Adaptive Kernel Estimation of the Spectral Density with Boundary Kernel Analysis

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Abstract. A hybrid estimator of the log-spectral density of a stationary time series is proposed. First, a multiple taper estimate is performed, followed by kernel smoothing the log-multitaper estimate. This procedure reduces the expected mean square error by $(\frac{\pi^2}{4})^8$ over simply smoothing the log tapered periodogram. The optimal number of tapers is $O(N^{8/15})$. A data adaptive implementation of a variable bandwidth kernel smoother is given. When the spectral density is discontinuous, one sided smoothing estimates are used.

§1. Introduction

We consider a discrete, stationary, Gaussian, time series $\{x_j, j = 1, \ldots N\}$ with a piecewise smooth spectral density, $S(f)$, that is bounded away from zero. The autocovariance is the Fourier transform of the spectral density:

$$\text{Cov} [x_j, x_k] = \int_{-1/2}^{1/2} S(f)e^{2\pi i(j-k)f} df.$$ Our goal is to estimate the log spectral density: $\theta(f) \equiv \ln[S(f)]$. We consider data adaptive kernel smoother estimators which self-consistently estimate the best local halfwidth for smoothing. When the spectral density is discontinuous at a point, the kernel estimate must be one-sided. We present new “boundary” kernels for one-sided estimation.

§2. Variance of multitapering and kernel smoothing

The multiple taper estimate of the spectral density is a quadratic estimate of the form:

$$\hat{S}_{MT}(f) = \sum_{m,n=1}^{N} Q_{mn} x_m x_n e^{2i(m-n)f} = \sum_{k=1}^{K} \mu_k \left| \sum_{n=1}^{N} \nu_n^{(k)} x_n e^{-2\pi i nf} \right|^2,$$

where the $\mu_k$ and $\nu_n^{(k)}$ are $K$ eigenvalues and orthonormal eigenvectors of $Q$. In the large $N$ limit, the sinusoidal tapers are optimal: $\nu_n^{(k)} = \sqrt{\frac{2}{N+1}} \sin \left( \frac{\pi km}{N+1} \right)$ [4]. Let $\mu_k \equiv 1/K$. For these tapers, the spectral estimate (1) reduces to
\[
\hat{S}_{MT}(f) = \frac{\Delta}{K} \sum_{k=1}^{K} |y(f + k\Delta) - y(f - k\Delta)|^2 ,
\]

where \(y(f)\) is the FT of \(\{x\}\): \(y(f) = \sum_{m=1}^{N} x_m e^{-2\pi imf}\) and \(\Delta \equiv 1/(2N+2)\). The sinusoidal multitaper estimate reduces the bias since the sidelobes of \(y(f + k\Delta)\) are partially cancelled by those of \(y(f - k\Delta)\).

To leading order in \(K/N\), the local white noise approximation holds: \(\hat{S}_{MT}(f)\) has a \(\chi^2_K\) distribution. Note \(\mathbb{E} [\ln(\chi^2_K)] = \psi(K) - \ln(K)\), \(\text{Var} [\ln(\chi^2_K)] = \psi'(K)\), where \(\psi\) is the digamma function.

We now consider kernel estimators of the \(q\)th derivative, \(\partial^q f S(f)\):

\[
\partial^q_f S(f) \equiv \frac{1}{h^{q+1}} \int_{-1/2}^{1/2} \kappa \left( \frac{f' - f}{h} \right) \hat{S}_{MT}(f') df' ,
\]

where \(\kappa(f)\) is a smooth kernel with support in \([-1, 1]\), and \(\kappa(\pm 1) = 0\) and \(h\) is the bandwidth parameter. We say a kernel is of order \((q, p)\) if \(\int f^m \kappa(f) df = q! \delta_{m, q} , m = 0, \ldots, p - 1\). We denote the \(p\)th moment of a kernel of order \((q, p)\) by \(B_{q,p} \equiv \int f^p \kappa(f) df = p! B_{q,p}\). For function estimation \((q = 0)\), we use \(p = 2\) and \(p = 4\). To estimate the second derivative, we use a kernel of order \((2,4)\).

The estimator (3) is a quadratic estimator as in (1) with \(Q_{mm} = \hat{k}_{m-n} \sum_{k=1}^{K} \nu_m^{(k)} \nu_n^{(k)}\), where \(\hat{k}_m \equiv h^{-(q+1)} \int \kappa(L m) e^{imf} df'\) is the FT of the kernel. We now consider the local white noise approximation:

\[
\text{Var} [\partial^q_f S(f)] / S(f)^2 = \text{tr}[QQ] = \sum_{k,k'=-1}^{K} \sum_{n=1}^{N} \sum_{m=1}^{N-n} \hat{k}_m^2 \nu_{n+m}^{(k)} \nu_n^{(k)} \nu_{n+m}^{(k')} \nu_n^{(k')} .
\]

(4)

For \(mh \gg 1\), note that \(\hat{k}_m \sim \mathcal{O}(||\hat{\kappa}||/(mh)^2)\). Since the \(k\)-th taper has a scale length of variation of \(N/k\), \(\nu_{n+m}^{(k)} \simeq \nu_n^{(k)} [1 + \mathcal{O}(\frac{m}{N})]\). We expand (4) in \(mk/N\) for \(|mh| < \mathcal{O}((Nh/K)^{1/5})\) and drop all terms with \(|mh| > \mathcal{O}((Nh/K)^{1/4})\):

\[
\text{Var} [\partial^q_f S(f)] \simeq S(f)^2 \sum_{k,k'=1}^{K} \left( \sum_{n=1}^{N} \nu_n^{(k)} |\nu_n^{(k')}|^2 \right) \left( \sum_{m=1}^{N-n} \hat{k}_m^2 \right) .
\]

(5)

The last line is valid to \(\mathcal{O}(1/(mh)^4) + \mathcal{O}(km/N)\), yielding a final accuracy of (5) of \(\mathcal{O}((K/Nh)^4/5)\). For the sinusoidal tapers, (5) reduces to

\[
\text{Var} [\partial^q_f S(f)] \simeq \frac{||\kappa||^2 S(f)^2}{N h^{(q+1)}} \left( 1 + \frac{1}{2K} \right) + \mathcal{O}((K/Nh)^4/5) ,
\]

where \(||\kappa||^2\) is the square integral of \(\kappa\). To calculate the local bias, we Taylor expand the spectral density. Note \(\int_{-1/2}^{1/2} |f'|^2 |V^{(k)}(f')|^2 df' = k^2/(4N^2)\), where \(V^{(k)}\) is the FT of the sinusoidal \(\nu^{(k)}\).
§3. Smoothed log-multitaper estimate

We define the multitaper estimate of the logarithm of the spectral density by $\hat{\theta}_{MT}(f) \equiv \ln(\hat{S}_{MT}(f)) - [\psi(K) - \ln(K)]/K$. By averaging the $K$ estimates prior to taking the logarithm, we reduce both the bias and the variance. The variance reduction factor from using $\ln(\hat{S}(f))$, instead of $\ln(\hat{S}(f))$ is $K\psi'(K)/\psi'(1)$. For large $K$, $K\psi'(K) \approx 1 + \frac{1}{2K}$, so the variance reduction factor is asymptotically $6/\pi^2$.

We define the smoothed multitaper ln-spectral estimate: $\overline{\partial_f^q \theta}(f)$ by kernel smoothing $\hat{\theta}_{MT}(f)$ analogous to Eq. (3). To evaluate the error in $\overline{\partial_f^q \theta}(f)$, we expand $\hat{\theta}_{MT}(f')$ about $\theta(f)$:$\hat{\theta}_{MT}(f') \simeq \ln[\theta(f)] + [\hat{S}_{MT}(f) - S(f')] / S(f')$, that is valid when $K \ll N, h \ll 1$, and $Nh \gg 1$. The leading order bias is

$$\text{Bias}[\overline{\partial_f^q \theta}(f)] \approx B_{q,p} \partial_f^p \theta(f) h^{p-q} + \partial_f^q [\theta'' + |\theta'|^2(f)] \frac{K^2}{24N^2}.$$  \hspace{1cm} (6)

The first term is the bias from kernel smoothing and the second term is from the sinusoidal multitaper estimate. To leading order in $1/K$, the variance of $\overline{\partial_f^q \theta}(f)$ reduces to the same calculation as the variance of $\overline{\partial_f^q S(f)}$. To this order, the variance inflation factor from the long tail of the $\ln[\chi^2_K]$ distribution is not visible. Since $\text{Cov}[\hat{\theta}_{MT}(f'), \hat{\theta}_{MT}(f'')] \leq [\psi'(K)/K] \times \text{Cov}[\hat{S}_{MT}(f'), \hat{S}_{MT}(f'')]$, we have

$$\text{Var} \left[ \overline{\partial_f^q \theta}(f) \right] \approx \frac{||\kappa||^2}{Nh^{2q+1}} \left( 1 + \frac{1}{2K} \right)^2.$$  \hspace{1cm} (7)

Using (6) and (7), the expected asymptotic square error (EASE) in $\overline{\partial_f^q \theta}$:

$$\text{E} \left[ \left| \overline{\partial_f^q \theta}(f_j) - \partial_f^q \theta(f_j) \right|^2 \right] \approx \text{Var} \left[ \overline{\partial_f^q \theta}(f) \right] + \text{Bias}^2[\overline{\partial_f^q \theta}(f)],$$  \hspace{1cm} (8)

where corrections are $O(h^{2(p-q)+1}) + O(\frac{1}{K}) + O((\frac{K}{Nh})^{4/5}) + O(\frac{1}{Nh})$. The benefit of multitapering (in terms of the variance reduction) tends rapidly to zero. Minimizing (8) with respect to $h$ and $K$ yields $K_{\text{opt}} \ll Nh_{\text{opt}}$ and that to leading order

$$h_{\text{opt}}(f) = \left[ \frac{2q + 1}{2(p-q)} \frac{||\kappa||^2}{B_{q,p} Nh |\partial_f^q \theta(f_j)|^2} \left( 1 + \frac{1}{2K} \right)^2 \right]^{\frac{1}{2p+1}},$$  \hspace{1cm} (9)

and $K_{\text{opt}} \sim N^{(3p+q+2)/(6p+3)}$. For kernels of order $(0,2)$, this reduces to $h_{\text{opt}} \sim N^{-1/5}$ and $K_{\text{opt}} \sim N^{8/15}$. Thus the ordering $1 \ll K \ll Nh$ is justified. The EASE depends only weakly on $K$ for $1 \ll K \ll Nh$ while
the dependence on the choice of bandwidth is strong. When the bandwidth, \( h_o \), satisfies (9), the leading order EASE reduces to

\[
\mathbb{E} \left[ (\partial_j^q \theta(f_j) - \partial_j^q \theta(f_j))^2 \right] \sim |B_{q,p} \partial_j^p \theta(f_j)|^{q+2 \over 2p+1} \left( \| \kappa \|^2 \over N \right)^{2(p-q) \over 2p+1}.
\]

(10)

Thus the EASE in estimating \( \partial_j^q \theta \) is proportional to \( N^{-2(p-q) \over 2p+1} \). The loss depends on the kernel shape through \( B_{q,p} \) and \( \| \kappa \|^2 \). In Sec. 5, we optimize the kernel shape subject to moment constraints. If \( K = 1 \) (a single taper), the variance term in (7) should be inflated by a factor of \( \pi^2 / 6 \). Therefore using a moderate level of multitapering prior to smoothing the logarithm reduces the EASE by a factor of \( \pi^2 / 6 \sum_{n=1}^{N} \nu_n^4 \), where we use \( \sum_{n=1}^{N} \nu_n^4 = 1.5 \).

§4. Data adaptive estimate

In practice, \( \theta''(f) \) is unknown and we use a data adaptive multiple stage kernel estimator where a pilot estimate of the optimal bandwidth is performed prior to estimating \( \theta(f) \). When the spectral range is large, it is often essential to allow the bandwidth to vary locally as a function of frequency. If computational effort is not important, set \( K = N^8 / 15 \); otherwise we set \( K \) by the computational budget. For nonparametric function estimation, data adaptive multiple stage schemes are given in [1-5]. Our scheme for spectral estimation has the following steps:

0) Compute the Fourier transform, \( y(f) \) on a grid of size \( 2N + 2 \) and \( \hat{\theta}_1(f) = \ln|y(f + \Delta) - y(f - \Delta)|^2 / 2(2N + 1) | \) on a grid of size \( N + 1 \). Evaluate \( \hat{\theta}_{MT}(f) \) on a grid of size \( 2N + 2 \).

1) Smooth the tapered log-periodogram, \( \hat{\theta}_1(f) \), a kernel of order (0,4). Choose the global halfwidth by either the Rice criterion [1] or by fitting the average square residual as a function of the global halfwidth to a two parameter model [3].

2) Estimate \( \theta''(f) \) by kernel smoothing the multitaper estimate \( \hat{\theta}_{MT} \) with global halfwidth \( h_{2,4} \). Relate the optimal (2,4) to the optimal (0,4) global halfwidth using the halfwidth quotient relation [1,5]: \( h_{2,4} = H(k_{2,4}, k_{0,4}) h_{0,4} \).

3) Estimate \( \theta(f) \) using the variable halfwidth given by substituting \( \hat{\theta}''(f) \) into the optimal halfwidth expression of Eq. (9).

An estimation scheme has a relative convergence rate of \( N^{-\alpha} \) if

\[
\mathbb{E} \left[ (\hat{\theta}(f|h_{0,2}) - \theta(f))^2 \right] \approx (1 + O(C^2 N^{-2\alpha})) \mathbb{E} \left[ (\hat{\theta}(f|h_{0,2}) - \theta(f))^2 \right],
\]

where \( h_{0,2} \) is the optimal halfwidth and \( \hat{h}_{0,2} \) is the estimated halfwidth. Our data-adaptive method has a convergence rate of \( N^{-4/5} \) and a relative convergence rate: \( N^{-2/9} \).
If multitapering were used in step 1, then \( \theta(f_n) \) would be correlated at neighboring Fourier frequency. The multitaper induced autocorrelation would then bias the estimate of the \( h_{o.4} \) halfwidth. We use a single taper in Step 1 and many tapers in Steps 2-3. To correct for this, we inflate the variance in the (0,4) kernel estimate. The halfwidth quotient relation relates the optimal halfwidth for derivative estimates, \( h_{o.4} \), to that of the (0,4) kernel using (9): 

\[
\hat{h}_{2,4} = H(\kappa_{2,4}, \kappa_{0,4}) \hat{h}_{o.4},
\]

where

\[
H(\kappa_{2,4}, \kappa_{0,4}) \equiv \left( \frac{10B^2_{0.4}\|\kappa_{2,4}\|^2}{B^2_{2,4}\|\kappa_{0,4}\|^2} \right)^{\frac{1}{3}} \left( \frac{\pi^2 \sum \nu_n^{(1)} |q|}{6} \right)^{\frac{1}{2}}.
\]

When \( \hat{\theta}''(f) \) is vanishingly small, the optimal halfwidth becomes large. Thus, \( \hat{h}_{o.2} \) needs to be regularized. Following Riedel & Sidorenko (1994), we determine the size of the regularization from \( \hat{h}_{o.4} \) in the previous stage.

§5. Discontinuities and boundary kernels

When \( S(f) \) or its derivatives are discontinuous, the kernel estimate needs to be one sided using only the data to the left (or right) of discontinuity, \( f_{\text{disc}} \). A similar problem occurs when we wish to estimate the spectral density near the boundary, in our case at \( f = 1/2 \) or \( f = 0 \) if \( S'(0) \neq 0 \). In these cases, the estimation point, \( f \), is not in the center of the kernel domain, that we denote as \( f_i \in [f_{\text{disc}}, f_{\text{disc}} + 2h] \). The kernel estimate is a weighted average of the \( \hat{\theta}_i \): 

\[
\partial^q_i \hat{\theta}(f) = \sum_i K(f, f_i) \hat{\theta}_i \quad \text{in the frequency interval,} \quad f_i \in [f_{\text{disc}}, f_{\text{disc}} + 2h].
\]

The kernel function, \( K(f, f_i) \), must still satisfy the moment conditions: 

\[
\sum_i K(f, f_i)(f_i - f)^j = q! \delta_{j,q}, \quad 0 \leq j < m.
\]

Thus \( K(f, f_i) \) is asymmetric and cannot be simply a function of \( f - f_i \). We now describe results in [6] on kernel estimation near a boundary or discontinuity.

We assume that the estimation point, \( f \), satisfies \( f \geq f_{\text{disc}} \). Far from the discontinuity, we use the standard kernel estimate (3) with \( h_{o}(f) \) given by (9). As \( f \) approaches \( f_{\text{disc}} \), the domain of the kernel touches the discontinuity when \( f - f_{\text{disc}} = h_{o}(f) \). This point is the start of the boundary region around the discontinuity. We call this point, “the right touch point”, \( f_{tp} \) as defined by the equation: 

\[
f_{tp} - f_{\text{disc}} = h_{o}(f_{tp}).
\]

In the boundary region between \( f_{\text{disc}} \) and \( f_{tp} \), we use a fixed halfwidth, \( h \) and modify the kernel shape to satisfy the moment conditions.

We define \( \bar{f} \equiv f_{\text{disc}} + h, \bar{f} \equiv (f - f_{\text{disc}})/h \). The “measurements” are the log multitaper values, that are evaluated on a grid of size \( 2N \): 

\[
\hat{\theta}_i \equiv \hat{\theta}_{MT}(f_i \equiv i/2N) \quad \text{We standardize the grid points:} \quad \tilde{z}_i \equiv (f_i - f_{\text{disc}})/h.
\]

The kernel estimate is a weighted average of the \( \hat{\theta}_i \) in the frequency interval, \( f_i \in [f_{\text{disc}}, f_{\text{disc}} + 2h] \). The total halfwidth is \( 2h \). We define orthonormal polynomials, \( P_j \) on \([f_{\text{disc}}, f_{\text{disc}} + 2h] \) by 

\[
\frac{1}{N h} \sum_i P_k(\tilde{z}_i) P_j(\tilde{z}_i) = g_k \delta_{kj} \quad \text{where} \quad g_k \text{ is a normalization. We have expanded the kernel function,} \ K(f, f_i) \text{ in the polynomials,} \ P_j:
\]
Among all boundary kernels with support \( \frac{h}{2} \), \( h \) is the actual halfwidth and \( h_0(f) \) is given in Eq. (9). Using \( \beta \) instead of \( \theta^{(p)}(f) \) is advantageous because we are interested in kernels that have a fixed halfwidth, \( h \) in the boundary region: \( h(f) = h_0(f_{tp}) \) and \( \beta = \frac{h_0(f_{tp})}{h_0(f)} \).

**Theorem.** Among all boundary kernels with support \([0, 2h]\), the kernel which minimizes the leading order EASE is \( K(f, f_i) = \frac{\gamma_q}{Nh^{q+1}} G\left(\tilde{f}, \tilde{z}_i\right) \) where

\[
G(\tilde{f}, \tilde{z}_i) = P_q(\tilde{z}_i) + (2q + 3)\tilde{f}P_{q+1}(\tilde{z}_i) + \frac{(2q+3)\tilde{f}^2 - 1}{2q+5} P_{q+2}(\tilde{z}_i),
\]

\( P_q, P_{q+1}, P_{q+2} \) are the Legendre polynomials, \( \beta = h/h_0(f) \) [6].

For \( h(f) = h_0(f) \), the optimal boundary kernel simplifies to

\[
G(\tilde{f}, \tilde{z}) = P_q(\tilde{z}) + (2q + 3)\tilde{f}P_{q+1}(\tilde{z}) + ((2q + 3)\tilde{f}^2 - 1) P_{q+2}(\tilde{z}).
\]

At the touch point, \( f = f_{tp} \equiv f_{disc} + h(f_{tp}) \) with \( h = h_0(f_{tp}) \), the optimal boundary kernel is identical to the optimal interior kernel:
Thus using the optimal boundary kernel guarantees the continuity of the estimate if at the touch point we apply the optimal interior kernel of the optimal halfwidth.

At the discontinuity, \((f = f_{\text{disc}}, \tilde{\theta} = -1, \tilde{z} = h_0(0))\), the kernel has a simple expression: 
\[
G(-1, \tilde{\theta}) = P_q(\tilde{\theta}) - (2q+3)P_{q+1}(\tilde{\theta}) + (2q+2)P_{q+2}(\tilde{\theta}) .
\]
The leading order EASE at the boundary is exactly \(4(q + 1)^2\) times larger than for the optimal interior kernel.

One method of constructing kernel shapes is to perform a local polynomial regression (LPR) in the neighborhood of \(f\). We model \(\theta(f)\) as a \(p\)th order polynomial: 
\[
\theta(f) = \sum_{j=0}^{p-1} a_j (f - f_i)^j ,
\]
in the region \(f_i \in [f_{\text{disc}}, f_{\text{disc}} + 2h]\). The \(p\) free parameters \(\{a_j\}\) are chosen by minimizing
\[
F(a_0, a_1, \ldots, a_{p-1}) = \sum_i w_i(f) \left( \sum_{j=0}^{p-1} a_j (f_i - f)^j - \theta_i \right)^2 .
\]
We take \(q!a_q\) as the estimate of \(\theta(q)(f)\). The weighting functions, \(w_i(f)\), are arbitrary and we choose them to minimize the EASE. The equivalence of LPR and kernel smoothing is given by

**Theorem.** A kernel of type \((q, p)\) is the equivalent kernel of local polynomial regression of order \(p - 1\) with non-negative weights if and only if the kernel has no more than \(p - 1\) sign changes.

It is known (Müller (1987), Fan(1993)) that the optimal interior kernel of type \((q, p)\), \(p - q \equiv 0 \mod 2\), in the continuum limit, is produced by the scaling weight function \(W(y) = 1 - y^2\). This choice is not unique!

**Theorem** Let \(p - q\) be even. If data points, \(f_i\), in the interval of support, \([f - h, f + h]\), are symmetric around the estimation point, \(t\), and their weights are chosen as \(w_i = W\left(\frac{f_i - t}{h}\right)\), then each of the functions \(W_1(z) = 1 - z\), \(W_2(z) = 1 + z\), \(W_3(z) = 1 - z^2\) produces the same estimator [6].

Because of the optimality in the interior, the Bartlett-Priestley weighting, \(W(z) = 1 - z^2\), is used often in the boundary region as well. This does not minimize the EASE [6]:

**Theorem.** The asymptotically optimal kernel is equivalent to a linear, nonnegative weighting function. At the boundary, the equivalent weighting equals \(2h - (z - f_{\text{disc}})\). For the intermediate estimation points, \(f_{\text{disc}} < f < f_{tp}\), the slope of the weighting line varies as \(t\) changes. For \(q = 0\), the equivalent weighting is \((1 - \tilde{f}^2)h + \left(\tilde{f} + \sqrt{1 - 3\tilde{f}^2 + 3\tilde{f}^4}\right)h\tilde{z}\).

§6. Summary

We have analyzed the expected asymptotic square error of the smoothed log multitapered periodogram and shown that multitapering reduces the
error by a factor of $\left[\frac{\pi^2}{4}\right]^{-8}$ for the sinusoidal tapers. The optimal rate of presmoothing prior to taking logarithms is $K \sim N^{8/15}$, but the expected loss depends only weakly on $K$ when $1 \ll K \ll Nh$.

We have proposed a data-adaptive multiple stage variable halfwidth kernel smoother. It has a relative convergence of $N^{-2/9}$, which can be improved to $N^{-1/4}$ if desired. The multiple stage estimate has the following steps. 0) Estimate $\hat{\theta}_{MT}(f) \equiv \ln[\hat{S}_{MT}(f)] - B_{K}/K$ as described in Sec. 2. 1) Estimate the optimal kernel halfwidth for a kernel of (0,4) for the log-single tapered periodogram. 2) Estimate $\theta''(f)$ using a kernel smoother of order (2,4). 3) Estimate $\theta(f)$ using a kernel smoother of order (0,2) with the halfwidth $h_{0}(f)$. The halfwidth is the evaluation of the asymptotically optimal halfwidth: $h(f) \sim c|\partial_{f}^{2}\theta|^{-2/5}N^{-1/5}$.

Acknowledgments. Work funded by U.S. Dept. of Energy Grant DE-FG02-86ER53223.

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