of normalized bin counts on $\mathcal{G}_N$ such that the $n_j = nZ_j \lambda(D_j)$ are independent Poisson counts with intensities $n(\mathcal{D}_N \mathcal{G}) \lambda(D_j)$, for some $g = \sum g_\nu \psi_\nu$ in $\mathcal{G}$. Write $Z = \sum \hat{Z}_\nu x_\nu^T y_\nu$. Let $\Gamma$ be the matrix with entries $\Gamma_{\nu,\rho} = \gamma_{\nu,\rho}$ if $\rho \in [\nu]$ and zero otherwise: this is the matrix representation of $\mathcal{D}_N$ relative to the bases $\{ \psi_\nu \}$ and $\{ x_\nu \}$, respectively. Denote by $g$ the vector of coefficients $g_\nu$, and use other boldface letters similarly; denote by $Z$ the vector of coefficients $\hat{Z}_\nu$.

It follows from the matching SVD assumption that

$$E_g Z = (\Gamma g)[\nu],$$

and by standard calculations that the covariance matrix, $V^g$, is given by, say,

$$n^{-1} V^g_{[\nu], [\nu]} = \text{cov}_g \{ \hat{Z}_{[\nu]}, \hat{Z}_{[\nu]} \} = n^{-1} \sum_i (\mathcal{D}_N \mathcal{G}) x_{[\nu], i} x_{[\nu], i} \lambda(D_i).$$

In the particular case where $g$ is the uniform density on $\mathcal{G}$ with respect to $\lambda$, so that $\mathcal{D}_N \mathbf{1} = 1$, the orthonormality of the $x_\nu$ implies that the covariance has the much simpler form

$$\text{cov}_1 \{ \hat{Z}_{[\nu]}, \hat{Z}_{[\nu]} \} = n^{-1} \delta_{[\nu], [\nu]},$$

so that $V^g$ is simply the identity matrix.

The composed mapping $\mathcal{D}_N \mathcal{P}$ aliases the $\phi_\nu$ for $\nu$ within each equivalence class, and so it is natural to restrict attention to estimators that take values in $\mathcal{F}^L$. In addition we consider those estimators that are linear.
functions on $\mathcal{G}_N$; some remarks about more general estimators are made below.

Let $\mathcal{T}_N$ be the class of linear functions from $\mathcal{G}_N$ to $\mathcal{F}^L$, and write $T_{jk}$ for the matrix representation of $T$ in $\mathcal{T}_N$ relative to the bases $\{x_{1}\}$ and $\{\phi_v : v \in \mathcal{L}_N^0\}$. The estimator corresponding to $T \in \mathcal{T}_N$ may be written as

$$\hat{T}(x) = \phi_0 + \sum_{v \in \mathcal{L}_N^0} \phi_v(x) \sum_{[\pi]} T_{\nu[\pi]} \hat{Z}_{[\pi]}.$$  \hfill (7)

Let $\mathcal{T}_N^0$ be the subclass consisting of those $T$ in $\mathcal{T}_N$ that have diagonal matrix representation, so that $T_{x \nu} = \lambda_{v\nu}$ for each $v$ in $\mathcal{L}_N^0$, and $T_{x[0]} = 0$.

2.2 Risk Functions

Let $g \in \mathcal{G}$ and let $B$ be the diagonal matrix with entries $b_v$ so that $g = Bf$. We use the notation $E_g$ to denote an expectation for normalized Poisson counts as above. Let $f = (f_v : v \neq 0)$. Making use of (5) and (6) above, the mean square error of an estimator $T$ in $\mathcal{T}_N$ can be written

$$M(T, f) = E_{\phi f} \|\hat{T} - f\|^2 = E_{\phi f} \|TE_{\phi f}Z - f + T(Z - E_{\phi f}Z)\|^2$$

$$= \|TBBf - f\|^2 + n^{-1} \text{tr } TV^{\phi f}T^T.$$  

Because of the complicated form (6) of $V^{\phi f}$, it is convenient to work in terms of a surrogate mean integrated square error $M^*(T, f)$, obtained by replacing the variance term by the corresponding variance term under the uniform distribution, to give

$$M^*(T, f) = \|TBBf - f\|^2 + n^{-1} \text{tr } TV^{\phi f}T^T.$$  

In order to discuss the relation between surrogate mean square error and true mean square error, it is helpful to consider a kernel estimator representation for $\hat{T}$. Let $J_i = j(Y_i)$ be a random variable indicating the bin into which $Y_i$ falls. We have the representation

$$\hat{Z}_{[\pi]} = \sum_j Z_j \chi_{[\pi]} \lambda(D_j) = n^{-1} \sum_j n_j \chi_{[\pi], j} = n^{-1} \sum_i \chi_{[\pi], J_i}$$

Substituting this into (7) gives

$$\hat{T}(x) = \phi_0(x) + n^{-1} \sum_i t(x, J_i),$$  \hfill (8)
where

\[ t(x, j) = \sum_{\nu \in \mathbb{Z}_N} \phi^*_\nu(x) \sum_{[\nu]} T_{\nu[\nu]} \chi_{[\nu]}. \]

From (8) and the Poisson structure of the data,

\[ \text{var}_g \hat{T}(x) = n^{-1} \int t^2(x, j(y)) g(y) d\lambda(y). \]  

(9)

Conditioning on \( n \) leads to an alternative form for the mean squared error

\[ M(T, f) = \int [(E_{gT}(x) - f(x))^2 + \text{var}_{gT}(x)] \mu(dx). \]

It now clear from this and (9) that if \( g \) is bounded above and below away from zero, then for all linear estimators \( T \),

\[ \inf_{\mathcal{F}} g(y) \leq M(T, f)/M^*(T, f) \leq \sup_{\mathcal{F}} g(y). \]  

(10)

Thus, under the condition

\[ 0 < \inf_{\mathcal{F}} g \leq \sup_{\mathcal{F}} g < \infty, \]

(11)

the ratio of surrogate to true mean integrated square error will be bounded above and below away from zero uniformly on \( \mathcal{F}_0 \), so that order of magnitude statements made for one will also be true for the other. We discuss validity of (11) in each of the examples below.

Our concern in this paper is with minimax risks over certain function classes and classes of estimators. Given a class of estimators \( \mathcal{T} \) and a function class \( \mathcal{F}_0 \), define

\[ M(\mathcal{T}, \mathcal{F}_0) = \inf_{\mathcal{T} \in \mathcal{T}} \sup_{f \in \mathcal{F}_0} M^*(T, f). \]

3. Optimizing the Minimax Risk

In this section we investigate the minimax risk \( M(\mathcal{T}_N, \mathcal{F}_0) \). Our basic technique is to provide bounds for the minimax risk in terms of the minimax risk for the problem where the maximum is confined to low-frequency functions \( f \). We begin by characterizing this risk by reference to previous results of Johnstone and Silverman (1990) which make use of work of Speckman (1985) and Pinsker (1980).
Lemma 1. With the definitions given in Section 2.2 above,

$$M(\mathcal{F}_N, \mathcal{F}_0^*) = n^{-1} \sum_{\nu \in \mathcal{F}_0^*} b_{\nu}^{-2} \gamma_{\nu}^{-2} (1 - \alpha^{1/2} a_{\nu})_+, \quad (12)$$

where $\alpha$ is chosen to ensure that

$$n^{-1} \sum_{\nu \in \mathcal{F}_0^*} b_{\nu}^{-2} \gamma_{\nu}^{-2} a_{\nu}^2 (\alpha^{-1/2} a_{\nu}^{-1} - 1)_+ = C^2. \quad (13)$$

The minimax estimator $T^*$ is given by setting

$$T^*_{\nu \pi} = \delta_{\nu \pi} b_{\nu}^{-1} \gamma_{\nu}^{-1} (1 - \alpha^{1/2} a_{\nu})_+, \quad (14)$$

for all $\nu$ in $\mathcal{F}_0^*$ and $\pi$ in $\mathcal{L}_N$.

Proof. The proof follows that of Lemma 4.2 of Johnstone and Silverman (1990).

We can now state and prove the main result of this section.

Theorem 1. Given any $\nu$ in $\mathcal{L}_N$, define

$$S_N(\nu) = \sum_{\rho \in (\nu) \cup \nu} a_{\rho}^{-2}. \quad (15)$$

Then

$$M(\mathcal{F}_N, \mathcal{F}_0^*) \leq M(\mathcal{F}_N, \mathcal{F}_0) \leq \sup_{f \in \mathcal{F}_0} M^*(T^*, f) \leq \{M(\mathcal{F}_N, \mathcal{F}_0^*)\}^{1/2} + \varepsilon(N)^{1/2},$$

where

$$\varepsilon(N) = C^2 \{\max_{\nu \in \mathcal{F}_0^*} S_N(\nu) + \max_{\rho \in \mathcal{L}_N} a_{\rho}^{-2}\}.$$

Proof. The first two inequalities in (15) are immediate from the definition of the minimax risk and the facts that $\mathcal{F}_0^* \subset \mathcal{F}_0$ and $T^* \in \mathcal{F}_N$. To prove the last inequality, write any $f$ in $\mathcal{F}$ as $\phi_0 + f^L + f^H$ where $f^L \in \mathcal{F}_0$ and $f^H \in \mathcal{F}_H$. We then have

$$M^*(T^*, f)^i - M^*(T^*, f^L)^i \leq \|(I - T^* \Gamma B)f^H\|$$

since, when positive, the left side is bounded above by $\|(I - T^* \Gamma B)f\| - \|(I - T^* \Gamma B)f^L\|$ (and when negative, the inequality is trivial). Since $f^H$ and $T^* \Gamma Bf^H$ are orthogonal,
\[ \| (I - T^* \Gamma B)t^H \|^2 = \| t^H \|^2 + \| T^* \Gamma B t^H \|^2 = \sum_{\rho \in \mathcal{N}} f_\rho^2 + \sum_{\rho \in \mathcal{N}} \left( \sum_{\nu \in \mathcal{N} \setminus \rho} T^*_{\nu \rho} \gamma_{\rho} f_\rho \right)^2. \] (17)

Now, for \( f \) in \( \mathcal{F}_0 \), so that \( \sum a_\rho^2 f_\rho^2 \leq C^2 \), we have
\[ \sum_{\rho \in \mathcal{N}} f_\rho^2 \leq C^2 \max_{\rho \in \mathcal{N}} a_\rho^{-2}. \] (18)

By the definition of the low-frequency class \( \mathcal{F}_L \) and the estimator \( T^* \), we have \( |T^*_{\nu \rho} \gamma_{\rho}| \leq 1 \) wherever \( \nu \in \mathcal{N} \) and \( \rho \sim \nu \). Hence, for any \( f \) in \( \mathcal{F}_0 \),
\[ \sum_{\nu \in \mathcal{N}} \left( \sum_{\rho \in \mathcal{N} \setminus \nu} T^*_{\nu \rho} \gamma_{\rho} f_\rho \right)^2 \leq \sum_{\nu \in \mathcal{N}} \left( \sum_{\rho \in \mathcal{N} \setminus \nu} a_\rho^{-2} \right) \left( \sum_{\rho \in \mathcal{N} \setminus \nu} a_\rho^2 f_\rho^2 \right) \leq C^2 \max_{\nu \in \mathcal{N}} S_\nu. \] (19)

Now substitute the bounds (18) and (19) into (17) and thence into (16) to obtain, for any \( f \) in \( \mathcal{F}_0 \),
\[ M^*(T^*, f)^{1/2} - \varepsilon(N)^{1/2} \leq M^*(T^*, f^L)^{1/2} \leq \sup_{f \in \mathcal{F}_0} M^*(T^*, f^L)^{1/2} \]
\[ = M(\mathcal{F}_N, \mathcal{F}_0^L)^{1/2}, \]
completing the proof of the theorem.

Our approach in the remainder of the paper is to explore, in a number of examples, when the term \( \varepsilon(N) \) can be neglected, so that the risks \( M(\mathcal{F}_N, \mathcal{F}_0^L) \) and \( M(\mathcal{F}_N, \mathcal{F}_0) \) are asymptotically equivalent and furthermore it can be concluded that the minimax risk over the full class \( \mathcal{F}_0 \) is attained by the estimator \( T^* \) obtained by reference to the restricted class \( \mathcal{F}_0^L \).

4. Some Specific Examples

In this section we begin the application of the previous theory to examples, focusing here on the histogram and deconvolution cases. First we study the matching SVD assumption, and then carry out the minimax risk computations in our discretization model.
4.1 Density Estimation from Binned Data

For simplicity we restrict attention to the periodic case, assuming that the observations are taken on the interval \([0, 2\pi]\) from a density \(f\) that satisfies periodic boundary conditions. Let \(\mathcal{B}\) and \(\mathcal{D}\) both be the space of functions on \([0, 2\pi]\) that are square integrable with respect to Lebesgue measure, and define the measures \(\lambda\) and \(\mu\) by \(d\lambda(t) = d\mu(t) = (2\pi)^{-1} dt\). Define the orthonormal bases \(\phi\) and \(\psi\) by

\[
\phi_\nu(t) = \psi_\nu(t) = e^{i\nu t}, \quad \nu = 0, \pm 1, \pm 2, \ldots
\]

so that the orthonormal expansion of a function \(f\) is its complex Fourier expansion.

Consider discretization into an odd number \(r = 2N + 1\) bins of equal size. Then, by the definition (1) of the discretization operator,

\[
(\mathcal{D}_N\psi_\nu)_j = (\mathcal{D}_N\phi_\nu)_j = (2\pi)^{-1} \int_{2(\nu-1)\pi/r}^{2\pi} e^{i\nu t} dt = \sin(\pi\nu/r) e^{2j(\nu-1/2)i\pi r}.
\]

It is easily checked that the vectors given in (20) are either orthogonal or parallel, so that the matching SVD assumption holds. To obtain the expression (3) explicitly, define \(\chi_\rho\) for \(\rho = 0, \pm 1, \pm 2, \ldots\) to be the vector with \(j\)-th element \(\exp\{2\rho(j - 1/2)\pi i/r\}\) and define \([\nu]\) for each \(\nu\) by \(-N \leq [\nu] \leq N\) and \([\nu] = \nu \pmod{r}\). The values \(\gamma_\nu\) are then given by

\[
\gamma_\nu = \sin(\pi\nu/r).
\]

4.2 Deconvolution

Consider, now, the problem of deconvolution where the spaces \(\mathcal{B}\) and \(\mathcal{D}\) are still both equal to the interval \([0, 2\pi]\) but the functions \(f\) and \(g\) are related by a convolution equation

\[
g(t) = (2\pi)^{-1} \int_0^{2\pi} f(t - s) d\beta(s),
\]

where \(\beta\) is a known probability distribution on \([0, 2\pi]\) and all arithmetic on the arguments of \(f\) and \(\beta\) is performed modulo \(2\pi\). Let \(\sum b_\nu\exp(ilt) dt\) be the formal Fourier expansion of \(d\beta(t)\). By standard calculations the mapping \(\mathcal{P}\) has singular value decomposition given by the singular functions \(\phi_\nu\) and \(\psi_\nu\) defined as in Section 4.1, with singular values \(b_\nu\). It has already
been shown in Section 4.1 that the matching SVD assumption will hold in this case.

We concentrate in this paper on the case $b^2 = |\nu + 1|^{-2b}$ for some index $b \geq 0$. Polya's criterion (see p. 509 of Feller, 1971) shows that this is indeed the Fourier expansion of a probability distribution $\beta$; for $b = 0$ we recover the density estimation example as a special case.

4.3 Minimax Risks

In this section we evaluate the minimax risks in the particular case of the deconvolution problem just described. The notation is as in the above two sections. It is assumed that the smoothness class is defined by setting $a_r = \alpha(a')^r$, for some $a > \frac{1}{2}$. By standard manipulations of Fourier series, it can be shown that, in the notation of condition (11),

$$\sup_{\gamma \in \mathcal{F}_0} \pm (g - 1) = 2C^2 \sum_{k=1}^{\infty} k^{-2(a+b)},$$

a quantity that is automatically less than 1 provided $C$ is small enough to ensure that $\mathcal{F}_0$ consists only of positive functions.

We first find the class $\mathcal{L}_N$. Suppose that $-N \leq \nu \leq N$ and $\rho \sim \nu$. Then, since $\rho/r$ and $\nu/r$ differ by an integer, $\sin^2(\pi \rho/r) = \sin^2(\pi \nu/r)$ and so $\rho_2 = \rho^{-2} \nu_2 \gamma_2^2 \leq \gamma_2^2$ with equality only if $\rho = \nu$; also, by definition, $b^2 > b^2$. Hence within each equivalence class $b^2_\rho \gamma_2^2$ will be maximized by choosing $-N \leq \nu \leq N$ and so $\mathcal{L}_N = [-N, -N + 1, \ldots, N - 1, N]$.

The quantity $S_N(\nu)$ as defined in Theorem 1 is given by

$$S_N(\nu) = \sum_{j \neq 0} |\nu + jr|^{-2a} = \sum_{j=0}^{\infty} \{(r + \nu + jr)^{-2a} + (r - \nu + jr)^{-2a}\}$$

$$\leq \sum_{j=0}^{\infty} \{(2N + 2Nj)^{-2a} + (N + 2Nj)^{-2a}\} = N^{-2a} \sum_{k=1}^{\infty} k^{-2a}.$$}

For $\rho \in \mathcal{L}_N$, we have $|\rho| > N$ and so the maximum value of $a_\rho^{-2}$ is $(N + 1)^{-2a}$. Therefore the bound $C(N)$ is exactly of order $N^{-2a}$.

We now consider the choice of $\alpha$ in Lemma 1. Let $\nu_\alpha = [\alpha^{-1/2a}]$ so that $\alpha^{1/2} a_\nu < 1$ if and only if $|\nu| < \nu_\alpha$. Then, provided $\nu_\alpha < N$ the choice of $\nu_\alpha$ is asymptotically equivalent to that of $\alpha$ and the condition (14) to

$$n^{-1} \sum_{\nu=1}^{\nu_\alpha} \frac{\nu^{2(a+b)}}{\text{sinc}^2(\pi \nu/r)} \{(\nu_\alpha/\nu)^a - 1\} = \frac{1}{2} C^2.$$

If $\alpha < N^{-2a}$ then the condition (14) becomes, asymptotically,

$$n^{-1} \sum_{\nu=1}^{N} \frac{\nu^{2(a+b)}}{\sin^2(\pi \nu/r)} \left( \alpha^{-1/2}\nu^{-a} - 1 \right) = \frac{1}{2} C^2.$$  \hspace{1cm} (21)$$

since $\alpha^{-1/2}\nu^{-a} > 1$ for all $\nu$ in $\mathbb{Z}^N$. 

In order to make the choice of $\alpha$, we consider three different asymptotic regimes in turn. 

4.3.1 The subcritical case. Suppose that $n = o(N^{2a+2b+1})$, so that the discretization index tends to infinity faster than $n^{1/(2a+2b+1)}$. Define $M$ by

$$M^{2a+b+1} = n(a + 2b + 1)(2a + 2b + 1)C^2/2a,$$

so that $M = o(N)$ as $n$ tends to infinity. Then, since the sinc terms converge uniformly to 1,

$$n^{-1} \sum_{\nu=1}^{M} \frac{\nu^{2(a+b)}}{\sin^2(\pi \nu/r)} \left( (M/\nu)^a - 1 \right) = n^{-1} \sum_{\nu=1}^{M} \nu^{2(a+b)} \left( (M/\nu)^a - 1 \right)$$

$$= n^{-1} \left( M^{a}(a + 2b + 1)^{-1} M^{a+2b+1} \right) - (2a + 2b + 1)^{-1} M^{2a+2b+1} = C^2/2.$$  \hspace{1cm} (22)$$

Here and below, the notation $a_n = b_n$ means that $a_n/b_n \to 1$ as $n \to \infty$. Thus $\nu_n^* = M$. To find the low-frequency minimax error $M(\mathcal{F}_N, \mathcal{F}^L_0)$, substitute back into (12) to obtain

$$M(\mathcal{F}_N, \mathcal{F}^L_0) \approx 2n^{-1} \sum_{\nu=1}^{M} \frac{\nu^{2b}}{\sin^2(\pi \nu/r)} \left( 1 - (\nu/M)^a \right)$$

$$\approx 2n^{-1} \sum_{\nu=1}^{M} \nu^{2b} \left( 1 - (\nu/M)^a \right)$$  \hspace{1cm} (23)$$

$$\approx 2n^{-1} a(2b + 1)^{-1} (a + 2b + 1)^{-1} M^{2b+1} \propto n^{-2a/(2a+2b+1)}.$$  

The asymptotic behavior of the error $\varepsilon(N)$ fits nicely with (23), because we have

$$\varepsilon(N) = O(N^{-2a}) = o(n^{-2a/(2a+2b+1)}) = o(M(\mathcal{F}_N, \mathcal{F}^L_0)).$$

Thus the full minimax error $M(\mathcal{F}_N, \mathcal{F}_0)$ is, by Theorem 1, asymptotically the same as the restricted minimax error $M(\mathcal{F}_N, \mathcal{F}^L_0)$. Indeed setting all the
\( \gamma \) equal to 1, and hence considering the case where there is no discretization, yields calculations leading to the same results as those of (22) and (23). Thus, at least as far the terms of leading order are concerned, the discretization has asymptotically no effect, either in the choice of estimator or in the mean square error obtained.

4.3.2 The critical case: Small \( c \). Now suppose that the discretization index tends to infinity precisely at the rate \( n^{1/(2a+2b+1)} \). For definiteness, we assume that \( n = C^{2c+2b+1} \) for some \( c, 0 < c < \infty \).

We define a family of increasing functions \( J_{p,q}(v) \) for \( 0 \leq v < \frac{1}{4} \) and \( p \) and \( q \geq 0 \) by

\[
J_{p,q}(v) = \int_0^v \frac{(u^p - u^p)u^q}{\sin^2(\pi u)} \, du = \int_0^v \frac{(u^p - u^p)u^{q+2}}{\sin^2(\pi u)} \, du.
\]

In this subsection we consider the case where \( c < 2C^{-2}J_{a,a+2b}(1) \); the case of \( c \) larger than this threshold is considered in Subsection 4.3.3 below.

In order to perform a calculation similar to (22), define \( U \) so that

\[
Ja,a+2b(U) = C^{2/2},
\]

and let \( M \) be the integer part of \( rU \). The assumption on \( c \) implies that \( 0 < U < \frac{1}{4} \) and so \( M \leq N \). A standard integral approximation argument then gives

\[
n^{-1} \sum_{v=1}^{M} \frac{v^{2(a+b)}}{\sin^2(\pi v/r)} \{(M/v)^a - 1\}
\]

\[
\approx n^{-1} r^{2a+2b+1} \int_0^U \frac{u^{2(a+b)}}{\sin^2(\pi u)} \{(U/u)^a - 1\} \, du
\]

\[
= c^{-1} Ja,a+2b(U) = C^{2}/2,
\]

by definition, so that \( \nu = M \). To find \( M(\mathcal{F}_N, \mathcal{F}_0^a) \), substitute back into (12) to obtain

\[
M(\mathcal{F}_N, \mathcal{F}_0^a) = 2n^{-1} \sum_{v=1}^{M} \frac{\nu^{2b}}{\sin^2(\pi \nu/r)} \left[ 1 - (\nu/M)^a \right]
\]

\[
= 2n^{-1} r^{1+2b} U^{-a} Ja,a(1) \propto n^{-2a(2a+2b+1)}, \quad (24)
\]

This is the same rate as in (23), but it should be noted that the constant of proportionality in (23) is independent of the discretization index, pro-
vided that the defining property is satisfied. This is not the case in (24), because both $r$ and $U$ depend on the constant $c$ in ways that do not cancel out. It can be shown that the constant of proportionality in (24) is strictly larger than that in (23) for all $c$ in the range considered in this subsection; thus, even before the high-frequency components are taken into account, the discretization will increase the asymptotic minimax risk. A fortiori, the full minimax risk $M(\mathcal{F}_N, \mathcal{F}_0)$ will be asymptotically larger than in the case where there is no discretization.

We now turn to the high-frequency effect. We have, in the same notation previously used,

$$\varepsilon(N) \propto N^{-2a} \propto n^{-2a(2a+2b+1)}$$

so that $\varepsilon(N)$ has the same order of magnitude as $M(\mathcal{F}_N, \mathcal{F}_0)$ and the ratio between the upper and lower bounds in (15) no longer tends to 1 as $n \to \infty$, though it does remain bounded.

Thus, to sum up, the behavior in this case is quite different from the previous regime. Although the optimum rate of convergence, $O(n^{-2a(2a+2b+1)})$, of the minimax risk is the same, the discretization will make itself felt both by increasing the low-frequency minimax risk and also by allowing the high-frequency error to make a significant contribution.

4.3.3 The critical case: Large $c$. Suppose, now, that $n = c r^{2a+2b+1}$ for some $c > 2C^{-2} J_{a,a+2b}(\frac{1}{2})$. Define a family of constants $I_p$ for $p \geq 0$ by

$$I_p = \int_{0}^{1/2} \frac{u^p}{\sin^2(\pi u)} \, du,$$

and define $\alpha_r$ such that

$$\alpha_r^{-1/2} = r^a I_{a+2b}^{-1} \left( \frac{1}{2} C^2 c + I_{2a+2b} \right).$$

Since $J_{a,a+2b}(\frac{1}{2}) = 2^{-a} I_{a+2b} - I_{2a+2b}$, it follows from the lower bound on $c$ that $\alpha_r \leq (\frac{1}{2} c)^{-2a} < N^{-2a}$. Set $\alpha = \alpha_r$ in (21) and perform a simple integral approximation to obtain

$$n^{-1} \sum_{\nu=1}^{N} \frac{\nu^{2(a+b)}}{\sin^2(\pi \nu/r)} \left( \alpha_r^{-1/2} \nu^{-a} - 1 \right)$$

$$\approx n^{-1} (r^{a+2b+1} \alpha_r^{-1/2} I_{a+2b} - r^{2a+2b+1} I_{2a+2b}) = C^2/2,$$

by the definition of $\alpha_r$. Thus condition (13) of Lemma 1 is satisfied with $\alpha \approx \alpha_r$. 
To calculate the minimax low-frequency risk \( M(\mathcal{F}_N, \mathcal{F}_0) \), substitute back into (12) and approximate the sums by integrals to obtain

\[
M(\mathcal{F}_N, \mathcal{F}_0) = 2n^{-1} \sum_{\nu=1}^{N} \frac{\nu^{2b}}{\text{sinc}^2(\pi\nu/r)} (1 - \alpha_r^{1/2} \nu^a)
\]

Just as in Subsection 4.3.2, this gives the same rate as in (23), but with a constant of proportionality depending on the constant \( c \). Because the high-frequency bound \( e(N) \) is still of the same order of magnitude, it follows that \( M(\mathcal{F}_N, \mathcal{F}_0) \) is of order \( n^{-2a/(2a+2b+1)} \), but with a larger constant of proportionality than in the case where there is no discretization; we have already remarked that this is true if \( c \) is small, and the effect for fixed \( n \) of increasing \( c \) is to reduce the number of bins, and hence to reduce the information available and to increase the minimax risk over the fixed function class \( \mathcal{F}_0 \).

It is of interest to point out that the constant of proportionality in (25) actually converges to zero as \( c \) tends to infinity. Therefore, for large \( c \), the value of \( \lim_{n \to \infty} n^{2a/(2a+2b+1)} M(\mathcal{F}_N, \mathcal{F}_0) \) will be smaller than its value in the subcritical and no-discretization cases. This apparent paradox is explained by the fact that the function class \( \mathcal{F}_0 \) will also be reduced in dimensionality as the number of bins is reduced, and so more of the error will be due to the high-frequency effects.

Finally we point out that Lemma 1 shows that the minimax estimator \( T^* \) corresponding to (25) has \( T^*_\nu \neq 0 \) for all \( \nu \) in \( \mathcal{L}_0^0 \) and so the estimate will involve all the coefficients \( \tilde{Z}_\nu \) for \( \nu \) in \( \mathcal{L}_0^0 \). This is not the case for the minimax estimators in the previous two subsections, which will have \( T^*_\nu = 0 \) for all \( |\nu| > \nu_\alpha \).

5. THE WICKSELL PROBLEM

In our treatment of the unfolding problem, we shall assume that the sphere radii, and hence the observed circle radii, all fall in an interval \([0, A]\) on the positive half-line. By redefining the units of measurement if necessary, we assume without loss of generality that \( A = 1 \), so that the spaces \( \mathcal{B} \) and \( \mathcal{D} \) are both equal to the unit interval. For reasons of mathematical tractability, we equip \( \mathcal{B} \) with the dominating measure \( \mu \) defined by \( d\mu(x) = (4x)^{-1} \, dx \) and \( \mathcal{D} \) with the dominating probability measure \( \lambda \) defined by \( d\lambda(y) = 4\pi^{-1} (1 - y^2)^{1/2} \, dy \). The spaces \( \mathcal{F} \) and \( \mathcal{G} \) are defined to be the sets of functions on \([0, 1]\) that are square integrable with respect to \( \mu \) and \( \lambda \) respectively.
Suppose the sphere radii come from a population with intensity $f$ with respect to $\mu$. Then, by a standard argument of stereology (Wicksell, 1925) the intensity (per unit area of the intersecting plane) of the observed circle radii with respect to Lebesgue measure on $\mathbb{S}$ will be $y \int_1 (x^2 - y^2)^{-1/2} f(x) d\mu(x)$. Hence the intensity with respect to the measure $\lambda$ will be

$$\mathcal{P}f(y) = \frac{1}{4} \pi y(1 - y^2)^{-1/2} \int_1 (x^2 - y^2)^{-1/2} f(x) d\mu(x). \quad (26)$$

5.1 The Singular Value Decomposition

We now display the SVD of the mapping $\mathcal{P}$ from $\mathcal{F}$ to $\mathcal{G}$ as defined in (26) above. For integers $\nu \geq 0$ define functions $\phi_\nu$ and $\psi_\nu$ on the unit interval by

$$\phi_\nu(x) = 4(\nu + 1)^{1/2} x^2 P^{0,1}_\nu(2x^2 - 1) \quad (27)$$

and

$$\psi_\nu(y) = 2y U_\nu(2y^2 - 1) = U_{2\nu+1}(y),$$

where $P^{0,1}_\nu$ is the Jacobi polynomial of type $(\alpha, \beta) = (0, 1)$ and order $\nu$ and $U_\nu$ is the second-kind Chebyshev polynomial of order $\nu$.

It follows from (27) by standard properties of Jacobi polynomials that $\{\phi_\nu\}$ form a complete orthonormal basis for $\mathcal{F}$ with respect to $\mu$; we have, substituting $u = 2x^2 - 1$,

$$\int_0^1 \phi_\nu(x)\phi_\nu(x) d\mu(x) = \frac{1}{2} (\nu + 1)^{1/2}(\nu' + 1)^{1/2} \int_{-1}^1 P^{0,1}_\nu(u)P^{0,1}_{\nu'}(u)(1 + u)du = \delta_{\nu\nu'}.$$

Completeness is proved by an argument involving the same change of variable. The orthonormality of the $\{\psi_\nu\}$ follows in a similar fashion.

It can now be shown that

$$\mathcal{P}\phi_\nu = \frac{1}{16} \pi (1 + \nu)^{-1/2} \phi_\nu \quad (28)$$

so that the orthonormal sequences $\{\phi_\nu\}$ and $\{\psi_\nu\}$ define the SVD of $\mathcal{P}$, with the singular values $b_\nu$ given by $b_\nu = (\pi/16)(1 + \nu)^{-1/2}$.

To prove (28) substitute the definition of $\phi_\nu$ into (26) and make the substitutions $\cos \theta = y$, $v = 2y^2 - 1 = \cos 2\theta$ and $u = 2x^2 - 1$ to obtain
\[ \mathcal{P} \phi_y(y) = \frac{1}{8} (\nu + 1)^{1/2} \pi y (1 - y^2)^{-1/2} \int_y^1 (x^2 - y^2)^{-1/2} P_{\nu}^{0,1}(2x^2 - 1) x \, dx \]

\[ = \frac{\sqrt{2}}{32} (\nu + 1)^{1/2} \pi y (1 - y^2)^{-1/2} \int_0^1 (u - v)^{-1/2} P_{\nu}^{0,1}(u) \, du. \]

The Jacobi polynomials \( P_{\nu}^{0,1} \) are connected to the more familiar Legendre polynomials \( P_{\nu} \) via the relation \( (2\nu + 1) P_{\nu} = (\nu + 1) P_{\nu}^{0,1} + \nu P_{\nu}^{0,1} \). The following identity may be derived then from formula (22.13.11) of Abramowitz and Stegun (1964) and the recurrence relation for second-kind Chebychev polynomials:

\[ \int_0^1 (u - v)^{-1/2} P_{\nu}^{0,1}(u) \, du = 2(\nu + 1)^{-1/2}(1 - v)^{1/2} U_{\nu}(v). \] (29)

Singular value decomposition (28) is an immediate consequence of formula (29).

Although we have outlined a direct verification of (28), it should be pointed out that the SVD was first derived by transforming (26) into an Abel integral operator equation, equivalent to half-order integration. The hypergeometric function in general, and Jacobi polynomials in particular, can be considered as fractional derivatives of beta densities; see Gel'fand and Shilov (1964). Since derivatives of different orders commute, one obtains a family of identities of which (29) is most appropriate for our analysis.

### 5.2 Discretization

We now consider the case where the circle radii are only observed in binned form. We divide the observation space \( \mathcal{G} \) into unequally sized bins, with respect to which the matching SVD property holds approximately. For \( j = 1, 2, \ldots, N \), define \( D_j \) to be the bin \( [\cos(j\pi/2N), \cos((j - 1)\pi/2N)] \). For convenience, we define angles \( \theta_j \) and \( \delta \) by

\[ \theta_j = \frac{(j - 1/2)\pi}{2N} \quad \text{and} \quad \delta = \frac{\pi}{4N}. \]

If we make the transformation \( y = \cos \theta \), then the bins are of equal size in \( \theta \) space, and have midpoints \( \theta_j \) and width \( 2\delta \).

Given any \( g \) in \( \mathcal{G} \), the discretization operator maps \( g \) to the vector of averages of \( g \) over the various bins,

\[ (\mathcal{G} \mathcal{G})_j = \mathcal{G}(D_j)^{-1} \int_{D_j} g(y) \, d\lambda(y) = \frac{\int_{\theta_j-\delta}^{\theta_j+\delta} g(\cos \theta) 4\pi^{-1} \sin^2 \theta \, d\theta}{\int_{\theta_j-\delta}^{\theta_j+\delta} 4\pi^{-1} \sin^2 \theta \, d\theta}. \] (30)
We equip the space $\mathcal{G}_N$ with a modified weighted vector inner product,

$$\langle a, b \rangle^* = 2N^{-1} \sum_{j=1}^{N} a_j b_j \sin^2 \theta_j. \quad (31)$$

This inner product is obtained from the inner product $\sum a_j b_j \lambda(D_j)$ by substituting the approximation

$$h(D_j) = \frac{1}{2} \int_{\theta_j}^{\theta_j+\delta} 4\pi^{-1} \sin^2 \theta \ d\theta = \frac{\sin^2 \theta_j}{\sin \theta_j} \delta.$$ \quad (32)

The accuracy of this approximation is discussed in more detail in Section 5.4 below.

In order to set out the approximate matching SVD property satisfied by $\mathcal{D}$ and $\mathcal{G}_N$ define $\chi_l$ in $\mathcal{G}_N$ for $l = 0, \ldots, N - 1$ by

$$\chi_l \equiv \frac{\sin((2l + 2)\theta_j)/\sin \theta_j}{2^{-1/2} \sin((2l + 2)\theta_j)/\sin \theta_j} \quad \text{if } l < N - 1$$

$$\chi_l \equiv 2^{-1/2} \sin((2l + 2)\theta_j)/\sin \theta_j \quad \text{if } l = N - 1.$$ 

Elementary trigonometric manipulations show that the $\{\chi_l\}$ form an orthonormal basis of $\mathcal{G}_N$ with respect to the modified inner product (31).

Given any $\nu \geq 0$ let $\nu' \equiv \nu \mod 2N$. There are two cases to consider. First, if $\nu' = 2N - 1$ then

$$\mathcal{D}_N \psi_\nu \approx 0,$$

so we define $\gamma_\nu = 0$, and, for definiteness, $[\nu] = 0$. If $\nu' < 2N - 1$ then define

$$[\nu] = \min(\nu', 2N - 2 - \nu')$$

and

$$\gamma_\nu = (-1)^{\nu-\nu' + 2N} \sin^2((\nu + 1)\pi/2N).$$

It is then the case that

$$\mathcal{D}_N \psi_\nu \approx \gamma_\nu \chi_{[\nu]}; \quad (33)$$

the derivation of this approximation is considered in Section 5.4 below.

5.3 Surrogate Risk Behavior

Since each of the $\psi_\nu$ has a first-order zero at $\gamma = 0$, it is clear that the lower bound part of (11) is not available for the Wicksell operator. How-
ever, we shall see that the ratio of surrogate to true mean integrated squared error can be bounded above and below away from zero uniformly over $\mathcal{F}_0$ at least for diagonal linear estimators.

**Proposition 1.** Let $\mathcal{F}_0 = \{ f \in \mathcal{F}: f_0 = 1, \sum_{v=0}^{\infty} f_v^2 (1 + v)^{\beta} \leq c^2 \}$. Let $\zeta(s) = \sum_{v=1}^{\infty} k^{-v}$. For every $g \in \mathcal{P} \mathcal{F}$, and every $y \in \mathcal{D}$,

$$\left| \frac{g(y)}{b_0 \psi_0(y)} - 1 \right| \leq c b_0^{-1} [\zeta(\beta - 1) - 1]. \quad (34)$$

**Proof.** Expanding $g = \mathcal{P} f$ in terms of $\psi_v$ and using the Chebyshev polynomial bound $|U_v(z)| \leq v + 1$ enables us to bound the left side of (34) by

$$\left| 1 - \sum_{v \neq 0} b_0^{-1} g_v \frac{\psi_v}{\psi_0} \right| \leq \left| \sum_{v \neq 0} b_0^{-1} g_v (v + 1) \right|.$$

The bound follows by maximizing this linear combination over the ellipsoid $\mathcal{P} \mathcal{F}_0 = \{ g : g_0 = b_0, \sum_{v \neq 0} (1 + v)^{\beta + 1} g_v^2 \leq c^2 \}$.

The proposition shows that $\mathcal{P} f$ is nonnegative for any $f \in \mathcal{F}_0$ so long as $c$ is small enough that the right side of (34) is less than 1. In turn, this implies the validity of the upper bound (10). For the lower bound, we first note that for $c$ small enough the proposition and (9) imply the existence of a constant $m(\beta, c)$ such that

$$n \text{var}_{\mathcal{F}_0} T(x) \geq m(\beta, c) \int t^2(x, j(y)) \psi_0(y) d\lambda(y). \quad (35)$$

Now restrict attention to estimators in $\mathcal{F}_0^0$, which have the form

$$t(x, j) = \sum_{v \in \mathcal{F}_0^0} T_{v\psi} \psi_0(x) \chi_{[v]}(j).$$

Integrating over $x$ in (35) and changing orders of integration gives

$$\int n \text{var}_{\mathcal{F}_0^0} \hat{T}(x) \mu(dx) = \sum_{v \in \mathcal{F}_0^0} T_{vv}^2 \int \chi_{[v]}(j(y)) \psi_0(y) d\lambda(y).$$

For the corresponding term in the surrogate risk $M^*(T, f)$, on the other hand, under the uniform density $g = 1$ on $\mathcal{D}$, we obtain simply

$$\text{tr} TT^T = \sum_{v \in \mathcal{F}_0^0} T_{vv}^2.$$
according to Gradshteyn and Ryzhik (1980, formula 7.345.5). For large $N$, this establishes that the ratio of true to surrogate risk is bounded away from zero over the class $\mathcal{F}_0$ for large $N$ and appropriate $(\beta, c)$.

5.4 Accuracy of the Discretization Approximation

In this section we discuss the approximations (32) and (33) in more detail. The approximations we justify are stated formally in the following proposition. The approximation (33) is obtained by dividing (37) by (36), with the error terms neglected.

**Proposition 2.** Given any $\nu \geq 0$, and any $j$, $1 \leq j \leq N$,

$$\lambda(D_j) = 2N^{-1} \sin^2 \theta_j + O(N^{-3}) \quad \text{uniformly over } j$$

and

$$\int_{D_j} \psi_r(y) d\lambda(y) = 2N^{-1} \gamma \sin(2[\nu] + 2) \theta_j \sin \theta_j + O(N^{-2})$$

uniformly over $j$ and $\nu$. \hfill (37)

**Proof.** A key step in the proof is the simple identity

$$\int_{\theta - \delta}^{\theta + \delta} \cos \theta \, d\theta = r^{-1} \{\sin r(\theta_j + \delta) - \sin r(\theta_j - \delta)\} = 2\delta \sin c \theta \cos r\theta.$$ \hfill (38)

We now have

$$\lambda(D_j) - 2N^{-1} \sin^2 \theta_j = 4\pi^{-1} \int_{\theta - \delta}^{\theta + \delta} (\sin^2 \theta - \sin^2 \theta_j) \, d\theta$$

$$= 2\pi^{-1} \int_{\theta - \delta}^{\theta + \delta} (\cos 2\theta_j - \cos 2\theta) \, d\theta$$

$$= 4\delta \pi^{-1} (1 - \sin c 2\delta) \cos 2\theta_j.$$

This last quantity is bounded in absolute value by $\pi^2 N^{-3/6}$ for all $j$, completing the proof of (36). To prove (37), use the definitions and the identity (38) to write

$$\int_{D_j} \psi_r \, d\lambda = 4\pi^{-1} \int_{\theta - \delta}^{\theta + \delta} \sin(2\nu + 2) \theta \sin \theta \, d\theta$$

$$= 2\pi^{-1} \int_{\theta - \delta}^{\theta + \delta} (\cos(2\nu + 1) \theta - \cos(2\nu + 3) \theta) \, d\theta$$

$$= N^{-1} \{\sin c(2\nu + 1) \delta \cos(2\nu + 1) \theta_j \}.$$
Replacing both the sinc terms by sinc(2ν + 2)δ incurs an error bounded by $2N^{-18} \sup |\text{sinc}'(x)| = O(N^{-2})$, so that

$$\int_{D_j} \psi_\nu \, d\lambda = N^{-1} \text{sinc}(2\nu + 2)\delta \{\cos(2\nu + 1)\theta_j - \cos(2\nu + 3)\theta_j\} + O(N^{-2})$$

$$= 2N^{-1} \text{sinc}(2\nu + 2)\delta \sin(2\nu + 2)\theta_j \sin \theta_j + O(N^{-2}).$$

Simple properties of trigonometric functions complete the proof of (37).

5.5 Minimax Risks

The appropriate matching SVD property that we have demonstrated can now be used to calculate approximate minimax risks in the Wicksell problem. We assume that $a_\nu = \nu^a$ for some $a \geq \frac{1}{2}$, as before. There are then very close similarities between the calculations of the approximate minimax risks and those performed in Section 4.3 above for the deconvolution problem, setting the index $b = \frac{1}{2}$ throughout.

In the deconvolution problem, we have $\gamma_\nu = \text{sinc}(\pi\nu/(2N + 1))$ while in the Wicksell problem $\gamma_\nu = \text{sinc}(\pi(\nu + 1)/2N)$, but this makes no material difference to the asymptotic calculations we perform; nor does the fact that the maximum value of $\nu$ in $L_N$ is $N - 1$ rather than $N$. The important differences are that in the Wicksell problem sums over $L_N$ involve only positive indices $\nu < N$, and the singular values $b_\nu$ are $(\pi/16)(1 + \nu)^{-1/2}$ rather than simply $(1 + \nu)^{-1/2}$. The effect of these differences is to replace $\frac{1}{4}C^2$ by $(\pi/16)^2 C^2$ throughout and in addition to multiply the expressions corresponding to (23), (24), and (25) by $\frac{1}{4}(\pi/16)^{-2}$. The only other change that needs to be made is to substitute $2N$ explicitly for $r$ as the discretization index.

Reworking Section 4.3 with these minor changes thus yields the following results, all subject to the approximations involved in Eq. (33) defining the matching SVD property for the Wicksell problem, and in Eq. (32) concerning the modification of the inner product on $s_N$. Firstly, if $n = o(N^{2+2a})$ then the minimax risk $M(F_N, \mathcal{F}_0)$ is asymptotically proportional to $n^{-a/(a+1)}$, with a constant of proportionality that does not depend on the discretization at all. In the critical case $n = c'N^{2a+2}$ the asymptotic power dependence of $n$ of the full minimax risk will be the same, but the constant of proportionality will be larger than that in the case of no discretization. As $c'$ increases, the low-frequency minimax estimator and risk will change in exactly the way discussed in Subsections 4.3.2 and 4.3.3 above.

6. Positron Emission Tomography

The detailed discussion of the PET problem has something in common with the Wicksell unfolding problem discussed above, and we set it out in a similar way; there is the additional complication of double subscripts on
the various families of vectors and functions. We begin by recapitulating the two-dimensional mathematical model of PET that was used by Johnstone and Silverman (1990). Further details on the relation between the actual tomographic problem and the model described here are given in that paper and in Shepp and Vardi (1982) and Vardi et al. (1985). Bickel and Ritov (1990) also address discretization issues in PET, concentrating on the estimation of linear functionals of the image.

6.1 The Continuous Formulation

As described in Section 1 above, the original radioactive emissions take place in a thin cylindrical section $\mathcal{B}$ that may be considered as being the unit disk in $\mathbb{R}^2$; we equip $\mathcal{B}$ with the dominating measure $\mu$ defined by $d\mu(x) = \pi^{-1}dx$. The emissions may be regarded as an i.i.d. sample from a density $f$ defined relative to $\mu$ and the space $\mathcal{F}$ will be the space of all $f$ for which $\int f^2d\mu$ is finite.

Each emission gives rise to a pair of photons that fly off from the emission point $X$ in opposite directions along a randomly directed line $Y$, which can be observed. The set of possible lines may be parametrized by the length $s$ and the orientation $\phi$ of the perpendicular from the center of the unit disk to the line, as shown in Fig. 1. Detector space $\mathcal{D}$ consists of all possible lines, given in coordinates by $\{(\phi, s): 0 \leq \phi \leq 2\pi, -1 \leq s \leq 1\}$. Note that there is a two-to-one indeterminacy in this description, since

Fig. 1. An emission within the detector circle, showing the line of flight of the photons and the detectors that are activated.
(\phi, s) and (\phi + \pi, -s) each describe the same actual line, and it is assumed that any particular line has probability 0.5 of being parametrized in each possible way. Sometimes it is convenient to use the alternative parametrization \{((\phi, \theta); 0 \leq \phi \leq 2\pi, 0 \leq \theta \leq \pi}\}, setting \(s = \cos \theta\).

Define the dominating measure \(\lambda\) on \(\mathcal{B}\) by

\[
d\lambda(\phi, s) = \pi^{-2}(1 - s^2)^{1/2}ds\ d\phi = \pi^{-2} \sin^2 \theta\ d\theta\ d\phi.
\] (39)

Let \(\mathcal{G}\) be the space of functions on \(\mathcal{B}\) that are square integrable with respect to \(\mu\) and that satisfy the condition \(g(\phi, s) = g(\phi + \pi, -s)\), to take account of the indeterminacy in the parametrization. The density \(g = \mathcal{G}f\) of lines in detector space arising from a population of emissions drawn from the density \(f\) over \(\mathcal{B}\) will then be given by the normalized Radon transform

\[
g(\phi, s) = \frac{1}{2} (1 - s^2)^{-1/2} \int_{\sqrt{1-t^2}}^{\sqrt{1-t^2}} f(s \cos \phi - t \sin \phi, s \sin \phi + t \cos \phi) dt.
\]

The SVD of the mapping \(\mathcal{P}\) from \(\mathcal{F}\) to \(\mathcal{G}\) is described in terms of a double index set

\[
\mathcal{N} = \{(j, k): j = 0, 1, 2, \ldots; k = 0, 1, 2, \ldots\}.
\]

Using polar coordinates \(x = (r \cos \alpha, r \sin \alpha)\) for points in \(\mathcal{B}\), define the orthonormal basis \(\phi_{\nu}\) for \(\mathcal{F}\) by

\[
\phi_{\nu}(x) = (j + k + 1)^{1/2} Z_{j+k}^{j-k}(r)e^{i(j-k)\alpha}
\]

for \(\nu = (j, k) \in \mathcal{N}\), where \(Z_{j+k}^{j-k}\) is the Zernike polynomial of degree \(j + k\) and order \(|j - k|\); see Marr (1974) and Johnstone and Silverman (1990). The corresponding orthonormal basis for \(\mathcal{G}\) is

\[
\psi_{\nu}(\phi, s) = e^{i(j-k)\phi} U_{j+k}(s) = e^{i(j-k)\phi} \frac{\sin(j + k + 1)\theta}{\sin \theta}
\]

for \(\nu = (j, k) \in \mathcal{N}\).

Here the \(U_{j+k}\) are the Chebychev polynomials of the second kind. We then have \(\mathcal{P}\phi_{\nu} = (j + k + 1)^{-1/2}\psi_{\nu}\) so that the singular values \(b_{\nu}\) are given by

\[
b_{\nu} = b_{jk} = (j + k + 1)^{-1/2} \quad \text{for} \ \nu = (j, k) \in \mathcal{N}.
\]
6.2 Discretization

In reality the photon lines cannot be observed exactly because of the finite size of the detectors. Suppose the unit circle is divided into an even number \( N \) detectors of equal size, the intervals having polar angular coordinate \((2\pi d/N, 2\pi (d + 1)/N)\) for \( d = 0, 1, \ldots, N - 1 \). Given a pair of detectors \( d_1 \) and \( d_2 \), define the corresponding detector tube to be the set of all lines in detector space \( \mathcal{D} \) that intersect the detectors \( d_1 \) and \( d_2 \).

In order to describe this detector tube explicitly, it is most convenient to work in \((\phi, \theta)\) coordinates. Given a particular detector tube, define \((\phi_1, \theta_1)\) and \((\phi_2, \theta_2)\) to be the two different parametrizations of the line joining the midpoints of the two detectors, so that \(\phi_1 = (d_1 + d_2 + 1)\pi/N\) and \(\phi_2 = \phi_1 + \pi \mod 2\pi\) and \(\theta_2 = \pi - \theta_1\). It can be seen from Fig. 1 that the angular coordinates of the points at which the line \( Y \) crosses the unit circle are simply \(\phi \pm \theta\). It follows that the line \( Y \) will fall within the detector tube if and only if either \(|\phi - \phi_1| + |\theta - \theta_1| < \pi/N\) or \(|\phi - \phi_2| + |\theta - \theta_2| < \pi/N\), interpreting arithmetic involving \(\phi\) modulo \(2\pi\).

Thus the detector tube consists of the union of two "diamonds" in \((\phi, \theta)\) space. Each diamond is a square in \((\phi, \theta)\) space rotated through \(45^\circ\); for example the one centered at \((\phi_1, \theta_1)\) will be bounded by the four lines \((\phi - \phi_1) \pm (\theta - \theta_1) = \pm \pi/N\).

It is convenient to index the set of all detector tubes in a slightly different way, by reference to the midpoints of the corresponding diamonds. Define

\[
\mathcal{M}_N = \{(l, m): 0 \leq l < 2N; 0 < m < N; l + m \text{ odd}\}.
\]

Then each possible diamond will have as midpoint a point of the form \((\phi_1, \theta_1) = (l\pi/N, m\pi/N)\) for \((l, m)\) in \(\mathcal{M}_N\), and the set of all detector tubes will be obtained by pairing diamonds whose \(l\)-indices differ by \(N\) and whose \(m\)-indices sum to \(N\). A natural way of doing this is to index the detector tubes by the set

\[
\mathcal{M}_N^* = \{(l, m): 0 \leq l < N; 0 < m < N; l + m \text{ odd}\}
\]

defining the tube \(D_{lm}\) to be the union of the two diamonds with indices \((l, m)\) and \((l + N, N - m)\) in \(\mathcal{M}_N\). Note that suffices of the form \(jk\) are attached to singular functions such as \(\phi_v = \phi_{jk}\) while suffices \(lm\) are attached to the bins \(D_{lm}\) into which the observation space \(\mathcal{D}\) is divided.

Given any \(g\) in \(\mathcal{G}\), the discretization operator maps \(g\) to the vector of averages of \(g\) over the various bins, in our case

\[
(\mathcal{D}_N g)_{lm} = \lambda(D_{lm})^{-1} \int_{D_{lm}} g(\phi, \theta) d\lambda(\phi, \theta) = \frac{\int_{D_{lm}} g(\phi, \theta) \sin^2 \theta \ d\phi \ d\theta}{\int_{D_{lm}} \sin^2 \theta \ d\phi \ d\theta}.
\] (40)
We equip the space \( \mathcal{D}_N \) with a modified weighted vector inner product, defining \( \langle a, b \rangle^* \) to be

\[
4N^{-2} \sum_{m,n} a_{lm} \overline{b}_{lm} \sin^2 \theta_m = 4N^{-2} \sum_{m,n} a_{lm} \overline{b}_{lm} \sin^2 m\pi/N. \tag{41}
\]

The weights involved in this inner product are a natural approximation to the \( \lambda(D_{lm}) \), obtained as before by replacing the density \( \pi^{-2} \sin^2 \theta \) in the definition (39) of \( \lambda \) by its value at the center of the diamond. Details of the closeness of the approximation of the inner product (41) to that defined using the exact weights \( \lambda(D_{lm}) \) are given in Section 6.3 below.

It is now the case that \( \mathcal{D} \) and \( \mathcal{D}_N \) approximately obey the matching SVD property. The space \( \mathcal{D}_N \) has dimension \( \frac{1}{2}N(N-1) \) and the relevant orthonormal basis with respect to the inner product (41) is most naturally indexed by the set \( \mathcal{N}_{N-1} = \{(j, k): j, k \geq 0, j + k \leq N - 2\} \). Define basis vectors \( \chi_{j,k} \) by restricting \( \chi_{j,k} \) to \( \mathcal{M}_N^* \):

\[
(\chi_{j,k})_{lm} = \psi_{jk}(\phi_l, \cos \theta_m) = e^{i(j-k)l/N} \sin((j + k + 1)m\pi/N) / \sin(m\pi/N)
\]

\( (l, m) \in \mathcal{M}_N^* \). \tag{42}

The vectors \( \{\chi_{j,k}, (j, k) \in \mathcal{N}_{N-1}\} \) form an orthonormal basis for \( \mathcal{D}_N \) relative to the inner product \( \langle \cdot, \cdot \rangle^* \): this remarkable fact is derived by Marr (1974) (a partial verification appears in Natterer (1986)).

The following easily verified identities show that for any \( (j, k) \in \mathcal{N}, \chi_{j,k} \) is aliased either to zero or a basis vector in \( \mathcal{D}_N \):

\[
\chi_{j+k,N-k,k} = (-1)^{n_1+n_2} \chi_{j,k},
\]

\[
\chi_{N-1-k,N-1-j} = -\chi_{j,k} \tag{43}
\]

from which follows

\[
\chi_{j,k} = 0 \quad \text{if } j + k = N - 1 \pmod{N}.
\]

We can now define the equivalence classes needed for the matching SVD property (3). Given any \( \nu_0 = (j_0, k_0) \) in \( \mathcal{N}_{N-1} \), define \( j_1 = N - 1 - k_0 \) and \( k_1 = N - 1 - j_0 \). Then the equivalence class of \( \nu_0 \) consists of all indices of the form \( (j_0 + r_j N, k_0 + r_k N) \) or \( (j_1 + r_j N, k_1 + r_k N) \) for nonnegative integers \( r_j \) and \( r_k \). In addition, all pairs \( (j, k) \) with \( j + k = N - 1 \pmod{N} \) are added to the equivalence class of \( (0, 0) \). It follows at once from the definitions that if \( \nu \sim \nu_0 \) then

\[
j_0 \leq j \quad \text{and} \quad k_0 \leq k. \tag{44}
\]
Finally (using \( \lfloor \cdot \rfloor \) to denote integer part) define
\[
\gamma_\nu = \begin{cases} 
0 & \text{if } j + k \equiv N - 1 \pmod{N} \\
(-1)^{(j+k)/N} \sin((2j + 1)\pi/2N) \sin((2k + 1)\pi/2N) & \text{otherwise.}
\end{cases}
\]

With these definitions, we can now state the approximation
\[
2_N \psi_\nu \approx \gamma_\nu \chi_\nu,
\]
whose derivation and accuracy is discussed next.

### 6.3 Accuracy of the Discretization Approximation

One possible quantification of the accuracy of the approximation (45) is given by the following proposition. The numerator and denominator of (40) are approximated separately.

**Proposition 3.** Given any \( \nu = (j, k) \in \mathcal{N} \) and any \( (l, m) \in \mathbb{Z}_N^* \),
\[
\int_{D_m} \psi_\nu(\phi, \cos \theta) d\lambda(\phi, \theta) = \gamma_\nu(\chi_\nu)lm 4N^{-1} \sin^2(m\pi/N) + R_{v,lm}.
\]
The error term satisfies the bounds
\[
\sup_{l,m} |R_{v,lm}| \leq \frac{2j + 2k + 3}{6} N^{-4} + O(N^{-6})
\]
\[
\sup_{v,l,m} |R_{v,l,m}| \leq 1.08\pi N^{-3}.
\]

**Proof.** The proof is elementary and is only sketched here. Begin with the left side of (46): changing variables \( \theta = \theta_k + t, \phi = \phi_l + u \), accounting for the two-to-one multiplicity and exploiting the symmetry of the domain of integration, we obtain
\[
\int_{D_m} \psi_\nu(\phi, \cos \theta) \sin^2 \theta d\phi d\theta
= e^{i(j-k)\phi_l} \int e^{i(j-k)u}[\cos(j+k)\theta_m \cos(j+k)t \\
- \cos(j+k+2)\theta_k \cos(j+k+2)t]dtdu,
\]
where the integral is taken over the set \( \{|t| + |u| < \pi N^{-1}\} \). Now apply the easily derived identity
\[
\int_{|t| + |u| < \pi N^{-1}} \cos(j-k)u \cos(j+k)t du dt
= 2\pi^2 N^{-2} \sin(j\pi/M) \sin(k\pi/N), \quad (j, k) \in \mathbb{Z}_2^2
\]
to rewrite the left side of (49) as
\[
\text{sinc} \left\{ \left( j + \frac{1}{2} \right) \pi / N \right\} \text{sinc} \left\{ \left( k + \frac{1}{2} \right) \pi / N \right\} \psi_s(\phi_l, \cos \theta_m) \, 4 \pi^2 N^{-2} \sin^2 \theta_m
\]
\[+ R_{v,lm}, \quad (50)\]

where
\[
R = 2 \pi^2 N^{-2} e^{(j-k) \phi_l} \left[ \varepsilon_{jk} \cos(j + k) \theta_m + \varepsilon_{j+1/2,k+1/2} \cos(j + k + 2) \theta_m \right],
\]
\[\varepsilon_{jk} = \text{sinc}\{j\pi/N\} \text{sinc}\{k\pi/N\} - \text{sinc} \left\{ \left( j + \frac{1}{2} \right) \pi / N \right\} \text{sinc} \left\{ \left( k + \frac{1}{2} \right) \pi / N \right\}.
\]

Using the definition (42) and relations (43) converts (50) to (46). Power series expansions of the sinc functions give the approximation
\[
\varepsilon_{jk} = \frac{1}{12} (2j + 2k + 1) N^{-2} + O(N^{-4}) \quad \text{for any fixed} \ j, k.
\]

A uniform bound over all \( j, k \) is given by applying the mean value theorem, to obtain the bound
\[
\sup_{j,k} |\varepsilon_{jk}| \leq (\pi/2N) \sup_{x,y} |\text{sinc} x \text{sinc}' y + \text{sinc}' x \text{sinc} y|\]
\[= 0.2701 \ldots \pi N^{-1}.
\]

The error bounds (47) and (48) follow immediately by using these inequalities for \( \varepsilon_{jk} \) and \( \varepsilon_{j+1/2,k+1/2} \).

### 6.4 The Minimax Risks

We are now able to carry out calculations of the minimax risks analogous to those performed for the other examples above. The basic principles of the calculations are the same, but the doubly subscripted arrays of singular functions and values make the details a little more complicated. Just as in the calculations outlined in Section 5.5 for the Wicksell example, all our conclusions are necessarily approximate, because the matching SVD assumption has only been demonstrated approximately for the PET problem, in Eq. (45) above, and the inner product on \( \Theta_N \) has been modified as set out in Eq. (41).

The relation between surrogate and true mean integrated square error for the formulation of the PET problem studied here is discussed in detail in Section 2 of Johnstone and Silverman (1990). It is shown there that the condition (11) for the ratio of the two errors to be uniformly bounded
above and below on $\mathcal{F}_0$ is satisfied provided $C < 2^{a - \frac{1}{2}}$, in our notation; this condition also ensures that $\mathcal{F}_0$ consists solely of positive functions.

The first step in our detailed calculations is to identify the set of low-frequency indices. Consider $\nu$ for which $\nu \neq (0,0)$, so that $\gamma_\nu \neq 0$. From the definitions we have

$$h^2\gamma^2_\nu = \frac{16N^4 \sin^2\{(2j + 1)\pi/2N\} \sin^2\{(2k + 1)\pi/2N\}}{\pi^4 (j + k + 1)(2j + 1)(2k + 1)^2}.$$ (51)

It is easy to check from the derivation of the equivalence classes that the numerator of (51) is invariant within each equivalence class, while the inequalities (44) show that replacing $j$ by $j_0$ and $k$ by $k_0$ can only decrease the denominator of (51). Hence the set $\mathcal{L}_N^0$ is precisely $\mathcal{N}_{N-1}(0,0)$.

The smoothness classes we consider are defined, as in Johnstone and Silverman (1990), by setting

$$a_{jk} = (j + 1)^a (k + 1)^a \quad \text{for } (j, k) \in \mathcal{N},$$

for some $a > \frac{1}{2}$. It is shown in Proposition 2.2 and the Appendix of Johnstone and Silverman (1990) that the classes will then consist of functions whose $2a$th derivatives satisfy a weighted square-integrability condition.

We now consider the bound on the high-frequency error. Take any $\nu = (j_0, k_0)$ in $\mathcal{L}_N^0$. Set $\zeta = \zeta(2a) = \sum_{n=1}^{\infty} n^{-2a}$, and define the function $a(j) = (j + 1)^{2a}$. Assume without loss of generality that $k_1 \geq j_1$, so that $k_1 \geq \frac{1}{2} N - 1$ and $1 + k - N + k_1 N \geq \frac{1}{2} k N$ for all $k \geq 1$. We now have

$$S_N(\nu) = \sum_{j,k=0}^{\infty} a(j_0 + jN) a(k_0 + kN)$$

$$+ \sum_{j,k=0}^{\infty} a(j_1 + jN) a(k_1 + kN) - a(j_0) a(k_0)$$

$$= \sum_{j,k=1}^{\infty} a(j_0 + jN) a(k_0 + kN) + \sum_{j,k=1}^{\infty} a(j_1 + jN) a(k_1 - N + kN)$$

$$+ a(k_0) \sum_{j=1}^{\infty} a(j_0 + jN) + a(j_0) \sum_{k=1}^{\infty} a(k_0 + kN)$$

$$+ a(j_1) \sum_{k=1}^{\infty} a(k_1 - N + kN)$$
\[ 5 \cdot (jN)^{-2a} + (jN)^{-2a} \left( \frac{kN}{2} \right)^{-2a} \]

\[ + \sum_{j=1}^{\infty} (jN)^{-2a} + \sum_{k=1}^{\infty} \left\{ (kN)^{-2a} + \left( \frac{kN}{2} \right)^{-2a} \right\} \]

\[ = (1 + 2^{2a}) \xi^2 N^{-4a} + (2 + 2^{2a}) \xi N^{-2a} = O(N^{-2a}). \]

Thus we have

\[ \sup_{v \in \mathcal{V}} S_N(v) = O(N^{-2a}). \]

To obtain the other term in the definition of \( e(N) \), note that if \( v \in \mathcal{L}_N \) then \( j + k \geq N - 1 \) and so \( (j + 1)(k + 1) \geq N \). Therefore \( a_v^{-2} \leq N^{-2a} \). Putting this together with the above bound for \( S_N(v) \) shows that \( e(N) = O(N^{-2a}) \).

We now consider the low-frequency minimax risk \( I_N(f, \mathfrak{F}_k) \). There are two distinct cases, depending on the asymptotic behavior of the discretization index.

6.4.1 The subcritical case. Assume in this subsection that \( n = o(N^{2a+2}) \), so that \( N^{-2a} = o(n^{-a(a+1)}) \) and the high-frequency error \( e(N) \) will satisfy \( e(N) = o(n^{-a(a+1)}) \).

By reference to the discussion following (4.18) of Johnstone and Silverman (1990), define \( M \) by

\[ M^{2a+2} = 6\pi^{-2}a^{-1}(a + 1)(a + 2)C^2n \]

so that \( M = o(N) \) as \( n \to \infty \). Define \( a_M = M^{-2a} \) and let \( \Sigma_{(M)} \) denote a sum over the set \( \mathcal{C}_M = \{(j, k): 1 < (j + 1)(k + 1) \leq M\} = \{(j, k): jk \neq 0 \text{ and } \alpha_{jk} \leq 1\} \). Since \( M = o(N) \), it follows that \( \mathcal{C}_M \subset \mathcal{K}_{N-1} \) for all sufficiently large \( n \), and that \( \gamma_{jk} \to 1 \) uniformly over \( \mathcal{C}_M \) as \( n \to \infty \).

Turning to Lemma 1, we now have

\[ n^{-1} \sum_{v \in \mathcal{V}_N} b_v^{-2} \gamma_v^{-2} a_v^2 (a_M^{-1/2} a_v^{-1} - 1) = n^{-1} \sum_{(M)} b_{jk}^{-2} \gamma_{jk}^{-2} a_{jk}^2 (a_M^{-1/2} a_{jk}^{-1} - 1) \]

\[ \approx n^{-1} \sum_{(M)} b_{jk}^{-2} a_{jk}^2 (a_M^{-1/2} a_{jk}^{-1} - 1) \approx C^2 \]

by (4.18) of Johnstone and Silverman (1990), so that \( a_M \) is asymptotically the required solution of (13). Substituting back into (12), and using the proof of Theorem 3.2 of Johnstone and Silverman (1990) to approximate the sum, now gives
Since we have already shown that $\varepsilon(N)$ is of smaller order, the unrestricted minimax risk $\mathcal{M}(\mathcal{F}_N, \mathcal{F}_0)$ will also satisfy (52) with the same constant of proportionality. Theorem 3.2 of Johnstone and Silverman (1990) shows that this is also true for the minimax risk where the undiscretized data are available. Thus, just as in the subcritical cases considered previously, the discretization has no first-order large sample effect.

6.4.2 The critical case. Now suppose that $n = cN^{2a+2}$ for some constant $c$, so that $\varepsilon(N)$ is exactly of order $n^{-a(a+1)}$. Using the same notation for summations as in Subsection 6.4.1 above, we define a function $J_a(u)$ for $0 < u < 1$ by

$$J_a(u) = \lim_{N \to \infty} N^{-2a-2} \sum_{n(N)} b_{jk}^2 \gamma_{jk}^{-2} (uN)^a - a_{jk}. \quad (53)$$

By an extension of the technique used in (4.16) of Johnstone and Silverman (1990), it can be shown that the limit exists (uniformly on closed subintervals of $u$ in $(0, 1)$) and that

$$J_a(u) = 2a^a \sum_{k=1}^\infty k^a \int_0^{u/k} x^{a+1} dx \frac{x}{\sin^2 \pi x} - 2a^a \sum_{k=1}^\infty k^{2a} \int_0^{u/k} x^{2a+1} dx \frac{x}{\sin^2 \pi x}; \quad (54)$$

the details are omitted. It is clear from (53) that $J_a(u)$ is a strictly increasing function of $u$. To investigate the behavior of $J_a(u)$ as $u \to 1$, note that the total contribution to the sums in (54) from the terms with $k \geq 2$ is bounded as $u \to 1$. So, restricting attention to the terms with $k = 1$, we have

$$J_a(u) = 2a^a \int_0^{u} x^{a+1} \frac{x^a - x^a}{\sin^2 \pi x} dx + O(1)$$

$$= -2a \log(1 - u) + O(1) \quad \text{as } u \to 1,$$

by elementary analysis, and so $J_a$ maps $(0, 1)$ to $(0, \infty)$.

Now define $U$ so that $J_a(U) = cC^2$. It follows straightforwardly from the definition of $J_a$ that (13) is asymptotically satisfied with $\alpha^{-1} = (UN)^{2a}$. Hence, by a limiting argument similar to that used to obtain (54),

$$\mathcal{M}(\mathcal{F}_N, \mathcal{F}_0) = 2n^{-2} \sum_{k=1}^\infty \int_0^{U/k} x(1 - U^{-a}k^a x^a) dx \frac{x}{\sin^2 \pi x} \sim n^{-a(a+1)}. $$
This term has the same order of magnitude as $\epsilon(N)$ and so the general conclusions for the critical regime in the previous cases still hold: although the discretization does not affect the order of magnitude of $M(\mathcal{T}_N, \mathcal{F}_0)$, it is felt in two separate ways, both by inflating the constant of proportionality for the low-frequency minimax risk, and also by yielding a nonnegligible bound $\epsilon(N)$ on the high-frequency contribution.

There are interesting differences between the PET example and the other examples considered in this paper. In the PET case, the critical case no longer divides into two separate cases according to the value of $c$, but the same form of calculation works for all values of $c$. In the other examples, for $c$ greater than some threshold value the minimax estimator $T^*$ has no zeros on its diagonal so that all the coefficients $\tilde{z}_{i1}$ contribute to the minimax estimate. In the PET example this is far from true. Of the $\frac{1}{2}N(N - 1)$ coefficients indexed by $\mathcal{N}_{N-1}$, only those with $(j + 1)(k + 1) < N$ can ever contribute to the minimax estimate; the number of these is asymptotically $N \log N$ and so in a certain sense the minimax estimate makes use of a vanishingly small proportion of the information available, no matter how large the value of $c$. This fascinating phenomenon is an obvious topic for further investigation.

REFERENCES


