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6 AUTOMATIC SMOOTHING OF THE LOG PERIODOGRAM

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Abstract

We consider an estimate of the log spectral density based on smoothing the log periodogram with a smoothing spline. This estimate is also a windowed estimate. We show that an unbiased estimate $\hat{R}(\lambda)$ of the expected integrated mean square error can be obtained as a function of the smoothing, or "bandwidth" parameter λ. The smoothing parameter is then chosen as that λ which minimizes $\hat{R}(\lambda)$. The degree of the smoothing spline (equivalently, the "shape" parameter of the window) can also be chosen this way. Results of some Monte Carlo experiments illustrating the effectiveness of the method are given.

Key words: log spectral density estimate, optimal choice of bandwidth parameter, spline spectral density estimate

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1. Introduction

In this note we report a simple and completely objective method for determining the appropriate amount of smoothing when smoothing the log periodogram for the purpose of estimating the log spectral density. Our estimate of the log spectral density is a smoothing spline fitted to the log periodogram. Smoothing splines for this purpose were suggested by Cogburn and Davis (1974) in the context of smoothing the periodogram. The resulting estimate is also a windowed estimate (see Parzen (1961)), and choosing the degree of smoothing is equivalent to choosing the "bandwidth" parameter, or window width. Engineers and scientists have been routinely computing windowed spectral density estimates for at least twenty years. For some applications see Bath (1974), Blackman and Tukey (1958). Early theoretical work concentrated on obtaining "windows" with good "shape" properties (see Blackman and Tukey (1958)), but it is now part of the folklore that the choice of window width is more important than the exact window shape. However, for at least twenty years it appears that a completely objective method for choosing window width has eluded researchers. An examination of popular books from 1958 to 1978 discussing the subject of spectral density estimation via smoothing the log periodogram or periodogram (Blackman and Tukey (1958), Bloomfield (1976), Brillinger (1974), Jenkins and Watts (1968), Koopmans (1974), Robinson and Silvia (1978), see also Anderson (1977)) reveal only subjective methods, which basically involve trying different values of the bandwidth parameter until one finds a value that results in a (subjectively) satisfactory estimate.

In this note we make the very simple observation: For the smoothing spline log spectral density estimate, an essentially unbiased estimate $\hat{R}(\lambda)$ of the expected integrated mean square error $ER(\lambda)$ can be written down, as a function of the smoothing or bandwidth parameter, λ. The bandwidth parameter is then choosen by finding the minimizer of $\hat{R}(\lambda)$. In Section 2 we present the details of this argument, and in Section 3 we present the results of some numerical experiments, which demonstrate how well the method works on some synthetic data where the true spectral density is known. In Section 4 we collect some miscellaneous remarks concerning the relation of the present method to cross-validation, to ridge estimates and Mallows C_L, and to autoregressive spectral estimates.

2. Optimally smoothed spline (OSS) log spectral density estimates.

Let $X(t)$, $t = \ldots -1,0,1,\ldots$ be a zero mean stationary Gaussian time series with (theoretical) covariance

$$r(\tau) = EX(s)X(s+\tau), \qquad \tau = \ldots -1,0,1,\ldots$$

independent of s. The spectral density function $f(\omega)$ of this process is

$$f(\omega) = \sum_{\tau=-\infty}^{\infty} r(\tau)e^{2\pi i\omega\tau}, \qquad -1/2\leq\omega\leq 1/2.$$

It is desired to estimate $g(\omega) \equiv \log f(\omega)$ from a record $X(1),X(2),\ldots,X(2N)$ of the process.

Define the periodogram

$$I(\omega) = \frac{1}{2N}\left|\sum_{\tau=1}^{2N} X(\tau)e^{2\pi i\omega\tau}\right|^2, \qquad -1/2\leq\omega\leq 1/2$$

and let $I_j = I(j/2N)$. Then $I_j = I_{-j}$, and, to a good approximation $I_j = f(j/2N)U_j$, where the U_j, $j = 1,2,\ldots,N-1$ are independently distributed as 1/2 times a chi-squared random variable, with two degrees of freedom, and U_0 and U_N are distributed as chi-squared with one degree of freedom. See Walker (1965). Thus, while I_j is approximately an unbiased estimate for $f(j/2N)$, its variance is a constant independent of N, and a plot of $I(\omega)$ or $\log I(\omega)$ will be uselessly wiggly. (See Section 3 for some plots of $\log I(\omega)$). We propose here a technique for smoothing the log periodogram to obtain an estimate of the log spectral density, where the optimum degree of smoothing to minimize expected mean square error can be estimated from the data.

Let $Y_j = \log I_j + C_j$, where $C_j = \gamma$, the Euler Mascheroni constant, $\gamma = .57721$ for $j = \pm 1, 2, \ldots, N-1$, and $C_0 = C_N = (\ln 2+\gamma)/\pi$. Then $Y_j = g(j/2N)+\epsilon_j$, $j = -(N-1),\ldots,N$, and $\epsilon_j = \log U_j + C_j$. Using Bateman (1954), vol.1, Sect.4.6, and the density of a chi-squared random variable, it can be shown that $E\epsilon_j = 0$, $j = -(N-1),\ldots,N$, $E\epsilon_j^2 = \pi^2/6$, $j = \pm 1, \pm 2, \ldots, \pm N-1$. See also Davis and Jones (1968).

The estimate $\hat{g}(\omega)$ for $g(\omega)$ that we use is

$$\hat{g}(\omega) \equiv \hat{g}_{N,m,\lambda}(\omega) = \sum_{\nu=-(N-1)}^{N} e^{2\pi i\nu\omega} \frac{\tilde{g}_\nu}{(1+\lambda(2\pi\nu)^{2m})}$$

where

$$\tilde{g}_\nu = \frac{1}{2N}\sum_{k=-(N-1)}^{N} e^{-2\pi i\nu k/2N}\, Y_k$$

and λ and possibly m are to be chosen. We make a few remarks concerning this estimate.

The $\tilde{g}_\nu$ are estimates of the fourier coefficients g_ν of $g(\omega)$

$$g(\omega) \sim \sum_{-\infty}^{\infty} e^{2\pi i\nu\omega}\, g_\nu ,$$

and it is implicitly being assumed that $g^{(m)}(\omega) \in L_2$, equivalently

$$\sum_{\nu=-\infty}^{\infty} (2\pi\nu)^{2m}\, |g_\nu|^2 < \infty . \tag{2.1}$$

The estimate $\hat{g}_{N,m,\lambda}$ is obtained by taking the sample fourier coefficients of the log periodogram (i.e. the "cepstrum" of Tukey (1962)), and damping the coefficient at frequency ν by the "filter function" $\phi(\nu) = 1/(1+\lambda(2\pi\nu)^{2m})$. Figure 2.1 shows $\phi(\cdot)$ for $m = 2$, $\lambda = 10^{-7}$ and 10^{-5}, and $m = 4$, $\lambda = 10^{-14}$ and 10^{-10}. It can be seen that λ controls the width of the filter, while m controls the steepness of the roll-off. This filter function for the OSS is the classical Butterworth filter.

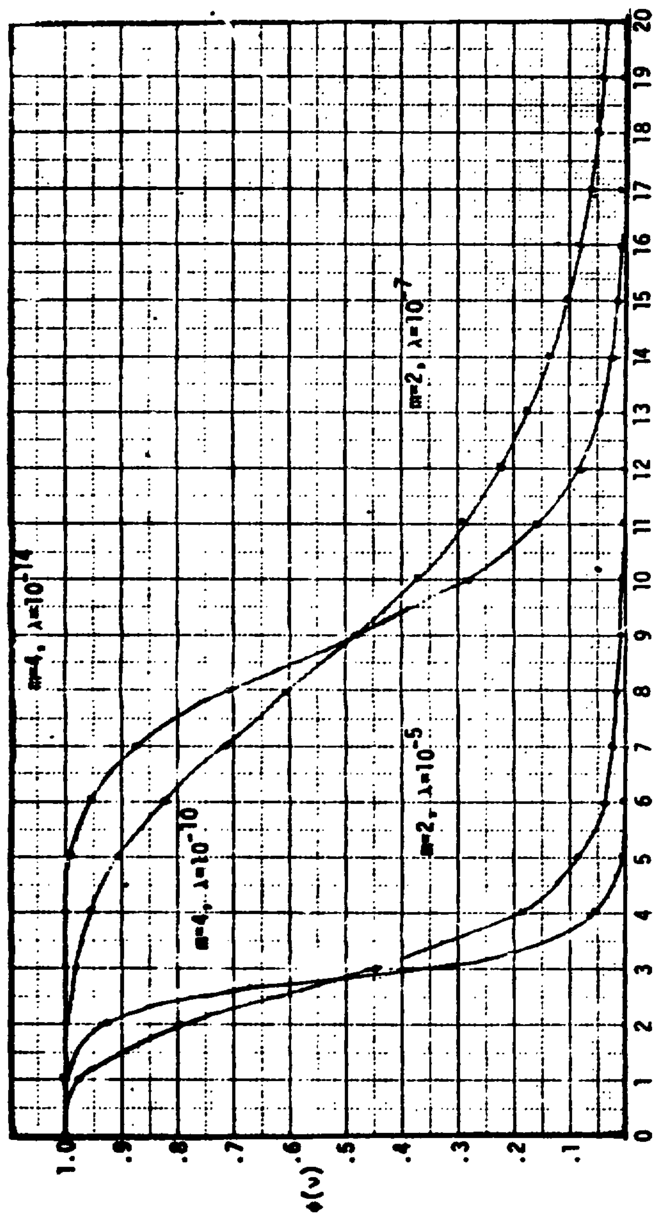
The estimate is a windowed estimate in the sense that

$$\hat{g}_{N,m,\lambda}(\omega) = \frac{1}{2N}\sum_{k=-(N-1)}^{N} Y_k\, W_{m,\lambda}(\omega - k/2N) ,$$

where the window $W_{m,\lambda}$ is given by

$$W_{m,\lambda}(\omega) = \sum_{\nu=-(N-1)}^{N} \frac{e^{2\pi i\nu\omega}}{1+\lambda(2\pi\nu)^{2m}} .$$

It is also the lattice smoothing spline of Cogburn and Davis (1974) and is, to a good approximation, the solution to the minimization problem: Find g in the reproducing kernel Hilbert space of



The filter function $\phi(\nu) = 1/(1+\lambda(2\pi\nu)^{2m})$.

Figure 2.1

functions $\{g: g, g, \ldots, g^{(m-1)}$ abs. cont., $g^{(\nu)}(-1/2) = g^{(\nu)}(1/2)$, $\nu = 0,1,\ldots,m-1$, $g^{(m)} \in L_2\}$ to minimize

$$\frac{1}{2N}\sum_{j=-N-1}^{N}(g(\tfrac{j}{2N})-Y_j)^2 + \lambda\int_{-1/2}^{1/2}(g^{(m)}(\omega))^2\,d\omega\ . \tag{2.2}$$

Define the integrated mean square error $R_N(\lambda,m)$ by

$$R_N(\lambda,m) = \int_{-1/2}^{1/2}[\hat{g}_{N,m,\lambda}(\omega)-g(\omega)]^2\,d\omega\ .$$

By Parseval's Theorem, we have

$$R_N(\lambda,m) = \sum_{\nu=-(N-1)}^{N}\left|g_\nu - \frac{\tilde{g}_\nu}{1+\lambda(2\pi\nu)^{2m}}\right|^2 + \sum_{\substack{\nu>N\\ \nu<-(N-1)}}|g_\nu|^2\ .$$

Assuming (2.1) is true, the second term can easily be shown to be negligible compared with the first, and we shall henceforth ignore it.

Now

$$E\,\tilde{g}_\nu = \frac{1}{2N}\sum_{k=-(N-1)}^{N}e^{-2\pi i\nu k/2N}g(k/2N)$$

$$= g_\nu$$

$$E|\tilde{g}_\nu|^2 = |g_\nu|^2 + \frac{1}{2N}\frac{\pi^2}{6} \tag{2.3}$$

and so

$$ER_N(\lambda,m) \approx \sum_{\nu=-(N-1)}^{N}|g_\nu|^2\left(1-\frac{1}{1+\lambda(2\pi\nu)^{2m}}\right)^2 + \frac{1}{2N}\left(\frac{\pi^2}{6}\right)\sum_{\nu=-(N-1)}^{N}\frac{1}{(1+\lambda(2\pi\nu)^{2m})^2}\ . \tag{2.4}$$

where $\approx$ means we are ignoring the fact that $E\epsilon_0^2 = E\epsilon_N^2 + \frac{\pi^2}{6}$, and neglecting terms of order

$$\sum_{|\nu|\geq N} |g_\nu|^2 . \qquad (2.5)$$

The main theoretical result of this paper is the following trivial but useful

Proposition:

Ignoring a factor $(1+o(1))$, an unbiased estimate of $ER_N(\lambda,m)$, is given by $\hat{R}_N(\lambda,m)$ defined by

$$\hat{R}_N(\lambda,m) = \sum_{\nu=-(N-1)}^{N} \left(|\hat{g}_\nu|^2 - \frac{1}{2N}\frac{\pi^2}{6}\right)\left(1 - \frac{1}{1+\lambda\,(2\pi\nu)^{2m}}\right)^2$$

$$+ \frac{1}{2N}\left(\frac{\pi^2}{6}\right) \sum_{\nu=-(N-1)}^{N} \frac{1}{(1+\lambda(2\pi\nu)^{2m})^2} . \qquad (2.6)$$

Proof:

Using (2.3) the proof is immediate.

We remark that it is clear that the same argument can be carried out for any estimate of the form

$$\hat{g}_\theta(\omega) = \sum_{\nu=-(N-1)}^{N} e^{2\pi i\nu\omega}\phi_\theta(\nu)\hat{g}_\nu ,$$

where $\phi_\theta(\cdot)$ is any filter function depending on a (low-dimentional) parameter vector θ. We believe that one bandwidth and one shape parameter are sufficient for practical purposes. Estimates based on filter functions of the form $\phi_\theta(\nu) = 1/(1+|\sum_{j=0}^{p}\alpha_j\nu^j|^2/|\sum_{k=0}^{q}\beta_k\nu^k|^2)$, $\nu \geq 0$, $\phi_\theta(\nu) = \phi_\theta(-\nu)$ will have the same large sample properties as those based on $\phi(\nu) = 1/(1+\lambda(2\pi\nu)^{2m})$, with $m = p-q$ and $\lambda = (2\pi)^{-2m}\alpha_p/\beta_q$. A Bayesian argument supporting the adequacy of this two parameter family of filter functions can be found in Wahba (1978).

3. Monte Carlo Experiments

A computer program was written to simulate autoregressive moving average time series according to a known spectral density, as follows. Let

$$X(t) = -\sum_{j=1}^{p} a_j X(t-j) + \sum_{k=0}^{q} b_j\epsilon(t-j) , \quad b_0 = 1 \qquad (3.1)$$

where the $\epsilon(j)$ are $N(0,1)$, and the $\{a_j\}$ and $\{b_j\}$ are given. Then

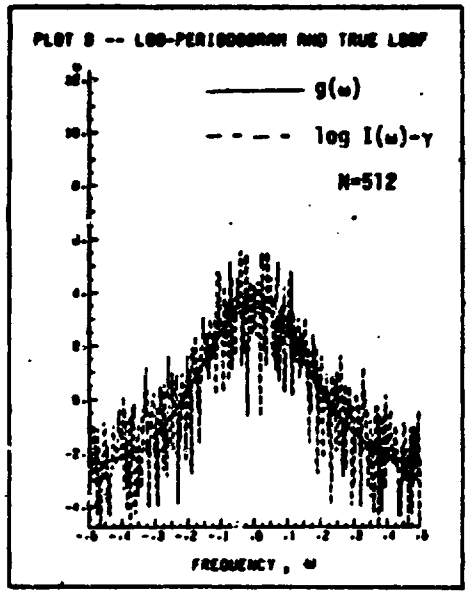
$$f(\omega) = |\sum_{k=0}^{q} b_j e^{2\pi i\omega k}|^2/|\sum_{j=0}^{p} a_j e^{2\pi i\omega j}|^2, \quad a_0 = 1.$$

Synthetic time series were generated by letting the ϵ's be pseudorandom normal numbers, using 0 for the p initial values of X(t), and computing X(t) as in (3.1). The first 10p values of X were then discarded so as to lessen the effects of the initial conditions.

The first example is an AR3 model, that is $p = 3$, $q = 0$, with $a_1 = -1.4256$, $a_2 = .7344$ and $a_3 = -0.1296$.

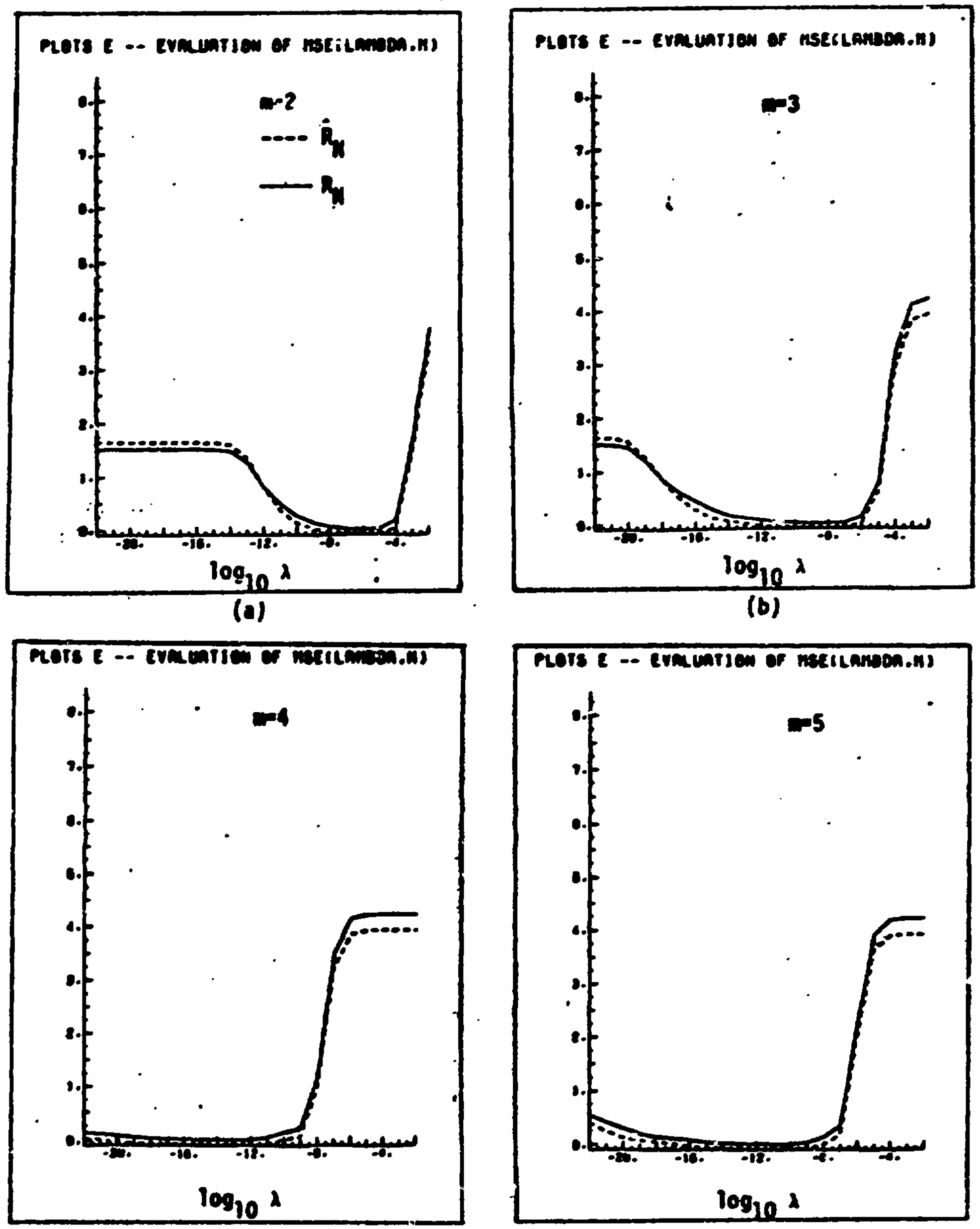
The wiggly line in Figure 3.1 is the scaled log periodogram (that is, γ has been subtracted), and the smooth curve is the true log spectral density, g. The sample size $N = 512$. The dashed lines in Figures 3.2(a), (b), (c), (d), are plots of $\hat{R}_N(\lambda,m)$ as a function of λ for $m = 2,3,4$, and 5. The solid lines in Figures 3.2(a), (b), (c), (d) are the observed integrated mean square error $R_N(\lambda,m)$, computed as

$$R_N(\lambda,m) = \frac{1}{2N}\sum_{j=-(N-1)}^{N}[\hat{g}_{N,m,\lambda}(j/2N)-g(j/2N)]^2 ,$$



Scaled log periodogram, log $I(\omega)-\gamma$, and true log spectral density, $g(\omega)$. AR3 model, N=512.

Figure 3.1



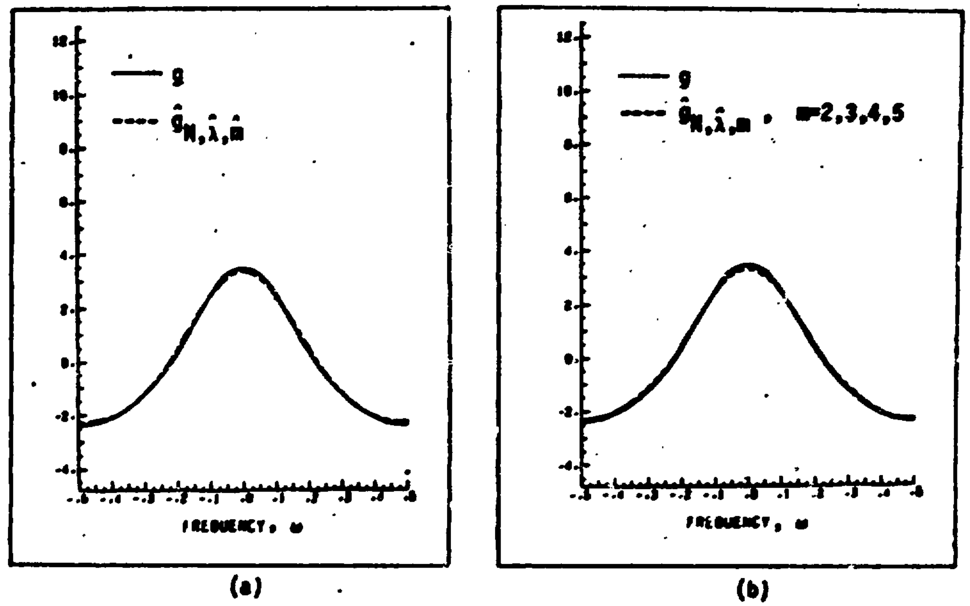
R_N and $\hat{R}_N$ for m = 2,3,4,5. AR3 model, N=512.

Figure 3.2

for $m = 2,3,4$ and 5. Note that $\hat{R}_N$ may be negative but that $\hat{R}_N$ tracks R_N in the neighborhood of the minimum. The minimum was achieved for $m = 4$, $\lambda = 10^{-14}$. The filter function $\phi(\nu)$ for $m = 4$, $\lambda = 10^{-14}$ is shown in Figure 2.1. Figure 3.3a gives $g(\omega)$ and $\hat{g}_{N,\hat{\lambda},\hat{m}}$, where $\hat{\lambda}$ and $\hat{m}$ are the minimizing values of $\hat{R}_N(\lambda,m)$, (among those values tried.) Figure 3.3b gives, for comparison, g and $\hat{g}_{N,\hat{\lambda},m}$, for $m = 2,3,4,5$. In this example it can be seen that the results are essentially the same for all four values of m tried.

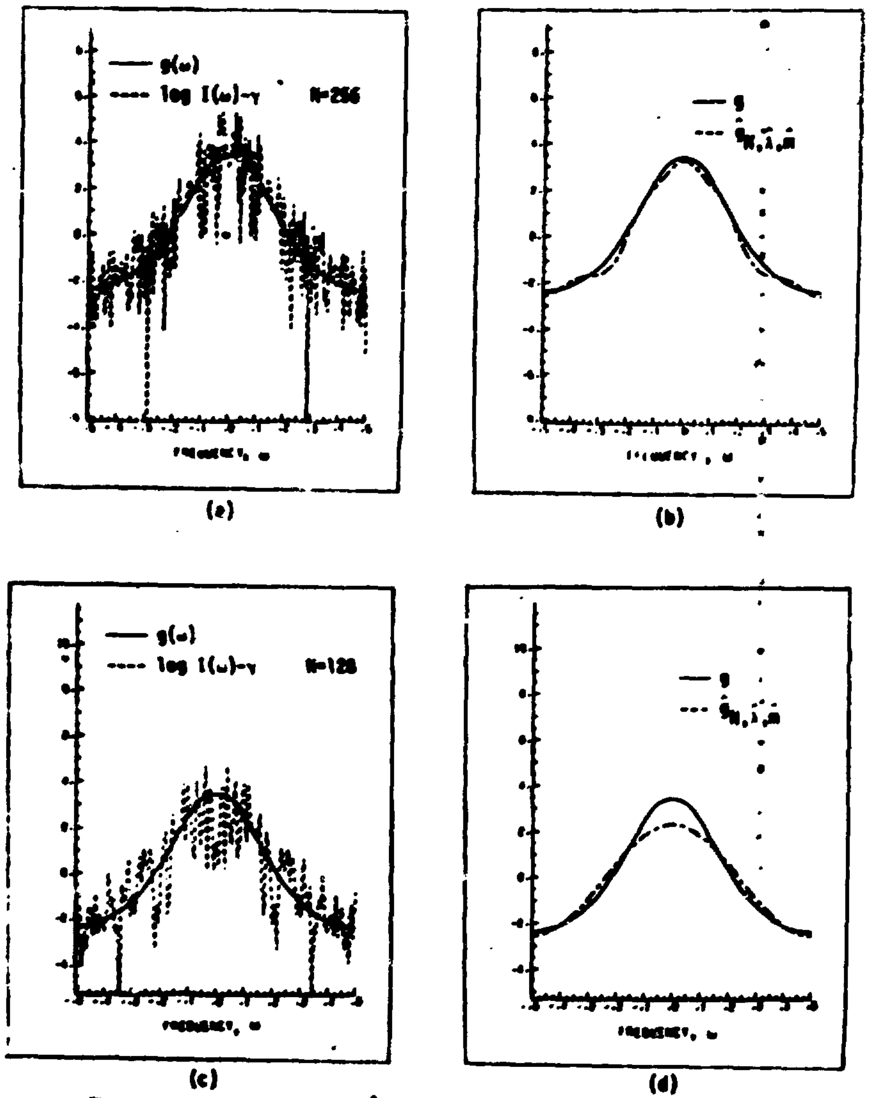
For smaller sample sizes, the results, as to be expected, are not as good. Figure 3.4 gives the figures corresponding to 3.1 and 3.3a for $N = 256$ and 128, respectively. For $N = 128$, $\hat{\lambda} = 10^{-10}$, $\hat{m} = 4$, and the corresponding filter function is also shown in Figure 2.1. Note that the "half power point" of this filter is between $\nu = 2$ and $\nu = 3$, so that the estimate $\hat{g}_{N,\hat{\lambda},\hat{m}}$ is essentially a linear combination of the first 3 or 4 complex exponentials.

Figure 3.5(a), (b), (c) and (d) give the figures corresponding to Figures 3.1 and 3.3(a) for an MA4 model with $N = 512$ and $N = 256$. Here $p = 0$, $q = 4$, and the coefficients are $b_1 = -.3$, $b_2 = -.6$, $b_3 = -.3$ and $b_4 = .6$. Figures 3.6(a) and (b) give the figures corresponding to Figures 3.1 and 3.3(a) for the same MA4 model with $N = 128$. In this example $\hat{R}_N$ with $m = 2$ had the smallest minimum. Figure 3.7(a) gives R_N and $\hat{R}_N$ for $m = 2$ and Figure 3.7(b) gives $\hat{g}_{N,\hat{\lambda},m}$ for $m = 2,3,4,5$. It can be seen that there is a slight difference in the estimates for different m. Figure 3.8(a), (b), (c) and (d) give the figures corresponding to Figures 3.1 and 3.3(a) for an AR12 model, with $a_1 = a_2 = a_3 = a_5 = a_6 = a_7 = a_9 = a_{10} = a_{11} = 0$



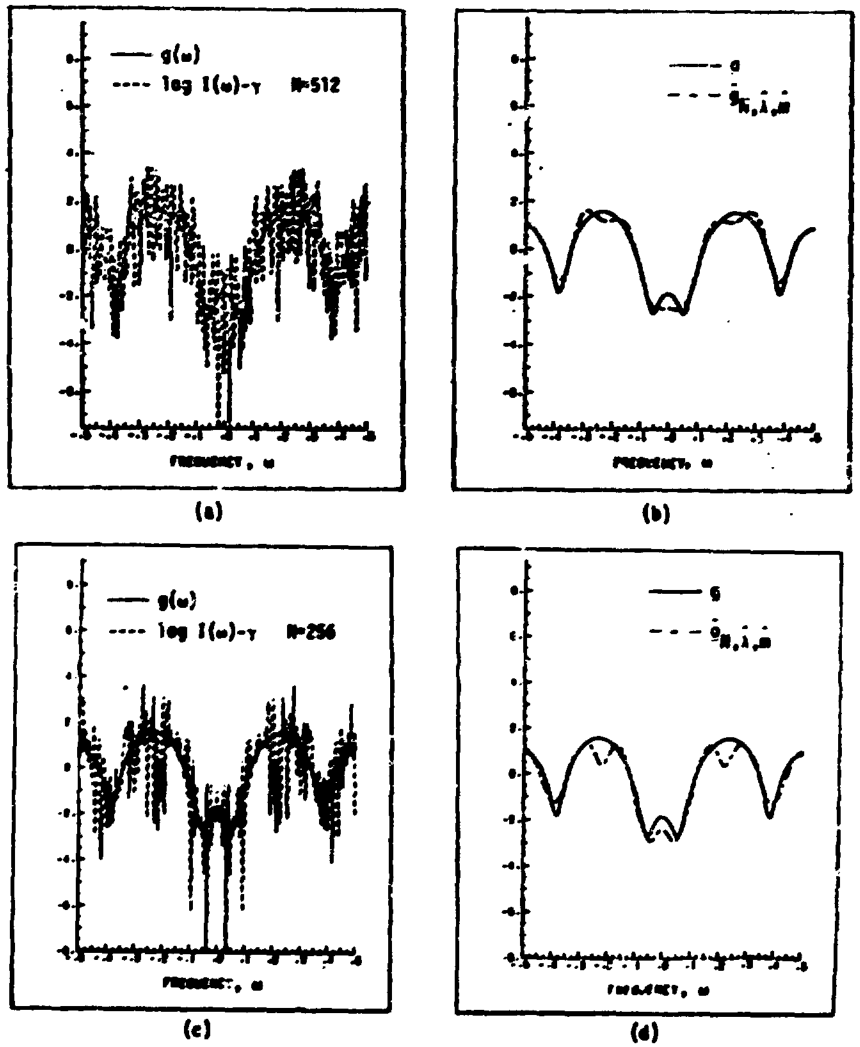
g and $\hat{g}_{N,\hat{\lambda},m}$ for (a) $m=\hat{m}$, (b) $m=2,3,4,5$. AR3 model, N=512.

Figure 3.3



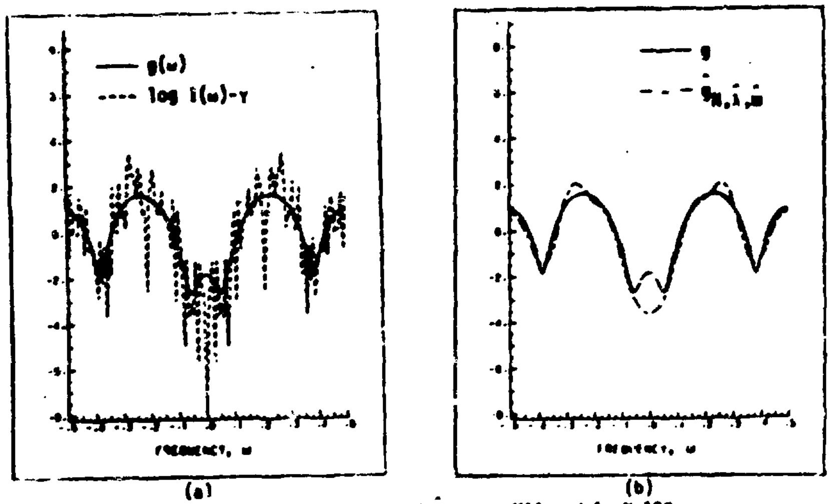
The log periodogram, g, and $\hat{g}_{N,\hat{\lambda},\hat{m}}$ for AR3 model, N=256 and 128.

Figure 3.4



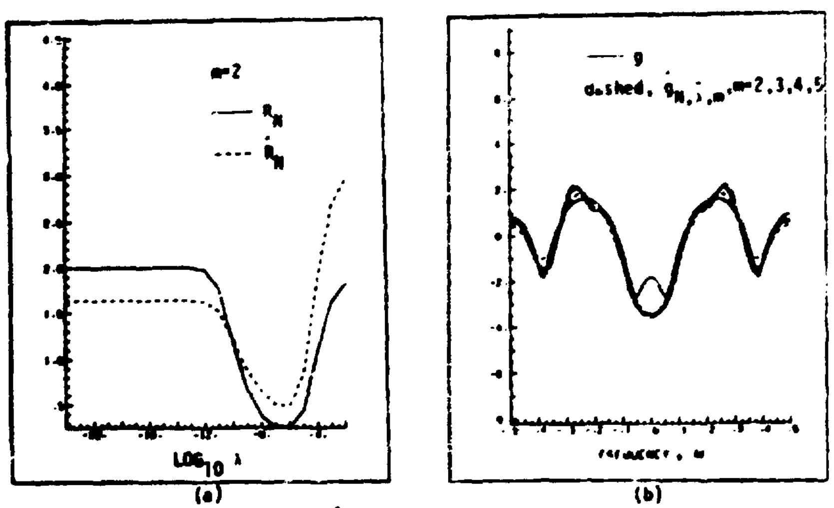
The periodogram, g and $\hat{g}_{N,\hat{\lambda},\hat{m}}$, MA4 model, N=512 and N=256.

Figure 3.5



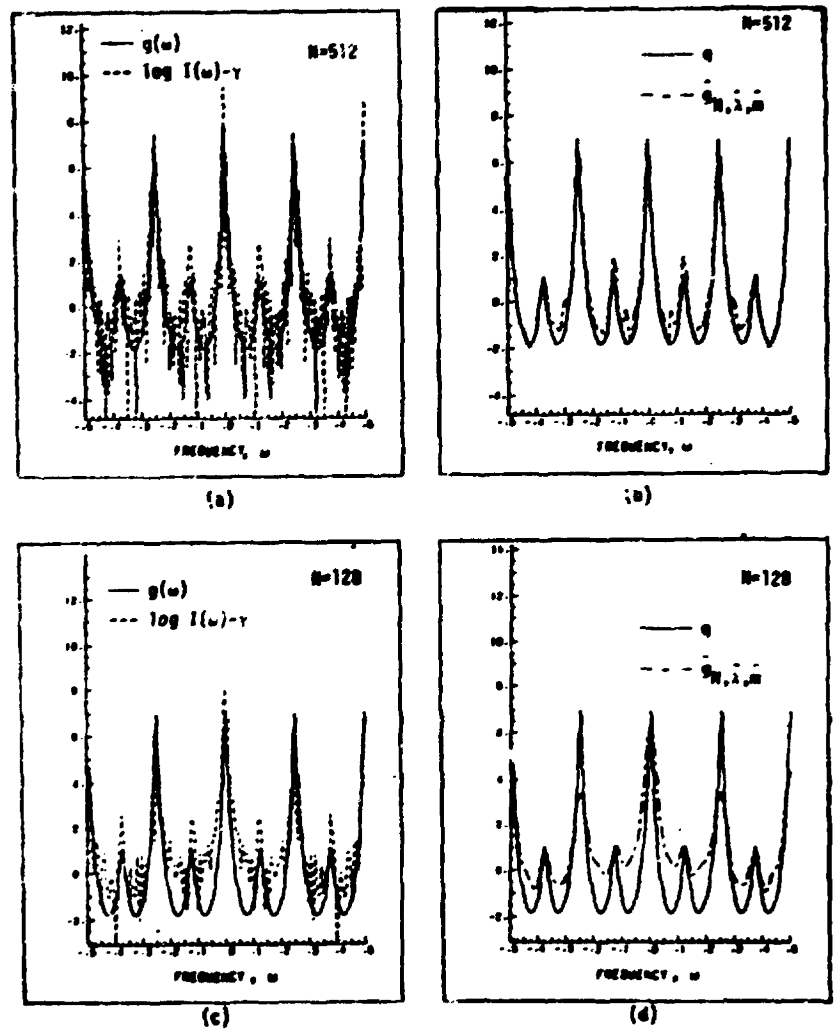
The periodogram, g and $\hat{g}_{N,\hat{\lambda},\hat{m}}$, MA4 model, N=128

Figure 3.6



R_N, $\hat{R}_N$, and g and $\hat{g}_{N,\hat{\lambda},\hat{m}}$ for m=2,3,4,5. MA4 model, N=128

Figure 3.7



g and $\hat{g}_{N,\hat{\lambda},\hat{m}}$, AR12 model, N=512 and N=128

Figure 3.8

$a_4 = -.9,\ a_8 = -.7,\ a_{12} = +.63.$

It can be seen that the minimizer of $\hat{R}_N$ is a good estimate of the minimizer of R_N and that for large sample sizes very good estimates of the log spectral density obtain. Minimizing in m as well as λ can improve the estimate (over using $m=2$, say), but, at least in these examples the effect is not large. The two leftmost filter function "curves" in Figure 2.1 are typical of those obtaining in these examples for $N=128$ whereas the two on the right are typical of our examples for $N=512$. For the larger sample size then the log spectral density estimate is a linear combination (roughly) of the first 10-20 complex exponentials) where for the smaller sample size the estimate is a linear combination of only, say the first 3-7 complex exponentials. Thus, one cannot expect to recover detailed structure of the log spectral density with a small sample size. However good large sample estimates can be obtained completely automatically.

4. Miscellaneous Remarks

In Wahba and Wold (1975), we suggested the use of cross validation for choosing the smoothing parameter in the smoothing spline log spectral density estimate, and showed that that method would, asymptotically, estimate the minimizer of the expected integrated mean square error $ER(\lambda)$. We believe (without having carried out numerical tests) that the present method is better, but probably not by very much. Basically in the present context, the cross validation function $V(\lambda)$ which is minimized in Wahba and

Wold satisfies $EV(\lambda)+\text{constant} = ER(\lambda)(1+o(1))$ where the $o(1)$ may tend to zero somewhat slower than N. (See also Craven and Wahba (1977).) Here $E\hat{R}(\lambda) = ER(\lambda)(1+o(1))$ where the $o(1)$ is very much smaller and due essentially only to aliasing.

We note that the minimization problem (2.2) to which the smoothing spline is the solution is formally similar to the minimization problem in Euclidean p-space which is solved by a ridge regression estimate. To see this consider the standard regression problem

$$y = X\beta + \epsilon\ , \qquad \epsilon \sim N(0,\sigma^2 I)$$

and the ridge estimate $\hat{\beta}_\lambda = (X^T X + n\lambda I)^{-1} X^T y$. $\hat{\beta}_\lambda$ is the solution to: Find $\beta \in E_p$ to minimize $\frac{1}{N}||y-X\beta||_N^2 + \lambda||\beta||_p^2$, where $||\cdot||_N$ and $||\cdot||_p$ are norms in Euclidean N and p space respectively, and this expression is to be compared with (2.2). Similarly, it can be seen that our estimate of the optimal smoothing parameter bears a similarity to Mallows (1973) C_L method for choosing the ridge parameter in a ridge regression estimate, see also Hudson (1974). The reader interested in pursuing the relationship between smoothing splines and ridge estimates can consult Wahba (1977) where the ridge regression geometry and smoothing spline geometry is discussed in parallel. Similarly, as ridge estimates are Bayes estimates, the same can be shown (roughly) for the smoothing splines, here. We omit the details, but the argument is carried out for certain analogous smoothed orthogonal series density estimates in Wahba (1978). Thus, the present method may be viewed as an empirical

Bayes method, while it is simultaneously in the tradition of non-parametric spectral density estimation. Within the past few years it has been suggested that the spectral density be estimated by fitting a low order autoregressive scheme to the time series and then estimating the spectral density as the spectral density of the estimated low order schemes (see Burg (1975), Parzen (1974) and Akaike (1974)). The length of the autoregressive scheme plays the role of the smoothing parameter, and Akaike (1974) and Parzen (1974) have both given objective criteria for choosing it. This autoregressive method has, in fact, become popular in geophysical applications. See Landers and Lacosse (1977), Griffiths and Prieto-Diaz (1977). We do not know how the two methods (OSS vs. autoregressive spectral estimation) compare in general. We conjecture that the answer will very much depend on what the true spectral density is as well as on the sample size. Our own very preliminary experimentation, which is presently restricted to simulated low order autoregressive moving average models, seems to suggest this.

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log spectral density estimate, optimal choice of bandwidth parameter, spline spectral density estimate

lambda

20. ABSTRACT (Continue on reverse side if necessary and identify by block number) We consider an estimate of the log spectral density based on smoothing the log periodogram with a smoothing spline. This estimate is also a windowed estimate. ~~We show that~~ an unbiased estimate $R(\lambda)$ of the expected integrated mean square error can be obtained as a function of the smoothing, or "bandwidth" parameter λ. The smoothing parameter is then chosen as that λ which minimizes $R(\lambda)$. The degree of the smoothing spline (equivalently, the "shape" parameter of the window) can also be chosen this way. Results of some Monte Carlo experiments illustrating the effectiveness of the method are given.

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